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**Análisis Numérico de algunos modelos
diferenciales acoplados de la Mecánica de
Fluidos**

Memoria presentada por

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INTRODUCCIÓN

La finalidad de esta tesis es aportar un mayor grado de entendimiento, desde el aspecto numérico, de diversos sistemas en derivadas parciales provenientes de la mecánica de fluidos. Más precisamente, estudiamos un modelo de Navier-Stokes con difusión de masa y un modelo de cristales líquidos. Como punto final analizamos un modelo estático de campo de fase para un proceso de solidificación de una mezcla binaria con propiedades térmicas.

Los dos primeros modelos son de tipo Navier-Stokes incompresible en formulación velocidad-presión, acoplados con una nueva ecuación de estado (bien de la densidad o bien del vector orientación de los cristales líquidos). Además de las dificultades bien conocidas del modelo de Navier-Stokes clásico (tratamiento del término no lineal convectivo, el acoplamiento velocidad-presión y la restricción de incompresibilidad), estos modelos presentan otras dificultades, como son: la nueva incógnita debe verificar un principio del máximo, tiene un orden de regularidad mayor que la velocidad y aparecen nuevas no linealidades que acoplan la incógnita de la ecuación de estado con la velocidad del fluido.

Modelos de Navier-Stokes con difusión de masa

En una gran parte de la tesis, nos centramos en los modelos de Navier-Stokes con difusión de masa. Para fijar ideas supongamos que el fluido ocupa un dominio acotado $\Omega \subset \mathbb{R}^d$ ($d = 2$ ó 3) de frontera Γ . Denotamos $Q = \Omega \times (0, T)$ y $\Sigma = \Gamma \times (0, T)$, donde $[0, T]$ es el intervalo temporal de observación, para $T > 0$. Las incógnitas para este modelo son $\mathbf{u} : Q \rightarrow \mathbb{R}^d$ el campo incompresible de velocidades del fluido, $q : Q \rightarrow \mathbb{R}$ una función potencial (relacionada con la presión) y $\rho : Q \rightarrow \mathbb{R}$ la concentración de masa del fluido, que verifican el siguiente sistema de

ecuaciones en derivadas parciales:

$$\left\{ \begin{array}{l} \rho [\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}] - \mu \Delta \mathbf{u} \\ -\lambda [(\nabla \rho \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \nabla \rho] + \nabla q = \rho \mathbf{f} \quad \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0 \quad \text{en } Q, \\ \rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0 \quad \text{en } Q, \end{array} \right. \quad (1)$$

donde \mathbf{f} es la fuerza externa sobre el sistema y, $\mu > 0$ y $\lambda > 0$ son los coeficientes de viscosidad y de difusión de masa, respectivamente.

La primera ecuación resulta de la conservación del momento lineal, la segunda ecuación de la incompresibilidad del fluido y la tercera está relacionada con la conservación de la masa del sistema.

Por ejemplo, este sistema modela la mezcla de dos fluidos newtonianos, viscosos, incompresibles y miscibles donde en el proceso de mezcla se produce un fenómeno de difusión de masa gobernado por la ley de Fick (ley formulada en 1855 por Adolf Eugen Fick).

Este fenómeno ocurre cuando colocamos agua y agua saturada de sal en un vaso, entonces las moléculas de sal se difunden por toda el agua.

Otros ejemplos prácticos relacionados con el modelo (1) son: endurecimiento de acero por gas carburizante (industria), movimiento de agua o de soluto a través de una membrana, ascenso de la savia por el xilema en los vegetales frente a la acción de la gravedad (biomecánica). Por otro lado, diremos que modelos algo más generales que (1) ayudan al entendimiento de avalanchas [15].

Para completar (1) supongamos que Γ es impermeable y no hay intercambio de masa a través de la frontera Γ entre la mezcla y el exterior, lo que se formula con las siguientes condiciones de contorno:

$$\mathbf{u}|_{\Sigma} = 0, \quad \frac{\partial \rho}{\partial \mathbf{n}} \Big|_{\Sigma} = 0, \quad (2)$$

donde \mathbf{n} es el vector unitario normal a Γ . Además, consideramos las condiciones iniciales

$$\rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad (3)$$

donde $\rho_0 : \Omega \rightarrow \mathbb{R}^+$ y $\mathbf{u}_0 : \Omega \rightarrow \mathbb{R}^d$ son funciones dadas.

Desde el punto de vista del análisis teórico, este sistema de ecuaciones ha sido tratado por numerosos autores. Fue introducido por *A. V. Kazhikhov* y *Sh. Smagulov* en 1977 ([25]), de aquí que sea conocido también como modelo de *Kazhikhov* y *Smagulov*, quienes probaron, bajo

existencia de solución fuerte local (y regularidad) de (5), y algunas estimaciones de error entre las soluciones del método iterativo y la solución exacta en diversas normas.

Se puede observar, al menos de manera formal, que cuando $\lambda = 0$ recuperamos el clásico sistema de Navier-Stokes con densidad variable:

$$\begin{cases} \rho [\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}] - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{f} & \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0, \quad \rho_t + \mathbf{u} \cdot \nabla \rho = 0 & \text{en } Q. \end{cases} \quad (6)$$

En este modelo, la ecuación de continuidad pierde su carácter parabólico para convertirse en una ecuación hiperbólica y en el sistema de momentos desaparecen algunos términos no lineales, aunque se sigue conservando el acoplamiento $\rho \mathbf{u}_t$.

P. Secchi en [35] para el caso bidimensional y *F. Guillén-González* ([21]) en el caso 3D y con densidad inicial sólo positiva, probaron el comportamiento asintótico, cuando $\lambda \rightarrow 0$, del modelo de Kazhikov-Smagulov hacia el problema de Navier-Stokes con densidad variable.

Las dificultades principales a la hora de diseñar esquemas numéricos estables y convergentes para (1) y (5), usando elementos finitos a lo más globalmente continuos, son: la falta de regularidad H^2 y la no verificación en general del principio del máximo para la densidad discreta, y la obtención de compacidad para la velocidad aproximada puesto que está directamente relacionada con poder estimar adecuadamente los términos fuertemente no lineales que aparecen en el sistema de momentos para \mathbf{u} .

Los antecedentes referente a los resultados numéricos para (1), (5) y (6) son escasos. El único resultado numérico, que conocemos hasta el momento, está hecho por *J. Étienne- P. Saramito* en [15], para un modelo más general que (1), con una reescritura en función de un campo de velocidades compresible. Se trata de un algoritmo numérico basado en un esquema de Euler retrógrado junto con el método de las características para la discretización en tiempo y elementos finitos en espacio. Este esquema es analizado en [15] bajo la perspectiva de estimaciones de error, donde los autores dan cotas de error optimal bajo ciertas restricciones sobre los parámetros de discretización y asumiendo hipótesis de bastante regularidad sobre la solución continua. Dicha regularidad exige, en particular, que se verifique una bien conocida condición de compatibilidad global para la presión en $t = 0$ (ver [24]), que no se puede comprobar en la práctica.

El esquema de [15] se describe, para el caso particular del modelo (1), como sigue: se considera una partición uniforme del intervalo $[0, T]$ de paso de tiempo $k = T/N$ con $N \in \mathbb{N}$, y una familia de triangulaciones \mathcal{T}_h de Ω asociada al parámetro h , con los espacios de elementos

finitos siguientes:

$$\begin{aligned} W_h &= \{\rho_h \in C^0(\bar{\Omega}) : \rho_h|_K \in \mathbb{P}_l, \forall K \in \mathcal{T}_h\}, \\ \mathbf{V}_h &= \{\mathbf{v}_h \in \mathbf{C}^0(\bar{\Omega}) : \mathbf{v}_h|_K \in \mathbb{P}_l, \forall K \in \mathcal{T}_h\} \cap \mathbf{H}_0^1(\Omega), \\ Q_h &= \{p_h \in L^2(\Omega) : p_h|_K \in \mathbb{P}_{l-1}, \forall K \in \mathcal{T}_h\}. \end{aligned}$$

Entonces una etapa de tiempo genérica del esquema se describe como:

Etapa $n + 1$: Dado $\mathbf{u}_h^n \in \mathbf{V}_h$, calcular la característica aproximada \mathbf{X}_h^n por

$$\mathbf{X}_h^n(\mathbf{x}) := \mathbf{x} - k \mathbf{u}_h^n(\mathbf{x}).$$

Esta aproximación se obtiene discretizando el sistema diferencial ordinario característico:

$$\begin{cases} \frac{d}{dt} \mathbf{X}(\mathbf{x}, s; t) = \mathbf{u}(\mathbf{X}(\mathbf{x}, s; t), t), \\ \mathbf{X}(\mathbf{x}, s; s) = \mathbf{x}, \end{cases}$$

particularizado para $s = t_{n+1}$ y $t = t_n$, usando un esquema de Euler explícito.

Dados $(\rho_h^n, \mathbf{u}_h^n) \in W_h \times \mathbf{V}_h$, hallar $\rho_h^{n+1} \in W_h$ tal que:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n \circ \mathbf{X}_h^n}{k}, \psi_h \right) + \lambda (\nabla \rho_h^{n+1}, \nabla \psi_h) = 0 \quad \forall \psi_h \in W_h.$$

Dados $(\rho_h^{n+1}, \mathbf{u}_h^n) \in W_h \times \mathbf{V}_h$, hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times Q_h$ tal que:

$$\begin{aligned} &\left(\rho_h^{n+1} \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n \circ \mathbf{X}_h^n}{k} \right) + \mu (\nabla \mathbf{u}_h^{n+1}, \nabla \mathbf{v}_h) - \lambda ((\nabla \rho_h^{n+1} \cdot \nabla) \mathbf{u}_h^{n+1}, \mathbf{v}_h) \\ &- \lambda (\rho_h^{n+1} (\nabla \mathbf{u}_h^{n+1})^t, \nabla \mathbf{v}_h) - (p_h^{n+1}, \nabla \cdot \mathbf{v}_h) = (\rho_h^{n+1} \mathbf{f}^{n+1}, \mathbf{v}_h) \quad \forall \mathbf{v}_h \in \mathbf{V}_h, \\ &(\nabla \cdot \mathbf{u}_h^{n+1}, q_h) = 0 \quad \forall q_h \in Q_h. \end{aligned}$$

Nótese que el término discreto $(\rho_h^{n+1} (\nabla \mathbf{u}_h^{n+1})^t, \nabla \mathbf{v}_h)$ proviene del término continuo $((\mathbf{u} \cdot \nabla) \nabla \rho, \mathbf{v})$ integrando por partes dos veces y usando la condición de incompresibilidad de la velocidad. Además, se desacopla el cálculo de la densidad ρ_h^{n+1} del par velocidad-presión $(\mathbf{u}_h^{n+1}, p_h^{n+1})$

Bajo las restricciones de los parámetros de discretización $l > d - 1$ (d la dimensión del espacio) y $k = C_0 h^r$ con $r : d < r < 2l + 2 - d$, se demuestra en [15], por recurrencia en la etapa de tiempo, que para cualquier $\varepsilon > 0$ existe $h_0 > 0$ tal que para $h \leq h_0$ se tiene primero la estimación puntual para la densidad $0 < m - \varepsilon \leq \rho_h^{n+1} \leq M + \varepsilon$ en Ω y segundo las estimaciones de error

$$\|\rho - \rho_{h,k}\|_{\ell^\infty(0,T;H^1(\Omega))} + \|\mathbf{u} - \mathbf{u}_{h,k}\|_{\ell^\infty(0,T;H^1(\Omega))} + \|p - p_{h,k}\|_{\ell^2(0,T;L^2(\Omega))} \leq C(k + h^l),$$

$$\|\rho - \rho_{h,k}\|_{\ell^\infty(0,T;L^2(\Omega))} + \|\mathbf{u} - \mathbf{u}_{h,k}\|_{\ell^\infty(0,T;L^2(\Omega))} \leq C(k + h^{l+1}).$$

Por otra parte, *C. Liu* y *N. J. Walkington* en [32] analizan un esquema numérico para el problema de Navier-Stokes con densidad variable (6), tomando además la viscosidad del fluido dependiente de la densidad $\mu = \mu(\rho)$ tal que $0 < c \leq \mu(\rho) \leq C$ y cambiando el término de difusión $-\mu\Delta\mathbf{u}$ por $-\nabla \cdot (\mu(\rho)\nabla\mathbf{u})$. Las incógnitas se aproximan usando un método de Galerkin discontinuo con polinómios de orden 0 para la ecuación hiperbólica de la densidad y un par de elementos finitos estables en velocidad-presión para el sistema de momentos:

$$W_h = \{\rho_h \in L^2(\Omega) : \rho_h|_K \in \mathbb{P}_0, \forall K \in \mathcal{T}_h\},$$

$$\mathbf{V}_h = \{\mathbf{v}_h \in \mathbf{C}^0(\bar{\Omega}) : \mathbf{v}_h|_K \in \mathbb{P}_l, \forall K \in \mathcal{T}_h\} \cap \mathbf{H}_0^1(\Omega),$$

$$Q_h = \{p_h \in L_0^2(\Omega) : p_h|_K \in \mathbb{P}_m, \forall K \in \mathcal{T}_h\},$$

de modo que (\mathbf{V}_h, Q_h) verifica la condición de Babuska-Brezzi (condición *inf-sup*). Una etapa genérica del esquema se define como sigue:

- Conocido $(\rho_h^n, \mathbf{u}_h^n) \in W_h \times \mathbf{V}_h$, hallar $\rho_h^{n+1} \in W_h$ tal que:

$$\int_K \rho_h^{n+1} \psi_h + k \int_{\partial K} ((\rho_h^{n+1})_-(\mathbf{u}_h^n \cdot \mathbf{n})^+ + (\rho_h^{n+1})_+(\mathbf{u}_h^{n-1} \cdot \mathbf{n})^-) \psi_h = \int_K \rho_h^n \psi_h,$$

para cada $K \in \mathcal{T}_h$ y $\psi_h \in \mathbb{P}_0$. Aquí, $\mathbf{u} \cdot \mathbf{n} = (\mathbf{u} \cdot \mathbf{n})^+ + (\mathbf{u} \cdot \mathbf{n})^-$ son la parte positiva y negativa de $\mathbf{u} \cdot \mathbf{n}$ y $\rho_\pm(\mathbf{x}) = \lim_{s \searrow 0} \rho^n(\mathbf{x} \pm s\mathbf{n})$.

- Conocido $(\rho_h^{n+1}, \mathbf{u}_h^n) \in W_h \times \mathbf{V}_h$, hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times Q_h$, tal que:

$$\begin{aligned} & \frac{1}{2} \int_\Omega \rho_h^n \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k} \right) \cdot \mathbf{v}_h + (\rho_h^{n+1} \mathbf{u}_h^n \cdot \nabla) \mathbf{u}_h^{n+1} \cdot \mathbf{v}_h + \left(\frac{\rho_h^{n+1} \mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n}{k} \right) \cdot \mathbf{v}_h, \\ & - \int_\Omega (\rho_h^{n+1} \mathbf{u}_h^n \cdot \nabla) \mathbf{v}_h - p_h^{n+1} \nabla \cdot \mathbf{v}_h + \mu(\rho_h^{n+1}) \nabla \mathbf{u}_h^{n+1} \cdot \nabla \mathbf{v}_h = \int_\Omega \rho_h^{n+1} \mathbf{f}^{n+1} \cdot \mathbf{v}_h \quad \forall \mathbf{v}_h \in \mathbf{V}_h, \end{aligned}$$

$$\int_\Omega \nabla \cdot \mathbf{u}_h^{n+1} q_h = 0 \quad \forall q_h \in Q_h,$$

donde \mathbf{f}^{n+1} es una media de \mathbf{f} en $[t^n, t^{n+1}]$.

Se observa que este esquema también desacopla el cálculo de la densidad ρ_h^{n+1} del par velocidad-presión $(\mathbf{u}_h^{n+1}, p_h^{n+1})$. Para este esquema se prueban las siguientes estimaciones puntuales para la densidad y de energía para la velocidad:

$$0 < m \leq \rho_h^n \leq M \quad (m \text{ y } M \text{ son las cotas de la densidad exacta}),$$

$$\int_{\Omega} \rho_h^n |\mathbf{u}_h^n|^2 + \sum_{i=1}^n \int_{\Omega} \rho_h^{i-1} |\mathbf{u}_h^i - \mathbf{u}_h^{i-1}|^2 + 2k \sum_{i=1}^n \int_{\Omega} \mu(\rho_h^i) |\nabla \mathbf{u}_h^i|^2 = \int_{\Omega} \rho_h^0 |\mathbf{u}_h^0|^2 + 2k \sum_{i=1}^n \int_{\Omega} \rho_h^i \mathbf{f}^i \cdot \mathbf{u}_h^i.$$

Además, para establecer la convergencia del esquema hacia un solución débil de (6) se prueba la estimación discreta de tipo derivada fraccionaria en tiempo siguiente:

$$k \sum_{m=0}^{N-r} \|\sqrt{\rho_h^{m+r}} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^2(\Omega)}^2 \leq C (rk)^\alpha, \quad \forall r : 0 \leq r \leq N,$$

para $\alpha \in (0, 1)$, que junto con las estimaciones de energía para la velocidad, implican la compacidad de la velocidad discreta en $\mathbf{L}^2(Q)$.

En [20] *J. L. Guermond* y *L. Quaterpelle* analizan dos métodos de proyección (semidiscretos en tiempo) para el sistema de Navier-Stokes con densidad variable (6). Los métodos de proyección separan el término de difusión de la restricción de incompresibilidad en dos pasos en cada etapa de tiempo. La idea es resolver, en cada etapa temporal, un problema para la velocidad, donde desaparece la condición de incompresibilidad y, posteriormente, “proyectar” esta velocidad sobre un espacio de divergencia nula, lo cual equivale a resolver un problema de Poisson para la presión. El primer método propuesto en [20] se describe como:

Método no incremental de proyección. Sean $\rho^0 = \rho_0$, $\sigma^0 = \sqrt{\rho^0}$ y $\mathbf{u}^0 = \mathbf{u}_0$.

Etapas $n + 1$: Conocido $(\rho^n, \sigma^n, \mathbf{u}^n, \hat{\mathbf{u}}^n, p^n)$, hallar:

- ρ^{n+1} como la solución del problema elíptico de Neumann:

$$\begin{cases} \frac{\rho^{n+1} - \rho^n}{k} + \mathbf{u}^n \cdot \nabla \rho^{n+1} + \frac{1}{2} (\nabla \cdot \mathbf{u}^n) \rho^{n+1} = 0 & \text{en } \Omega, \\ \frac{\partial \rho^{n+1}}{\partial \mathbf{n}} = 0 & \text{sobre } \partial\Omega, \end{cases}$$

- $\sigma^{n+1} = \sqrt{\rho^{n+1}}$,

- la velocidad intermedia \mathbf{u}^{n+1} como la solución del problema de Dirichlet homogéneo:

$$\begin{cases} \sigma^{n+1} \frac{\sigma^{n+1} \mathbf{u}^{n+1} - \sigma^n \mathbf{u}^n}{k} - \mu \Delta \mathbf{u}^{n+1} + (\rho^{n+1} \mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1} \\ \quad + \frac{1}{2} \nabla \cdot (\rho^{n+1} \mathbf{u}^n) \mathbf{u}^{n+1} = \rho^{n+1} \mathbf{f}^{n+1} & \text{en } \Omega, \\ \mathbf{u}^{n+1} = 0 & \text{sobre } \partial\Omega, \end{cases}$$

- la velocidad final y la presión $(\hat{\mathbf{u}}^{n+1}, p^{n+1})$ con la etapa de proyección:

$$\begin{cases} \rho^{n+1} \frac{\hat{\mathbf{u}}^{n+1} - \mathbf{u}^{n+1}}{k} + \nabla p^{n+1} = 0 & \text{en } \Omega, \\ \nabla \cdot \hat{\mathbf{u}}^{n+1} = 0 & \text{en } \Omega, \\ \hat{\mathbf{u}}^{n+1} \cdot \mathbf{n} = 0 & \text{sobre } \partial\Omega. \end{cases}$$

Este esquema es incondicionalmente estable, en el sentido que, no se impone ninguna restricción sobre el paso de tiempo k para conseguir las siguientes estimaciones:

$$\|\rho^n\|_{L^2(\Omega)} \leq \|\rho^0\|_{L^2(\Omega)},$$

$$\|\sigma^n \mathbf{u}^n\|_{L^2(\Omega)}^2 + 2\mu k \sum_{i=1}^n \|\nabla \mathbf{u}^i\|_{L^2(\Omega)}^2 \leq \|\sigma^0 \mathbf{u}^0\|_{L^2(\Omega)}^2.$$

Sin embargo, en este artículo [20] no se hace referencia sobre el principio del máximo para la densidad discreta ni se analiza la convergencia hacia una solución débil de (6).

En [20] también se describe el **método incremental de proyección**:

Etapa $n + 1$: Conocidos $(\rho^n, \sigma^n, p^n, \mathbf{u}^n, q^n)$, hallar:

- ρ^{n+1} como antes,
- $\sigma^{n+1} = \sqrt{\rho^{n+1}}$,
- p^{n+1} tal que

$$\begin{cases} -\nabla \cdot \left(\frac{1}{\rho^{n+1}} \nabla p^{n+1} \right) = -\nabla \cdot \left(\frac{1}{\sigma^n \sigma^{n+1}} \nabla q^n \right) & \text{en } \Omega, \\ \frac{1}{\sigma^{n+1}} \frac{\partial p^{n+1}}{\partial \mathbf{n}} = \frac{1}{\sigma^n} \frac{\partial q^n}{\partial \mathbf{n}} & \text{sobre } \partial\Omega, \end{cases}$$

- \mathbf{u}^{n+1} tal que

$$\begin{cases} \sigma^{n+1} \frac{\sigma^{n+1} \mathbf{u}^{n+1} - \sigma^n \mathbf{u}^n}{k} - \mu \Delta \mathbf{u}^{n+1} + (\rho^{n+1} \mathbf{u}^n \cdot \nabla) \mathbf{u}^{n+1} \\ + \frac{1}{2} \nabla \cdot (\rho^{n+1} \mathbf{u}^n) \mathbf{u}^{n+1} + \nabla p^{n+1} + \frac{\sigma^{n+1}}{\sigma^n} \nabla (q^n - p^n) = \rho^{n+1} \mathbf{f}^{n+1} & \text{en } \Omega, \\ \mathbf{u}^{n+1} = 0 & \text{sobre } \partial\Omega, \end{cases}$$

- q^{n+1} tal que

$$\begin{cases} -\nabla \cdot \left(\frac{1}{\rho^{n+1}} \nabla (q^{n+1} - p^{n+1}) \right) = -\frac{1}{k} \nabla \cdot \mathbf{u}^{n+1} & \text{en } \Omega, \\ \frac{\partial (q^{n+1} - p^{n+1})}{\partial \mathbf{n}} = 0 & \text{sobre } \partial\Omega. \end{cases}$$

Al igual que para el método de proyección no incremental, se prueba en [20] que este método de proyección incremental tiene las siguientes estimaciones de estabilidad:

$$\|\rho^{n+1}\|_{L^2(\Omega)} \leq \|\rho^0\|_{L^2(\Omega)},$$

$$\|\sigma^n \mathbf{u}^n\|_{L^2(\Omega)}^2 + k^2 \left\| \frac{\nabla q^n}{\sigma^n} \right\|_{L^2(\Omega)}^2 + 2\mu k \sum_{i=1}^n \|\nabla \mathbf{u}^i\|_{L^2(\Omega)}^2 \leq \|\sigma_0 \mathbf{u}^0\|_{L^2(\Omega)}^2 + k^2 \left\| \frac{\nabla q^0}{\sigma^0} \right\|_{L^2(\Omega)}^2.$$

Por último reseñar que los modelos de difusión de masa y Navier-Stokes con densidad variable abarcan un amplio rango de situaciones físicas que el sistema de Navier-Stokes tradicional no alcanza a modelar, en particular, cuando se trata de gobernar la mezcla de fluidos con distintas densidades. Sin embargo, estos modelos se encuentran bastante por explotar desde el punto de vista del análisis numérico, ya que los resultados que se conocen para el problema de Navier-Stokes clásico (con densidad constante), no se pueden extender en general a estos problemas.

Modelos de cristales líquidos nemáticos

Los *cristales líquidos* (CL) son mesofases de la materia, es decir, fases intermedias entre un líquido y un sólido. Se trata de materiales con una microestructura en la que se mantienen correlaciones orientacionales típicas de los sólidos cristalinos, pero cuyas moléculas no ocupan las posiciones fijas de una red, sino que tienen la movilidad característica de los líquidos. Existen dos grandes familias dentro de los cristales líquidos: Los *termotrópicos*, que son aquellos en los que las mesofases se generan por efecto de la temperatura, y los *liotrópicos*, que están formados por mezclas de al menos dos sustancias (un mesógeno y un disolvente) y en los que las mesofases se producen por variación de la composición de la mezcla. También se conocen CL obtenidos a partir de polímeros.

Los CL desempeñan un papel fundamental en los organismos vivos (el ADN forma diversas fases líquido-cristalinas); se utilizan para fabricar dispositivos electrónicos (indicadores electro-ópticos de calculadoras y relojes electrónicos); han permitido fabricar pantallas de TV extraordinariamente delgadas, son esenciales para fabricar nuevos materiales (fibras de alta resistencia) y son de gran utilidad en la recuperación del petróleo.

Los CL termotrópicos tienen fases estables en un intervalo dado de temperatura y son los más usados en la práctica. Por ejemplo, gracias a las propiedades ópticas de estos materiales, pueden permitir el paso de la luz o pueden bloquearla inducidos por la acción de un campo eléctrico, y por ello sirven para el desarrollo de pantallas planas. Las moléculas del cristal líquido termotrópico pueden ser largas, con forma de barra (caso *calamítico*) o redondas y planas (caso *discótico*). Un campo eléctrico puede guiar estas moléculas, y así controlar los rayos de luz que circulen a través de ellas.

De acuerdo con el tipo de arreglos moleculares que pueden formar, Friedel (1922) clasificó los cristales líquidos termotrópicos en tres grandes clases: *nemáticos*, *esméticos* y *colestéricos*. En los nemáticos las moléculas conservan sólo el orden en la orientación, mientras que en los

esméticos y colestéricos, también se conserva cierto orden en la posición de las moléculas.

El modelo que estudiaremos es una simplificación, introducida por *F. H. Lin* ([27]), del modelo propuesto por Ericksen-Leslie para modelar el comportamiento dinámico de los cristales líquidos nemáticos. Las incógnitas son: \mathbf{u} el campo de velocidades incompresible, p la presión del fluido y \mathbf{d} la orientación de las macromoléculas de cristales líquidos, y verifican el siguiente problema en derivadas parciales:

$$\left\{ \begin{array}{l} \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \lambda \nabla \cdot (\nabla \mathbf{d} \odot \nabla \mathbf{d}) = \mathbf{0} \quad \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0 \quad \text{en } Q, \\ \partial_t \mathbf{d} + \mathbf{u} \cdot \nabla \mathbf{d} - \gamma \Delta \mathbf{d} - \gamma |\nabla \mathbf{d}|^2 \mathbf{d} = \mathbf{0} \quad \text{en } Q, \\ |\mathbf{d}| = 1 \quad \text{en } Q, \end{array} \right. \quad (7)$$

donde $\nabla \mathbf{d} \odot \nabla \mathbf{d}$ es la matriz $(\nabla \mathbf{d} \odot \nabla \mathbf{d})_{i,j} = \sum_{k=1}^3 \partial_i d_k \partial_j d_k$, junto con las condiciones de contorno

$$\mathbf{u} = 0, \quad \mathbf{d} = \mathbf{l} \quad \text{sobre } \Sigma, \quad (8)$$

donde $\mathbf{l} : \Sigma \rightarrow \mathbb{R}^d$ es el dato de contorno, y las condiciones iniciales

$$\mathbf{d}(\mathbf{x}, 0) = \mathbf{d}_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad \mathbf{x} \in \Omega, \quad (9)$$

donde $\mathbf{u}_0 : \Omega \rightarrow \mathbb{R}^d$ y $\mathbf{d}_0 : \Omega \rightarrow \mathbb{R}^d$ son los datos iniciales. La constante $\nu > 0$ representa la viscosidad del fluido, $\lambda > 0$ es la constante de elasticidad y el parámetro $\gamma > 0$ depende del tiempo de relajación.

La primera ecuación representa la conservación del momento lineal. Esta ecuación es de tipo Navier-Stokes la cual describe el movimiento de un fluido isotrópico junto con el término de acoplamiento no lineal $\lambda \nabla \cdot (\nabla \mathbf{d} \odot \nabla \mathbf{d})$ que determina el comportamiento anisótropo. La segunda ecuación indica que el fluido es incompresible y la tercera proviene de la conservación del momento angular. La restricción $|\mathbf{d}| = 1$ indica que \mathbf{d} es un vector orientación.

Imponiendo que $|\mathbf{d}_0| = 1$ en Ω y $|\mathbf{l}| = 1$ sobre Σ , se tiene la existencia de solución global en tiempo de (7) con la siguiente regularidad:

$$\mathbf{d} \in L^\infty(0, T; \mathbf{H}^1(\Omega)), \quad \mathbf{u} \in L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)).$$

Esta solución fue encontrada por *F. Guillén-González* y *M. A. Rojas-Medar* en [23], mediante un proceso asintótico, a partir de un modelo penalizado de tipo Ginzburg-Landau, que se obtiene de (7) relajando la restricción $|\mathbf{d}| = 1$ por $|\mathbf{d}| \leq 1$, y en el sistema para \mathbf{d} cambiando los términos

más no lineales $|\nabla \mathbf{d}|^2 \mathbf{d}$ por el término de penalización $\mathbf{f}_\varepsilon(\mathbf{d}) = \varepsilon^{-2}(|\mathbf{d}|^2 - 1)\mathbf{d}$ (asociado al parámetro de penalización $\varepsilon > 0$) que es el gradiente de la función escalar

$$F_\varepsilon(\mathbf{d}) = \frac{1}{4\varepsilon^2}(|\mathbf{d}|^2 - 1)^2,$$

es decir, $\mathbf{f}_\varepsilon(\mathbf{d}) = \nabla_{\mathbf{d}}(F_\varepsilon(\mathbf{d}))$ para todo $\mathbf{d} \in \mathbb{R}^N$:

$$\left\{ \begin{array}{l} |\mathbf{d}| \leq 1, \quad \mathbf{d}_t + \mathbf{u} \cdot \nabla \mathbf{d} + \gamma(\mathbf{f}_\varepsilon(\mathbf{d}) - \Delta \mathbf{d}) = \mathbf{0} \quad \text{en } Q, \\ \mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \lambda \nabla \cdot (\nabla \mathbf{d} \odot \nabla \mathbf{d}) = \mathbf{0} \quad \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0 \quad \text{en } Q. \end{array} \right. \quad (10)$$

El espacio para obtener dicha solución débil se encuentra en la igualdad de energía conseguida por *F. H. Lin* y *C. Lui* en [29] para (10) considerando la condición frontera para el vector de orientación \mathbf{d} independiente del tiempo (i.e. $\mathbf{l} = \mathbf{l}(\mathbf{x})$) que es la traza del dato inicial \mathbf{d}_0 :

$$\frac{d}{dt} \left(\frac{1}{2} \|\mathbf{u}\|_{L^2(\Omega)}^2 + \frac{\lambda}{2} \|\nabla \mathbf{d}\|_{L^2(\Omega)}^2 + \lambda \int_{\Omega} F_\varepsilon(\mathbf{d}) d\mathbf{x} \right) + \nu \|\nabla \mathbf{u}\|_{L^2(\Omega)}^2 + \lambda \gamma \|\mathbf{f}_\varepsilon(\mathbf{d}) - \Delta \mathbf{d}\|_{L^2(\Omega)}^2 = 0, \quad (11)$$

que se obtiene eligiendo $\lambda(\mathbf{f}(\mathbf{d}) - \Delta \mathbf{d})$ y \mathbf{u} como funciones test en (10)_a y (10)_b, respectivamente. Esta expresión refleja la relación entre la energía cinética y la elástica e indica que la energía del sistema decrece con el tiempo. Además, muestra el acoplamiento entre el término de transporte y el tensor $\nabla \cdot (\nabla \mathbf{d} \odot \nabla \mathbf{d})$.

La idea clave en [23] para pasar al límite $\varepsilon \rightarrow 0$ es obtener la compacidad del gradiente del vector de orientación en $\mathbf{L}^2(Q)$, usando técnicas de optimización para caracterizar el vector de orientación penalizado y su límite. Esta compacidad permite pasar al límite en el término $\nabla \cdot (\nabla \mathbf{d} \odot \nabla \mathbf{d})$ de (10)_b.

Respecto a los resultados teóricos conocidos para el modelo penalizado (10), en [29] *F. H. Lin* y *C. Lui* probaron mediante un método de semi-Galerkin, considerando en dimensión finita sólo la velocidad para asegurar el principio del máximo del vector de orientación $|\mathbf{d}| \leq 1$, la existencia global de solución débil

$$\mathbf{d} \in L^\infty(0, T; \mathbf{H}^1(\Omega)) \cap L^2(0, T; \mathbf{H}^2(\Omega)), \quad \mathbf{u} \in L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)),$$

tomando la condición frontera para el vector de orientación independiente del tiempo y el parámetro de penalización ε fijo. Además, se consiguen resultados locales en tiempo de regularidad y unicidad.

Las principales dificultades para diseñar esquemas numéricos estables y convergentes para el modelo penalizado (10) son, además de las clásicas del sistema de Navier-Stokes: aproximar \mathbf{d} con elementos finitos a lo más globalmente continuos aunque la regularidad del límite \mathbf{d} es H^2 y obtener la restricción $|\mathbf{d}| \leq 1$ en el límite aunque el esquema no verifique puntualmente dicha restricción.

En [30] *C. Lui* y *J. N. Walkington* construyen un esquema numérico no lineal usando diferencias finitas implícitas en tiempo y un método de elementos finitos $C^0(\bar{\Omega})$ y $C^1(\bar{\Omega})$ para aproximar la velocidad y el vector de orientación, respectivamente; tomando independiente del tiempo la condición de Dirichlet \mathbf{l} para el vector de orientación \mathbf{d} . La aproximación $C^1(\bar{\Omega})$ es considerada para conservar la ley de energía (11) ya que en la obtención de la misma se usa la función test $\Delta \mathbf{d}$. La convergencia del esquema se establece bajo apropiadas hipótesis de regularidad de la solución continua. El esquema estudiado en [30] es el siguiente: conocidos $(\mathbf{u}_h^n, p_h^n, \mathbf{d}_h^n)$, hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}, \mathbf{d}_h^{n+1}) \in \mathbf{V}_h \times Q_h \times \mathbf{D}_h$ con $\mathbf{d}_h^{n+1}|_{\partial\Omega} = \mathbf{l}_h$ tal que

$$\begin{aligned} & \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\mathbf{u}_h^n \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \nu \left(\nabla \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ & + \lambda \left((\nabla \mathbf{d}_h^{n+1})^t \Delta \mathbf{d}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0 \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \\ & \left(\bar{p}_h, \nabla \cdot \mathbf{u}_h^{n+1} \right) = 0 \quad \forall \bar{p}_h \in Q_h, \\ & \left(\frac{\nabla(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)}{k}, \nabla \bar{\mathbf{d}}_h \right) - \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^{n+1}, \Delta \bar{\mathbf{d}}_h \right) + \gamma \left(\Delta \mathbf{d}_h^{n+1} - \mathbf{f}_\varepsilon(\mathbf{d}_h^{n+1}), \Delta \bar{\mathbf{d}}_h \right) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}, \end{aligned} \quad (12)$$

donde $\mathbf{V}_h \times Q_h \times \mathbf{D}_{0h}$ son aproximaciones de $\mathbf{H}_0^1 \times L_0^2 \times (\mathbf{H}^2 \cap \mathbf{H}_0^1)$. Además, se ha usado la identidad

$$\nabla \cdot (\nabla \mathbf{d} \odot \nabla \mathbf{d}) = \frac{1}{2} \nabla (|\nabla \mathbf{d}|^2) + (\nabla \mathbf{d})^t \Delta \mathbf{d},$$

donde el término de gradiente se absorbe en la presión modificada $p \sim p + \frac{1}{2} |\nabla \mathbf{d}|^2$.

Observar que (12) es una aproximación de la formulación variacional de la ecuación para el vector de orientación tomando como función test $-\Delta \bar{\mathbf{d}}_h$.

Se consiguen las siguientes estimaciones de error:

$$\begin{aligned} & \|\mathbf{u}_h^n - \mathbf{u}(t_n)\|_{L^2(\Omega)}^2 + \|\mathbf{d}_h^n - \mathbf{d}(t_n)\|_{H^1(\Omega)}^2 + k \sum_{m=0}^N \left(\|\mathbf{u}^m - \mathbf{u}(t_m)\|_{H^1(\Omega)}^2 + \|\mathbf{d}_h^m - \mathbf{d}(t_m)\|_{H^2(\Omega)}^2 \right) \\ & \leq C k^2 + C \|\mathbf{u}_h^0 - \mathbf{u}(0)\|_{L^2(\Omega)}^2 + C \|\mathbf{d}_h^0 - \mathbf{d}(0)\|_{H^1(\Omega)}^2 + C \max_{0 \leq m \leq N} \left[\inf_{\mathbf{v}_h \in \mathbf{V}_h} \|\mathbf{u}(t_m) - \mathbf{v}_h\|_{H^1(\Omega)}^2 \right. \\ & \left. + \inf_{p_h \in Q_h} \|p(t_m) - p_h\|_{L^2(\Omega)}^2 + \inf_{\mathbf{d}_h \in \mathbf{D}_h} \|\mathbf{d}(t_m) - \mathbf{d}_h\|_{H^2(\Omega)}^2 \right] \end{aligned}$$

donde la constante $C > 0$ depende del parámetro de penalización ε . Además se exhiben resultados numéricos sobre el buen comportamiento del esquema en la aniquilación de singulares (que son puntos $\mathbf{x} \in \Omega$ donde $|\mathbf{d}_0(\mathbf{x})| = 0$).

En un segundo trabajo [31], *C. Liu* y *J. N. Walkington* relajan la hipótesis $C^1(\bar{\Omega})$ para aproximar el vector de orientación por $C^0(\bar{\Omega})$ definiendo una formulación mixta para la ecuación (7)_c introduciendo la variable auxiliar $\mathbf{w} = \nabla \mathbf{d}$ con la que reescriben el sistema (10) en la forma:

$$\begin{cases} \mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \lambda (\nabla \mathbf{d})^t \nabla \cdot \mathbf{w} = \mathbf{0} & \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0, \quad \nabla \mathbf{d} = \mathbf{w} & \text{en } Q, \\ \mathbf{w}_t + \nabla \left((\mathbf{u} \cdot \nabla) \mathbf{d} - \gamma (\nabla \cdot \mathbf{w} - f_\varepsilon(\mathbf{d})) \right) = \mathbf{0} & \text{en } Q, \end{cases} \quad (13)$$

considerando las condiciones de contorno

$$\mathbf{u} = 0, \quad \mathbf{d} = \mathbf{l} \quad \text{sobre } \Sigma,$$

y las condiciones iniciales

$$\mathbf{w}(\mathbf{x}, 0) = \nabla \mathbf{d}_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega.$$

Hemos de hacer notar que $\Delta \mathbf{d} = \nabla \cdot \mathbf{w}$ y que no se ha reemplazado $\nabla \mathbf{d}$ por \mathbf{w} en los términos $\lambda (\nabla \mathbf{d})^t \nabla \cdot \mathbf{w}$ y $(\mathbf{u} \cdot \nabla) \mathbf{d}$. Se tiene la estabilidad del siguiente esquema no lineal, de tipo Euler totalmente implícito para la formulación débil de (13):

Etapa $n + 1$: Dado $(\mathbf{u}_h^n, \mathbf{w}_h^n, \mathbf{d}_h^n)$, calcular $(\mathbf{u}_h^{n+1}, p_h^{n+1}, \mathbf{w}_h^{n+1}, \mathbf{d}_h^{n+1}) \in (\mathbf{V}_h, Q_h, \mathbf{W}_h, \mathbf{D}_h)$,

$$\begin{aligned} & \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\mathbf{u}_h^n \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \nu \left(\nabla \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ & - \lambda \left((\nabla \mathbf{d}_h^{n+1})^t \nabla \cdot \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0, \end{aligned}$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0,$$

$$\left(\frac{\mathbf{w}_h^{n+1} - \mathbf{w}_h^n}{k}, \bar{\mathbf{w}}_h \right) - \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^{n+1}, \nabla \cdot \bar{\mathbf{w}}_h \right) + \gamma \left(\nabla \cdot \mathbf{w}_h^{n+1} - f_\varepsilon(\mathbf{d}_h^{n+1}), \nabla \cdot \bar{\mathbf{w}}_h \right) = 0,$$

$$\left(\nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{d}}_h \right) - \left(\nabla \cdot \mathbf{w}_h^{n+1}, \bar{\mathbf{d}}_h \right) = 0,$$

para todo $(\bar{\mathbf{u}}_h, \bar{p}_h, \bar{\mathbf{w}}_h, \bar{\mathbf{d}}_h) \in \mathbf{V}_h \times Q_h \times \mathbf{W}_h \times \mathbf{D}_{0h}$, con $\mathbf{D}_{0h} := \mathbf{D}_h \cap \mathbf{H}_0^1(\Omega)$. Las incógnitas velocidad, presión y vector de orientación son calculadas con espacios de elementos finitos de funciones globalmente continuas $\mathbf{V}_h \times Q_h \times \mathbf{D}_h$ aproximaciones de $\mathbf{H}_0^1(\Omega) \times L_0^2(\Omega) \times \mathbf{H}^1(\Omega)$ y \mathbf{W}_h se construye con un elemento finito de tipo Raviart-Thomas, aproximación de $\mathbf{H}(\Omega, \text{div})$.

En [31] se deducen las estimaciones de estabilidad:

$$\begin{aligned} & \|\mathbf{u}_h^n\|_{L^2(\Omega)} + \|\mathbf{w}_h^n\|_{L^2(\Omega)}^2 + k \sum_{m=1}^n \left(\nu \|\nabla \mathbf{u}_h^m\|_{L^2(\Omega)}^2 + \lambda \gamma \|\nabla \cdot \mathbf{w}_h^m\|_{L^2(\Omega)}^2 \right) \\ & \leq C(F_\varepsilon, \varepsilon) \left(\|\mathbf{u}_h^0\|_{L^2(\Omega)}^2 + \|\mathbf{w}_h^0\|_{L^2(\Omega)}^2 \right) + C(\mathbf{d}_0, F_\varepsilon, \varepsilon). \end{aligned}$$

y las tasas de convergencias:

$$\begin{aligned} & \max_{1 \leq n \leq N} \left\{ \|\mathbf{u}_h^n - \mathbf{u}(t_n)\|_{L^2(\Omega)} + \|\mathbf{w}_h^n - \nabla \mathbf{d}(t_n)\|_{H^1(\Omega)} \right\} \\ & + \left(k \sum_{n=0}^N \left(\|\mathbf{u}^n - \mathbf{u}(t_n)\|_{H^1(\Omega)}^2 + \|\nabla \cdot \mathbf{w}_h^n - \Delta \mathbf{d}(t_n)\|_{L^2(\Omega)}^2 \right) \right)^{1/2} \leq C(k + h^l) \end{aligned}$$

y

$$\max_{1 \leq n \leq N} \|\mathbf{d}_h^n - \mathbf{d}(t_n)\|_{H^1} \leq h^l,$$

bajo adecuadas hipótesis de regularidad para la solución continua $(\mathbf{u}, p, \mathbf{d})$ y los espacios discretos son tales que contienen polinomios de grado $\leq l$ para \mathbf{V}_h y \mathbf{D}_h , polinomios de grado $\leq l - 1$ para Q_h y, finalmente, \mathbf{W}_h se genera con elementos finitos $BDFM_l$, [11].

La introducción de la nueva variable $\mathbf{w} = \nabla \mathbf{d}$ incrementa el número de incógnitas y la complicación de la implementación del esquema.

En [19], *V. Girault* y *F. Guillén-González* introducen un esquema (lineal) con una variable auxiliar $\mathbf{w} = -\Delta \mathbf{d}$ para el problema penalizado (10). Dicho esquema resulta ser incondicionalmente estable y convergente, obteniéndose además estimaciones de error óptimas y convergencia de métodos iterativos para desacoplar el esquema en cada etapa de tiempo ya que éste resulta totalmente acoplado.

Primero, se considera \mathbf{l}_h^n una aproximación en el tiempo $t = t_n$ del dato de contorno de Dirichlet $\mathbf{l} = \mathbf{l}(\mathbf{x}, t)$ asociado al vector de orientación que se supone en esta ocasión dependiente de la variable temporal. Entonces, se define $\tilde{\mathbf{d}}_h^n \in \mathbf{D}_h$ como la solución del problema elíptico discreto siguiente:

$$\tilde{\mathbf{d}}_h^n|_{\partial\Omega} = \mathbf{l}_h^n \quad \text{y} \quad \left(\nabla \tilde{\mathbf{d}}_h^n, \nabla \mathbf{g}_h \right) = 0 \quad \forall \mathbf{g}_h \in \mathbf{D}_{0h}.$$

Inicialización: Sean $(\mathbf{u}_h^0, \mathbf{d}_h^0) \in (\mathbf{V}_h, \mathbf{D}_h)$ determinadas aproximaciones de $(\mathbf{u}_0, \mathbf{d}_0)$. Se define $\hat{\mathbf{d}}_h^0 \in \mathbf{D}_{0h}$ tal que $\mathbf{d}_h^0 = \hat{\mathbf{d}}_h^0 + \tilde{\mathbf{d}}_h^0$.

Etapas $n+1$: Dado $(\mathbf{u}_h^n, \hat{\mathbf{d}}_h^n) \in (\mathbf{V}_h, \mathbf{D}_{0h})$ (y $\mathbf{d}_h^n = \hat{\mathbf{d}}_h^n + \tilde{\mathbf{d}}_h^n$), encontrar $(\mathbf{u}_h^{n+1}, \mathbf{w}_h^{n+1}) \in \mathbf{V}_h \times \mathbf{W}_h$ y $(p_h^{n+1}, \hat{\mathbf{d}}_h^{n+1}) \in Q_h \times \mathbf{D}_{0h}$ (con $\mathbf{d}_h^{n+1} = \hat{\mathbf{d}}_h^{n+1} + \tilde{\mathbf{d}}_h^{n+1}$) solución del sistema lineal algebraico:

$$\begin{aligned} & \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\mathbf{u}_h^n \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \nu \left(\nabla \mathbf{u}^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ & - \lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0 \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_{0h}, \end{aligned}$$

$$\begin{aligned}
& \left(\bar{p}_h, \nabla \cdot \mathbf{u}_h^{n+1} \right) = 0, \quad \forall \bar{p}_h \in Q_{0h}, \\
& \left(\frac{\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n}{k}, \bar{\mathbf{w}}_h \right) + \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n, \bar{\mathbf{w}}_h \right) + \gamma \left(\mathbf{f}_\varepsilon(\mathbf{d}_h^n) + \mathbf{w}_h^{n+1}, \bar{\mathbf{w}}_h \right) = 0 \quad \forall \bar{\mathbf{w}}_h \in \mathbf{W}_h, \\
& \left(\nabla \widehat{\mathbf{d}}_h^{n+1}, \nabla \bar{\mathbf{d}}_h \right) - \left(\mathbf{w}_h^{n+1}, \bar{\mathbf{d}}_h \right) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h},
\end{aligned}$$

donde los espacios de elementos finitos usados para aproximar las incógnitas son:

$$\mathbf{X}_h \sim (\mathbb{P}_1 + \text{burbuja}) \text{ y } \mathbf{V}_h = \mathbf{X}_h \cap \mathbf{H}_0^1 \text{ (velocidad),}$$

$$L_h \sim \mathbb{P}_1 \text{ y } Q_h = L_h \cap L_0^2 \text{ (presión),}$$

$$\mathbf{W}_h \sim \mathbb{P}_0 \text{ (función auxiliar),}$$

$$\mathbf{D}_h \sim \mathbb{P}_1 \text{ y } \mathbf{D}_{0h} = \mathbf{D}_h \cap \mathbf{H}_0^1 \text{ (orientación de los cristales).}$$

Este esquema reduce los grados de libertad a calcular respecto a los esquemas anteriores de [30] y [31] para (10) lo que implica una coste computacional menor, además de ser un esquema lineal.

En [28], *P. Lin* y *C. Liu* proponen dos esquemas numéricos lineales usando elementos finitos $C^0(\bar{\Omega})$ y sin usar ninguna variable auxiliar para dominios bidimensionales, lo que reduce el coste computacional significativamente y facilita la implementación. Sin embargo, estos esquemas no son analizados desde el punto de vista de estabilidad y convergencia, o estimaciones de error, pero recuperan los resultados numéricos obtenidos en [30]. Los algoritmos son implementados con la ayuda del software *Freefem++*.

El primer esquema que se analiza en [28], desacopla el cálculo del par velocidad-presión y el vector de orientación considerando el término de acoplamiento del sistema de momentos de forma explícita y de forma semi-implícita el término de penalización. Así, el esquema en una etapa de tiempo $n + 1$ resulta:

Conocidos $(\mathbf{u}_h^n, p_h^n, \mathbf{d}_h^n)$, hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}, \mathbf{d}_h^{n+1}) \in \mathbf{V}_h \times Q_h \times \mathbf{D}_h$ con $\mathbf{d}_h^{n+1}|_{\partial\Omega} = \mathbf{l}_h$ tal que,

$$\begin{aligned}
& \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\mathbf{u}_h^n \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \nu \left(\nabla \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\
& - \lambda \left((\nabla \mathbf{d}_h^n)^t \nabla \mathbf{d}_h^n, \nabla \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0 \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \\
& \left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0 \quad \forall \bar{p}_h \in Q_h, \\
& \left(\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k}, \bar{\mathbf{d}}_h \right) + \left((\mathbf{u}_h^n \cdot \nabla) \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h \right) \\
& + \left(\nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{d}}_h \right) + \frac{\gamma}{\varepsilon^2} \left((|\mathbf{d}_h^n|^2 - 1) \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h \right) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h},
\end{aligned}$$

donde el espacio para la velocidad y el vector de orientación $(\mathbf{V}_h, \mathbf{D}_h)$ son elementos finitos cuadráticos y el espacio de la presión Q_h son polinomios lineales a trozos.

Para el segundo esquema de [28] se plantea una discretización de la derivada material usando el método de las características como sigue:

$$\begin{aligned} & \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n(\mathbf{X}_h^n)}{k}, \bar{\mathbf{u}}_h \right) + \nu (\nabla \mathbf{u}^{n+1}, \nabla \bar{\mathbf{u}}_h) \\ & - \lambda \left((\nabla \mathbf{d}_h^n)^t \nabla \mathbf{d}_h^n, \nabla \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0 \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \\ & \left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0 \quad \forall \bar{p}_h \in Q_h, \\ & \left(\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n(\mathbf{X}_h^{n+1})}{k}, \bar{\mathbf{d}}_h \right) + (\nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{d}}_h) + \frac{\gamma}{\varepsilon^2} \left((|\mathbf{d}_h^n|^2 - 1) \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h \right) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}, \end{aligned}$$

donde $\mathbf{X}_h^n := \mathbf{x} + k \mathbf{u}_h^n(\mathbf{x})$ y $\mathbf{X}_h^{n+1} := \mathbf{x} + k \mathbf{u}_h^{n+1}(\mathbf{x})$ (discretización de tipo Euler retrógrado en tiempo y actualización de la velocidad de la característica en el sistema para \mathbf{d}_h^{n+1} , dado el carácter secuencial del esquema, respectivamente) aproximando con los mismos espacios de elementos finitos $(\mathbf{V}_h, Q_h, \mathbf{D}_h)$ antes mencionados.

Por último en [13], *Q. Du, B. Guo* y *J. Shen*, usando aproximaciones de Fourier espectral, demuestran existencia de solución del modelo penalizado (10) y estimaciones de error para las aproximaciones de Fourier totalmente discretas junto con experiencias numéricas de aniquilación de singularidades. Este método es eficiente para dominios rectangulares y condiciones de frontera periódicas.

Cuando se trata de construir esquemas numéricos estables y convergentes hacia (7) a través del modelo penalizado, haciendo tender $\varepsilon \rightarrow 0$ junto con los parámetros discretos en espacio y tiempo (h, k) , nos encontramos principalmente con las siguientes dificultades: Obtener estimaciones de estabilidad independientes de ε , ya que no está claro que para los esquemas anteriormente descritos puedan obtenerse tales estimaciones. Se pierde la estimación H^2 para \mathbf{d} , que dificulta: primero, la compacidad en $\mathbf{L}^2(Q)$ para \mathbf{u} , que es la clave en el paso al límite en el sistema para \mathbf{d} , y segundo, la compacidad en $\mathbf{L}^2(Q)$ para $\nabla \mathbf{d}$, fundamental para pasar al límite en el sistema de momentos.

Modelo estático de campo de fase

Por último, estudiamos un modelo estático de campo de fase para un proceso de solidificación de una mezcla binaria con propiedades térmicas, en el cual veremos que algunas de las técnicas

desarrolladas en los modelos anteriores permiten el desarrollo numérico de esquemas para este modelo.

Un motivo por el cual los modelos de campo de fase son aceptados para tratar los fenómenos de solidificación, es que cubren situaciones más generales que el clásico modelo de Stefan de frontera libre. El modelo de Stefan gobierna la interfase sólido-líquido suponiéndola que es una hipersuperficie suave con posición desconocida y las ecuaciones son formuladas en cada una de las fases independientemente, basadas en principios de conservación y una condición extra impuesta a la interfase (llamada condición de Stefan).

Los modelos de campo de fase son usados en tratamientos de fenómenos tales como crecimiento de cristales, en la fusión y en el ensamblamiento de materiales. El carácter anisótropo de algunos modelos lo hace una herramienta poderosa para el estudio de situaciones con estructuras complejas de crecimiento como son el crecimiento de dendritas en las neuronas. Aplicaciones industriales como la fabricación de nuevos materiales llevan un proceso de campo de fase asociado.

Supongamos $\Omega \subseteq \mathbb{R}^d$ ($d = 2$ ó 3) una región abierta acotada con frontera Γ . Consideramos el modelo diferencial de campo de fase:

$$\begin{cases} \alpha \varepsilon^2 \phi_t - \varepsilon^2 \Delta \phi = -f(\phi) + \beta(\theta - \theta_{Ac} - \theta_B(1 - c)) & \text{en } Q, \\ C_V \theta_t + \frac{l}{2} \phi_t = \nabla \cdot [K_1(\phi) \nabla \theta] & \text{en } Q, \\ c_t = K_2(\Delta c + M \nabla \cdot [c(1 - c) \nabla \phi]) & \text{en } Q, \end{cases} \quad (14)$$

donde f es la derivada de una función potencial que toma sus mínimos globales en ± 1 . Un ejemplo clásico es

$$f(\phi) = \nabla_\phi F(\phi) \quad \text{con} \quad F(\phi) = \frac{1}{4}(\phi^2 - 1)^2.$$

La ecuación (14)_a es una ecuación de Ginzburg-Landau/Allen-Cahn que gobierna la difusión de la fase sólida, la ecuación (14)_b plantea el balance de energía en la interfase, se conoce como ecuación de Stefan y por último (14)_c representa la conservación de la masa de sistema.

La incógnitas para este modelo son: $\phi : Q \rightarrow \mathbb{R}$ (campo de fase) es la variable estado que caracteriza las diferentes fases de modo que $\phi = 1$ representa la fase líquida y $\phi = -1$ representa la fase sólida, $\theta : Q \rightarrow \mathbb{R}$ es la temperatura de la mezcla, $c : Q \rightarrow [0, 1]$ (concentración) representa la fracción de uno de los dos materiales en la mezcla. El parámetro $\alpha > 0$ es el tiempo de relajación (tiempo característico que tarda el sistema en volver de un estado de energía más elevado a un estado de equilibrio de energía inferior); el parámetro β es dado por $\beta = \varepsilon[s]/3\sigma$,

donde $\varepsilon > 0$ es la medida del grosor de la interfase, σ es la tensión superficial y $[s]$ es la diferencia de la densidad de la entropía entre las fases (mide la parte de la energía que no puede utilizarse para producir el cambio de fase); $C_V > 0$ es el calor específico (indica la mayor o menor dificultad que presenta la mezcla para experimentar cambios de temperatura bajo el suministro de calor); la constante $l > 0$ es el calor latente (calor absorbido por la mezcla en el cambio de fase); θ_A, θ_B son las respectivas temperaturas de fusión de cada una de los dos materiales en la mezcla; $K_2 > 0$ es la difusión del soluto; M es una constante relativa a las pendientes de las líneas de sólido y líquido; $K_1 = K_1(\phi)$ modela la conductividad térmica.

Se supone que $K_1 = K_1(\phi)$ es una función continua tal que existe $b > 0$ con $0 \leq K_1(r) \leq b$ para todo $r \in \mathbb{R}$.

Este modelo es completado con las condiciones fronteras de tipo Neumann homogéneas

$$\left. \frac{\partial \phi}{\partial \mathbf{n}} \right|_{\Sigma} = 0, \quad (K_1(\phi) \nabla \theta) \cdot \mathbf{n} \Big|_{\Sigma} = 0, \quad \left. \frac{\partial c}{\partial \mathbf{n}} \right|_{\Sigma} = 0 \quad (15)$$

y las condiciones iniciales

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \quad \theta(\mathbf{x}, 0) = \theta_0(\mathbf{x}), \quad c(\mathbf{x}, 0) = c_0(\mathbf{x}) \quad \mathbf{x} \in \Omega. \quad (16)$$

En los últimos años los modelos de cambio de fase han generados una enorme cantidad de literatura. Las principales dificultades de (14)-(16) son: determinar la posición y la deformación de la interfase entre las dos componentes, la verificación de un principio del máximo para la variable concentración y la singularidad de la ecuación de la temperatura al ser $K_1 \geq 0$.

En [4], *J. L. Boldrini* y *G. Planas* prueban la existencia de una solución débil para (14) vía la introducción de problemas aproximados regularizantes, seguido por la obtención de estimaciones adecuadas y la aplicación de argumentos de compacidad.

En [16], *X. Feng* y *A. Prohl* consideran un modelo más simple que (14), donde no se considera la ecuación para la concentración:

$$\begin{cases} \varepsilon \alpha(\varepsilon) \phi_t - \varepsilon \Delta \phi = \frac{1}{\varepsilon} (\phi - (\phi)^3) + \beta(\varepsilon) \theta & \text{en } Q, \\ C_V(\varepsilon) \theta_t - \Delta \theta = -\phi_t & \text{en } Q. \end{cases}$$

Aquí, el tiempo de relajación $\alpha = \alpha(\varepsilon)$ y el calor específico $C_V = C_V(\varepsilon)$ dependen del ancho de la interfase ε y la conductividad térmica K_1 se toma constante (e igual a uno). En [16] se analiza el siguiente esquema numérico no lineal totalmente discreto para X_h una aproximación conforme de $H^1(\Omega)$.

Etapa $n + 1$: Dado $(\phi_h^n, \theta_h^n) \in X_h \times X_h$.

Hallar $\phi_h^{n+1} \in X_h$ como la solución del problema:

$$\begin{aligned} & \alpha \varepsilon^2 \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) + \varepsilon^2 (\nabla \phi_h^{n+1}, \nabla x_h) + ((\phi_h^{n+1})^3, x_h) \\ & = (\phi_h^n, x_h) + \varepsilon \beta(\varepsilon) (\theta_h^n, x_h), \quad \forall x_h \in X_h. \end{aligned}$$

Hallar $\theta_h^{n+1} \in X_h$ como la solución del problema variacional desacoplado:

$$C_V \left(\frac{\theta_h^{n+1} - \theta_h^n}{k}, x_h \right) + (\nabla \theta_h^{n+1}, \nabla x_h) = -\frac{l}{2} \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right), \quad \forall x_h \in X_h.$$

Para este esquema se obtienen estimaciones de error optimales prestando especial atención en la dependencia del parámetro ε . En particular, se muestran cotas de error que dependen sólo de forma polinomial de $\frac{1}{\varepsilon}$ cuando ε es pequeño.

Finalmente, las estimaciones de error son usadas para establecer la convergencia de las soluciones discretas hacia soluciones de interfase límite singulares del modelo de campo de fase, cuando $\varepsilon \rightarrow 0$, bajo diferentes escalas de los coeficientes.

En [6], *J. L. Boldrini* y *C. Vaz* proponen un esquema semi-discreto en tiempo no lineal considerando únicamente la ecuación para la temperatura tomando $K_1(\phi) = \kappa > 0$ y reemplazando la fracción de masa sólida $\frac{l}{2}\phi_t$ por $\frac{l}{2}g_s(\theta, \phi)_t$ y la ecuación para el campo de fase eligiendo como potencial $f(\phi) = a(\mathbf{x})\phi + b(\mathbf{x})\phi^2 - \phi^3$, donde $a(\mathbf{x})$ y $b(\mathbf{x})$ son funciones conocidas en $L^\infty(\Omega)$. Además, $g_s \in C_b^{1,1}(\mathbb{R}^2)$ tal que $0 \leq g_s(y, z) \leq 1$ para todo $(y, z) \in \mathbb{R}^2$ y tal que para cada z la función $y \mapsto g_s(y, z)$ es no decreciente.

Etapa $n + 1$: Dado $(\phi^n, \theta^n) \in H^2(\Omega) \times H^2(\Omega)$.

Hallar $(\phi^{n+1}, \theta_h^{n+1}) \in H^2(\Omega) \times H^2(\Omega)$ como la solución del problema acoplado:

$$\begin{aligned} \frac{\phi^{n+1} - \phi^n}{k} - \alpha \Delta \phi^{n+1} - a(\mathbf{x})\phi^{n+1} - b(\mathbf{x})(\phi^{n+1})^2 + (\phi^{n+1})^3 + \theta^{n+1} &= 0 \quad \text{en } \Omega, \\ \frac{\theta^{n+1} - \theta^n}{k} + \kappa \Delta \theta^{n+1} + \frac{l}{2} \frac{g_s(\theta^{n+1}, \phi^{n+1}) - g_s(\theta^n, \phi^n)}{k} &= 0 \quad \text{en } \Omega, \\ \theta^{n+1} = 0, \quad \frac{\partial \phi^{n+1}}{\partial n} &= 0 \quad \text{sobre } \Gamma. \end{aligned}$$

Se prueba convergencia de las soluciones semi-discretas hacia una solución débil y resultados de regularidad de la solución obtenida.

En [7], *E. Burman*, *D. Kessler* y *J. Rappaz* muestran estimaciones de error de un esquema no lineal para un modelo general isoterma de campo de fase anisótropo para mezclas binarias:

$$\begin{cases} \phi_t - \nabla \cdot (A(\nabla \phi) \nabla \phi) - S(c, \phi) = 0 & \text{en } Q, \\ c_t - \nabla \cdot (D_1(\phi) \nabla c + D_2(c, \phi) \nabla \phi) = 0 & \text{en } Q, \end{cases}$$

junto con las condiciones fronteras

$$A(\nabla\phi)\nabla\phi \cdot \mathbf{n} = 0 \quad \text{y} \quad (D_1(\phi)\nabla c + D_2(c, \phi)\nabla\phi) \cdot \mathbf{n} = 0 \quad \text{sobre} \quad \Gamma$$

donde A es la matriz anisótropa, $S = S(c, \phi)$, $D_1 = D_1(\phi)$ y $D_2 = D_2(c, \phi)$ son funciones continuas y lipschitzinas, con primeras derivadas respecto de ϕ y c uniformemente acotadas y satisfacen $S(c, 0) = S(c, 1) = 0$, $0 < D_s \leq D_1(\phi) < D_l < \infty$ y $D_2(c, \phi) = 0$ para $c = 0, 1$ y $\phi = 0, 1$.

En [26], *D. Kessler* y *J. F. Scheid* demuestran estimaciones de error de un esquema totalmente discreto no lineal asociado al modelo general isoterma de campo de fase isótropo para mezclas binarias:

$$\begin{cases} \phi_t = M\Delta\phi + F_1(\phi) + cF_2(\phi) & \text{en } Q, \\ c_t = \nabla \cdot (D_1(\phi)\nabla c + D_2(c, \phi)\nabla\phi) & \text{en } Q. \end{cases}$$

En [33] y [5], *J. L. Boldrini* and *G. Planas* demuestran la existencia de solución débil global bi y tridimensional, respectivamente, para un modelo de campo de fase con fluido no estático para un proceso de mezcla binaria con propiedades térmicas. Se trata del modelo (14) acoplado con una ecuación de Navier-Stokes la cual modela el movimiento de la parte fluida de la mezcla:

$$\left\{ \begin{array}{ll} \mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nu\Delta\mathbf{u} + \nabla p + k(g_s(\phi))\mathbf{u} = \mathbf{f} & \text{en } Q_{ml}, \\ \nabla \cdot \mathbf{u} = 0 & \text{en } Q_{ml}, \\ \mathbf{u} = 0 & \text{en } Q_s, \\ \alpha\varepsilon^2\phi_t + \alpha\varepsilon^2\mathbf{u} \cdot \nabla\phi - \varepsilon^2\Delta\phi \\ -\frac{1}{2}(\phi - (\phi)^3) - \beta(\theta - \theta_{Ac} - \theta_B(1 - c)) = 0 & \text{en } Q, \\ C_V\theta_t + C_V\mathbf{u} \cdot \nabla\theta - \frac{l}{2}\phi_t - \nabla \cdot [K_1(\phi)\nabla\theta] = 0 & \text{en } Q, \\ c_t + \mathbf{u} \cdot \nabla c K_2(\Delta c + M\nabla \cdot [c(1 - c)\nabla\phi]) = 0 & \text{en } Q. \end{array} \right.$$

El dominio Q se descompone en tres regiones Q_s , Q_m y Q_l . La primera región representa la parte totalmente sólida, la segunda es la parte blanda o mixta y la tercera es la parte totalmente líquida. Estas regiones se describen en función de g_s (fracción sólida) como:

$$Q_s = \{(\mathbf{x}, t) \in Q : g_s(\phi(\mathbf{x}, t)) = 1\},$$

$$Q_m = \{(\mathbf{x}, t) \in Q : 0 < g_s(\phi(\mathbf{x}, t)) < 1\},$$

$$Q_l = \{(\mathbf{x}, t) \in Q : g_s(\phi(\mathbf{x}, t)) = 0\}$$

y $Q_{ml} = Q_j \cup Q_m$ se refiere a la zona no sólida que gobierna la ecuación de tipo *Navier-Stokes*.

Este modelo es un problema de frontera libre donde hay que determinar para cada tiempo $t \in [0, T]$

$$\Omega_{ml}(t) = \{\mathbf{x} \in \Omega : 0 \leq g_s(\phi(\mathbf{x}, t)) < 1\}$$

bajo las condiciones fronteras

$$\frac{\partial \phi}{\partial \mathbf{n}} \Big|_{\Sigma} = 0, \quad \frac{\partial \theta}{\partial \mathbf{n}} \Big|_{\Sigma} = 0, \quad \frac{\partial c}{\partial \mathbf{n}} \Big|_{\Sigma} = 0, \quad \mathbf{v} = 0 \text{ sobre } \partial Q_{ml}$$

y las condiciones iniciales

$$\phi(0) = \phi_0, \quad \theta(0) = \theta_0, \quad c(0) = c_0 \quad \text{en } \Omega, \quad \mathbf{v}(0) = \mathbf{v}_0 \text{ en } \Omega_{ml}(0).$$

Para este modelo se asumen las hipótesis:

- k es una función no decreciente de clase $C^1([0, 1])$ con $k(0) = 0$ y $\lim_{x \rightarrow 1^-} k(x) = +\infty$.
- g_s y g'_s son funciones continuas y Lipschitzianas definidas en \mathbb{R} y satisfaciendo $0 \leq g_s(r) \leq 1$ para $r \in \mathbb{R}$.
- K_1 es una función continua y Lipschitziana definida en \mathbb{R} tal que $0 < a \leq K_1(r) \leq b$, $\forall r \in \mathbb{R}$,
- \mathbf{f} es dada en $L^2(Q)$.

Principales aportaciones originales de la Memoria

A continuación, describiremos los principales resultados de esta tesis. La tesis está compuesta de 7 capítulos de los cuales 4 de ellos están destinados al modelo de Kazhikov-Smagulov, el quinto trata un problema de cristales líquidos nemáticos, el sexto sobre un modelo de campo de fase, y, en el séptimo y último, presentamos algunas simulaciones numéricas concernientes al problema de cristales nemáticos.

Capítulo 1

El primer capítulo tiene como objetivo desarrollar un esquema numérico totalmente discreto (en espacio y tiempo) para aproximar la única solución débil del modelo de Kazhikov-Smagulov (1) en dominios bidimensionales. De hecho, el esquema propuesto es el primero que conocemos para (1) que se analiza desde el punto de vista de estabilidad y convergencia hacia una solución débil cualquiera del modelo, a diferencia del esquema presentado para un modelo más general que (1) en [15], donde se estudia desde la perspectiva de estimaciones de error respecto de una solución suficientemente regular. La filosofía de la discretización es:

- considerar elementos finitos continuos de grado 1 para aproximar la densidad a pesar de que ésta tendrá regularidad H^2 , evitando usar elementos finitos globalmente $C^1(\bar{\Omega})$.
- usar una variable auxiliar (que no aparece explícitamente en el esquema) para “capturar” a nivel discreto algunas propiedades de la regularidad H^2 de la densidad,
- considerar un par elementos finitos estables para el par velocidad-presión.

Entonces, si elegimos una partición uniforme de $[0, T]$ de parámetro $k = T/N$, ($t_n = nk$), con $N \in \mathbb{N}$ y espacios de elementos finitos a lo más de funciones globalmente continuas $(W_h, \mathbf{V}_h, M_h) \subset H^1 \times \mathbf{H}_0^1 \times L_0^2$ para la densidad, la velocidad y la presión respectivamente, proponemos el siguiente esquema:

Inicialización: Fijamos el par $(\rho_h^0, \mathbf{u}_h^0) \in W_h \times \mathbf{V}_h$ determinadas aproximaciones de (ρ_0, \mathbf{u}_0) , cuando $h \rightarrow 0$.

Etapa $n + 1$: Dado $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Encontrar $\rho_h^{n+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + (\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h) + \lambda (\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h) = 0. \quad (17)$$

2. Encontrar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1}, \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h), \end{array} \right. \quad (18)$$

$$(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h) = 0, \quad (19)$$

donde definimos

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu (\nabla \mathbf{u}, \nabla \mathbf{v}) + \lambda \int_{\Omega} \left(\frac{M+m}{2} - \rho \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} \, d\mathbf{x}$$

$$c(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \frac{1}{2} \left[((\mathbf{u} \cdot \nabla) \mathbf{v}, \mathbf{w}) - ((\mathbf{u} \cdot \nabla) \mathbf{w}, \mathbf{v}) \right],$$

y dada $w_h \in W_h$ se define $[w_h]_T \in W_h$ tal que:

$$[w_h]_T(\mathbf{x}_i) = \begin{cases} w_h(\mathbf{x}_i) & \text{si } w_h(\mathbf{x}_i) \in [m, M], \\ m & \text{si } w_h(\mathbf{x}_i) < m, \\ M & \text{si } w_h(\mathbf{x}_i) > M, \end{cases}$$

donde \mathbf{x}_i son los nodos de la malla \mathcal{T}_h .

El esquema (17)-(19) ha sido diseñado siguiendo la idea de un esquema en tiempo de tipo Euler retrógrado, implícito en difusión y semi-implícito en convección para la velocidad y explícito para la densidad (e implícito para el resto de términos), donde al sistema de momentos le hemos añadido los términos estabilizadores

$$\frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n, \nabla(\bar{\mathbf{u}}_h \cdot \mathbf{u}_h^{n+1}) \right) + \frac{\lambda}{2} \left(\nabla \rho_h^{n+1}, \nabla(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right), \quad (20)$$

$$\lambda \int_{\Omega} \frac{M+m}{2} (\nabla \mathbf{u}_h^{n+1})^t : (\nabla \bar{\mathbf{u}}_h) dx. \quad (21)$$

Los términos de (20) están directamente relacionados con la ecuación de la densidad, y el término de (21) con la ecuación de incompresibilidad.

Otra peculiaridad de este esquema es la aproximación del término $\rho(t_{n+1})\mathbf{u}_t(t_{n+1})$ por el cociente $\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}$ en lugar de $\rho_h^{n+1} \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}$ que sería en principio un cálculo más actualizado. Esta elección queda justificada considerando en los dos primeros términos de (18) la función test $\bar{\mathbf{u}}_h = \mathbf{u}_h^{n+1}$, llegando

$$\begin{aligned} & \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \mathbf{u}_h^{n+1} \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \mathbf{u}_h^{n+1} \right) \\ &= \frac{1}{2k} \left(\|\sqrt{[\rho_h^{n+1}]_T} \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 - \|\sqrt{[\rho_h^n]_T} \mathbf{u}_h^n\|_{L^2(\Omega)}^2 + \|\sqrt{[\rho_h^n]_T} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)\|_{L^2(\Omega)}^2 \right), \end{aligned} \quad (22)$$

que es una versión discreta de la igualdad en continuo

$$\left(\rho \frac{d}{dt} \mathbf{u}, \mathbf{u} \right) + \frac{1}{2} \left(\frac{d}{dt} \rho, \mathbf{u} \cdot \mathbf{u} \right) = \frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2.$$

La presencia del operador de truncamiento por nodos $[\cdot]_T$, aplicado a determinadas densidades que aparecen en el sistema de momentos discreto (18), garantiza estimaciones puntuales y positividad, que por otra parte no podemos verificar para la densidad discreta directamente. La positividad de las densidades discretas truncadas $[\rho_h^n]_T$ y $[\rho_h^{n+1}]_T$ estabiliza los términos relacionados con las derivadas temporales en el sistema de momentos discreto, gracias a (22).

Desde el punto de vista de la implementación, la discretización temporal elegida nos proporciona un esquema secuencial donde en cada etapa de tiempo hay que resolver dos sistemas lineales cuadrados desacoplados, el primero relacionado con una ecuación de difusión discreta para la densidad y segundo con un problema de Stokes discreto en formulación mixta velocidad-presión, además del cálculo de la densidad discreta truncada.

Para asegurar buenas propiedades de estabilidad y convergencia para este esquema, consideramos las siguientes condiciones de regularidad para los datos, aproximación de los espacios discretos y regularidad de la frontera del dominio:

(H1) O bien

$$\mathbf{u}_0 \in \mathbf{H}, \rho_0 \in H^1(\Omega) \quad \text{y} \quad \mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega)) \quad \text{para } p > 1 \quad \text{con } k/h^2 \leq C,$$

o bien

$$\mathbf{u}_0 \in \mathbf{V}, \rho_0 \in H_N^2(\Omega), \quad \text{y} \quad \mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega)) \quad \text{para algún } p > 1.$$

(H2) La frontera de Ω es poligonal tal que se tiene la condición de dependencia continua en norma H^2 del problema de *Poisson-Neumann*.

(H3) La triangulación de Ω y los espacios discretos verifican:

- Las desigualdades inversas:

$$\begin{aligned} \|\nabla \bar{\rho}_h\|_{L^4(\Omega)} &\leq C h^{-1/2} |\nabla \bar{\rho}_h|, \quad \forall \bar{\rho}_h \in W_h, \\ \|\nabla \bar{\rho}_h\|_{L^2(\Omega)} &\leq C h^{-1} \|\bar{\rho}_h\|_{L^2(\Omega)}, \quad \forall \bar{\rho}_h \in W_h, \end{aligned}$$

- Los errores de interpolación:

$$\|\bar{\rho} - I_h \bar{\rho}\|_{H^1(\Omega)} + h^{1/2} \|\bar{\rho} - I_h \bar{\rho}\|_{W^{1,4}(\Omega)} \leq C h \|\bar{\rho}\|_{H^2(\Omega)}, \quad \forall \bar{\rho} \in H^2(\Omega),$$

$$\|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{H^1(\Omega)} \leq C h \|\bar{\mathbf{u}}\|_{H^2(\Omega)}, \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$\|\bar{p} - K_h \bar{p}\|_{L^2(\Omega)} \leq C h \|\bar{p}\|_{H^1(\Omega)}, \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega),$$

donde J_h , K_h y I_h son operadores de interpolaciones de $\mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ en \mathbf{V}_h , $H^1(\Omega) \cap L_0^2(\Omega)$ en M_h y $H^2(\Omega)$ en W_h respectivamente.

(H4) La condición Inf-sup. Existe una constante $\beta > 0$ (independiente de h) tal que $\forall \bar{p}_h \in M_h$

$$\|\bar{p}_h\|_{L_0^2(\Omega)} \leq \beta \sup_{\bar{\mathbf{u}}_h \in \mathbf{V}_h \setminus \{0\}} \frac{(\bar{p}_h, \nabla \cdot \bar{\mathbf{u}}_h)}{\|\bar{\mathbf{u}}_h\|_{H_0^1(\Omega)}}$$

En las condiciones anteriores encontramos que el esquema numérico (17)-(19) verifica las siguientes estimaciones de estabilidad:

Lema 1 Si $\lambda < 2\mu(M - m)^{-1}$ entonces, la solución del esquema discreto (17), (18)-(19) satisface las siguientes estimaciones:

$$\begin{aligned} \text{i)} \max_{0 \leq n \leq N} \|\mathbf{u}_h^n\|_{L^2(\Omega)} &\leq C, & \text{ii)} k \sum_{n=0}^N \|\nabla \mathbf{u}_h^n\|_{L^2}^2 &\leq C, & \text{iii)} \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n\|_{L^2(\Omega)}^2 &\leq C, \\ \text{iv)} \max_{0 \leq n \leq N} \|\nabla \rho_h^n\|_{L^2(\Omega)} &\leq C, & \text{v)} k \sum_{n=0}^N \|\nabla \rho_h^n\|_{L^4(\Omega)}^4 &\leq C, & \text{vi)} \sum_{n=0}^{N-1} \|\nabla(\rho_h^{n+1} - \rho_h^n)\|_{L^2(\Omega)}^2 &\leq C, \end{aligned}$$

con $C > 0$ independiente de k y h .

La hipótesis $\lambda < 2\mu(M - m)^{-1}$ no se debe al diseño del propio esquema numérico, ya se imponía en el resultado de existencia de solución débil de (4).

La clave para obtener las estimaciones para la densidad discreta es usar la versión discreta de la desigualdad de tipo *Gagliardo-Nirenberg* para dominios $2D$

$$\|\nabla \rho\|_{L^4(\Omega)} \leq C \|\nabla \rho\|_{L^2(\Omega)}^{1/2} \|\Delta \rho\|_{L^2(\Omega)}^{1/2},$$

en lugar de la desigualdad de interpolación (que se usa en los resultados analíticos)

$$\|\nabla \rho\|_{L^4(\Omega)} \leq C \|\rho\|_{L^\infty(\Omega)}^{1/2} \|\Delta \rho\|_{L^2(\Omega)}^{1/2},$$

para eludir la necesidad de tener estimaciones puntuales para la densidad discreta (que por otra parte no se pueden asegurar). Para la versión discreta de esta desigualdad, se considera el laplaciano discreto $-\Delta_h \rho_h^{n+1}$ definido como

$$-\Delta_h \rho_h^{n+1} \in W_h \quad \text{tal que} \quad - \left(\Delta_h \rho_h^{n+1}, \bar{\rho}_h \right) = \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) \quad \forall \bar{\rho}_h \in W_h. \quad (23)$$

En la demostración del Lema 1 conseguimos la estimación del laplaciano discreto

$$k \sum_{n=0}^{N-1} \|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}^2 \leq C,$$

que implicará la estimación **v)** del Lema 1 de tipo $\ell^4(W^{1,4}(\Omega))$.

Como es habitual en estos tipos de problemas no lineales, precisamos de la convergencia fuerte de las aproximaciones para identificar el límite de los términos no lineales, cuando los parámetros de discretización (h, k) van a cero.

Para la densidad discreta, la compacidad en $L^\infty(0, T; L^p(\Omega))$ con $1 \leq p < \infty$ vendrá dada como resultado de la acotación de la derivada discreta en tiempo

$$k \sum_{n=0}^N \left\| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right\|_{L^2(\Omega)}^2 \leq C.$$

Una consecuencia directa de esta estimación y de las propiedades del operador de truncamiento discreto $[\cdot]_T$ restringido a elementos finitos localmente \mathbb{P}_1 , es la estimación

$$k \sum_{n=0}^N \left\| \frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k} \right\|_{L^2(\Omega)}^2 \leq C, \quad (24)$$

que será necesaria para pasar al límite en el segundo término de (18).

Por último, se mejora la convergencia fuerte de la densidad discreta hasta $L^2(0, T; H^1(\Omega))$ a través de la ecuación del laplaciano discreto (23). Con tal compacidad pasaremos al límite en el término de la forma trilineal $c(\cdot, \cdot, \cdot)$ que involucra $\nabla \rho_h^{n+1}$.

La estimación de la derivada discreta en tiempo para la densidad truncada (24) jugará un papel crucial en la consecución de la compacidad de la velocidad discreta, basada en la siguiente acotación de una derivada en tiempo discreta de tipo fraccionaria:

$$k \sum_{m=0}^{N-r} \left\| \sqrt{[\rho_h^{m+r}]_T} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right\|_{L^2(\Omega)}^2 \leq C (rk)^{1/2}, \quad \forall r : 0 \leq r \leq N.$$

El procedimiento para probar esta acotación difiere del modo analítico-continuo hecho en [9], en que primero no conseguimos un principio del máximo y segundo no tenemos a nuestra disposición la ecuación de la densidad discreta de forma puntual para escribir el sistema de momentos en forma conservativa, que se usa para conformar la estimación de dicha derivada fraccionaria.

De las estimaciones a priori de la velocidad discreta en $L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega))$ junto con esta estimación fraccionaria para la velocidad, podemos aplicar de nuevo un resultado de compacidad de tipo *Aubin-Lions*, obteniendo convergencia fuerte en $\mathbf{L}^2(Q)$ de la velocidad.

La pregunta que sigue a la compacidad de la densidad y de la velocidad es qué hay acerca de la convergencia fuerte de la densidad discreta truncada (para pasar al límite en la forma trilineal $a(\cdot, \cdot, \cdot)$) y si converge a quién converge. La respuesta vendrá dada pasando al límite en la ecuación de la densidad discreta, encontrando que la densidad límite, ρ , tiene regularidad $\rho \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega))$ y verifica puntualmente la correspondiente ecuación de convección-difusión, con lo que se obtiene un principio del máximo $0 < m \leq \rho(\mathbf{x}, t) \leq M < \infty$ en casi todo $(\mathbf{x}, t) \in Q$, y usando que el operador de truncamiento por nodos $[\cdot]_T$ es un operador continuo de $L^2(Q)$ en $L^2(Q)$.

En resumidas cuentas, definiendo en $[0, T]$ las funciones auxiliares $\mathbf{u}_{k,h}, \rho_{h,k}$ constantes por subintervalos tal que $\mathbf{u}_{h,k}, \rho_{h,k}|_{(t_{n-1}, t_n]} = \mathbf{u}_h^n, \rho_h^n$ respectivamente, llegamos al resultado de convergencia:

Teorema 2 Si $\lambda < 2\mu(M - m)^{-1}$, entonces toda la sucesión $(\mathbf{u}_{h,k}, \rho_{h,k})$ converge hacia la (única) solución débil (\mathbf{u}, ρ) del problema (1) en el siguiente sentido: en $L^2(0, T; \mathbf{L}^2(\Omega) \times H^1(\Omega))$ fuerte, en $L^\infty(0, T; \mathbf{L}^2(\Omega) \times H^1(\Omega))$ débil- \star y en $L^2(0, T; \mathbf{H}_0^1(\Omega)) \times L^4(0, T; W^{1,4}(\Omega))$ débil.

Una variante del modelo *Kazhikhov-Smagulov*, donde los resultados anteriormente descritos nos proporcionan las herramientas necesarias para desarrollar esquemas numéricos incondicionalmente estables y convergentes, resulta cambiando la difusión lineal $-\mu\Delta\mathbf{u}$ por una difusión no lineal de tipo $-\lambda\nabla(\rho\nabla\mathbf{u})$ en el sistema de momentos. Luego, el sistema diferencial a considerar se describe como:

$$\begin{cases} \rho\mathbf{u}_t + ((\rho\mathbf{u} - \lambda\nabla\rho) \cdot \nabla)\mathbf{u} - \nabla \cdot (\mu\nabla\mathbf{u} - \lambda\rho(\nabla\mathbf{u})^t) + \nabla p = \rho\mathbf{f} & \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0 & \text{en } Q, \quad \rho_t + \mathbf{u} \cdot \nabla\rho - \lambda\Delta\rho = 0 & \text{en } Q, \end{cases}$$

junto con las condiciones mismas de contorno e iniciales.

Este tipo de modelo está relacionado con modelos de polución [8, 9].

El esquema que proponemos se obtiene siguiendo la línea del esquema numérico anterior, donde hemos sustituido el término estabilizador del sistema de momentos

$$-\lambda \int_{\Omega} \frac{M+m}{2} (\nabla\mathbf{u}_h^{n+1})^t : \nabla\bar{\mathbf{u}}_h \, dx$$

por el término $\frac{\lambda m}{2} (\nabla \cdot \mathbf{u}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h)$. Además, se ha truncado la densidad que aparece acoplada a la difusión. Así, llegamos al esquema numérico en la etapa $n+1$:

Dado $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Encontrar $\rho_h^{n+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + (\mathbf{u}_h^n \cdot \nabla\rho_h^n, \bar{\rho}_h) + \lambda(\nabla\rho_h^{n+1}, \nabla\bar{\rho}_h) = 0. \quad (25)$$

2. Encontrar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\begin{cases} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + \tilde{a}([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1}\mathbf{u}_h^n - \lambda\nabla\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h), \end{cases} \quad (26)$$

$$(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h) = 0, \quad (27)$$

donde

$$\tilde{a}(\rho, \mathbf{u}, \mathbf{v}) = \lambda \left(\rho (\nabla \mathbf{u} - (\nabla \mathbf{u})^t), \nabla \mathbf{v} \right) + \lambda m \left(\nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v} \right).$$

Para dar sentido al término estabilizador $\lambda m \left(\nabla \cdot \mathbf{u}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right)$, se parte primero de la igualdad

$$\int_{\Omega} \rho \left(|\nabla \mathbf{u}|^2 - (\nabla \mathbf{u})^t : \nabla \mathbf{u} \right) d\mathbf{x} = \int_{\Omega} \rho |\mathbf{rot} \mathbf{u}|^2 d\mathbf{x}.$$

y segundo de

$$\int_{\Omega} |\nabla \mathbf{u}|^2 d\mathbf{x} = \int_{\Omega} |\nabla \cdot \mathbf{u}|^2 + \int_{\Omega} |\mathbf{rot} \mathbf{u}|^2 d\mathbf{x}.$$

Por lo tanto,

$$\tilde{a}([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{n+1}) \geq m\lambda \|\nabla \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2.$$

Usando esta acotación inferior para $\tilde{a}(\cdot, \cdot, \cdot)$, del mismo tipo que para la forma trilineal para el modelo anterior $a(\cdot, \cdot, \cdot)$, se puede ver que todos los enunciados anteriormente descritos son válidos para el esquema (25)-(27).

Capítulo 2

El segundo capítulo de esta tesis concierne al estudio numérico del modelo de difusión de masa (1) en su versión tridimensional. Una de las claves del éxito de los esquemas bidimensionales, radica en el cambio de desigualdad de interpolación, diferente a la que se utiliza en los resultados teóricos que requiere un principio del máximo para obtener las estimaciones fuerte de la densidad. Pero esta interpolación es exclusiva del caso bidimensional, luego tenemos que cambiar de estrategia en dimensión tres.

Ahora el análisis teórico del modelo nos dicta el camino a seguir, obtener un principio del máximo discreto para la densidad, que verifica un esquema donde la velocidad de convección (que actúa como dato) tiene la estimación débil del problema de Navier-Stokes. Esta estimación no es suficiente para que los esquemas numéricos existentes en la literatura para ecuaciones de convección-difusión que verifican un principio de máximo discreto, debido a que estos precisan de estimación $L^\infty(Q)$ (al menos). Además, de dicho esquema se deben obtener estimaciones fuertes para la densidad discreta.

A lo largo de este capítulo asumiremos los siguientes hipótesis de trabajo sobre el dominio y los espacios:

(S) Condición de estabilidad:

$$\lim_{(h,k) \rightarrow 0} \frac{h}{k} = 0.$$

(H0) Hipótesis para los datos: Sea $\mathbf{u}_0 \in \mathbf{V}$, $\rho_0 \in H^1(\Omega)$ con $0 < m \leq \rho_0 \leq M$ en Ω y $\mathbf{f} \in L^2(0, T; \mathbf{L}^{6/5}(\Omega))$. Fijamos $\widetilde{M}, \widetilde{m}$ con $\widetilde{M} > M$ y $0 < \widetilde{m} < m$ tal que $\lambda \frac{\widetilde{M} - \widetilde{m}}{2} < \mu$ (esto es posible gracias a (4)).

(H1) Supongamos Ω un dominio acotado de \mathbb{R}^3 , con frontera poliédrica y tal que se tenga la dependencia continua en la norma de H^2 del problema de *Poisson-Neumann* y en norma de $\mathbf{H}^2 \times H^1$ del problema de Stokes.

(H2) La triangulación de Ω y los espacios discretos verifican:

- las desigualdades inversas:

$$\begin{aligned} \|\nabla \bar{\rho}_h\|_{L^2(\Omega)} &\leq C h^{-1} |\bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h, \\ \|\bar{\rho}_h\|_{L^\infty(\Omega)} + \|\nabla \bar{\rho}_h\|_{L^3(\Omega)} &\leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)} \quad \forall \bar{\rho}_h \in W_h, \end{aligned}$$

- y los errores de interpolación:

$$\|\bar{\mathbf{u}} - \widetilde{J}_h \bar{\mathbf{u}}\|_{H^1(\Omega)} + \|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{H^1(\Omega)} \leq C h \|\bar{\mathbf{u}}\|_{H^2(\Omega)} \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$\|\bar{p} - \widetilde{K}_h \bar{p}\|_{L^2(\Omega)} + \|\bar{p} - K_h \bar{p}\|_{L^2(\Omega)} \leq C h \|\bar{p}\|_{H^1(\Omega)} \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\|\bar{\rho} - I_h \bar{\rho}\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{1/2} \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),$$

$$\|\bar{\rho} - I_h \bar{\rho}\|_{L^2(\Omega)} + h \|\bar{\rho} - I_h \bar{\rho}\|_{H^1(\Omega)} \leq C h^2 \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),$$

donde $J_h, \widetilde{J}_h, K_h, \widetilde{K}_h$ y I_h son operadores de interpolación de $\mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ en \mathbf{V}_h , $\mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ en $\widetilde{\mathbf{V}}_h$, $H^1(\Omega) \cap L_0^2(\Omega)$ en M_h , $H^1(\Omega) \cap L_0^2(\Omega)$ en \widetilde{M}_h y $H^2(\Omega)$ en W_h , respectivamente.

(H3) Condición Inf-sup para (\mathbf{V}_h, M_h) y $(\widetilde{\mathbf{V}}_h, \widetilde{M}_h)$.

(H4) Condición de compatibilidad entre \widetilde{M}_h y W_h :

$$(W_h \cdot W_h) \cap L_0^2(\Omega) \subset \widetilde{M}_h,$$

es decir,

$$\forall \bar{\rho}_h^1, \bar{\rho}_h^2 \in W_h, \quad \bar{\rho}_h^1 \bar{\rho}_h^2 - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h^1(\mathbf{x}) \bar{\rho}_h^2(\mathbf{x}) d\mathbf{x} \in \widetilde{M}_h.$$

La propuesta de esquema para (1) en dominios tridimensionales parte del esquema (17)-(19) desarrollado para los dominios bidimensionales reemplazando el término convección explícito

$$\left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h \right)$$

del esquema para la densidad discreta (17) por el término convectivo semi-implícito

$$\left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right),$$

siendo \mathbf{w}_h^n una proyección de \mathbf{u}_h^n sobre un espacio de divergencia discreta nula adecuado con más grados de libertad que \mathbf{V}_h . También modificamos las cotas de corte del operador de truncamiento $[\cdot]_T$, que consideramos continuo en esta ocasión, que no serán exactamente la mínima y la máxima de la densidad inicial sino una perturbación de las mismas por exceso de la máxima y por defecto de la mínima. Con todo ello, llegamos al siguiente esquema numérico:

Etapa (n + 1): Dado $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Encontrar $\mathbf{w}_h^n \in \widetilde{\mathbf{V}}_h$ tal que para cada $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$:

$$\begin{cases} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0. \end{cases} \quad (28)$$

2. Encontrar $\rho_h^{n+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (29)$$

3. Encontrar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\begin{cases} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a \left([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{cases} \quad (30)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0, \quad (31)$$

donde la forma trilineal $c(\cdot, \cdot, \cdot)$ es definida como antes,

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu \left(\nabla \mathbf{u}, \nabla \mathbf{v} \right) + \lambda \int_{\Omega} \left(\frac{\widetilde{M} + \widetilde{m}}{2} - \rho \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} \, dx$$

y el operador de truncamiento ahora es

$$[w_h]_T(\mathbf{x}) = \begin{cases} w_h(\mathbf{x}) & \text{si } w_h(\mathbf{x}) \in [\tilde{m}, \tilde{M}], \\ \tilde{m} & \text{si } w_h(\mathbf{x}) < \tilde{m}, \\ \tilde{M} & \text{si } w_h(\mathbf{x}) > \tilde{M}, \end{cases}$$

con $\tilde{M} > M$, $0 < \tilde{m} < m$ tal que $\lambda \frac{\tilde{M} - \tilde{m}}{2} < \mu$ (ver (4)).

Este esquema bajo las condiciones impuestas a los espacios discretos de estabilidad (H3) y compatibilidad (H4) es incondicionalmente estable respecto de las estimaciones débiles para la velocidad y la densidad

Lema 3 *La solución del esquema (28)-(31) verifica las siguientes estimaciones:*

$$\begin{aligned} \text{i)} \max_{0 \leq n \leq N} \|\mathbf{u}_h^n\|_{L^2(\Omega)} \leq C, \quad \text{ii)} k \sum_{n=0}^N \|\nabla \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \leq C, \quad \text{iii)} \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \leq C, \\ \text{iv)} \max_{0 \leq n \leq N} \|\rho_h^n\|_{L^2(\Omega)} \leq C, \quad \text{v)} \lambda k \sum_{n=0}^{N-1} \|\nabla \rho_h^{n+1}\|_{L^2(\Omega)}^2 \leq C \quad \text{vi)} \sum_{n=0}^{N-1} \|\rho_h^{n+1} - \rho_h^n\|_{L^2(\Omega)}^2 \leq C, \end{aligned}$$

donde $C > 0$ es independiente de k, h y λ .

Ahora se trata de probar que la densidad discreta del esquema truncado (28)-(31) tiene estimaciones puntuales por exceso y por defecto respecto de las cotas máxima y mínima de la densidad inicial ρ_0 . Más precisamente, veremos que $\tilde{m} \leq \rho_h^n \leq \tilde{M}$ para cualquier k y h suficientemente pequeño satisfaciendo la restricción (S). Luego, podremos prescindir de aplicar el operador de truncamiento $[\cdot]_T$ en el sistema de momentos discreto (30).

Para ello, introducimos un esquema semi-discreto en tiempo de una ecuación de convección-difusión con velocidad de convección totalmente discreta proveniente del esquema truncado (28)-(31). Más concretamente, definimos la sucesión (ρ^n) con el siguiente esquema:

Inicialización: Sea $\rho^0 = \rho_0$.

Etapa $n + 1$: Dado ρ^n , calculamos $\rho^{n+1} \in H^2(\Omega)$ verificando el problema elíptico:

$$\begin{cases} \frac{\rho^{n+1} - \rho^n}{k} + \mathbf{w}_h^n \cdot \nabla \rho^{n+1} - \lambda \Delta \rho^{n+1} = 0 & \text{en } \Omega, \\ \frac{\partial \rho^{n+1}}{\partial \mathbf{n}} = 0 & \text{sobre } \Gamma. \end{cases} \quad (32)$$

Las propiedades que deseamos extraer de este esquema semi-discreto son: un principio del máximo, es decir, $0 < m \leq \rho^n(\mathbf{x}) \leq M$ para $\mathbf{x} \in \Omega$ y la estimación de regularidad

$k \sum_{n=0}^N \|\rho^n\|_{H^2(\Omega)}^2 \leq C$. A primera vista no se sigue directamente un principio del máximo para (32) dada la poca regularidad en tiempo de la velocidad discreta. Por esta razón, definimos el siguiente esquema no lineal, cuyas soluciones serán denotadas, como antes, por ρ^n para abreviar notación:

Inicialización: Sea $\rho^0 = \rho_0$.

Etapa $n + 1$: Dado ρ^n , calculamos $\rho^{n+1} \in H^2(\Omega)$ verificando el problema elíptico:

$$\begin{cases} \frac{\rho^{n+1} - \rho^n}{k} + \mathbf{w}_h^n \cdot \nabla K_m^M \rho^{n+1} - \lambda \Delta \rho^{n+1} = 0 & \text{in } \Omega, \\ \frac{\partial \rho^{n+1}}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0, \end{cases} \quad (33)$$

donde

$$K_m^M \rho^{n+1}(\mathbf{x}) = \begin{cases} \rho^{n+1}(\mathbf{x}) & \text{si } \rho^{n+1}(\mathbf{x}) \in [m, M], \\ m & \text{si } \rho^{n+1}(\mathbf{x}) < m, \\ M & \text{si } \rho^{n+1}(\mathbf{x}) > M. \end{cases}$$

Mediante un argumento de punto fijo y compacidad se prueba existencia de solución para (33). Además, es fácil comprobar que este esquema no lineal tiene estimaciones puntuales, es decir, $0 < m \leq \rho^n(\mathbf{x}) \leq M$ con lo que el operador de truncamiento puntual $K_m^M \rho^n = \rho^n$. Entonces, los esquemas (32) y (33) coinciden y se puede establecer el siguiente resultado de regularidad gracias a la hipótesis sobre el dominio discreto (H1) para (32):

Lema 4 Sea $\{\mathbf{w}_h^n\}_{n=0}^N \subset \mathbf{H}_0^1(\Omega)$ tal que $k \sum_{n=0}^N \|\mathbf{w}_h^n\|_{H^1(\Omega)}^2 \leq C$. Entonces, existe una única solución $\rho^{n+1} \in H^2(\Omega)$ de (32) que verifica:

$$0 < m \leq \rho^{n+1}(\mathbf{x}) \leq M, \quad \forall \mathbf{x} \in \Omega, \quad \forall n,$$

$$\lambda^2 k \sum_{n=0}^{N-1} \|\rho^{n+1}\|_{H^2(\Omega)}^2 \leq C,$$

donde $C > 0$ es una constante independiente de k, h y λ .

Ahora, realizando un estudio de error entre el esquema de la densidad totalmente discreto (29) y el esquema semi-discreto (32), obtenemos

$$\|\rho_h^{n+1} - \rho^{n+1}\|_{L^\infty(\Omega)} \leq C \frac{1}{\lambda} \sqrt{\frac{h}{k}},$$

gracias a la regularidad de (ρ^n) , a las hipótesis de aproximación, las interpolaciones inversas del espacio discreto de la densidad W_h y la estabilidad (H4) entre los espacios (W_h, \widetilde{M}_h) . Como consecuencia de este error y del principio del máximo encontrado para (ρ^n) , llegamos al

Teorema 5 *Existen $h \leq h_0$, $k \leq k_0$ satisfaciendo la condición (S) tal que la densidad discreta del esquema truncado (28)-(31) verifica las estimaciones puntuales*

$$0 < \widetilde{m} \leq \rho_h^{n+1} \leq \widetilde{M}.$$

Luego, como se mencionó, podemos prescindir del operador de truncamiento en el sistema de momentos discreto (30) resultando el esquema como sigue:

Etapa $(n+1)$: Dado $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Encontrar $\mathbf{w}_h^n \in \widetilde{\mathbf{V}}_h$ tal que para cada $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$:

$$\begin{cases} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0. \end{cases} \quad (34)$$

2. Encontrar $\rho_h^{n+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (35)$$

3. Encontrar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\begin{cases} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a \left(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{cases} \quad (36)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0, \quad (37)$$

Por último, usando una versión discreta de la desigualdad de interpolación

$$\|\nabla \rho\|_{L^\infty(\Omega)} \leq C \|\rho\|_{L^\infty(\Omega)}^{1/2} \|\Delta \rho\|_{L^\infty(\Omega)}^{1/2} \quad \forall \rho \in H_N^2(\Omega),$$

obtenemos las estimaciones fuertes para la densidad discreta:

Teorema 6 *Bajo las hipótesis del Teorema 5, la solución ρ_h^{n+1} del esquema discreto (35) verifica las siguientes estimaciones, para h y k suficientemente pequeños:*

$$\begin{aligned} \text{vii)} \quad & \lambda \max_{0 \leq n \leq N} \|\nabla \rho_h^n\|_{L^2(\Omega)}^2 \leq C, & \text{viii)} \quad & \lambda^2 \sum_{n=0}^N k \|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}^2 \leq C, \\ \text{ix)} \quad & \lambda \sum_{n=0}^{N-1} \|\nabla(\rho_h^{n+1} - \rho_h^n)\|_{L^2(\Omega)}^2 \leq C, \end{aligned}$$

donde $C > 0$ independiente de h , k y λ .

Recopilando la información conseguida se puede establecer el siguiente resultado de convergencia para el esquema (34)-(37):

Teorema 7 *Supongamos las hipótesis (S), (H0)-(H4). Entonces existe una subsucesión convergente de $(\mathbf{u}_{h,k}, \rho_{h,k})$ (denota de la misma manera) cuando $(h, k) \rightarrow 0$ hacia una solución débil (\mathbf{u}, ρ) del problema (1), (2)-(3) en el siguiente sentido: $(\mathbf{u}_{h,k}, \rho_{h,k}) \rightarrow (\mathbf{u}, \rho)$ en $L^2(0, T; \mathbf{L}^2(\Omega)) \times L^2(0, T; H^1(\Omega))$ -fuerte, en $L^\infty(0, T; \mathbf{L}^2(\Omega)) \times (H^1(\Omega) \cap L^\infty(\Omega))$ -débil* y en $L^2(0, T; \mathbf{H}_0^1(\Omega)) \times L^4(0, T; W^{1,3}(\Omega))$ -débil. Además, $\tilde{m} \leq \rho_{h,k} \leq \tilde{M}$.*

Los resultados descritos en este capítulo se pueden adaptar, al igual que ocurría en el caso bidimensional, al caso de considerar una difusión no lineal $-\lambda \nabla \cdot (\rho \nabla \mathbf{u})$ para dominios tridimensionales.

Resulta natural a este nivel de información sobre el esquema plantearse si el esquema (34)-(37) aproxima una solución débil del problema de Navier-Stokes con densidad variable (6) cuando el parámetro de difusión converge a cero junto con los parámetros de discretización (h, k) (como ya se hizo en [35] y en [21] para el caso continuo). Por ello, en todo el capítulo hemos tenido especial cuidado con la dependencia de las estimaciones con respecto a λ . El grado de dependencia encontrado nos aportarán la información suficiente para que las no lineales del esquema (34)-(37) que depende de λ vayan a cero cuando λ va a cero, $\lambda \rightarrow 0$, junto con los parámetros de discretización en espacio y tiempo, $(h, k) \rightarrow 0$. En el camino nos encontraremos que tenemos que imponer una nueva condición de estabilidad que relaciona los parámetros de discretización y difusión que reemplace la condición (S) por

$$(S') \quad \lim_{(\lambda, h, k) \rightarrow 0} \frac{1}{\lambda} \sqrt{\frac{h}{k}} = 0,$$

y completar (H2) con una propiedad de aproximación adicional para W_h :

$$(H2') \quad \|\bar{\rho} - I_h \bar{\rho}\|_{L^2(\Omega)} \leq C h^{2/3} \|\bar{\rho}\|_{W^{1,3/2}(\Omega)} \quad \forall \bar{\rho} \in W^{1,3/2}(\Omega).$$

Por lo tanto, una vez que sabemos cómo se comportan las estimaciones en relación con el parámetro de difusión λ nos queda por saber la compacidad para pasar al límite hacia una solución débil del sistema de Navier-Stokes con densidad variable (6). De nuevo acotamos una derivada fraccionaria discreta para la convergencia fuerte de la velocidad teniendo cuidado con la dependencia del parámetro de difusión:

$$k \sum_{m=0}^{N-r} \|\sqrt{\rho_h^{m+r}} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^2(\Omega)}^2 \leq C (rk)^{1/2}, \quad \forall r : 0 \leq r \leq N,$$

Obsérvese que las estimaciones de energía para la velocidad discreta no depende de la difusión λ , luego como se probó en el caso de λ fijo, las aproximaciones de la velocidad son compactas en $L^2(Q)$.

Por otro lado, ahora se pierde la convergencia fuerte de la densidad discreta en $L^2(0, T; H^1(\Omega))$. Aún así podemos pasar al límite en (28)-(31) reescribiéndolo en forma conservativa, luego en particular en el término convectivo $c(\rho_h^{n+1}, \mathbf{u}_h^n, \bar{\mathbf{u}}_h)$ de (36) se transforma en $(\rho_h^{n+1} \mathbf{u}_h^n \cdot \nabla) \bar{\mathbf{u}}_h, \mathbf{u}_h^{n+1}$, y llegamos al siguiente resultado de convergencia:

Teorema 8 *Cambiando (S) por (S') y extendiendo (H2) por (H2'), entonces existe una subsecuencia convergente de $(\mathbf{u}_{h,k,\lambda}, \rho_{h,k,\lambda})$ cuando $(h, k, \lambda) \rightarrow 0$ hacia una solución débil (\mathbf{u}, ρ) del problema de Navier-Stokes con densidad variable en el siguiente sentido: $\mathbf{u}_{h,k,\lambda} \rightarrow \mathbf{u}$ en $L^2(0, T; \mathbf{L}^2(\Omega))$ -fuerte, en $L^\infty(0, T; \mathbf{L}^2(\Omega))$ -débil* y en $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -débil, y $\rho_{h,k,\lambda} \rightarrow \rho$ en $L^\infty(Q)$ -débil*.*

Capítulo 3

En el capítulo 3 nos centramos en extender los resultados obtenidos en el capítulo 2 al modelo completo de difusión de masa (5) que incluye el término $\lambda^2 \nabla \cdot \left(\frac{1}{\rho} \nabla \rho \otimes \nabla \rho \right)$. Este término introduce nuevas dificultades ya que las estimaciones fuertes de la densidad discreta ahora no se consiguen de modo independiente de las estimaciones débiles para la velocidad y la densidad sino que están relacionadas. Por esta razón la estrategia de apoyarse en un esquema truncado similar a (28)-(31) para posteriormente garantizar un principio del máximo para la densidad aproximada no funciona. Ahora consideremos directamente el esquema sin truncar:

Initialization: Sea $(\mathbf{u}_h^0, \rho_h^0) \in \mathbf{V}_h \times W_h$ aproximaciones de (\mathbf{u}_0, ρ_0) cuando $h \rightarrow 0$.

Etapa $n + 1$: Dado $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

- Encontrar $\mathbf{w}_h^n \in \widetilde{\mathbf{V}}_h$ tal que para cada $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$:

$$\begin{cases} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0. \end{cases} \quad (38)$$

- Hallar $\rho_h^{n+1} \in W_h$ tal que, para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + c(\mathbf{u}_h^n, \rho_h^{n+1}, \bar{\rho}_h) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (39)$$

- Hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que, para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left(\frac{\rho_h^n \mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k} \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + a \left(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + \lambda^2 \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^n, \nabla \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{array} \right. \quad (40)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, q_h \right) = 0. \quad (41)$$

La técnica para probar estabilidad de este esquema será mediante un proceso de inducción en la etapa de tiempo bajo una serie de restricciones. En el paso de inducción primero se prueba un principio del máximo discreto y, luego estimaciones débiles para la velocidad discreta y estimaciones fuertes para la densidad discreta. Todo esto será posible gracias al carácter secuencial que muestra este esquema.

Para este esquema asumimos las mismas hipótesis que para el capítulo 2 cambiando la hipótesis de regularidad para los datos iniciales y de pequeñez de los parámetros (λ, μ) de (H0) por

(H0) Regularidad para los datos:

$$\mathbf{u}_0 \in \mathbf{V}, \rho_0 \in H_N^2(\Omega) \text{ con } 0 < m \leq \rho_0 \leq M \text{ en } \Omega \text{ y } \mathbf{f} \in L^2(0, T; \mathbf{L}^{6/5}(\Omega)).$$

Asumimos λ/μ suficientemente pequeño.

También se amplía la hipótesis (H2) sobre la triangulación y los espacios discretos, por la desigualdad inversa:

$$\|\nabla \bar{\rho}_h\|_{L^4(\Omega)} \leq C h^{-3/4} \|\nabla \bar{\rho}_h\|_{L^2(\Omega)} \quad \forall \bar{\rho}_h \in W_h,$$

y el error de interpolación:

$$\|\bar{\rho} - I_h \bar{\rho}\|_{W^{1,4}(\Omega)} \leq C h^{1/4} \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),$$

donde I_h es el operador de interpolación de $H^2(\Omega)$ en W_h .

En una primera etapa, como ya se vió en el capítulo 2, bajo una acotación de la velocidad discreta en $L^2(0, T; \mathbf{H}^1(\Omega))$ podemos asegurar un principio del máximo para la densidad aproximada.

Lema 9 Fijado $n : 0 \leq n \leq N - 1$, si la velocidad discreta satisface $k \sum_{l=0}^n \|\nabla \mathbf{u}_h^l\|_{L^2(\Omega)}^2 \leq C_d$ con $C_d > 0$ independiente de h, k, n y λ , entonces existen h_0 y k_0 (independiente de n) tal que

para cualquier $h \leq h_0$, $k \leq k_0$ satisfaciendo (S), el esquema de la densidad (39) tiene una única solución ρ_h^{n+1} que verifica la estimación puntual

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M} \quad \text{en } \Omega.$$

A continuación, asumiendo estimaciones puntuales para las densidades discretas ρ_h^n y ρ_h^{n+1} y acotaciones sobre las normas $\|\Delta_h \rho_h^n\|_{L^2(\Omega)}$ y $\|\nabla \mathbf{u}_h^n\|_{L^2(\Omega)}$ establecemos dos desigualdades, primero para $\|\mathbf{u}_h^{n+1}\|_{L^2(\Omega)}$ y $\|\nabla \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}$, luego para $\|\nabla \rho_h^{n+1}\|_{L^2(\Omega)}$ y $\|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}$ en función de la densidad y la velocidad en la etapa n :

Lema 10 Fijado $n : 0 \leq n \leq N - 1$, suponemos

$$0 < \tilde{m} \leq \rho_h^n, \rho_h^{n+1} \leq \tilde{M} \quad \text{en } \Omega$$

y

$$\frac{1}{16 C_2} \lambda^2 \mu k \|\Delta_h \rho_h^n\|_{L^2(\Omega)}^2 + \frac{1}{2} \mu k \|\nabla \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \leq C_d,$$

con $C_d > 0$ independiente de h , k , n y λ . Entonces, existen h_0 y k_0 de modo que para cualquier $h \leq h_0$, $k \leq k_0$ satisfaciendo (S), el esquema (38)-(41) tiene una única solución $(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1})$ que verifica las siguientes estimaciones:

$$\begin{cases} \|\sqrt{\rho_h^{n+1}} \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 - \|\sqrt{\rho_h^n} \mathbf{u}_h^n\|_{L^2(\Omega)}^2 + \|\sqrt{\rho_h^n} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)\|_{L^2(\Omega)}^2 + \frac{\mu}{2} k \|\nabla \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 \\ \leq k C_1 \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 + \varepsilon \mu \lambda^2 k \left(\|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}^2 + \|\Delta_h \rho_h^n\|_{L^2(\Omega)}^2 \right), \end{cases} \quad (42)$$

$$\lambda \|\nabla \rho_h^{n+1}\|_{L^2(\Omega)}^2 - \lambda \|\nabla \rho_h^n\|_{L^2(\Omega)}^2 + \lambda \|\nabla (\rho_h^{n+1} - \rho_h^n)\|_{L^2(\Omega)}^2 + \frac{\lambda^2}{2} k \|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}^2 \leq C_2 k \|\nabla \mathbf{u}_h^n\|_{L^2(\Omega)}^2, \quad (43)$$

con $C_1, C_2 > 0$ independientes de h , k , n y λ , y $\varepsilon > 0$ arbitrariamente pequeño (también independiente de h , k y λ).

Finalmente, imponiendo sobre las aproximaciones iniciales las hipótesis de los lemas anteriores, se prueba por un proceso de inducción sobre la etapa tiempo, el siguiente resultado:

Teorema 11 Existen $h_0 > 0$ y $k_0 > 0$ (dependiente de λ) de modo que para cualquier $h \leq h_0$, $k \leq k_0$, y para cada $n = 0, \dots, N - 1$, el problema discreto (38)-(41) tiene una única solución $(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1})$ que verifica las siguientes desigualdades:

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M} \quad \text{en } \Omega \quad (44)$$

y

$$\begin{aligned}
& \frac{1}{4C_2} \mu \lambda \|\nabla \rho_h^{n+1}\|_{L^2(\Omega)}^2 + \|\sqrt{\rho_h^{n+1}} \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 - \left(\frac{1}{4C_2} \mu \lambda \|\nabla \rho_h^n\|_{L^2(\Omega)}^2 + \|\sqrt{\rho_h^n} \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \right) \\
& + \|\sqrt{\rho_h^n} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)\|_{L^2(\Omega)}^2 + \frac{1}{4C_2} \mu \lambda \|\nabla (\rho_h^{n+1} - \rho_h^n)\|_{L^2(\Omega)}^2 + \frac{3\mu}{4} k \|\nabla \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 \\
& + \frac{1}{8C_3} \mu \lambda^2 k \|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}^2 \leq C_1 k \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 + \varepsilon \mu \lambda^2 k \|\Delta_h \rho_h^n\|_{L^2(\Omega)}^2 + \frac{1}{4} \mu k \|\nabla \mathbf{u}_h^n\|_{L^2(\Omega)}^2.
\end{aligned} \tag{45}$$

donde $C_1 > 0$ y $C_2 > 0$ son constantes independientes de h , k , n y λ , y $\varepsilon > 0$ es suficientemente pequeño (el cual aparece en el Lema 10).

Como consecuencia inmediata se consiguen las estimaciones globales de estabilidad.

Corolario 12 *Bajo las hipótesis del Teorema 16, la solución $(\rho_h^{n+1}, \mathbf{u}_h^{n+1})$ del problema discreto (38)-(41) verifica las siguientes estimaciones:*

$$\begin{aligned}
& \text{i) } \max_{0 \leq n \leq N} \|\mathbf{u}_h^n\|_{L^2(\Omega)} \leq C, & \text{ii) } k \sum_{n=0}^N \|\nabla \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \leq C, \\
& \text{iii) } \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \leq C, & \text{iv) } \max_{0 \leq n \leq N} \left(\|\rho_h^n\|_{L^\infty}^2 + \lambda \|\nabla \rho_h^n\|_{L^2(\Omega)}^2 \right) \leq C, \\
& \text{v) } \lambda^2 k \sum_{n=0}^{N-1} \|\Delta_h \rho_h^{n+1}\|_{L^2(\Omega)}^2 \leq C, & \text{vi) } \lambda \sum_{n=0}^{N-1} \|\nabla (\rho_h^{n+1} - \rho_h^n)\|_{L^2(\Omega)}^2 \leq C,
\end{aligned}$$

donde $C > 0$ es una constante dependiente únicamente de los datos $(\mathbf{f}, \mathbf{u}_0, \rho_0, \mu)$ e independiente de k , h y λ .

De nuevo aprovechando la dependencia de las estimaciones que nos da el Corolario anterior con respecto al parámetro de difusión λ , que de hecho son del mismo tipo que para el esquema (34)-(37), se consigue la convergencia del esquema (40)-(41) hacia una solución débil del problema de Navier-Stokes con densidad variable (6), cuando $(h, k, \lambda) \rightarrow 0$.

Capítulo 4

En el capítulo cuatro realizamos un estudio de error de un esquema numérico para el modelo de difusión de masa (1) para el cual no proyectamos la velocidad del término convectivo de la ecuación de la densidad. Este estudio de error se apoyará en una solución regular cuya regularidad no exige que se verifique una condición de compatibilidad no local de la presión en el tiempo $t = 0$ que depende de los datos iniciales \mathbf{u}_0 , ρ_0 y $\mathbf{f}(0)$ (ver [24]) que no se puede verificar en la práctica. Como consecuencia no se obtendrá orden de error optimal respecto del parámetro de discretización en tiempo. Esta condición de compatibilidad es impuesta en los resultados de [15]

para un esquema que usa el método de la características para discretizar la derivada en tiempo y el término convectivo del sistema de momentos y de la ecuación de conservación de la masa. Probaremos estimaciones de error para las normas débiles conjuntamente para la velocidad y la densidad de $O(k^{1/2} + h)$. Para las normas fuerte de la densidad se mantendrá el mismo orden. Estas estimaciones de error no optimales en tiempo se pueden mejorar imponiendo mejor regularidad para la velocidad exacta, más concretamente para la segunda derivada en tiempo de la velocidad.

Consideramos las siguientes hipótesis a lo largo del capítulo:

(S) Condición de estabilidad: $\lim_{(h,k)=0} \frac{h}{k} \rightarrow 0$.

(H0) *Regularidad para los datos*: Supongamos $\lambda \frac{M-m}{2} < \mu$ y sean $\widetilde{M} > M$ y $0 < \widetilde{m} < m$ tal que $\lambda \frac{\widetilde{M}-\widetilde{m}}{2} < \mu$.

Sea $\mathbf{u}_0 \in \mathbf{V} \cap \mathbf{H}^2(\Omega)$, $\rho_0 \in H_N^3(\Omega)$ con $0 < m \leq \rho_0 \leq M$ en Ω , $\mathbf{f} \in L^2(0, T; \mathbf{H}^1(\Omega))$ y $\mathbf{f}_t \in L^2(0, T; \mathbf{L}^{6/5}(\Omega))$.

Regularidad para la solución: Supongamos que (ρ, \mathbf{u}) es la única solución del problema (1), (2)-(3) en $(0, T)$ con la siguiente regularidad:

$$(\rho, \mathbf{u}) \in L^\infty(0, T; H^3(\Omega) \times \mathbf{H}^2(\Omega)), \quad p \in L^\infty(0, T, H^1(\Omega))$$

$$(\rho_t, \mathbf{u}_t) \in (L^\infty(0, T; H^1) \cap L^2(0, T; H^2)) \times L^\infty(0, T; \mathbf{L}^2(\Omega)),$$

$$(\rho_{tt}, \sigma^{1/2} \mathbf{u}_{tt}) \in L^2(0, T; L^2(\Omega) \times \mathbf{H}^{-1}(\Omega)),$$

donde $\sigma(t) = \min\{1, t\}$.

Suponemos aproximaciones $(\rho_h^0, \mathbf{u}_h^0)$ de los datos iniciales (ρ_0, \mathbf{u}_0) tales que

$$|\mathbf{u}_0 - \mathbf{u}_h^0| \leq G_1 h,$$

$$|\nabla \mathbf{u}_h^0| \leq G_2,$$

$$|\rho_0 - \rho_h^0| + h \|\rho_0 - \rho_h^0\|_{H^1(\Omega)} \leq G_3 h^2,$$

$$0 < \widetilde{m} \leq \rho_h^0(\mathbf{x}) \leq \widetilde{M},$$

para G_i constantes positivas que dependen de \mathbf{u}_0, ρ_0 y Ω .

(H2) La frontera de Ω es un poliedro tal que se verifique la dependencia continua en la norma H^2 del problema de *Poisson-Neumann*.

(H2) The triangulación de Ω y los espacios discretos verifican:

- la desigualdad inversa:

$$\|\bar{\rho}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)} \quad \forall \bar{\rho}_h \in W_h,$$

- y los errores de interpolación:

$$\inf_{\bar{\mathbf{u}}_h \in \mathbf{V}_h} \{ \|\bar{\mathbf{u}} - \bar{\mathbf{u}}_h\|_{L^2(\Omega)} + h \|\bar{\mathbf{u}} - \bar{\mathbf{u}}_h\|_{H^1(\Omega)} \} \leq C h^2 \|\bar{\mathbf{u}}\|_{H^2(\Omega)} \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$\inf_{\bar{p}_h \in M_h} \|\bar{p} - \bar{p}_h\|_{L^2(\Omega)} \leq C h \|\bar{p}\|_{H^1(\Omega)} \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\inf_{\bar{\rho}_h \in W_h} \{ \|\bar{\rho} - \bar{\rho}_h\|_{L^2(\Omega)} + h \|\bar{\rho} - \bar{\rho}_h\|_{H^1(\Omega)} \} \leq C h^2 \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),$$

$$\inf_{\bar{\rho}_h \in W_h} \|\bar{\rho} - \bar{\rho}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{1/2} \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega).$$

(H3) Condición inf-sup para (\mathbf{V}_h, M_h) .

(H4) Los espacios discretos en velocidad \mathbf{V}_h y en densidad W_h satisfacen $\mathbf{V}_h \cdot \mathbf{V}_h \subset W_h$, es decir,

$$\forall \bar{\mathbf{u}}_h^1, \bar{\mathbf{u}}_h^2 \in \mathbf{V}_h, \quad \bar{\mathbf{u}}_h^1 \cdot \bar{\mathbf{u}}_h^2 \in W_h.$$

Una primera observación con respecto a las hipótesis de compatibilidad (H4) de los esquemas de los capítulos 3 y 4 y la hipótesis (H4) de este capítulo es que son en cierto sentido opuestas, ya que si por simplificar suponemos $\mathbf{V}_h = \widetilde{\mathbf{V}}_h$ y $M_h = \widetilde{M}_h$, llegamos a las siguientes inclusiones desde el punto de vista de los grados de libertad de los espacios:

$$(\mathbf{V}_h \cdot \mathbf{V}_h \cdot \mathbf{V}_h \cdot \mathbf{V}_h) \subset (W_h \cdot W_h) \subset M_h \subset \mathbf{V}_h$$

(la última inclusión es debido a la condición *inf-sup* entre (\mathbf{V}_h, M_h)) las cuales son contradictorias.

El esquema que presentamos es como sigue:

Inicialización: Se define $(\mathbf{u}_h^0, \rho_h^0) \in \mathbf{V}_h \times W_h$ aproximaciones de (\mathbf{u}_0, ρ_0) , cuando $h \rightarrow 0$.

Etapa $n + 1$: Dados $\rho_h^n \in W_h$ y $\mathbf{u}_h^n \in \mathbf{V}_h$, hallar $\rho_h^{n+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) - \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (46)$$

Dados $\rho_h^n, \rho_h^{n+1} \in W_h$ y $\mathbf{u}_h^n \in \mathbf{V}_h$, hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left(\frac{\rho_h^n \mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + \frac{1}{2} \left((\nabla \cdot \mathbf{u}_h^n) \rho_h^{n+1} \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}(t_{n+1}), \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{array} \right. \quad (47)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0, \quad (48)$$

donde

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu (\nabla \mathbf{u}, \nabla \mathbf{v}) - \lambda \int_{\Omega} \left(\rho - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} \, dx$$

con

$$\widetilde{M} > M, \quad 0 < \widetilde{m} < m \quad \text{tales que} \quad \lambda \frac{\widetilde{M} - \widetilde{m}}{2} < \mu.$$

Para conseguir las tasas de error del esquema procederemos por inducción en la etapa de tiempo (con una idea similar a la desarrollada en el Capítulo 3 para probar la estabilidad del esquema para el modelo de difusión de masa completo, con los términos de $O(\lambda^2)$). Un primer resultado para la etapa $n + 1$, conocida la información de la etapa n , es el siguiente principio del máximo discreto.

Lema 13 *Para $n = 0, \dots, N - 1$, supongamos que $\|\nabla \mathbf{u}_h^l\|_{L^2(\Omega)} \leq C_s$, con $l = 0, \dots, n$, siendo $C_s > 0$ una constante independiente de los parámetros de discretización (k, h) y de n . Si imponemos la hipótesis (S), entonces para h/k suficientemente pequeño (independiente de la etapa de tiempo n) la densidad discreta del esquema (46) verifica*

$$0 < \widetilde{m} \leq \rho_h^{l+1} \leq \widetilde{M}, \quad \forall l : 0 \leq l \leq n.$$

La obtención de este principio del máximo es semejante al conseguido para el esquema (35), que difiere del esquema (46), que ahora proponemos, en que la velocidad del término convectivo no es proyectada en un espacio mejor de aquí que tengamos que pedir a la velocidad discreta la estimación $\|\nabla \mathbf{u}_h^l\|_{L^2(\Omega)} \leq C$ en lugar de $k \sum_{l=0}^n \|\nabla \mathbf{u}_h^l\|_{L^2(\Omega)}^2 \leq C$. Esta regularidad en tiempo de tipo ℓ^∞ se alcanzará de la estimación de error del esquema (46)-(48).

Definición 14 *Consideramos las siguientes definiciones:*

$$\begin{aligned} \mathbf{e}_{\mathbf{u}}^n &= e_{d,\mathbf{u}} + \mathbf{e}_{i,\mathbf{u}}, \quad \text{donde } e_{d,\mathbf{u}} = \mathbf{u}_h^n - I_h \mathbf{u}(t_n) \text{ y } \mathbf{e}_{i,\mathbf{u}} = I_h \mathbf{u}(t_n) - \mathbf{u}(t_n), \\ e_p^n &= e_{d,p} + e_{i,p}, \quad \text{donde } e_{d,p} = p_h^n - J_h p(t_n) \text{ y } e_{i,p} = J_h p(t_n) - p(t_n), \\ e_\rho^n &= e_{d,\rho} + e_{i,\rho}, \quad \text{donde } e_{d,\rho} = \rho_h^n - K_h \rho(t_n) \text{ y } e_{i,\rho} = K_h \rho(t_n) - \rho(t_n). \end{aligned}$$

A continuación usando el principio del máximo discreto anterior para la densidad discreta, establecemos una desigualdad recursiva para los errores, que jugará un papel esencial en el proceso de inducción.

Lema 15 *Supongamos $0 < \tilde{m} \leq \rho_h^n, \rho_h^{n+1} \leq \tilde{M}$ en Ω . Entonces, para k y h suficientemente pequeño y $h \leq Ck$ (gracias a la hipótesis (S)), existe una constante $A > 0$ (dependiente de la solución exacta) tal que se verifica la desigualdad*

$$\left\{ \begin{array}{l} \left(\|\sqrt{\rho_h^{n+1}} \mathbf{e}_u^{n+1}\|_{L^2(\Omega)}^2 + A \|e_\rho^{n+1}\|_{L^2(\Omega)}^2 \right) - \left(\|\sqrt{\rho_h^n} \mathbf{e}_u^n\|_{L^2(\Omega)}^2 + A \|e_\rho^n\|_{L^2(\Omega)}^2 \right) \\ + \left(\frac{\tilde{m}}{2} \|\mathbf{e}_u^{n+1} - \mathbf{e}_u^n\|_{L^2(\Omega)}^2 + \frac{A}{2} \|e_\rho^{n+1} - e_\rho^n\|_{L^2(\Omega)}^2 \right) + k \frac{3}{4} \left(\mu_1 \|\nabla \mathbf{e}_u^{n+1}\|_{L^2(\Omega)}^2 + A \lambda \|\nabla e_\rho^{n+1}\|_{L^2(\Omega)}^2 \right) \\ \leq C_1 k \left(\tilde{m} \|\mathbf{e}_u^n\|_{L^2(\Omega)}^2 + A \|e_\rho^n\|_{L^2(\Omega)}^2 \right) + k \frac{1}{4} \left(\mu_1 \|\nabla \mathbf{e}_u^n\|_{L^2(\Omega)}^2 + A \lambda \|\nabla e_\rho^n\|_{L^2(\Omega)}^2 \right) \\ + C k \left(\|\mathbf{e}_{i,\mathbf{u}}^{n+1}\|_{H^1(\Omega)}^2 + \|e_{i,\rho}^{n+1}\|_{H^1(\Omega)}^2 \right) + C \left(\|\mathbf{e}_{i,\mathbf{u}}^{n+1}\|_{L^2(\Omega)}^2 + \|e_{i,\rho}^{n+1}\|_{L^2(\Omega)}^2 \right) \\ + C k^2 \int_{t_n}^{t_{n+1}} \left(\|\rho_{tt}(s)\|_{H^1(\Omega)'}^2 + \|\rho_{tt}(s)\|_{L^{6/5}(\Omega)}^2 + \|\mathbf{u}_t(s)\|_{L^2(\Omega)}^2 \right) ds \\ + C k \int_{t_n}^{t_{n+1}} (s - t_n) \|\mathbf{u}_{tt}(s)\|_{L^{6/5}(\Omega)}^2 ds, \end{array} \right. \quad (49)$$

donde C y C_1 son constantes positivas independientes de los parámetros de discretización (h, k) y dependientes de la solución exacta.

Al menos de manera formal, si suponemos que hemos probado la desigualdad (49) para toda etapa de tiempo, la convergencia $O(k^{1/2} + h)$ es evidente para las normas débiles para la velocidad y la densidad.

Teorema 16 *Asumiendo las hipótesis (H0)-(H4) y la restricción (S), se tienen las siguientes estimaciones de error, para k y h suficientemente pequeño:*

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M}, \quad \forall n : 0 \leq n \leq N - 1, \quad (50)$$

$$\left\{ \begin{array}{l} \max_{0 \leq n \leq N-1} \left(\tilde{m} \|\mathbf{e}_u^{n+1}\|_{L^2(\Omega)}^2 + A \|e_\rho^{n+1}\|_{L^2(\Omega)}^2 \right) + \sum_{n=0}^{N-1} \left(\frac{\tilde{m}}{2} \|\mathbf{e}_u^{n+1} - \mathbf{e}_u^n\|_{L^2(\Omega)}^2 + \frac{A}{2} \|e_\rho^{n+1} - e_\rho^n\|_{L^2(\Omega)}^2 \right) \\ + k \sum_{n=0}^{N-1} \left(\frac{\mu_1}{2} \|\nabla \mathbf{e}_u^{n+1}\|_{L^2(\Omega)}^2 + A \lambda \|\nabla e_\rho^{n+1}\|_{L^2(\Omega)}^2 \right) \leq C (k + h^2). \end{array} \right. \quad (51)$$

Ahora podemos mejorar el error para la densidad a normas de un orden más de regularidad en espacio, donde la regularidad H^2 queda representada por el laplaciano discreto, cuyo error entre el laplaciano continuo en $t = t_{n+1}$, $-\Delta \rho(t_{n+1})$, lo definimos como e_Δ^{n+1} . El orden de convergencia que extraeremos es el mismo que en el Teorema anterior.

Teorema 17 En las hipótesis del Teorema 16, se tienen las siguientes estimaciones de error para h suficientemente pequeño:

$$\max_{0 \leq n \leq N-1} \|\nabla e_\rho^{n+1}\|_{L^2(\Omega)}^2 + \sum_{n=0}^{N-1} \|\nabla(e_\rho^{n+1} - e_\rho^n)\|_{L^2(\Omega)}^2 + k \sum_{n=0}^{N-1} \|e_\Delta^{n+1}\|_{L^2(\Omega)}^2 \leq C(k + h^2). \quad (52)$$

Además en este capítulo presentamos dos métodos iterativos para aproximar en cada etapa de tiempo a $(\mathbf{u}_h^{n+1}, p_h^{n+1}, \rho_h^{n+1})$, donde en cada etapa de los dos métodos iterativos hay que resolver sistema lineales de matrices constantes.

Método iterativo para el problema (46). Conocidos $(\rho_h^n, \mathbf{u}_h^n)$, se aproxima ρ_h^{n+1} solución de (46) por la sucesión $(\rho_h^{n+1,i})_i$ definida como:

Inicialización: Sean $\rho_h^{n+1,0} = \rho_h^n$.

Etapas $i + 1$: Conocido $\rho_h^{n+1,i}$, hallar $\rho_h^{n+1,i+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1,i+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1,i+1}, \nabla \bar{\rho}_h \right) = \left(\rho_h^{n+1,i} \mathbf{u}_h^n, \nabla \bar{\rho}_h \right).$$

Método iterativo para el problema (47). Conocidos $(\rho_h^n, \rho_h^{n+1}, \mathbf{u}_h^n)$, se aproxima \mathbf{u}_h^{n+1} solución de (47) por la sucesión $(\mathbf{u}_h^{n+1,i})_i$ definida como:

Inicialización: Sea $\mathbf{u}_h^{n+1,0} = \mathbf{u}_h^n$.

Etapas $i + 1$: Conocido $\mathbf{u}_h^{n+1,i}$, hallar $(\mathbf{u}_h^{n+1,i+1}, p_h^{n+1,i+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left(\frac{\rho_{\tilde{m}}^{\tilde{M}} \mathbf{u}_h^{n+1,i+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \mu \left(\nabla \mathbf{u}_h^{n+1,i+1}, \nabla \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1,i+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ = - \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \mathbf{u}_h^{n+1,i}, \bar{\mathbf{u}}_h \right) - \lambda \int_0^T \left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) (\nabla \mathbf{u}_h^{n+1,i})^t : \nabla \bar{\mathbf{u}}_h \\ - \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1} \mathbf{u}_h^{n+1,i}, \bar{\mathbf{u}}_h \right) + \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(\left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^n \right) \frac{\mathbf{u}_h^{n+1,i} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right), \\ \left(\nabla \cdot \mathbf{u}_h^{n+1,i}, \bar{p}_h \right) = 0, \end{array} \right.$$

donde $\rho_{\tilde{m}}^{\tilde{M}} = \frac{\tilde{M} + \tilde{m}}{2}$.

Probaremos con un argumento de punto fijo que ambos esquemas iterativos convergen hacia $(\mathbf{u}_h^{n+1}, p_h^{n+1}, \rho_h^{n+1})$ cuando $i \rightarrow \infty$.

Capítulo 5

El capítulo 5 aborda la construcción de un esquema numérico basado en la formulación débil del modelo penalizado de tipo Ginzburg- Landau (10) para aproximar el modelo de cristales

líquidos nemáticos (7). La idea general es una discretización en tiempo de modo que nos permita obtener un esquema lineal para el cual se tenga una versión discreta de la desigualdad de energía (11). En esta ocasión, para conseguir un esquema estable y convergente para dominios tridimensionales, usaremos un algoritmo con una variable auxiliar para aproximar $-\Delta \mathbf{d}$, que deberá considerarse en un espacio de elementos finitos relacionado mediante una condición de compatibilidad con los espacios de aproximación de la velocidad y el vector de orientación. Sin embargo, en el caso de encontrarnos en un dominios bidimensional, esta hipótesis de estabilidad para el espacio de la variable auxiliar se puede debilitarse, manteniendo el esquema correspondiente las mismas propiedades que para el caso tridimensional (linealidad, estabilidad y convergencia).

Requerimos las siguientes propiedades para el dominio, los parámetros de discretización y los espacios de aproximación:

(S) Condiciones de estabilidad:

$$(S1) \quad \lim_{(h,k,\varepsilon) \rightarrow 0} \frac{k}{h^2 \varepsilon^6} = 0 \quad \text{y} \quad (S2) \quad \lim_{(h,k,\varepsilon) \rightarrow 0} \frac{h}{\varepsilon^4} = 0.$$

(H0) Hipótesis sobre los datos: $\mathbf{u}_0 \in \mathbf{V}$, $\mathbf{d}_0 \in \mathbf{H}^1(\Omega)$ con $|\mathbf{d}_0| = 1$ en Ω , $\mathbf{l} \in H^{3/2}(\partial\Omega)$ con $|\mathbf{l}| \leq 1$ sobre Σ

(H1) $\partial\Omega$ es poliédrico tal que se tiene la dependencia continua en las normas $\mathbf{W}^{2,r} \times W^{1,r}$ del problema de *Stokes* con $r > 3$ y la dependencia continua en la norma H^2 del problema de *Laplace-Dirichlet* no homogéneo.

(H2) La triangulación de Ω y los espacios discretos satisfacen:

- las desigualdades inversas:

$$\begin{aligned} \|\nabla \bar{\mathbf{u}}_h\|_{L^\infty(\Omega)} &\leq C h^{-3/2} |\nabla \bar{\mathbf{u}}_h|, \quad \forall \bar{\mathbf{u}}_h \in \mathbf{X}_h, \\ \|\bar{\mathbf{d}}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} &\leq C h^{-1/2} \|\bar{\mathbf{d}}_h\|_{H^1(\Omega)}, \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_h, \end{aligned}$$

- las propiedades de aproximación:

$$\begin{aligned} \|\mathbf{u} - J_h \mathbf{u}\|_{H^1(\Omega)} &\leq C h^2 \|\mathbf{u}\|_{H^3(\Omega)}, \quad \forall \mathbf{u} \in \mathbf{H}^3(\Omega) \cap \mathbf{H}_0^1(\Omega), \\ \|\mathbf{u} - J_h \mathbf{u}\|_{W^{1,\infty}(\Omega)} &\leq C h^{1/2} \|\mathbf{u}\|_{H^3(\Omega)}, \quad \forall \mathbf{u} \in \mathbf{H}^3(\Omega), \\ \|p - K_h p\|_{L^2(\Omega)} &\leq C h \|p\|_{H^1(\Omega)}, \quad \forall p \in H^1(\Omega) \cap L_0^2(\Omega), \end{aligned}$$

$$\|\mathbf{d} - I_h \mathbf{d}\|_{H^1(\Omega)} \leq C h \|\mathbf{d}\|_{H^2(\Omega)}, \quad \forall \mathbf{d} \in \mathbf{H}^2(\Omega),$$

$$\|\mathbf{d} - I_h \mathbf{d}\|_{L^2(\Omega)} \leq C h \|\mathbf{d}\|_{H^1(\Omega)}, \quad \forall \mathbf{d} \in \mathbf{H}^1(\Omega),$$

$$\|I_h \mathbf{d} - \mathbf{d}\|_{L^4(\Omega)} \leq C h^{1/4} \|\mathbf{d}\|_{H^1(\Omega)}, \quad \forall \mathbf{d} \in \mathbf{H}^1(\Omega),$$

donde J_h , K_h y I_h son operadores de interpolación en \mathbf{X}_h , Q_h y \mathbf{D}_h , respectivamente.

(H3) La condición *Inf-Sup* (\mathbf{X}_h, Q_h).

(H4) Condiciones de compatibilidad entre ($\mathbf{X}_h, \mathbf{W}_h, \mathbf{D}_h$):

$$(\mathbf{X}_h \cdot \nabla) \mathbf{D}_h \subset \mathbf{W}_h \quad \text{y} \quad \mathbf{D}_h \subset \mathbf{W}_h.$$

Para la resolución numérica del modelo de cristales líquidos nemáticos (7), como se dijo antes, partimos de un esquema numérico sobre el modelo penalizado de tipo Girsburg-Laundau (10) con traza para el vector de orientación independiente del tiempo que desafortunadamente será totalmente acoplado, pero por contra será lineal:

Inicialización: Sea $(\mathbf{u}_h^0, \mathbf{d}_h^0) \in (\mathbf{X}_h, \mathbf{D}_h)$ adecuadas aproximaciones de los datos iniciales $(\mathbf{u}_0, \mathbf{d}_0)$.

Etapa $n+1$: Dado $(\mathbf{u}_h^n, \mathbf{d}_h^n) \in (\mathbf{V}_h, \mathbf{D}_h)$, encontrar $(\mathbf{u}_h^{n+1}, \bar{p}_h^{n+1}, \mathbf{w}_h^{n+1}, \mathbf{d}_h^{n+1}) \in \mathbf{V}_h \times Q_h \times \mathbf{W}_h \times \mathbf{D}_h$ solución del sistema lineal algebraico:

$$\begin{aligned} & \left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + c\left((\mathbf{u}_h^n \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \nu \left(\nabla \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ & - \lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) + \lambda \left(\nabla \cdot \bar{\mathbf{u}}_h, F_\varepsilon(\mathbf{d}_h^n) \right) - \left(\bar{p}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0 \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \end{aligned} \quad (53)$$

$$\left(\bar{p}_h, \nabla \cdot \mathbf{u}_h^{n+1} \right) = 0 \quad \forall \bar{p}_h \in Q_h, \quad (54)$$

$$\left(\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k}, \bar{\mathbf{w}}_h \right) + \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n, \bar{\mathbf{w}}_h \right) + \gamma \left(\mathbf{f}_\varepsilon(\mathbf{d}_h^n) + \mathbf{w}_h^{n+1}, \bar{\mathbf{w}}_h \right) = 0 \quad \forall \bar{\mathbf{w}}_h \in \mathbf{W}_h, \quad (55)$$

$$\begin{cases} \left(\nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{d}}_h \right) = \left(\mathbf{w}_h^{n+1}, \bar{\mathbf{d}}_h \right), & \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}, \\ \mathbf{d}_h^{n+1}|_{\partial\Omega} = \mathbf{l}_h, \end{cases} \quad (56)$$

donde $\bar{p}_h^{n+1} = p_h^{n+1} + \lambda F_\varepsilon(\mathbf{d}_h^n)$ es una presión modificada debido a la introducción del término estabilidad de tipo potencial $\lambda \left(\nabla \cdot \bar{\mathbf{u}}_h, F_\varepsilon(\mathbf{d}_h^n) \right)$ y hemos introducido la forma trilineal $c(\cdot, \cdot, \cdot)$ definida por

$$c(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \left((\mathbf{u} \cdot \nabla) \mathbf{v}, \mathbf{w} \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u} \mathbf{v}, \mathbf{w} \right), \quad \mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbf{H}_0^1(\Omega),$$

la cual es antisimétrica $c(\mathbf{u}, \mathbf{v}, \mathbf{v}) = 0$, que suple que no se tenga la condición de incompresibilidad de manera puntual.

Debido a que en esta ocasión no podemos asegurar la restricción $|\mathbf{d}_h^{n+1}| \leq 1$, o al menos de manera aproximada, que junto con la estimación de $\|\nabla \mathbf{d}_h^{n+1}\|_{L^2(\Omega)}$ proporcionaría que $\|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)}$ está acotado independientemente de los parámetros de discretización, realizamos un levantamiento discreto del problema (55)-(56) transformándolo en $\mathbf{d}_h^{n+1} = \widehat{\mathbf{d}}_h^{n+1} + \widetilde{\mathbf{d}}_h$ tal que:

$$\widetilde{\mathbf{d}}_h|_{\partial\Omega} = \mathbf{l}_h \quad \text{y} \quad (\nabla \widetilde{\mathbf{d}}_h, \nabla \bar{\mathbf{d}}_h) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}.$$

$$\left(\frac{\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n}{k}, \bar{\mathbf{w}}_h \right) + \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n, \bar{\mathbf{w}}_h \right) + \gamma \left(\mathbf{f}_\varepsilon(\mathbf{d}_h^n) + \mathbf{w}_h^{n+1}, \bar{\mathbf{w}}_h \right) = 0 \quad \forall \bar{\mathbf{w}}_h \in \mathbf{W}_h,$$

$$(\nabla \widehat{\mathbf{d}}_h^{n+1}, \nabla \bar{\mathbf{d}}_h) - (\mathbf{w}_h^{n+1}, \bar{\mathbf{d}}_h) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h},$$

Con ayuda de este levantamiento discreto probaremos que $\|\nabla \widehat{\mathbf{d}}_h^{n+1}\|_{L^2(\Omega)}$ (o equivalentemente $\|\widehat{\mathbf{d}}_h^{n+1}\|_{H^1(\Omega)}$) está acotado independientemente de los parámetros de discretización. Por otro lado, se tiene que $\|\widetilde{\mathbf{d}}_h\|_{H^1}$ está acotado respecto del parámetro de espacio (y que no depende de tiempo). De ambas acotaciones concluimos que $\|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)}$ está acotado uniformemente respecto de n y h .

La prueba de la estabilidad del esquema (53)-(54) se realiza en dos pasos: en la primera etapa probamos una desigualdad de energía discreta para el tiempo $t = t_{n+1}$, imponiendo estimaciones sobre las aproximaciones de la etapa anterior como constata el siguiente resultado:

Lema 18 *Supongamos que existe una constante $C_d > 0$ independiente de h , k y ε tal que*

$$\|\mathbf{u}_h^n\|_{L^2(\Omega)}^2 + \lambda \|\nabla \widehat{\mathbf{d}}_h^n\|_{L^2(\Omega)}^2 \leq C_d.$$

Entonces, existen $h_0 > 0$, $k_0 > 0$ y $\varepsilon_0 > 0$ tal que para cada $h \leq h_0$, $k \leq k_0$ y $\varepsilon \leq \varepsilon_0$ satisfaciendo la hipótesis (S), la correspondiente solución $(\mathbf{u}_h^{n+1}, \mathbf{d}_h^{n+1}, \mathbf{w}_h^{n+1})$ del problema discreto (53)-(56) verifica la siguiente desigualdad:

$$\left\{ \begin{array}{l} \left(\|\mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 - \|\mathbf{u}_h^n\|_{L^2(\Omega)}^2 + \|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \right) + \nu k \|\nabla \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 \\ + \lambda \left(\|\nabla \widehat{\mathbf{d}}_h^{n+1}\|_{L^2(\Omega)}^2 - \|\nabla \widehat{\mathbf{d}}_h^n\|_{L^2(\Omega)}^2 + \|\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)\|_{L^2(\Omega)}^2 \right) + \lambda \gamma k \|P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n) + \mathbf{w}_h^{n+1})\|_{L^2(\Omega)}^2 \\ + 2\lambda \int_{\Omega} (F_\varepsilon(\mathbf{d}_h^{n+1}) - F_\varepsilon(\mathbf{d}_h^n)) + \frac{\lambda}{\varepsilon^2} \int_{\Omega} \left(\frac{1}{4} (\|\mathbf{d}_h^{n+1}\|_{L^2(\Omega)}^2 - \|\mathbf{d}_h^n\|_{L^2(\Omega)}^2)^2 + \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{L^2(\Omega)}^2 \right) \leq 0, \end{array} \right.$$

donde P_h es la proyección ortogonal en $L^2(\Omega)$ sobre \mathbf{W}_h .

En un segundo paso, por un proceso de inducción en la etapa de tiempo y bajo adecuadas estimaciones de los datos iniciales que verifiquen las condiciones del lema anterior, llegamos al

Teorema 19 *Existen h_0 , k_0 y ε_0 de modo que para cualquier $h \leq h_0$, $k \leq k_0$ y $\varepsilon \leq \varepsilon_0$ satisfaciendo la condición de estabilidad (S1), la correspondiente solución $(\mathbf{u}_h^{n+1}, \mathbf{d}_h^{n+1}, \mathbf{w}_h^{n+1})$ del problema discreto (53)-(56) verifica las estimaciones:*

$$\begin{aligned}
i) \quad & \max_{0 \leq n \leq N} \|\mathbf{u}_h^n\|_{L^2(\Omega)} \leq C, & ii) \quad & k \sum_{n=0}^{N-1} \|\nabla \mathbf{u}_h^{n+1}\|_{L^2(\Omega)}^2 \leq C, \\
iii) \quad & \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n\|_{L^2(\Omega)}^2 \leq C, & iv) \quad & \max_{0 \leq n \leq N} \|\mathbf{d}_h^n\|_{H^1(\Omega)} \leq C, \\
v) \quad & k \sum_{n=0}^{N-1} \|P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}\|_{L^2(\Omega)}^2 \leq C, & vi) \quad & \sum_{n=0}^{N-1} \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{H^1(\Omega)}^2 \leq C, \\
vii) \quad & \max_{0 \leq n \leq N} \int_{\Omega} F_\varepsilon(\mathbf{d}_h^n) \leq C & viii) \quad & \frac{1}{\varepsilon^2} \sum_{n=0}^{N-1} \int_{\Omega} \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{L^2(\Omega)}^2 \leq C,
\end{aligned}$$

donde $C > 0$ es independiente de (h, k, ε) .

Una vez establecidas las estimaciones de estabilidad pasamos a los resultados de compacidad para las aproximaciones. Para el vector de orientación, acotando la derivada discreta

$$k \sum_{n=0}^{N-1} \left\| \frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k} \right\|_{L^{3/2}(\Omega)}^2 \leq C,$$

se obtiene la compacidad en $L^q(0, T; L^r(\Omega))$ donde $1 \leq r < 6$ y $1 \leq q < \infty$. Para la velocidad tendremos que aplicar un resultado de compacidad por perturbación dado por *P. Azérad* y *F. Guillen-González* en [2]. Para ello, usando la estabilidad en $\mathbf{W}^{1,\infty}(\Omega) \times L^\infty(\Omega)$ (velocidad-presión) del operador de *Stokes* discreto ([18]), podemos acotar las derivada fraccionaria:

$$k \sum_{m=0}^{N-r} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{\mathbf{V}'_h}^2 \leq C (r k)^{1/2} \quad \forall \delta : 0 < \delta < T.$$

Observar que la norma en espacio de la derivada fraccionaria es en \mathbf{V}'_h (dual de \mathbf{V}_h) donde $\mathbf{V}_h = \{\mathbf{v}_h \in \mathbf{X}_h : (\nabla \cdot \mathbf{v}_h, q_h) = 0, \forall q_h \in Q_h\}$, que se mueve con respecto al parámetro de discretización de espacio. La siguiente operación será encontrar una estimación fraccionaria en tiempo, a partir de la anterior, cuyo norma en espacio no dependa del parámetro de espacio. Usando el operador ortogonal $R_h : \mathbf{V}_h \rightarrow \mathbf{V}$ definido como $(\nabla(R_h \mathbf{u}_h - \mathbf{u}_h), \nabla \mathbf{v}) = 0$ para todo $\mathbf{v} \in \mathbf{V}$, encontramos

$$k \sum_{m=0}^{N-r} \|R_h(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{\mathbf{V}'}^2 \leq C (r k)^{1/2} + C h^2.$$

Aplicando un teorema de compacidad por perturbación tendremos que $R_h \mathbf{u}_h^n$ es una sucesión compacta en $\mathbf{L}^2(Q)$ cuando los parámetros $(k, h, \varepsilon) \rightarrow 0$. De aquí, se prueba la compacidad de la velocidad discreta en $\mathbf{L}^2(Q)$.

Para pasar al límite en el tensor $-\lambda((\nabla \mathbf{d}^n)^t \mathbf{w}^{n+1}, \bar{\mathbf{u}}_h)$, integramos por parte de modo discreto consiguiendo

$$-\lambda((\nabla \mathbf{d}^n)^t \mathbf{w}^{n+1}, \bar{\mathbf{u}}_h) = -\lambda((\nabla \mathbf{d}^n)^t \nabla \mathbf{d}^{n+1}, \bar{\mathbf{u}}_h) + \text{Términos residuales.}$$

Luego, necesitamos probar que el gradiente del vector de orientación converge fuerte al menos en $\mathbf{L}^2(Q)$. La idea original de la compacidad del gradiente del vector de orientación (en el caso continuo) se encuentra en [23]. Definimos el problema de mínimos discreto asociado a $\mathbf{z}_{h,k,\varepsilon}(t) = \mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^{n+1}))$ y $\mathbf{d}_{h,k,\varepsilon}(t) = \mathbf{d}_h^{n+1}$ si $t \in (t_n, t_{n+1}]$ como

$$J_{h,k,\varepsilon}(\mathbf{d}_{h,k,\varepsilon}(t)) = \min_{\mathbf{d}_h \in \mathbf{D}_{l_h}} J_{h,k,\varepsilon}(\mathbf{d}_h)$$

siendo $J_{h,k,\varepsilon} : \mathbf{D}_{l_h} \rightarrow \mathbb{R}$ definido como

$$J_{h,k,\varepsilon}(\mathbf{d}_h) = \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{d}_h|^2 + F_\varepsilon(\mathbf{d}_h) - \mathbf{z}_{h,k,\varepsilon} \cdot \mathbf{d}_h \right)$$

y

$$\mathbf{D}_{l_h} = \{\mathbf{d}_h \in \mathbf{D}_h : \mathbf{d}_h = l_h \text{ sobre } \partial\Omega\}.$$

y el problema de mínimos continuo

$$J(\mathbf{d}(t)) = \min_{\{\bar{\mathbf{d}} \in \mathbf{H}_1, |\bar{\mathbf{d}}|=1\}} J(\bar{\mathbf{d}})$$

siendo \mathbf{d} el límite encontrado por la estabilidad de esquema y

$$J(\mathbf{d}) = \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{d}|^2 - \mathbf{z}(t) \cdot \mathbf{d} \right).$$

Relacionando estos dos problemas probamos que $\int_0^T J_{h,k,\varepsilon}(\mathbf{d}_{h,k,\varepsilon}(t)) dt \rightarrow \int_0^T J(\mathbf{d}(t)) dt$ cuando $(h, k, \varepsilon) \rightarrow 0$. Por otra parte, ya sabíamos que $\int_0^T (z_{h,k,\varepsilon}, \mathbf{d}_{h,k,\varepsilon}) dt \rightarrow \int_0^T (z_{h,k,\varepsilon}, \mathbf{d}_{h,k,\varepsilon})$ y se prueba que $\int_{F_\varepsilon}(\mathbf{d}_{h,k,\varepsilon}) \rightarrow 0$ cuando $(h, k, \varepsilon) \rightarrow 0$. Luego, deducimos que el vector de orientación es compacto en $L^2(0, T; \mathbf{H}^1(\Omega))$.

Finalmente, se llega al siguiente resultado:

Teorema 20 *Supongamos las hipótesis (S), (H0)-(H4). Entonces, existe una subsucesión convergente de aproximaciones definidas por el problema discreto (53)-(56) cuando $(h, k, \varepsilon) \rightarrow 0$*

hacia una solución débil (\mathbf{u}, \mathbf{d}) del problema (7), (8)-(9), en el siguiente sentido: la velocidad discreta en $L^2(0, T; \mathbf{L}^2(\Omega))$ -fuerte, en $L^\infty(0, T; \mathbf{L}^2(\Omega) \times)$ -débil* y en $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -débil y el vector de orientación discreto en $L^2(0, T; \mathbf{H}^1(\Omega))$ -fuerte y en $L^\infty(0, T; \mathbf{H}^1(\Omega))$ -débil*.

Capítulo 6

En este capítulo presentamos dos esquemas numéricos para el modelo de campo de fase para un proceso de solidificación de una mezcla binaria con propiedades térmicas (14) junto con las condiciones de contorno (15) e iniciales (16). El primer esquema que construimos es no lineal, incondicionalmente estable y convergente. Concretamente, proponemos una discretización no lineal de la ecuación para la variable campo de fase (14)₁, siendo las dos restantes ecuaciones (para la temperatura y la concentración) desacopladas y lineales. Con este esquemas recuperamos las estimaciones obtenidas en el trabajo teórico [4] de existencia de solución para (14) de *J.L. Boldrini* y *G. Planas*.

En el segundo esquema consideramos una discretización lineal de la ecuación que caracteriza el campo de fase, llegando a un algoritmo totalmente lineal, condicionalmente estable y convergente. Luego, la linealidad de la ecuación de la variable campo de fase nos cuesta una restricción entre los parámetros espacio y tiempo. Si observamos los algoritmos numéricos desarrollados para los modelos de campo de fase descritos anteriormente, vemos que todos ellos resultan ser no lineales aunque estos esquemas son propuestos incluso para modelos más simples que el que consideramos en esta tesis. La estabilidad de este esquema lineal es consecuencia de la similitud que presenta la ecuación para el campo de fase (14)₁ y la del vector de orientación del modelo de cristales líquidos penalizado (7)₂ dado que el potencial $f(\phi) = \frac{1}{2\varepsilon^2}(\phi^2 - 1)\phi$ asociado a (14)₁ es similar al término de penalización de (7)₂.

Para ambos esquemas usamos un operador de truncamiento discreto para preservar el principio del máximo de la variable de concentración.

Sea una partición uniforme del intervalo temporal $[0, T]$ de paso k y sea X_h el espacio de elementos finitos continuos que sobre cada elemento de la triangulación es un polinomio de grado 1. Entonces el esquema no lineal que presentamos se describe como:

Inicialización: Sean $(\phi_h^0, \theta_h^0, c_h^0) \in X_h \times X_h \times X_h$ determinadas aproximaciones de (ϕ_0, θ_0, c_0) cuando $h \rightarrow 0$.

Etapa $n + 1$: Dado $(\phi_h^n, \theta_h^n, c_h^n) \in X_h \times X_h \times X_h$.

Hallar $\phi_h^{n+1} \in X_h$ como la solución del problem:

$$\begin{cases} \alpha \varepsilon^2 \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) + \varepsilon^2 (\nabla \phi_h^{n+1}, \nabla x_h) + \frac{1}{2} ((\phi_h^{n+1})^3, x_h) \\ = \frac{1}{2} (\phi_h^n, x_h) + \beta (\theta_h^n - \theta_A c_h^n - \theta_B (1 - c_h^n), x_h) \quad \forall x_h \in X_h. \end{cases} \quad (57)$$

Hallar $\theta_h^{n+1} \in X_h$ y $c_h^{n+1} \in X_h$ como las soluciones de los problemas variacionales desacoplados:

$$C_V \left(\frac{\theta_h^{n+1} - \theta_h^n}{k}, x_h \right) + (K_1^k (\phi_h^{n+1}) \nabla \theta_h^{n+1}, \nabla x_h) = -\frac{l}{2} \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) \quad \forall x_h \in X_h, \quad (58)$$

$$\left(\frac{c_h^{n+1} - c_h^n}{k}, x_h \right) + K_2 (\nabla c_h^{n+1}, \nabla x_h) = -K_2 M ([c_h^n]_T (1 - [c_h^n]_T) \nabla \phi_h^n, \nabla x_h) \quad \forall x_h \in X_h. \quad (59)$$

Aquí, $K_1^k = K_1 + k$ y $[\cdot]_T$ es un operador de truncamiento por nodos definido como sigue: dado $x_h \in X_h$, entonces $[x_h]_T \in X_h$ tal que:

$$[x_h]_T(\mathbf{x}_i) = \begin{cases} x_h(\mathbf{x}_i) & \text{si } x_h(\mathbf{x}_i) \in [0, 1], \\ 0 & \text{si } x_h(\mathbf{x}_i) < 0, \\ 1 & \text{si } x_h(\mathbf{x}_i) > 1, \end{cases}$$

donde \mathbf{x}_i son los nodos de la malla \mathcal{T}_h .

Tomando como funciones test ϕ_h^{n+1} , $\frac{\phi_h^{n+1} - \phi_h^n}{k}$, $-\Delta_h \phi_h^{n+1}$ en (57), θ_h^{n+1} en (58) y c_h^{n+1} en (59), llegamos a las estimaciones:

Lema 21 *La solución discreta del esquema (57)-(59) verifica las siguientes estimaciones:*

$$\begin{aligned} i) \max_{0 \leq n \leq N} \|\phi_h^n\|_{H^1(\Omega)} &\leq C, & ii) \sum_{n=0}^{N-1} \|\phi_h^{n+1} - \phi_h^n\|_{H^1(\Omega)}^2 &\leq C, \\ iii) k \sum_{n=0}^{N-1} \left\| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right\|_{L^2(\Omega)}^2 &\leq C, & iv) \max_{0 \leq n \leq N} \|\theta_h^n\|_{L^2(\Omega)} &\leq C, \\ v) \sum_{n=0}^{N-1} \|\theta_h^{n+1} - \theta_h^n\|_{L^2(\Omega)}^2 &\leq C, & vi) k \sum_{n=0}^{N-1} \|\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}\|_{L^2(\Omega)}^2 &\leq C, \\ vii) \max_{0 \leq n \leq N} \|c_h^n\|_{L^2(\Omega)} &\leq C, & viii) \sum_{n=0}^{N-1} \|c_h^{n+1} - c_h^n\|_{L^2(\Omega)}^2 &\leq C, \\ ix) k \sum_{n=0}^{N-1} \|\nabla c_h^{n+1}\|_{L^2(\Omega)}^2 &\leq C, \end{aligned}$$

donde $C > 0$ depende únicamente de los datos (ϕ_0, θ_0, c_0) .

A continuación, definiendo $\tilde{\phi}_{h,k}$, $\tilde{\theta}_{h,k}$ y $\tilde{c}_{h,k}$ como funciones lineales y continuas que toman los valores $\tilde{\phi}_{h,k}(t_n) = \phi_h^n$, $\tilde{\theta}_{h,k}(t_n) = \theta_h^n$ y $\tilde{c}_{h,k}(t_n) = c_h^n$ respectivamente, probamos el

Lema 22 *Se tienen las siguientes estimaciones:*

$$\int_0^T \|\partial_t \tilde{\theta}_{h,k}(t)\|_{H^1(\Omega)'}^2 dt \leq C, \quad (60)$$

$$\int_0^T \|\partial_t \tilde{c}_{h,k}(t)\|_{H^1(\Omega)'}^2 dt \leq C, \quad (61)$$

donde $C > 0$ es independiente de (h, k) .

Como consecuencia de los Lemas 21 y 22, se puede probar mediante un resultado de compacidad las estimaciones fuertes cuando $(h, k) \rightarrow 0$:

$$\tilde{\theta}_{h,k} \rightarrow \theta \quad \text{fuerte en } L^2(0, T; H^1(\Omega)'),$$

$$\tilde{c}_{h,k} \rightarrow c \quad \text{fuerte en } L^2(Q),$$

$$\tilde{\phi}_{h,k} \rightarrow \phi \quad \text{fuerte en } L^2(Q).$$

Usando la definición del laplaciano discreto y la compacidad en $L^2(Q)$ mejoramos la compacidad en $L^2(Q)$ de $\{\tilde{\phi}_{h,k}\}_{h,k}$ a

$$\{\tilde{\phi}_{h,k}\}_{h,k} \quad \text{es compacta en } L^2(0, T; H^1(\Omega)).$$

Finalmente, de la compacidad de $\{\tilde{c}_{h,k}\}_{h,k}$ en $L^2(Q)$ conseguimos el siguiente resultado para el operador de truncamiento:

Proposición 23 *Se tienen las siguientes convergencias*

$$[c_{h,k}]_T, [\hat{c}_{h,k}]_T \rightarrow T_0^1 c \quad \text{en } L^2(0, T; L^2(\Omega))\text{-fuerte, cuando } (h, k) \rightarrow 0. \quad (62)$$

donde T_0^1 es el operador de truncamiento definido como:

$$T_0^1 c(\mathbf{x}, t) = \begin{cases} c(\mathbf{x}, t) & \text{si } c(\mathbf{x}, t) \in [0, 1], \\ 0 & \text{si } c(\mathbf{x}, t) < 0, \\ 1 & \text{si } c(\mathbf{x}, t) > 1. \end{cases}$$

Por último, para pasar al límite en (59) no apoyamos en el siguiente resultado que asegura que la función límite c , a la que converge la concentración discreta, verifica el principio del máximo $0 \leq c \leq 1$ eliminando el operador de truncamiento T_0^1 de la función límite de la concentración discreta.

Lema 24 *Las dos siguientes ecuaciones son equivalentes:*

$$c_t = K_2(\Delta c + M\nabla \cdot [T_0^1 c(1 - T_0^1 c)\nabla\phi]) \quad \text{en } Q, \quad (63)$$

y

$$0 \leq c \leq 1, \quad c_t = K_2(\Delta c + M\nabla \cdot [c(1 - c)\nabla\phi]) \quad \text{en } Q,$$

En (57) y (58) se pasa al límite de forma estándar.

Ahora, definimos $f(\phi) = \frac{1}{2\varepsilon^2}(\phi^2 - 1)\phi$ asociada a la función potencial $\frac{1}{8\varepsilon^2}F(\phi) = (\phi^2 - 1)^2$.

Entonces, proponemos el siguiente esquema lineal:

Inicialización: Sean $(\phi_h^0, \theta_h^0, c_h^0) \in X_h \times X_h \times X_h$ determinadas aproximaciones de (ϕ_0, θ_0, c_0) as $h \rightarrow 0$.

Etapa $n + 1$: Dado $(\phi_h^n, \theta_h^n, c_h^n) \in X_h \times X_h \times X_h$.

Hallar $\phi_h^{n+1} \in X_h$ como la solución del problema:

$$\begin{aligned} & \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) + \frac{1}{\alpha} \left(\nabla \phi_h^{n+1}, \nabla x_h \right) \\ &= -\frac{1}{\alpha} \left(f(\phi_h^n), x_h \right) + \frac{\beta}{\varepsilon^2 \alpha} \left(\theta_h^n - \theta_A c_h^n - \theta_B (1 - c_h^n), x_h \right), \quad \forall x_h \in X_h. \end{aligned} \quad (64)$$

Hallar $\theta_h^{n+1} \in X_h$ y $c_h^{n+1} \in X_h$ como las soluciones de los problemas desacoplados:

$$C_V \left(\frac{\theta_h^{n+1} - \theta_h^n}{k}, x_h \right) + \left(K_1^k(\phi_h^{n+1}) \nabla \theta_h^{n+1}, \nabla x_h \right) = -\frac{l}{2} \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right), \quad \forall x_h \in X_h, \quad (65)$$

$$\left(\frac{c_h^{n+1} - c_h^n}{k}, x_h \right) + K_2 \left(\nabla c_h^{n+1}, \nabla x_h \right) = -K_2 M \left([c_h^n]_T (1 - [c_h^n]_T) \nabla \phi_h^n, \nabla x_h \right), \quad \forall x_h \in X_h. \quad (66)$$

Al igual que en el caso de cristales líquidos, la estabilidad del esquema (64)-(66) se prueba por un proceso de inducción en la etapa de tiempo n en dos pasos. Primero, asumiendo cierta restricción sobre los parámetros de discretización y acotación para la solución discreta en la etapa n encontramos las siguientes desigualdades tomando como funciones test $f(\phi_h^n) - \Delta \phi_h^{n+1}$, $\frac{\phi_h^{n+1} - \phi_h^n}{k}$ y ϕ_h^{n+1} en (64), θ_h^{n+1} en (65) y c_h^{n+1} en (66).

Lema 25 *Supongamos la restricción:*

$$(S) \quad \lim_{(h,k) \rightarrow 0} k/h = 0.$$

Si existe una constante $C_d > 0$ (independiente de n) tal que

$$\|\phi_h^n\|_{H^1(\Omega)}^2 + \frac{\alpha C_V^2}{8l^2} \|\theta_h^n\|_{L^2(\Omega)}^2 + \|c_h^n\|_{L^2(\Omega)}^2 \leq C_d.$$

Entonces, existen $k_0, h_0 > 0$ suficientemente pequeños, pero independiente de n tal que para cualquier $k \leq k_0$ y $h \leq h_0$, se tiene las siguientes desigualdades

$$\left\{ \begin{array}{l} \|\phi_h^{n+1}\|_{H^1(\Omega)}^2 - \|\phi_h^n\|_{H^1(\Omega)}^2 + \frac{1}{2}\|\phi_h^{n+1} - \phi_h^n\|_{H^1(\Omega)}^2 \\ + \frac{\alpha C_V^2}{8l^2} \left(\|\theta_h^{n+1}\|_{L^2(\Omega)}^2 - \|\theta_h^n\|_{L^2(\Omega)}^2 + \|\theta_h^{n+1} - \theta_h^n\|_{L^2(\Omega)}^2 \right) \\ + \frac{1}{4\epsilon^2} \int_{\Omega} \left((|\phi_h^{n+1}|^2 - 1)^2 - (|\phi_h^n|^2 - 1)^2 + \frac{1}{2}(|\phi_h^{n+1}|^2 - |\phi_h^n|^2)^2 \right) \\ + \frac{\alpha}{16} k \left\| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right\|_{L^2(\Omega)}^2 + \frac{k}{2\alpha} \|f(\phi_h^n) - \Delta \phi_h^{n+1}\|_{L^2(\Omega)}^2 + \frac{\alpha C_V k}{4l^2} \|\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}\|_{L^2(\Omega)}^2 \\ \leq C k \|\theta_h^n\|^2 + C k \|\phi_h^n\|_{L^2(\Omega)}^2 + C k \|c_h^n\|_{L^2(\Omega)}^2 + C k, \end{array} \right. \quad (67)$$

$$\|c_h^{n+1}\|_{L^2(\Omega)}^2 - \|c_h^n\|_{L^2(\Omega)}^2 + \|c_h^{n+1} - c_h^n\|_{L^2(\Omega)}^2 + k K_2 \|\nabla c_h^{n+1}\|_{L^2(\Omega)}^2 \leq C k \|\nabla \phi_h^n\|_{L^2(\Omega)}^2. \quad (68)$$

Claramente, si admitimos que las desigualdades (67) y (68) se tienen para cualquier etapa de tiempo n basta aplicar un lema de Gronwall para establecer las siguientes estimaciones de estabilidad del esquema lineal (64)-(66):

Lema 26 *La solución discreta del esquema (64)-(66) verifica las siguientes estimaciones:*

$$\begin{array}{lll} \text{i)} \max_{0 \leq n \leq N} \|\phi_h^n\|_{H^1(\Omega)} \leq C, & \text{ii)} \sum_{n=0}^{N-1} \|\phi_h^{n+1} - \phi_h^n\|_{H^1(\Omega)}^2 \leq C, & \text{iii)} k \sum_{n=0}^{N-1} \left\| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right\|_{L^2(\Omega)}^2 \leq C, \\ \text{iv)} \max_{0 \leq n \leq N} \|\theta_h^n\|_{L^2(\Omega)} \leq C, & \text{v)} \sum_{n=0}^{N-1} \|\theta_h^{n+1} - \theta_h^n\|_{L^2(\Omega)}^2 \leq C, & \text{vi)} k \sum_{n=0}^{N-1} \|\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}\|_{L^2(\Omega)}^2 \leq C, \\ \text{vii)} \max_{0 \leq n \leq N} \|c_h^n\| \leq C, & \text{viii)} \sum_{n=0}^{N-1} \|c_h^{n+1} - c_h^n\|_{L^2(\Omega)}^2 \leq C, & \text{ix)} k \sum_{n=0}^{N-1} \|\nabla c_h^{n+1}\|_{L^2(\Omega)}^2 \leq C, \end{array}$$

donde $C > 0$ es independiente de h, k .

La convergencia del esquema lineal (64)-(66) se realiza de forma totalmente análoga a esquema no lineal (57)-(59)

Capítulo 7

En este capítulo, presentamos algunas simulaciones numéricas del modelo simplificado de cristales líquidos nemáticos (7)-(9), usando el esquema numérico (53)-(56) desarrollado en el capítulo 5.

La literatura sobre simulaciones numéricas de cristales líquidos no es muy amplia. Los tests numéricos que realizamos son extraídos del trabajo [30] de *Liu* y *Walkington*, con los que comparamos los resultados. Estos tests exhiben el curioso comportamiento de los flujos

de cristales líquidos en presencia de singularidades. Además, también, mostramos otros tests numéricos inspirados en los realizados en [13], aunque con distintas condiciones de contorno.

Todos los ejemplos numéricos que se exhiben son computados en un dominio bidimensional $\Omega = (-1, 1) \times (-1, 1)$. El par velocidad y presión (\mathbf{u}, p) es aproximado usando el par de elementos finitos estable conocido como mini-elemento $(\mathbb{P}_1 + \text{burbuja}, \mathbb{P}_1)$. El par vector de orientación y su laplaciano $(\mathbf{d}, -\Delta \mathbf{d})$ es aproximado usando el par de elementos finitos $(\mathbb{P}_1, \mathbb{P}_0)$. Además, estos ejemplos son calculados sobre una malla uniforme de 32×32 y 160 pasos por unidad de tiempo (i.e. $h = 1/16$ y $k = 1/160$). Como en [30], seleccionamos los parámetros λ , ν y γ iguales a uno. Respecto al parámetro de penalización ε asociado a la función \mathbf{f}_ε haremos varias elecciones. Veremos que para $\varepsilon = 0.05$ (elegido en [30]) el esquema (53)-(56) es no convergente para ninguno de los ejemplos propuestos. Sin embargo para $\varepsilon = 0.06$ y $\varepsilon = 0.07$ nuestros resultados muestran el mismo comportamiento cualitativo para el vector de orientación que los de [30] aunque para $\varepsilon = 0.06$ la velocidad muestra un comportamiento distinto, siendo análogo para $\varepsilon = 0.07$. Las nuevas experiencias que proponemos son ejecutadas para $\varepsilon = 0.06$ y $\varepsilon = 0.08$ para un vector de orientación inicial con dos singularidades que se repelen hasta entrar en equilibrio con las condiciones de contorno impuestas para el vector de orientación (son las que provienen del vector de orientación inicial) y $\varepsilon = 0.06$ para una vector de orientación con una singularidad en el origen de coordenadas de orden cuatro para el cual observamos como la singularidad original de descomponen en cuatro singularidades que se van separando a las esquinas del dominio Ω donde permanecen.

Como hito a destacar son los tiempos de cálculos para los tests de [30] de una unidad de tiempo, donde nuestro esquema, lineal y totalmente acoplado, es con diferencia mucho menos costoso que el propuesto en [30], que es no lineal usando elementos finitos globalmente diferenciables para el vector de orientación.

La resolución numérica se lleva a cabo con la ayuda del software de *Freefem++* usando una formulación penalizada en norma L^2 de la presión en la ecuación de la divergencia discreta nula siendo el parámetro de penalización del orden de 10^{-6} . El sistema lineal que queda en cada etapa de tiempo es resuelto usando el método directo de sistemas lineales LU.

Los cálculos han sido ejecutados con un procesador Intel(R) Core(TM)2 CPU 4300 @ 1.80 GHz 1.80 GHz.

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Capítulo 1

Unconditional stability and convergence of fully discrete schemes for $2D$ viscous fluids models with mass diffusion

Unconditional stability and convergence of fully discrete schemes for $2D$ viscous fluids models with mass diffusion

F. Guillén-González*, J.V. Gutiérrez-Santacreu*

Abstract

In this work we develop fully discrete (in time and space) numerical schemes for two-dimensional incompressible fluids with mass diffusion, also called Kazhikhov-Smagulov models. We propose at most H^1 -conformed finite elements (only globally continuous functions) to approximate all unknowns (velocity, pressure and density), although the limit density (solution of continuous problems) will have the H^2 -regularity. A backward Euler in time scheme is considered decoupling the computation of the density from the velocity and pressure.

Unconditional stability and convergence of schemes towards the (unique) global in time weak solution of models are proved. Since a discrete maximum principle cannot be ensured, we must use a different interpolation inequality to obtain strong estimates for the discrete density, from the used one in the continuous case. This inequality is a discrete version of the *Gagliardo-Nirenberg* interpolation inequality in $2D$ domains. Moreover, the discrete density is truncated in some adequate terms of the velocity-pressure problem.

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Keywords: Kazhikhov-Smagulov models, Finite Elements, stability, convergence.

1 Introduction

1.1 The models

Let $\Omega \subseteq \mathbb{R}^2$ be a bounded domain with boundary Γ that is regular enough, and $[0, T]$ ($0 < T < \infty$) the time interval of observation. We will use the notation $Q = \Omega \times (0, T)$, $\Sigma = \Gamma \times (0, T)$.

We are going to study two models, which can be deduced from the following compressible Navier-Stokes system in Q :

$$\begin{cases} (\rho \mathbf{v})_t + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) - \mu \nabla \cdot (\Psi(\rho) \nabla \mathbf{v}) - (\mu + \tilde{\lambda}) \nabla (\nabla \cdot \mathbf{v}) + \nabla q = \rho \mathbf{f}, \\ \rho_t + \nabla \cdot (\rho \mathbf{v}) = 0, \end{cases} \quad (1)$$

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This model is related to a pollution problem [3, 4].

Note that the main differences with respect to the previous system (3) are that now the λ^2 -terms are all of potential type (included into the modified pressure $p = q - \lambda(\tilde{\lambda} + \lambda)\Delta \log \rho$) and the diffusion becomes nonlinear, changing $-\mu \nabla \cdot (\nabla \mathbf{u})$ by $-\lambda \nabla \cdot (\rho \nabla \mathbf{u})$ in the momentum system.

We complete these models with the following boundary conditions

$$\mathbf{u}|_{\Sigma} = 0, \quad \frac{\partial \rho}{\partial \mathbf{n}} \Big|_{\Sigma} = 0 \quad (9)$$

(where $\mathbf{n}(\mathbf{x})$ is the outwards unit normal vector on the boundary Γ) and the initial conditions

$$\rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega. \quad (10)$$

1.2 Known results

Concerning the reduced model (7), Kazhikhov and Smagulov ([12]) proved, via a semi-Galerkin method, existence of global weak solutions under the following hypothesis about the viscosity and diffusion coefficients $\lambda < 2\mu/(M - m)$ and existence and uniqueness of local strong solutions (which is global in time in the $2D$ case). On the other hand, Salvi([13]) proved existence of weak solutions in non-cylindrical domains. Secchi ([15]) studied the case $\Omega = \mathbb{R}^3$, proving existence and uniqueness of strong solutions, using a fixed point argument.

With respect to the full model (3), Beirão da Veiga ([2]) and Secchi ([14]) established local existence of strong solutions by means of linearization and fixed point argument. In ([14]), Secchi proved existence and uniqueness of global weak solutions in $2D$ domains imposing smallness on λ/μ and the asymptotic behavior towards a weak solution of the Navier-Stokes problem with variable density. Recently, in ([10]), by means of an iterative method, existence of strong solutions (and some error estimates) has been proved.

For the pollutant model (8), Guillén-González and Sy prove existence of strong solutions of (8) and find some error estimates by means of an iterative method in [11].

From the point of view of numerical analysis, a numerical algorithm is developed in [6, 7], for a compressible version of a Kazhikhov-Smagulov model, without using explicitly the decomposition of the compressible velocity in terms of an incompressible part. The scheme under consideration uses a discrete method of characteristics in time and finite elements in space. The authors get optimal error estimates assuming enough regularity for the continuous solution. It is important to remark that in these works, the analysis of unconditional stable, convergent schemes towards weak solutions is not considered.

1.3 Main results of the paper

The task of this paper is to design fully discrete schemes, unconditionally stable and convergent, by using only C^0 -finite elements for the two problems (7) and (8).

The main question to treat is: *Is it possible to approximate the weak solution of mass diffusion problems with only C^0 -finite elements?*

The answer is positive for models (7) and (8). Moreover, unconditional stability will be founded.

We will look for schemes using first order finite difference in time and C^0 -finite elements in space. The key idea is to find an adequate reformulation of continuous problems, adding “stabilized terms” such that the corresponding Galerkin finite element gives us an unconditionally stable scheme. Namely, in the case of problem (7), (9) and (10), we will arrive at the following variational formulation: a.e. $t \in (0, T)$,

$$\begin{aligned} & \left(\frac{d}{dt} \rho(t), \bar{\rho} \right) + \left(\mathbf{u}(t) \cdot \nabla \rho(t), \bar{\rho} \right) + \lambda \left(\nabla \rho(t), \nabla \bar{\rho} \right) = 0, \quad \forall \bar{\rho} \in H^1(\Omega), \\ & \begin{cases} \left([\rho]_T(t) \frac{d}{dt} \mathbf{u}(t), \bar{\mathbf{u}} \right) + \frac{1}{2} \left(\frac{d}{dt} [\rho]_T(t) \mathbf{u}(t), \bar{\mathbf{u}} \right) + a \left([\rho]_T(t), \mathbf{u}(t), \bar{\mathbf{u}} \right) \\ + c \left(\rho(t) \mathbf{u}(t) - \lambda \nabla \rho(t), \mathbf{u}(t), \bar{\mathbf{u}} \right) = \left([\rho]_T(t) \mathbf{f}(t), \bar{\mathbf{u}} \right) + \left(p(t), \nabla \cdot \bar{\mathbf{u}} \right), \quad \forall \bar{\mathbf{u}} \in \mathbf{H}_0^1(\Omega), \\ \left(\nabla \cdot \mathbf{u}(t), \bar{p} \right) = 0, \quad \forall \bar{p} \in L_0^2(\Omega), \end{cases} \end{aligned}$$

where we have defined

$$[\rho]_T(\mathbf{x}, t) = \begin{cases} \rho(\mathbf{x}, t) & \text{if } \rho(\mathbf{x}, t) \in [m, M], \\ m & \text{if } \rho(\mathbf{x}, t) < m, \\ M & \text{if } \rho(\mathbf{x}, t) > M, \end{cases}$$

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu \left(\nabla \mathbf{u}, \nabla \mathbf{v} \right) + \lambda \int_{\Omega} \left(\frac{M+m}{2} - \rho \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} dx$$

and

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) = \frac{1}{2} \left[\left((\mathbf{w} \cdot \nabla) \mathbf{u}, \mathbf{v} \right) - \left((\mathbf{w} \cdot \nabla) \mathbf{v}, \mathbf{u} \right) \right]$$

which verify adequate properties of continuity and coercivity for $a(\cdot, \cdot, \cdot)$ and antisymmetric for $c(\cdot, \cdot, \cdot)$, see (24), (25), (26) and (27) below.

Then, if we choose a partition of $(0, T)$ of parameter k , ($t_n = nk$), and take $(W_h, \mathbf{V}_h, M_h) \subset H^1 \times \mathbf{H}_0^1 \times L_0^2$ finite-element spaces for approximating the density, velocity and pressure, the following scheme is proposed:

Initialization: Let $(\mathbf{u}_h^0, \rho_h^0) \in (\mathbf{V}_h, W_h)$ be suitable approximations of (\mathbf{u}_0, ρ_0) , as $h \rightarrow 0$.

Time step $(n+1)$: Given $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Find $\rho_h^{n+1} \in W_h$ such that for each $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h \right).$$

2. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\begin{cases} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h), \\ (\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h) = 0. \end{cases}$$

Defining in $[0, T]$ the step functions $\mathbf{u}_{k,h}, \rho_{k,h}$ as $\mathbf{u}_{k,h}(t) = \mathbf{u}_h^n$ and $\rho_{k,h}(t) = \rho_h^n$ on $(t_{n-1}, t_n]$, respectively, we arrive at the following main result.

Theorem 1 *Let $\mathbf{u}_0 \in \mathbf{V}$, $\rho_0 \in H_N^2(\Omega)$ (see (11) and (12) in the next section) satisfying (13) and $\mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega))$ with $p > 1$. Suppose the constraint on the constants λ, μ, m and M : $\lambda < 2\mu(M-m)^{-1}$. Then, the whole sequence $(\mathbf{u}_{k,h}, \rho_{k,h})$ converges towards the (unique) weak solution (\mathbf{u}, ρ) of problem (7), (9) and (10) (see Definition 3), strongly in $L^2(0, T; \mathbf{L}^2(\Omega) \times H^1(\Omega))$, weak-star in $L^\infty(0, T; \mathbf{L}^2(\Omega) \times H^1(\Omega))$ and weakly in $L^2(0, T; \mathbf{H}_0^1(\Omega)) \times L^4(0, T; W^{1,4}(\Omega))$.*

Remark 2 *The fourth term of the velocity-pressure scheme $c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h)$ can be changed by $c(\rho_h^n \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h)$, keeping all results of this paper.*

After a justification of the choice of the scheme made in Sections 2 and 3, we give the proof of the previous convergence Theorem from Sections 4 to Section 7. An analogous result for the second problem (8), (9)-(10) will be also obtained in Section 8. Moreover, a generalization of this second model will be presented in Section 9, obtaining an unconditionally stable scheme, but its convergence remains as an open problem.

2 Analysis of a Kazhikhov-Smagulov model

In this section, we focus on system (7), completed with the boundary conditions (9) and the initial conditions (10). The unknowns are: $\rho : Q \rightarrow \mathbb{R}^+$ the density, $\mathbf{u} : Q \rightarrow \mathbb{R}^2$ the (averaged) velocity of the fluid and $p : Q \rightarrow \mathbb{R}$ a potential function (modified pressure).

Standard notation is adopted for the Lebesgue spaces, $L^p(\Omega)$, and the Sobolev spaces, $W^{m,p}(\Omega)$ or $H^m(\Omega)$.

To define the concept of weak solution, we introduce the following function spaces:

$$\begin{aligned} \mathbf{H} &= \{ \mathbf{u} : \mathbf{u} \in \mathbf{L}^2(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \Gamma \}, \\ \mathbf{V} &= \{ \mathbf{u} : \mathbf{u} \in \mathbf{H}_0^1(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \}, \\ L_0^2(\Omega) &= \left\{ p : p \in L^2(\Omega), \int_\Omega p(\mathbf{x}) d\mathbf{x} = 0 \right\}, \end{aligned} \tag{11}$$

$$H_N^2(\Omega) = \left\{ \rho \in H^2(\Omega) : \frac{\partial \rho}{\partial \mathbf{n}} = 0 \text{ on } \Gamma, \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x} \right\}. \quad (12)$$

In \mathbf{V} , the $\|\mathbf{u}\|_{H^1(\Omega)}$ and $\|\nabla \mathbf{u}\|_{L^2(\Omega)}$ norms are equivalent, which we will denote by $\|\cdot\|$. $H_N^2(\Omega)$ is an affine space, $H_N^2(\Omega) = \frac{1}{|\Omega|} \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x} + H_{N,0}^2(\Omega)$ where

$$H_{N,0}^2(\Omega) = \left\{ \rho \in H^2(\Omega) : \frac{\partial \rho}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega, \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = 0 \right\}.$$

In the $H_N^2(\Omega)$ space, the $\|\nabla \rho\|_{H^1(\Omega)}$ semi-norm is equivalent to the $\|\Delta \rho\|_{L^2(\Omega)}$ semi-norm.

We denote the norm and the scalar product in $L^2(\Omega)$ by $|\cdot|$ and (\cdot, \cdot) , respectively.

Throughout this work, we assume the hypothesis (strictly positive density)

$$0 < m \leq \rho_0(\mathbf{x}) \leq M \quad \text{in } \Omega. \quad (13)$$

Definition 3 A pair (ρ, \mathbf{u}) is called a weak solution of (7), (9)-(10) in $(0, T)$ if:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$,

$$\rho \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H_N^2(\Omega)), \quad 0 < m \leq \rho(\mathbf{x}, t) \leq M, \quad \text{a.e. } (\mathbf{x}, t) \in Q.$$

b) $\forall \phi \in C^1([0, T]; \mathbf{V})$ such that $\phi(T) = 0$,

$$\begin{aligned} & \int_0^T \left\{ -(\mathbf{u}, \rho \phi_t + (\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla \phi) + (\mu \nabla \mathbf{u} - \lambda \rho (\nabla \mathbf{u})^t, \nabla \phi) \right\} dt \\ &= \int_0^T (\rho \mathbf{f}, \phi) dt + (\rho_0 \mathbf{u}_0, \phi(0)). \end{aligned}$$

c) The equation of mass diffusion (7)_c is verified almost everywhere in Q .

Remark 4 As usual, the pressure p can be obtained by using b) and de Rham's lemma ([17]).

The existence and uniqueness of (global in time) weak solutions of (7), (9)-(10) was demonstrated in [12, 1].

Theorem 5 Let $\mathbf{u}_0 \in \mathbf{H}$, $\rho_0 \in H^1(\Omega)$ satisfying (13) and $\mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega))$ with $p > 1$. Suppose the constraint on the constants λ , μ , m and M :

$$\lambda < 2\mu(M - m)^{-1}. \quad (14)$$

Then, there exists a (unique) weak solution of (7), (9)-(10) in $(0, T)$.

For the reader's convenience, we will give an outline of the existence proof, via a semi-Galerkin method. Here, we introduce a little difference with respect to the proofs given in [12, 1], which consists in replacing the interpolation inequality $\|\nabla \rho\|_{L^4(\Omega)}^2 \leq C \|\rho\|_{L^\infty(\Omega)} |\Delta \rho|$ used to get the $L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega))$ regularity for the density by the *Gagliardo-Nirenberg* interpolation inequality in 2D domains $\|\nabla \rho\|_{L^4(\Omega)}^2 \leq C |\nabla \rho| |\Delta \rho|$, in order to avoid the use of the

maximum principle for the density. Moreover, we think that this proof will help to the reader to understand the statement of our scheme.

Proof. We only argue in a formal manner. Let us suppose that we have a regular enough solution (ρ, \mathbf{u}) of (7), (9)-(10).

First, thanks to the maximum principle applied to the parabolic problem for the density (7)_c and using (13), we can deduce that

$$0 < m \leq \rho(\mathbf{x}, t) \leq M \quad \text{in } Q.$$

To obtain a priori estimates for the velocity we need to add to the momentum equation (7)_a multiplied by $\mathbf{v} \in \mathbf{V}$ and integrated over Ω , the density equation multiplied by $\frac{1}{2}\mathbf{u} \cdot \mathbf{v}$ and integrated over Ω , resulting the variational equality:

$$\begin{aligned} & \left(\rho \mathbf{u}_t, \mathbf{v} \right) + \left((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla, \mathbf{u}, \mathbf{v} \right) + \left(\mu \nabla \mathbf{u} - \lambda \rho (\nabla \mathbf{u})^t, \nabla \mathbf{v} \right) \\ & + \frac{1}{2} \left(\rho_t, \mathbf{u} \cdot \mathbf{v} \right) - \frac{1}{2} \left(\rho \mathbf{u} - \lambda \nabla \rho, \nabla (\mathbf{u} \cdot \mathbf{v}) \right) = \left(\rho \mathbf{f}, \mathbf{v} \right). \end{aligned}$$

Choosing as a test function $\mathbf{v} = \mathbf{u}$, we get the following energy relation:

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2 d\mathbf{x} + \mu \|\mathbf{u}\|^2 = \lambda \int_{\Omega} \rho (\nabla \mathbf{u})^t : \nabla \mathbf{u} d\mathbf{x} + \left(\rho \mathbf{f}, \mathbf{u} \right). \quad (15)$$

Making use of the equality

$$\int_{\Omega} (\nabla \mathbf{v})^t : \nabla \mathbf{v} d\mathbf{x} = 0, \quad \forall \mathbf{v} \in \mathbf{V},$$

one can rewrite the first term on the right-hand side of (15) as

$$\int_{\Omega} \rho (\nabla \mathbf{u})^t : \nabla \mathbf{u} d\mathbf{x} = \int_{\Omega} \left(\rho - \frac{M+m}{2} \right) (\nabla \mathbf{u})^t : \nabla \mathbf{u} d\mathbf{x}.$$

Since $m \leq \rho \leq M$, the inequality $|\rho - (M+m)/2| \leq (M-m)/2$ holds almost everywhere in Q ; therefore

$$\lambda \int_{\Omega} \rho (\nabla \mathbf{u})^t : \nabla \mathbf{u} d\mathbf{x} \leq \lambda \frac{M-m}{2} \|\mathbf{u}\|^2. \quad (16)$$

Imposing the restriction on the coefficients, $\lambda < 2\mu(M-m)^{-1}$, this gives $\mu - \frac{\lambda}{2}(M-m) = \mu_1/2 > 0$. Then, from (15), (16) and the upper bound for the density,

$$\frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2 d\mathbf{x} + \mu_1 \|\mathbf{u}\|^2 \leq 2 \left(\rho \mathbf{f}, \mathbf{u} \right) \leq \varepsilon \|\mathbf{u}\|^2 + C_{\varepsilon} \|\mathbf{f}\|_{L^p(\Omega)}^2. \quad (17)$$

where $p > 1$. Therefore, integrating (17) over $(0, t) \forall t \leq T$ and applying the lower bound of the density, we arrive at the estimate

$$\max_{0 \leq t \leq T} |\mathbf{u}(t)|^2 + \int_0^T \|\mathbf{u}(t)\|^2 dt \leq C.$$

Multiplying the density equation (7)_c by $-\Delta \rho$, bounding the convective term thanks to the 2D interpolation inequalities

$$\|\mathbf{u}\|_{L^4(\Omega)} \leq C |\mathbf{u}|^{1/2} |\nabla \mathbf{u}|^{1/2} \quad \text{and} \quad \|\nabla \rho\|_{L^4(\Omega)} \leq C |\nabla \rho|^{1/2} |\Delta \rho|^{1/2},$$

(which are a consequence of *Gagliardo-Nirenberg's* inequality and the $\|\mathbf{u}\|_{H^1(\Omega)}$ and $|\nabla \mathbf{u}|_{L^2(\Omega)}$ norms and the $\|\nabla \rho\|_{H^1(\Omega)}$ and $|\Delta \rho|$ semi-norms are equivalent), we arrive at

$$\frac{1}{2} \frac{d}{dt} |\nabla \rho|^2 + \lambda |\Delta \rho|^2 \leq C \|\mathbf{u}\|_{L^4} \|\nabla \rho\|_{L^4} |\Delta \rho| \leq \varepsilon |\Delta \rho|^2 + C |\mathbf{u}|^2 |\nabla \mathbf{u}|^2 |\nabla \rho|^2.$$

Therefore, from Gronwall's Lemma, we get the estimate

$$\max_{0 \leq t \leq T} |\nabla \rho(t)|^2 + \lambda \int_0^T |\Delta \rho(t)|^2 dt \leq C.$$

Through a quite technical argument ([1]), one arrives at the following estimate of the “fractional in time derivative”

$$\int_0^{T-\delta} |\mathbf{u}(t+\delta) - \mathbf{u}(t)|^2 dt \leq C \delta^{1/2}, \quad \forall \delta \in (0, T).$$

This estimate implies ([16]) compactness for the velocity \mathbf{u} in $L^2(0, T; \mathbf{L}^2(\Omega))$. From here, it is rather standard to obtain existence of weak solutions of ([1]), using for instance the *Faedo-Galerkin* method. \square

3 Design of the numerical scheme

This section is devoted to designing an unconditionally stable, convergent scheme, using the backward Euler scheme in time (considered for simplicity a uniform partition of $[0, T]$ with time step $k = T/N$: $(t_n = nk)_{n=0}^{n=N}$), and finite elements in space.

In order to get an easy implementation, we are going to define a linear scheme which decouples the problems for (\mathbf{u}, p) and for ρ in each time step. Concerning the space discretization, we only choose at most H^1 -conformed finite element spaces for the density, velocity and pressure, which we denote by $(W_h, \mathbf{V}_h, M_h) \subset H^1 \times \mathbf{H}_0^1 \times L_0^2$ with the density space W_h generated by \mathbb{P}_1 continuous finite elements and velocity-pressure spaces (\mathbf{V}_h, M_h) satisfying the stability Babuska-Bezzi condition ([8]).

To start of these requirements, a first attempt would be the following scheme.

Let $\rho_h^n \in W_h$ and $\mathbf{u}_h^n \in \mathbf{V}_h$ be given.

1. Find $\rho_h^{n+1} \in W_h$ such that for each $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h \right). \quad (18)$$

2. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ + \left(\mu \nabla \mathbf{u}_h^{n+1} - \lambda \rho_h^{n+1} (\nabla \mathbf{u}_h^{n+1})^t, \nabla \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right), \end{array} \right. \quad (19)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0, \quad (20)$$

where $\mathbf{f}^{n+1} = \frac{1}{k} \int_{t_n}^{t_{n+1}} \mathbf{f}(t) dt$.

Remark 6 The approximation of $(\rho \mathbf{u}_t)(t_{n+1})$ by $\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}$ is justified by means of the equality:

$$\begin{aligned} & \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \mathbf{u}_h^{n+1} \right) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \mathbf{u}_h^{n+1} \right) \\ & = \frac{1}{2} \left(\int_{\Omega} \frac{\rho_h^{n+1} |\mathbf{u}_h^{n+1}|^2 - \rho_h^n |\mathbf{u}_h^n|^2}{k} + \int_{\Omega} \rho_h^n \frac{|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2}{k} \right), \end{aligned}$$

which is a discrete version of the continuous relation:

$$\left(\rho \frac{d}{dt} \mathbf{u}, \mathbf{u} \right) + \frac{1}{2} \left(\frac{d}{dt} \rho, \mathbf{u} \cdot \mathbf{u} \right) = \frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2.$$

Throughout this work we assume the following hypotheses:

(H1) Either

$$\mathbf{u}_0 \in \mathbf{H} \text{ and } \rho_0 \in H^1(\Omega) \text{ with } k/h^2 \leq C,$$

or

$$\mathbf{u}_0 \in \mathbf{V} \text{ and } \rho_0 \in H_N^2(\Omega).$$

(H2) The boundary of Ω is a polygon such that the continuous dependency in the H^2 -norm of the *Poisson-Neumann* problem holds (see (35)). This is true, for instance, if Ω is convex ([8]).

(H3) The triangulation of Ω and the discrete spaces. Let $\{\mathcal{T}_h\}_{h>0}$ be a regular, quasi-uniform family of triangulations of Ω , with $h = \max_{K \in \mathcal{T}_h} h_K$ (h_K =diameter of K), and

$$W_h = \{x_h \in C^0(\bar{\Omega}) : x_h|_K \in \mathbb{P}_1(K), \forall K \in \mathcal{T}_h\}.$$

In particular, this discrete space verifies the following properties which we are going to use in this paper:

- the inverse inequalities:

$$\begin{aligned} \|\nabla \bar{\rho}_h\|_{L^4(\Omega)} & \leq C h^{-1/2} |\nabla \bar{\rho}_h|, \quad \forall \bar{\rho}_h \in W_h, \\ |\nabla \bar{\rho}_h| & \leq C h^{-1} |\bar{\rho}_h|, \quad \forall \bar{\rho}_h \in W_h, \end{aligned}$$

- and the interpolation errors:

$$\|\bar{\rho} - I_h \bar{\rho}\|_{H^1(\Omega)} + h^{1/2} \|\bar{\rho} - I_h \bar{\rho}\|_{W^{1,4}(\Omega)} \leq C h \|\bar{\rho}\|_{H^2(\Omega)}, \quad \forall \bar{\rho} \in H^2(\Omega),$$

where I_h is the interpolation operator from $H^2(\Omega)$ into W_h .

On the other hand, we choose (V_h, M_h) verifying the interpolation errors:

$$\|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{H^1(\Omega)} \leq C h \|\bar{\mathbf{u}}\|_{H^2(\Omega)}, \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$\|\bar{p} - K_h \bar{p}\| \leq C h \|\bar{p}\|_{H^1(\Omega)}, \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega),$$

where J_h and K_h are interpolation operators from $\mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ into \mathbf{V}_h and from $H^1(\Omega) \cap L_0^2(\Omega)$ into M_h , respectively.

(H4) Inf-sup condition. There is a constant $\beta > 0$ (independent of h) such that $\forall \bar{p}_h \in M_h$,

$$\|\bar{p}_h\|_{L_0^2(\Omega)} \leq \beta \sup_{\bar{\mathbf{u}}_h \in \mathbf{V}_h \setminus \{0\}} \frac{(\bar{p}_h, \nabla \cdot \bar{\mathbf{u}}_h)}{\|\bar{\mathbf{u}}_h\|_{H^1(\Omega)}}.$$

For instance, a manner of defining the discrete spaces (\mathbf{V}_h, M_h) verifying (H3) and (H4) is:

$$M_h = W_h \cap L_0^2(\Omega)$$

and to select \mathbf{V}_h there are several possibilities ([8]). For instance:

1. (*Taylor-Hood*)

$$\mathbf{V}_h = \{v_h \in C^0(\bar{\Omega}) : v_h|_K \in \mathbb{P}_2(K), \forall K \in \mathcal{T}_h\}^2 \cap \mathbf{H}_0^1(\Omega).$$

2. (*Mini-element*) Define $\mathcal{P}(K) = [\mathbb{P}_1(K)]^2 \oplus \alpha_K \lambda_1 \lambda_2 \lambda_3$ with $\alpha_K \in \mathbb{R}^2$ and $\lambda_i \in \mathbb{P}_1$ such that $\lambda_i(a_j) = \delta_{ij}$, with a_j being the vertices of the triangle K . Then, we consider

$$\mathbf{V}_h = \{v_h \in C^0(\bar{\Omega}) : v_h|_K \in \mathcal{P}(K), \forall K \in \mathcal{T}_h\}^2 \cap \mathbf{H}_0^1(\Omega).$$

To obtain estimates for scheme (18)-(20), the idea is to follow the proof of the existence Theorem 5, but we find the following main difficulties:

1. We cannot assure the maximum principle for the discrete density ρ_h^n .
2. The density equation doesn't hold pointwise (as used in the proof of Theorem 5), or more concretely, we cannot take $\bar{\rho}_h = \frac{1}{2} \mathbf{u}_h^{n+1} \cdot \mathbf{u}_h^{n+1}$ in (18), because in general $\mathbf{u}_h^{n+1} \cdot \mathbf{u}_h^{n+1} \notin W_h$.
3. The incompressibility condition doesn't hold pointwise; therefore $\int_{\Omega} (\nabla \mathbf{u}_h^{n+1})^t : \nabla \mathbf{u}_h^{n+1} \neq 0$ in general.

4. We are not going to get strong H^2 estimates for the discrete density ρ_h^n , since we are approximating in H^1 (or at most in $W^{1,\infty}$), but not in H^2 .

To treat difficulty 1, i.e. the absence of the maximum principle, we define the following truncating (by nodes) operator : Given $w_h \in W_h$, one defines $[w_h]_T \in W_h$ such that:

$$[w_h]_T(\mathbf{x}_i) = \begin{cases} w_h(\mathbf{x}_i) & \text{if } w_h(\mathbf{x}_i) \in [m, M], \\ m & \text{if } w_h(\mathbf{x}_i) < m, \\ M & \text{if } w_h(\mathbf{x}_i) > M, \end{cases}$$

where \mathbf{x}_i are the nodes of the mesh \mathcal{T}_h .

To treat difficulty 2, we add to the discrete momentum system (19) the following terms:

$$\frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right),$$

where we have only truncated the discrete densities in the first term. Then, we change (19) by

$$\left\{ \begin{aligned} & \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) \\ & + \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right) \\ & + \left(\mu \nabla \mathbf{u}_h^{n+1} - \lambda [\rho_h^{n+1}]_T (\nabla \mathbf{u}_h^{n+1})^t, \nabla \bar{\mathbf{u}}_h \right) = \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{aligned} \right. \quad (21)$$

where we have also truncated the discrete density in the term $\int_{\Omega} \rho_h^{n+1} (\nabla \mathbf{u}_h^{n+1})^t : \nabla \bar{\mathbf{u}}_h \, d\mathbf{x}$ and $(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h)$. This last truncation is considered to reduce the hypothesis on the external force \mathbf{f} acting on the system.

With respect to difficulty 3, in order to “control” the term $-\lambda \int_{\Omega} [\rho_h^{n+1}]_T (\nabla \mathbf{u}_h^{n+1})^t : (\nabla \bar{\mathbf{u}}_h) \, d\mathbf{x}$ we add to (21) the term:

$$\lambda \int_{\Omega} \frac{M+m}{2} (\nabla \mathbf{u}_h^{n+1})^t : (\nabla \bar{\mathbf{u}}_h) \, d\mathbf{x}.$$

Then, taking $\bar{\mathbf{u}}_h = \mathbf{u}_h^{n+1}$ in (21), we obtain the following estimate (equivalent to (16)):

$$\left| \lambda \int_{\Omega} \left([\rho_h^{n+1}]_T - \frac{M+m}{2} \right) (\nabla \mathbf{u}_h^{n+1})^t : (\nabla \mathbf{u}_h^{n+1}) \, d\mathbf{x} \right| \leq \lambda \frac{M-m}{2} \|\mathbf{u}_h^{n+1}\|^2. \quad (22)$$

On the other hand, applying Leibnitz’s rule in the term

$$-\frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right),$$

we rewrite (21) as:

$$\left\{ \begin{aligned} & \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ & + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{aligned} \right. \quad (23)$$

where we have defined

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu(\nabla \mathbf{u}, \nabla \mathbf{v}) + \lambda \int_{\Omega} \left(\frac{M+m}{2} - \rho \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} \, dx$$

and

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) = \frac{1}{2} \left[\left((\mathbf{w} \cdot \nabla) \mathbf{u}, \mathbf{v} \right) - \left((\mathbf{w} \cdot \nabla) \mathbf{v}, \mathbf{u} \right) \right],$$

which verify the properties:

$$a([\rho]_T, \mathbf{u}, \mathbf{u}) \geq \frac{\mu_1}{2} \|\mathbf{u}\|^2 \quad \text{where} \quad \frac{\mu_1}{2} = \mu - \lambda \frac{M-m}{2} (> 0), \quad (\text{using (14)}), \quad (24)$$

$$a([\rho]_T, \mathbf{u}, \mathbf{v}) \leq C \|\mathbf{u}\| \|\mathbf{v}\| \quad (\text{using } \|\rho\|_{L^\infty(\Omega)} \leq M), \quad (25)$$

$$c(\mathbf{w}, \mathbf{u}, \mathbf{u}) = 0, \quad (26)$$

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) \leq C \|\mathbf{w}\|_{L^3(\Omega)} \|\mathbf{u}\| \|\mathbf{v}\|. \quad (27)$$

Finally, we will see that difficulty 4 can be circumvented.

In conclusion, we define the following numerical scheme:

Initialization: Let $(\mathbf{u}_h^0, \rho_h^0) \in (\mathbf{V}_h, W_h)$ be suitable approximations of (\mathbf{u}_0, ρ_0) , as $h \rightarrow 0$.

Time step $(n+1)$: Given $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Find $\rho_h^{n+1} \in W_h$ such that for each $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda (\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h) = -(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h). \quad (28)$$

2. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h), \end{array} \right. \quad (29)$$

$$(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h) = 0. \quad (30)$$

From the computational point of view, we propose a scheme where in each time step we have to solve two (decoupled) linear systems: the diffusion problem (28) for ρ_h^{n+1} and the problem of Stokes type (29)-(30) for $(\mathbf{u}_h^{n+1}, p_h^{n+1})$.

To conclude this section, we shall see that the linear systems (28) and (29)-(30) are well-posed; that is, existence and uniqueness of a solution hold. Indeed, as they can be written as algebraic linear systems, it suffices to verify the uniqueness of the solution for each problem, which will be deduced in particular from the a priori scheme estimates in the next section.

4 A priori scheme estimates (Unconditional stability)

In order to get stability estimates in strong norms for the density, we will need a discrete version of the 2D inequality interpolation $\|\nabla\rho\|_{L^4(\Omega)}^2 \leq C|\nabla\rho||\Delta\rho|$. For this, we first introduce the discrete Laplacian using the following auxiliary problem:

Given $(\mathbf{u}_h^n, \rho_h^n) \in \mathbf{V}_h \times W_h$, find $(\rho_h^{n+1}, \omega_h^{n+1}) \in W_h \times W_h$ such that:

$$\begin{cases} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\omega}_h \right) + \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\omega}_h \right) + \lambda \left(\omega_h^{n+1}, \bar{\omega}_h \right) = 0, \\ \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = \left(\omega_h^{n+1}, \bar{\rho}_h \right), \end{cases} \quad (31)$$

for each $(\bar{\omega}_h, \bar{\rho}_h) \in W_h \times W_h$. It is easy to prove that (31) has a unique solution.

Lemma 7 *Problems (31) and (28) are equivalent.*

Proof: Suppose that $(\rho_h^{n+1}, \omega_h^{n+1})$ is the solution of (31). Then, replacing (31)_b into (31)_a for $\bar{\rho}_h = \bar{\omega}_h$, this gives that ρ_h^{n+1} is solution of (28).

On the other hand, suppose that ρ_h^{n+1} is the solution of (28). We shall define $\omega_h^{n+1} \in W_h$ as the solution of:

$$\lambda \left(\omega_h^{n+1}, \bar{\omega}_h \right) = - \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\omega}_h \right) - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\omega}_h \right), \quad \forall \bar{\omega}_h \in W_h. \quad (32)$$

Comparing (28) and (32) for $\bar{\rho}_h = \bar{\omega}_h$, we arrive at

$$\left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = \left(\omega_h^{n+1}, \bar{\rho}_h \right), \quad \forall \bar{\rho}_h \in W_h.$$

Consequently $(\rho_h^{n+1}, \omega_h^{n+1})$ is the solution of (31). \square

Remark 8 *Taking $\bar{\rho}_h = 1$ as a test function in (31)_b, one has that $\int_{\Omega} \omega_h^{n+1}(\mathbf{x}) d\mathbf{x} = 0$.*

Lemma 9 *Let $\omega_h \in W_h \cap L_0^2(\Omega)$ and $\rho_h \in W_h$ such that:*

$$\left(\nabla \rho_h, \nabla \bar{\rho}_h \right) = \left(\omega_h, \bar{\rho}_h \right), \quad \forall \bar{\rho}_h \in W_h. \quad (33)$$

Then, there exists $C > 0$ (independent of h) such that:

$$\|\nabla \rho_h\|_{L^4(\Omega)}^2 \leq C |\nabla \rho_h| |\omega_h|. \quad (34)$$

Proof. We define $\rho(h) \in H^2(\Omega)$ as the solution of the following continuous problem:

$$-\Delta \rho(h) = \omega_h \quad \text{in } \Omega, \quad \frac{\partial \rho(h)}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0, \quad \int_{\Omega} \rho(h) d\mathbf{x} = 0. \quad (35)$$

Since the compatibility condition $\int_{\Omega} \omega_h(\mathbf{x}) d\mathbf{x} = 0$ holds, problem (35) is well-posed and verifies the continuous dependency property

$$\|\rho(h)\|_{H^2(\Omega)} \leq C |\omega_h|.$$

Now, we decompose

$$\begin{aligned} \|\nabla \rho_h\|_{L^4(\Omega)} &\leq \|\nabla \rho_h - \nabla I_h(\rho(h))\|_{L^4(\Omega)} \\ &\quad + \|\nabla I_h(\rho(h)) - \nabla \rho(h)\|_{L^4(\Omega)} + \|\nabla \rho(h)\|_{L^4(\Omega)}, \end{aligned} \quad (36)$$

where I_h is the interpolation operator from $H^1(\Omega)$ into W_h . By approximation properties of this interpolation operator ([5]), we have

$$\|\nabla I_h(\rho(h)) - \nabla \rho(h)\|_{L^4(\Omega)} \leq C h^{1/2} \|\rho(h)\|_{H^2(\Omega)} \leq C h^{1/2} |\omega_h|. \quad (37)$$

On the other hand, multiplying (35) by $\bar{\rho}_h \in W_h$ and integrating by parts,

$$\left(\nabla \rho(h), \nabla \bar{\rho}_h \right) = \left(\omega_h, \bar{\rho}_h \right). \quad (38)$$

Comparing (38) and (31)_b, one gets

$$\left(\nabla \rho_h - \nabla \rho(h), \nabla \bar{\rho}_h \right) = 0, \quad \forall \bar{\rho}_h \in W_h.$$

Adding and subtracting $\nabla I_h(\rho(h))$ and considering $\bar{\rho}_h = \rho_h - I_h(\rho(h)) \in W_h$, we obtain

$$\begin{aligned} |\nabla \rho_h - \nabla I_h(\rho(h))|^2 &= -\left(\nabla I_h(\rho(h)) - \nabla \rho(h), \nabla \rho_h - \nabla I_h(\rho(h)) \right) \\ &\leq |\nabla I_h(\rho(h)) - \nabla \rho(h)| |\nabla \rho_h - \nabla I_h(\rho(h))|, \end{aligned}$$

whence

$$|\nabla \rho_h - \nabla I_h(\rho(h))| \leq |\nabla I_h(\rho(h)) - \nabla \rho(h)| \leq C h \|\rho(h)\|_{H^2(\Omega)} \leq C h |\omega_h|. \quad (39)$$

Therefore, using the inverse inequality ([5])

$$\|\nabla \rho_h - \nabla I_h(\rho(h))\|_{L^4(\Omega)} \leq C h^{-1/2} |\nabla \rho_h - \nabla I_h(\rho(h))|$$

and (39), we arrive at

$$\|\nabla \rho_h - \nabla I_h(\rho(h))\|_{L^4(\Omega)} \leq C h^{1/2} |\omega_h|. \quad (40)$$

Next, by using *Gagliardo-Nirenberg's* inequality in $2D$ domains in the last term on the right-hand side of (36), we have

$$\|\nabla \rho(h)\|_{L^4(\Omega)} \leq C |\nabla \rho(h)|^{1/2} \|\rho(h)\|_{H^2(\Omega)}^{1/2} \leq C |\nabla \rho(h)|^{1/2} |\omega_h|^{1/2}. \quad (41)$$

Thus, applying (37), (40) and (41) in (36), one obtains

$$\|\nabla \rho_h\|_{L^4(\Omega)} \leq C h^{1/2} |\omega_h| + C |\nabla \rho(h)|^{1/2} |\omega_h|^{1/2}. \quad (42)$$

From (39) and the interpolation error $|\nabla I_h(\rho(h)) - \nabla \rho(h)| \leq C h \|\rho(h)\|_{H^2(\Omega)}$, one has

$$|\nabla \rho_h - \nabla \rho(h)| \leq |\nabla \rho_h - \nabla I_h(\rho(h))| + |\nabla I_h(\rho(h)) - \nabla \rho(h)| \leq C h |\omega_h|.$$

Accordingly,

$$|\nabla \rho(h)| \leq h |\omega_h| + |\nabla \rho_h|.$$

Replacing this last inequality in (42), we get

$$\|\nabla \rho_h\|_{L^4(\Omega)} \leq C h^{1/2} |\omega_h| + |\nabla \rho_h|^{1/2} |\omega_h|^{1/2}. \quad (43)$$

On the other hand, taking $\bar{\rho}_h = \omega_h$ in (33) we arrive at

$$|\omega_h|^2 = \left(\nabla \rho_h, \nabla \omega_h \right) \leq |\nabla \rho_h| |\nabla \omega_h|.$$

Using the inverse inequality ([5]) $|\nabla \omega_h| \leq C h^{-1} |\omega_h|$, one has

$$|\omega_h| \leq C h^{-1} |\nabla \rho_h|. \quad (44)$$

Combining estimates (43) and (44), one arrives at (34). \square

Now, we are in position to prove stability estimates for the scheme.

Lemma 10 *Suppose $\mathbf{u}_0 \in \mathbf{V}$, $\rho_0 \in H_N^2(\Omega)$ and $\mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega))$ with $p > 1$. Then, the solution of the discrete scheme (28), (29)-(30) satisfies the following estimates:*

$$\begin{aligned} \text{i)} \quad \max_{0 \leq n \leq N} |\mathbf{u}_h^n| &\leq C, & \text{ii)} \quad \sum_{n=0}^N k \|\mathbf{u}_h^n\|^2 &\leq C, & \text{iii)} \quad \sum_{n=0}^{N-1} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 &\leq C, \\ \text{iv)} \quad \max_{0 \leq n \leq N} |\nabla \rho_h^n| &\leq C, & \text{v)} \quad \sum_{n=0}^N k \|\nabla \rho_h^n\|_{L^4(\Omega)}^4 &\leq C, & \text{vi)} \quad \sum_{n=0}^{N-1} |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 &\leq C, \end{aligned}$$

with $C > 0$ depending only on $(\rho_0, \mathbf{u}_0, \mathbf{f})$.

Notice that, although the discrete density does not have the H^2 -regularity, v) implies that the discrete density conserves the $L^4(0, T; W^{1,4}(\Omega))$ -regularity.

Proof. First, we obtain a priori estimates for the velocity (\mathbf{u}_h^n) . Taking $\bar{\mathbf{u}}_h = 2k\mathbf{u}_h^{n+1}$ and $\bar{p}_h = p_h^{n+1}$ in (29)-(30), using the identity $(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2$ and the properties (24) and (26), and taking into account Remark 6, one has

$$\begin{aligned} &|\sqrt{[\rho_h^{n+1}]_T} \mathbf{u}_h^{n+1}|^2 - |\sqrt{[\rho_h^n]_T} \mathbf{u}_h^n|^2 + |\sqrt{[\rho_h^n]_T} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 + \mu_1 k \|\mathbf{u}_h^{n+1}\|^2 \\ &\leq 2k \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \mathbf{u}_h^{n+1} \right) \leq 2k \|\rho_h^{n+1}\|_{L^\infty(\Omega)} \|\mathbf{f}^{n+1}\|_{L^p(\Omega)} \|\mathbf{u}_h^{n+1}\|_{L^q(\Omega)} \\ &\leq \frac{\mu_1 k}{2} \|\mathbf{u}_h^{n+1}\|^2 + Ck \|\mathbf{f}^{n+1}\|_{L^p(\Omega)}^2, \end{aligned}$$

where q is the conjugate of p such that $\frac{1}{p} + \frac{1}{q} = 1$. Therefore,

$$|\sqrt{[\rho_h^{n+1}]_T \mathbf{u}_h^{n+1}}|^2 - |\sqrt{[\rho_h^n]_T \mathbf{u}_h^n}|^2 + |\sqrt{[\rho_h^n]_T (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)}|^2 + \frac{\mu_1}{2} k \|\mathbf{u}_h^{n+1}\|^2 \leq Ck \|\mathbf{f}^{n+1}\|_{L^p(\Omega)}^2. \quad (45)$$

Adding (45) for $n = 0, \dots, r$ with $r < N$, the estimates for the velocity **i**), **ii**) and **iii**) hold.

To obtain a priori estimates of the discrete density, we write scheme (28) as (31). Taking $\bar{\omega}_h = 2k\omega_h^{n+1}$ in (31)_a and $\bar{\rho}_h = 2(\rho_h^{n+1} - \rho_h^n)$ in (31)_b, we arrive at:

$$|\nabla \rho_h^{n+1}|^2 - |\nabla \rho_h^n|^2 + |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 + 2\lambda k |\omega_h^{n+1}|^2 = -2k \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \omega_h^{n+1} \right). \quad (46)$$

Bounding the right-hand side term of (46) as

$$\begin{aligned} 2k \left| \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \omega_h^{n+1} \right) \right| &\leq 2k \|\mathbf{u}_h^n\|_{L^4(\Omega)} \|\nabla \rho_h^n\|_{L^4(\Omega)} |\omega_h^{n+1}| \\ &\leq \lambda k |\omega_h^{n+1}|^2 + \frac{k}{\lambda} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^2 \|\nabla \rho_h^n\|_{L^4(\Omega)}^2, \end{aligned}$$

we get the inequality

$$|\nabla \rho_h^{n+1}|^2 - |\nabla \rho_h^n|^2 + |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 + \lambda k |\omega_h^{n+1}|^2 \leq \frac{k}{\lambda} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^2 \|\nabla \rho_h^n\|_{L^4(\Omega)}^2. \quad (47)$$

Note that ω_h^n is defined for $n \geq 1$ in scheme (31). For $n = 0$, it suffices to define ω_h^0 as an approximation in $M_h \subset L_0^2(\Omega)$ of $-\Delta \rho_0$, and therefore to define ρ_h^0 based on ω_h^0 using (31)_b jointly with the additional condition $\int_{\Omega} \rho_h^0 = \int_{\Omega} \rho_0$. Of course, this initialization is possible in the case of initial density sufficiently regular, concretely $\rho_0 \in H^2(\Omega)$. For the case $\rho_0 \in H^1(\Omega)$, see Remark 13 below.

Using the discrete Gagliardo-Nirenberg inequality (34) in (47), one has

$$|\nabla \rho_h^{n+1}|^2 - |\nabla \rho_h^n|^2 + |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 + \lambda k |\omega_h^{n+1}|^2 \leq Ck \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 |\nabla \rho_h^n|^2 + \frac{\lambda}{2} k |\omega_h^n|^2. \quad (48)$$

Adding (48) for $n = 0, \dots, r$ with any $r < N$, we arrive at

$$|\nabla \rho_h^{r+1}|^2 + \lambda k \sum_{n=0}^r |\omega_h^{n+1}|^2 \leq C \sum_{n=0}^r k \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 |\nabla \rho_h^n|^2 + \frac{\lambda}{2} k \sum_{n=0}^r |\omega_h^n|^2 + |\nabla \rho_h^0|^2.$$

Therefore,

$$|\nabla \rho_h^{r+1}|^2 + \frac{\lambda}{2} k \sum_{n=0}^r |\omega_h^{n+1}|^2 \leq C \sum_{n=0}^r k \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 |\nabla \rho_h^n|^2 + \frac{\lambda}{2} k |\omega_h^0|^2 + |\nabla \rho_h^0|^2. \quad (49)$$

Now, applying the discrete *Gronwall* lemma and using that

$$k \sum_{n=0}^N \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 \leq |\mathbf{u}_h^N|^2 k \sum_{n=0}^N \|\mathbf{u}_h^n\|^2 \leq C$$

(where \mathbf{i}) and \mathbf{ii}) are used) we obtain \mathbf{iv}), \mathbf{vi}) and

$$k \sum_{n=0}^N |\omega_h^n|^2 \leq C. \quad (50)$$

Finally, from (34) and estimate \mathbf{iv}) and (50), one gets \mathbf{v}). \square

Remark 11 When in the discrete density equation (28), the convective term is considered in a semi-implicit form, i.e. changing $(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho})$ by $(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho})$ in (28), then the estimates for the discrete density \mathbf{iv}), \mathbf{v}) and \mathbf{vi}) are obtained by imposing $Ch/k^2 < 1$, which is independent of the regularity of the data. Indeed, we consider $C \sum_{n=0}^r k \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 |\nabla \rho_h^{n+1}|^2$ instead of $C \sum_{n=0}^r k \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 |\nabla \rho_h^n|^2$ in (49). Then, in order to apply the generalized discrete Gronwall lemma, we need to get that $Ck \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 < 1$ which holds by using an inverse inequality,

$$Ck \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 \leq C \frac{k}{h^2} \|\mathbf{u}_h^n\|_{L^2(\Omega)}^4 \leq C \frac{k}{h^2} < 1.$$

Remark 12 One also holds the estimate $k \sum_{n=0}^n \|\rho_h^n\|_{W^{1,p}(\Omega)}^2 \leq C$ for $p : 2 < p < \infty$. For this, it suffices to see $\|\rho_h^n\|_{W^{1,p}(\Omega)} \leq C|\omega_h^n|$ and to apply (50). Indeed,

$$\|\rho_h^n\|_{W^{1,p}(\Omega)} \leq \|\rho_h^n - I_h(\rho(h))\|_{W^{1,p}(\Omega)} + \|I_h(\rho(h)) - \rho(h)\|_{W^{1,p}(\Omega)} + \|\rho(h)\|_{W^{1,p}(\Omega)}.$$

Using the inverse inequality $\|\bar{\omega}_h\|_{W^{1,p}(\Omega)} \leq Ch^{-(p-2)/p} \|\bar{\omega}_h\|_{H^1(\Omega)}$ and (39), we bound

$$\begin{aligned} \|\rho_h^n - I_h(\rho(h))\|_{W^{1,p}(\Omega)} &\leq Ch^{-(p-2)/p} \|\rho_h^n - I_h(\rho(h))\|_{H^1(\Omega)} \leq Ch^{1-(p-2)/p} |\omega_h^n| \leq C|\omega_h^n|, \\ \|\rho(h) - I_h(\rho(h))\|_{W^{1,p}(\Omega)} &\leq C \|\rho(h)\|_{H^2(\Omega)} \leq C|\omega_h^n|, \\ \|\rho(h)\|_{W^{1,p}(\Omega)} &\leq C \|\rho(h)\|_{H^2(\Omega)} \leq |\omega_h^n|; \end{aligned}$$

hence $\|\rho_h^n\|_{W^{1,p}(\Omega)} \leq C|\omega_h^n|$ holds. \square

Remark 13 Since $(\mathbf{u}_0, \rho_0) \in \mathbf{V} \times H_N^2(\Omega)$ has been imposed, then $\|\mathbf{u}_h^0\| \leq C\|\mathbf{u}_0\|$ and ω_h^0 was defined based on $\Delta\rho_0$ and verifying $|\omega_h^0| \leq C|\Delta\rho_0|$. Imposing only $(\mathbf{u}_0, \rho_0) \in \mathbf{H} \times H^1(\Omega)$, the construction of ω_h^0 must change. Firstly, we consider $\rho_h^0 \in W_h$ as an approximation of ρ_0 in $H^1(\Omega)$ and, afterwards, we define ω_h^0 from (31)_b. Therefore, using the inverse inequality $|\nabla \omega_h^0| \leq Ch^{-1}|\omega_h^0|$ it is easy to prove that $|\omega_h^0| \leq Ch^{-1}|\nabla \rho_h^0|$. Accordingly, to obtain the a priori estimates from (49), it is necessary to impose the constraint $k/h^2 \leq C$ (since then, $k|\omega_h^0|^2 \leq C(k/h^2)|\nabla \rho_h^0|^2 \leq C|\nabla \rho_0|$). An analogous way is used to make the estimate $k\|\mathbf{u}_h^0\|_{L^4(\Omega)}^2 \leq C(k/h^2)|\mathbf{u}_h^0|^2 \leq C\|\mathbf{u}_0\|^2$, which is necessary to bound the first term of the sum $Ck \sum_{n=0}^r \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 |\nabla \rho_h^n|^2$.

Corollary 14 (Estimates for $\int_{\Omega} \rho_h^{n+1}$) *It follows that*

$$\left| \int_{\Omega} \rho_h^{n+1} \right| \leq C$$

where $C > 0$ is a constant independent of n and h .

Proof: Choosing $\bar{\rho}_h = 1$ in (18), we get

$$\int_{\Omega} \rho_h^{n+1} = \int_{\Omega} \rho_h^n - k \int_{\Omega} \mathbf{u}_h^n \cdot \nabla \rho_h^n.$$

Summing for $n = 0, \dots, r < N$, one has

$$\int_{\Omega} \rho_h^{r+1} = \int_{\Omega} \rho_h^0 - k \sum_{n=0}^r \int_{\Omega} \mathbf{u}_h^n \cdot \nabla \rho_h^n.$$

Finally, applying Hölder's inequality to the last term of the previous equality, this gives

$$\left| \int_{\Omega} \rho_h^{r+1} \right| \leq \left| \int_{\Omega} \rho_h^0 \right| + \left(k \sum_{n=0}^r |\mathbf{u}_h^n|^2 \right)^{1/2} \left(k \sum_{n=0}^r |\nabla \rho_h^n|^2 \right)^{1/2} \leq C,$$

using the estimates of Lemma 10. □

Remark 15 *If the density and pressure are approximated by the same space (i.e. $W_h \cap L_0^2(\Omega) = M_h$), then the average of the density is conserved, i.e. $\int_{\Omega} \rho_h^n = \int_{\Omega} \rho_h^0$, for each n (this property is the discrete version of the continuous one $\int_{\Omega} \rho(\mathbf{x}, t_1) d\mathbf{x} = \int_{\Omega} \rho(\mathbf{x}, t_2) d\mathbf{x}$ for any $t_1, t_2 \in [0, T]$, whose physical meaning is the conservation of mass). To prove it, let us see first that $(\nabla \cdot \mathbf{u}_h^n, \bar{\rho}_h) = 0$, for each $\bar{\rho}_h \in W_h$. Indeed, taking $\bar{\rho}_h - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h \in M_h$ as a test function in (28), one has*

$$0 = \left(\nabla \cdot \mathbf{u}_h^n, \bar{\rho}_h - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h \right) = \left(\nabla \cdot \mathbf{u}_h^n, \bar{\rho}_h \right) - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h \int_{\Omega} \nabla \cdot \mathbf{u}_h^n.$$

Since $\int_{\Omega} \nabla \cdot \mathbf{u}_h^n = 0$, because $\mathbf{u}_h^n = 0$ on $\partial\Omega$, one gets $(\nabla \cdot \mathbf{u}_h^n, \bar{\rho}_h) = 0$. Therefore, if we choose $\bar{\rho}_h = 1$ in (28) and apply that $(\mathbf{u}_h^n \cdot \nabla \rho_h^n, 1) = -(\nabla \cdot \mathbf{u}_h^n, \rho_h^n) = 0$, one arrives at $\int_{\Omega} \rho_h^{n+1} = \int_{\Omega} \rho_h^n$, hence reasoning by induction $\int_{\Omega} \rho_h^n = \int_{\Omega} \rho_h^0$, for each n .

5 Weak convergences

In order to study the convergence of scheme (28), (29)-(30) towards the (unique) weak solution of (7), (9)-(10), we consider the following:

Definition 16 We define the auxiliary functions:

$$\begin{aligned}
\mathbf{u}_{h,k} &: [0, T] \rightarrow \mathbf{V}_h \text{ such that } \mathbf{u}_{h,k}(t) = \mathbf{u}_h^{n+1}, t_n < t \leq t_{n+1}, \\
\widehat{\mathbf{u}}_{h,k} &: [0, T] \rightarrow \mathbf{V}_h \text{ such that } \widehat{\mathbf{u}}_{h,k}(t) = \mathbf{u}_h^n, t_n < t \leq t_{n+1}, \\
\rho_{h,k} &: [0, T] \rightarrow W_h \text{ such that } \rho_{h,k}(t) = \rho_h^{n+1}, t_n < t \leq t_{n+1}, \\
\widehat{\rho}_{h,k} &: [0, T] \rightarrow W_h \text{ such that } \widehat{\rho}_{h,k}(t) = \rho_h^n, t_n < t \leq t_{n+1}, \\
p_{h,k} &: [0, T] \rightarrow M_h \text{ such that } p_{h,k}(t) = p_h^{n+1}, t_n < t \leq t_{n+1}, \\
\widetilde{\rho}_{h,k} &: [0, T] \rightarrow W_h \text{ such that} \\
&\quad \widetilde{\rho}_{h,k}(t) = \rho_h^{n+1} + \frac{\rho_h^{n+1} - \rho_h^n}{k}(t - t_{n+1}), t_n \leq t < t_{n+1}, \\
w_{h,k} &: [0, T] \rightarrow W_h \text{ such that } w_{h,k}(t) = w_h^{n+1}, t_n < t \leq t_{n+1}.
\end{aligned} \tag{51}$$

Using Lemma 10, Corollary 14 and the generalized Poincaré inequality

$$\|\rho\|_{H^1(\Omega)} \leq C \left(|\nabla \rho| + \left| \int_{\Omega} \rho \right| \right),$$

we arrive at the following:

Lemma 17 The following estimates (independent of h and k) hold:

$$\{\mathbf{u}_{h,k}\}_{h,k}, \{\widehat{\mathbf{u}}_{h,k}\}_{h,k} \text{ is bounded in } L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)), \tag{52}$$

$$\{\rho_{h,k}\}_{h,k}, \{\widehat{\rho}_{h,k}\}_{h,k} \text{ is bounded in } L^\infty(0, T; H^1(\Omega)) \cap L^4(0, T; W^{1,4}(\Omega)), \tag{53}$$

$$\{w_{h,k}\}_{h,k} \text{ is bounded in } L^2(0, T; L^2(\Omega)). \tag{54}$$

Moreover,

$$\|\mathbf{u}_{h,k} - \widehat{\mathbf{u}}_{h,k}\|_{L^2(0, T; L^2(\Omega))}^2 \leq Ck \quad \text{and} \quad \|\rho_{h,k} - \widehat{\rho}_{h,k}\|_{L^2(0, T; H^1(\Omega))}^2 \leq Ck. \tag{55}$$

Taking into account estimates (52)-(53) given in Lemma 17, there exists a subsequence (denoted in the same way) with the corresponding weak convergences towards limit functions \mathbf{u} , $\widehat{\mathbf{u}}$, ρ , $\widehat{\rho}$. Moreover, thanks to (55), the identities of the limits $\mathbf{u} = \widehat{\mathbf{u}}$ and $\rho = \widehat{\rho}$ hold.

Lemma 18 There exist a subsequence of $\{\mathbf{u}_{h,k}\}_{h,k}$, $\{\widehat{\mathbf{u}}_{h,k}\}_{h,k}$, $\{\rho_{h,k}\}_{h,k}$, $\{\widehat{\rho}_{h,k}\}_{h,k}$ (denoted in the same way) and limit functions \mathbf{u} , ρ verifying the following weak convergences as $(h, k) \rightarrow 0$:

$$\begin{aligned}
\mathbf{u}_{h,k} &\rightarrow \mathbf{u} \text{ and } \widehat{\mathbf{u}}_{h,k} \rightarrow \mathbf{u} \text{ in } \begin{cases} L^2(0, T; \mathbf{H}_0^1(\Omega))\text{-weak} , \\ L^\infty(0, T; \mathbf{L}^2(\Omega))\text{-weak*}, \end{cases} \\
\rho_{h,k} &\rightarrow \rho \text{ and } \widehat{\rho}_{h,k} \rightarrow \rho \text{ in } \begin{cases} L^4(0, T; W^{1,4}(\Omega))\text{-weak} , \\ L^\infty(0, T; H^1(\Omega))\text{-weak*}, \end{cases} \\
w_{h,k} &\rightarrow w \text{ in } L^2(0, T; L^2(\Omega))\text{-weak} .
\end{aligned}$$

6 Strong convergences

As usual in this type of nonlinear systems, to obtain the convergence of the scheme we must get strong convergence for the approximations in some suitable space in order to identify the limit of the nonlinear terms.

6.1 Strong Convergence for the density in $L^2(\Omega)$

Lemma 19

$$k \sum_{n=0}^N \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^2 \leq C,$$

where $C > 0$ depend only on $(\rho_0, \mathbf{u}_0, \mathbf{f})$.

Proof: Taking $\bar{\rho}_h = \frac{\rho_h^{n+1} - \rho_h^n}{k}$ in (28) and using the identity $(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2$, we arrive at

$$\left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^2 + \frac{\lambda}{2k} (|\nabla \rho_h^{n+1}|^2 - |\nabla \rho_h^n|^2 + |\nabla \rho_h^{n+1} - \nabla \rho_h^n|^2) = - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \frac{\rho_h^{n+1} - \rho_h^n}{k} \right). \quad (56)$$

We estimate the right-hand side as follows:

$$\left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \frac{\rho_h^{n+1} - \rho_h^n}{k} \right) \leq \frac{1}{2} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^2 \|\nabla \rho_h^n\|_{L^4(\Omega)}^2 + \frac{1}{2} \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^2. \quad (57)$$

Multiplying (56) by $2k$, incorporating (57) and summing for $n = 0, \dots, N - 1$ one gets

$$k \sum_{n=0}^{N-1} \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^2 + \lambda |\nabla \rho_h^N|^2 \leq k \sum_{n=0}^{N-1} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^2 \|\nabla \rho_h^n\|_{L^4(\Omega)}^2 + \lambda |\nabla \rho_h^0|^2,$$

where $k \sum_{n=0}^{N-1} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^2 \|\nabla \rho_h^n\|_{L^4(\Omega)}^2 \leq \frac{1}{2} \left(k \sum_{n=0}^{N-1} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 + k \sum_{n=0}^{N-1} \|\nabla \rho_h^n\|_{L^4(\Omega)}^4 \right) \leq C$, thanks to the estimates from Lemma 10. \square

Remark 20 As a consequence of the previous corollary, one has

$$\left\| \frac{d}{dt} \tilde{\rho}_{h,k} \right\|_{L^2(0,T;L^2(\Omega))} \leq C.$$

On the other hand, by Lemma 10, $\|\tilde{\rho}_{h,k}\|_{L^\infty(0,T;H^1(\Omega))} \leq C$ holds. Then, applying a compactness theorem of Aubin-Lions type,

$$\tilde{\rho}_{h,k} \rightarrow \rho \text{ in } L^\infty(0,T;L^p(\Omega)) \text{ as } (h,k) \rightarrow 0, \quad \text{with } 1 \leq p < \infty.$$

From this convergence we deduce that

$$\rho_{h,k}, \hat{\rho}_{h,k} \rightarrow \rho \text{ in } L^2(0,T;L^2(\Omega)) \text{ as } (h,k) \rightarrow 0,$$

using that $\|\tilde{\rho}_{h,k} - \rho_{k,h}\|_{L^2(0,T;L^2(\Omega))}^2 \leq \|\hat{\rho}_{h,k} - \rho_{k,h}\|_{L^2(0,T;L^2(\Omega))}^2 = k \sum_{n=0}^{N-1} |\rho_h^{n+1} - \rho_h^n|^2 \leq Ck$.

Corollary 21 *It follows that*

$$k \sum_{n=0}^N \left| \frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k} \right|^2 \leq C.$$

Proof: Using Lemma 19, it suffices to prove that $|\rho_h^{n+1}(\mathbf{x}, t)_T - [\rho_h^n(\mathbf{x}, t)]_T| \leq |\rho_h^{n+1}(\mathbf{x}, t) - \rho_h^n(\mathbf{x}, t)|$ pointwise in Q (here $|\cdot|$ denotes the absolute value function). But, this pointwise estimate is easy to verify taking into account that the approximations for the density are finite elements of degree 1. \square

6.2 Strong convergence for the density in $H^1(\Omega)$

Using the compactness of the discrete density in $L^2(0, T; \mathbf{L}^2(\Omega))$, we are going to improve the strong convergence for the discrete density to the space $L^2(0, T; H^1(\Omega))$. For this, we firstly have to identify $w = -\Delta\rho$. Indeed, let $\eta \in C_c^\infty(Q)$. We consider η_h^n as the interpolated function of $\eta(t_n)$ in W_h and define $\eta_{h,k} \in L^\infty(0, T; W_h)$ as the piecewise constant function taking values η_h^{n+1} in $(t_n, t_{n+1}]$. Then $\eta_{h,k} \rightarrow \eta$ in $L^\infty(0, T; H^1(\Omega))$ strongly as $(h, k) \rightarrow 0$. Therefore, setting $\bar{\rho}_h = \eta_h^{n+1}$ in (31)_b, multiplying by k , summing over n and doing $(h, k) \rightarrow 0$, we get

$$\int_Q (\nabla\rho, \nabla\eta) \leftarrow \int_Q (\nabla\rho_{h,k}, \nabla\eta_{h,k}) = \int_Q (w_{h,k}, \eta_{h,k}) \rightarrow \int_Q (w, \eta).$$

Therefore, it is clear that $w = -\Delta\rho$ in $L^2(Q)$, and consequently $\rho \in L^2(0, T; H^2(\Omega))$.

Next, taking $\eta \in C^\infty(Q)$ and proceeding in the same manner, we recover the boundary condition $\frac{\partial\rho}{\partial\mathbf{n}} = 0$ on Σ .

Corollary 22 *One has that $\|\rho_{h,k} - \rho\|_{L^2(0, T; H^1(\Omega))} \rightarrow 0$ as $(h, k) \rightarrow 0$.*

Proof: Considering $\bar{\rho}_h = \rho_h^{n+1}$ in (31)_b, multiplying by k and summing over n , one has

$$\int_0^T |\nabla\rho_{h,k}|^2 = \int_0^T (w_{h,k}, \rho_{h,k}) \rightarrow - \int_0^T (\Delta\rho, \rho) = \int_0^T |\nabla\rho|^2 \quad \text{as } (h, k) \rightarrow 0$$

because of $\{\rho_{h,k}\} \rightarrow \rho$ strongly in $L^2(0, T; L^2(\Omega))$ and $\{w_{h,k}\} \rightarrow -\Delta\rho$ weakly in $L^2(0, T; L^2(\Omega))$.

Therefore, since $\|\rho_{h,k}\|_{L^2(Q)} \rightarrow \|\rho\|_{L^2(Q)}$ as $(h, k) \rightarrow 0$ by Remark 20, we have obtained that $\|\rho_{h,k}\|_{L^2(0, T; H^1(\Omega))} \rightarrow \|\rho\|_{L^2(0, T; H^1(\Omega))}$ as $(h, k) \rightarrow 0$. Finally, from $\rho_{h,k} \rightarrow \rho$ weakly in $L^2(0, T; H^1(\Omega))$ by Lemma 18, we infer the desired result. \square

Taking into account estimate *iv*) of Lemma 10, it is easy to check that

$$\hat{\rho}_{h,k} \rightarrow \rho \text{ in } L^2(0, T; H^1(\Omega)) \text{ as } (h, k) \rightarrow 0.$$

6.3 Convergence for the density scheme

At this point, we study the convergence (as $(h, k) \rightarrow 0$) for the incompressible condition and for the density scheme.

Proposition 23 *The limit function \mathbf{u} satisfies*

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \times (0, T).$$

Proof: Let $q \in C^0([0, T]; H^1(\Omega))$ be such that $\int_{\Omega} q(x) dx = 0$. We define q_h^n as the interpolated into M_h of $q(t_n)$ and by $q_{h,k} \in L^\infty(0, T; M_h)$ the piecewise constant function taking values q_h^{n+1} on $(t_n, t_{n+1}]$. Then, one has

$$q_{k,h} \rightarrow q \quad \text{in } L^\infty(0, T; L^2(\Omega)). \quad (58)$$

Taking $p_h^{n+1} = q_h^{n+1}$ as a test function in (30), multiplying by k and adding for n ,

$$\int_0^T (\nabla \cdot \mathbf{u}_{h,k}, q_{h,k}) dt = 0. \quad (59)$$

Thus, taking the limit in (59) as $(h, k) \rightarrow 0$ and using that

$$\nabla \cdot \mathbf{u}_{h,k} \rightarrow \nabla \cdot \mathbf{u} \quad \text{in } L^2(0, T; L^2(\Omega))\text{-weak, as } (h, k) \rightarrow 0,$$

one arrives at

$$0 = \lim_{(h,k) \rightarrow 0} \int_0^T (\nabla \cdot \mathbf{u}_{h,k}, q_{h,k}) dt = \int_0^T (\nabla \cdot \mathbf{u}, q) dt.$$

Consequently, $\nabla \cdot \mathbf{u} = 0$ holds in Q . □

Proposition 24 *The limit function $\rho \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H_N^2(\Omega))$ satisfies:*

$$\rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0 \quad \text{a.e. in } Q \quad (60)$$

and the pointwise estimate

$$0 < m \leq \rho(\mathbf{x}, t) \leq M < \infty \quad \text{in } Q.$$

Proof: Let $\eta \in C^0([0, T]; C_c^\infty(\Omega))$. We define η_h^n as the interpolated function of $\eta(t_n)$ into W_h . We define $\eta_{h,k} \in L^\infty(0, T; W_h)$ as the piecewise constant function taking values η_h^{n+1} on $(t_n, t_{n+1}]$. One can also prove the following strong convergences as $(h, k) \rightarrow 0$:

$$\eta_{k,h} \rightarrow \eta \quad \text{in } L^\infty(0, T; H^1(\Omega)). \quad (61)$$

Taking $\bar{\rho}_h = \eta_h^{n+1}$ as test function in (28), multiplying by k and summing over n , we arrive at

$$- \int_0^T \left(\frac{d}{dt} \rho_{h,k}, \eta_{h,k} \right) dt + \int_0^T \left(\hat{\mathbf{u}}_{h,k} \cdot \nabla \hat{\rho}_{h,k}, \eta_{h,k} \right) dt + \lambda \int_0^T \left(\nabla \rho_{h,k}, \nabla \eta_{h,k} \right) dt = 0. \quad (62)$$

Taking the limit as $(h, k) \rightarrow 0$ in (62) and using the following convergences as $(h, k) \rightarrow 0$:

- $\widehat{\mathbf{u}}_{h,k} \rightarrow \mathbf{u}$ in $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -weak,
- $\widehat{\rho}_{h,k} \rightarrow \rho$ in $L^2(0, T; H^1(\Omega))$ -strong, $\frac{d}{dt}\rho_{h,k} \rightarrow \frac{d}{dt}\rho$ in $L^2(0, T; L^2(\Omega))$ -weak,

the proof is concluded by using the additional regularity $\rho \in L^2(0, T; H^2(\Omega))$. \square

6.4 Strong Convergence in $L^2(\Omega)$ for the truncated density

Using Proposition 24, we establish the following compactness result.

Proposition 25

$$[\rho_{h,k}]_T, [\widehat{\rho}_{h,k}]_T \rightarrow \rho \text{ in } L^2(0, T; L^2(\Omega))\text{-strong, as } (h, k) \rightarrow 0. \quad (63)$$

Proof: We will show the proof for $\rho_{h,k}$, and analogously it can be shown for $\widehat{\rho}_{h,k}$. We define the following pointwise truncating operator:

$$T_m^M \rho_{h,k}(\mathbf{x}, t) = \begin{cases} \rho_{h,k}(\mathbf{x}, t) & \text{if } \rho_{h,k}(\mathbf{x}, t) \in [m, M], \\ m & \text{if } \rho_{h,k}(\mathbf{x}, t) < m, \\ M & \text{if } \rho_{h,k}(\mathbf{x}, t) > M. \end{cases}$$

Notice that, in general, $T_m^M \rho_{h,k} \notin W_h$. Let us see first that $T_m^M \rho_{h,k} \rightarrow \rho$ in $L^2(0, T; L^2(\Omega))$ -strong as $(h, k) \rightarrow 0$. Indeed, since $\rho_{h,k} \rightarrow \rho$ in $L^2(0, T; L^2(\Omega))$ -strong, as $(h, k) \rightarrow 0$, one can extract a subsequence (denoted in the same way) such that:

$$\rho_{h,k}(\mathbf{x}, t) \rightarrow \rho(\mathbf{x}, t) \text{ a.e. } (\mathbf{x}, t) \in Q, \text{ as } (h, k) \rightarrow 0.$$

Therefore, if we consider $(\mathbf{x}, t) \in Q$ such that $\rho(\mathbf{x}, t) \in (m, M)$, then there exist $h_0(\mathbf{x}, t) > 0$ and $k_0(\mathbf{x}, t) > 0$ so that $\rho_{h,k}(\mathbf{x}, t) \in (m, M)$ holds for all $h \leq h_0(\mathbf{x}, t)$ and $k \leq k_0(\mathbf{x}, t)$. Thus, $\rho_{h,k}(\mathbf{x}, t) = T_m^M \rho_{h,k}(\mathbf{x}, t)$ and $T_m^M \rho_{h,k}(\mathbf{x}, t) \rightarrow \rho(\mathbf{x}, t)$ as $(h, k) \rightarrow 0$.

On the other hand, if $(\mathbf{x}, t) \in Q$ is such that $\rho(\mathbf{x}, t) = m$, then

$$\forall \varepsilon > 0, \exists (h_0, k_0)(\mathbf{x}, t) \text{ such that } \forall (h, k) \leq (h_0, k_0)(\mathbf{x}, t) \text{ one has}$$

$$|\rho_{h,k}(\mathbf{x}, t) - m| = |\rho_{h,k}(\mathbf{x}, t) - \rho(\mathbf{x}, t)| < \varepsilon.$$

If we choose $\varepsilon < M - m$ this gives $T_m^M \rho_{h,k}(\mathbf{x}, t) = \rho_{h,k}(\mathbf{x}, t)$ or $T_m^M \rho_{h,k}(\mathbf{x}, t) = m$. Therefore, $\forall \varepsilon > 0$ (with $\varepsilon < M - m$) and $\forall (h, k) \leq (h_0, k_0)(\mathbf{x}, t)$ one has

$$|T_m^M \rho_{h,k}(\mathbf{x}, t) - \rho(\mathbf{x}, t)| < \varepsilon.$$

Finally, the remaining case of $(\mathbf{x}, t) \in Q$ such that $\rho(\mathbf{x}, t) = M$ is proved in the same manner.

Consequently, we have that $T_m^M \rho_{h,k}(\mathbf{x}, t) \rightarrow \rho(\mathbf{x}, t)$ a.e. $(\mathbf{x}, t) \in Q$ as $(h, k) \rightarrow 0$. Therefore, using that $|T_m^M \rho_{h,k}(\mathbf{x}, t)| \leq M$ a.e. $(\mathbf{x}, t) \in Q$, we can apply the Dominated Convergence Theorem, obtaining

$$T_m^M \rho_{h,k} \rightarrow \rho \text{ in } L^2(0, T; L^2(\Omega))\text{-strong, as } (h, k) \rightarrow 0. \quad (64)$$

Using the interpolation operator I_h from $H^1(\Omega) \cap C^0(\Omega)$ into W_h , it is easy to check that

$$[\rho_{h,k}]_T = I_h(T_m^M \rho_{h,k});$$

hence we can write

$$[\rho_{h,k}]_T - \rho = I_h(T_m^M \rho_{h,k}) - I_h(\rho) + I_h(\rho) - \rho. \quad (65)$$

It is verified that

$$I_h(T_m^M \rho_{h,k}) - I_h(\rho) \rightarrow 0 \text{ in } L^2(0, T; L^2(\Omega)). \quad (66)$$

Indeed, taking the norm in $L^2(\Omega)$,

$$\begin{aligned} |I_h(T_m^M \rho_{h,k}) - I_h(\rho)| &= |I_h(T_m^M \rho_{h,k} - \rho)| \\ &\leq |I_h(T_m^M \rho_{h,k} - \rho) - (T_m^M \rho_{h,k} - \rho)| + |T_m^M \rho_{h,k} - \rho| \\ &\leq C h \|T_m^M \rho_{h,k} - \rho\|_{H^1(\Omega)} + |T_m^M \rho_{h,k} - \rho|. \end{aligned}$$

Next, taking the norm in $L^2(0, T)$,

$$\|I_h(T_m^M \rho_{h,k}) - I_h(\rho)\|_{L^2(0, T; L^2(\Omega))} \leq C h \|T_m^M \rho_{h,k} - \rho\|_{L^2(0, T; H^1(\Omega))} + \|T_m^M \rho_{h,k} - \rho\|_{L^2(0, T; L^2(\Omega))}.$$

Therefore, using (64) and that $T_m^M \rho_{h,k}$ is bounded in $L^2(0, T; H^1(\Omega))$ (thanks to $|\nabla T_m^M \rho_{h,k}| \leq |\nabla \rho_{h,k}|$ and $\{\rho_{h,k}\}_{h,k}$ is bounded in $L^2(0, T; H^1(\Omega))$), (66) holds.

As well $I_h(\rho) - \rho \rightarrow 0$ in $L^2(0, T; L^2(\Omega))$, thanks to $|I_h(\rho) - \rho| \leq C h \|\rho\|_{H^1(\Omega)}$; hence

$$\|I_h(\rho) - \rho\|_{L^2(0, T; L^2(\Omega))} \leq C h \|\rho\|_{L^2(0, T; H^1(\Omega))}.$$

From (65), we arrive at (63). □

6.5 Strong convergence for the velocity

Proposition 26 *The following “fractional in time” estimate holds:*

$$\int_0^{T-\delta} \left| \sqrt{[\rho_{h,k}]_T(t+\delta)} (\mathbf{u}_{h,k}(t+\delta) - \mathbf{u}_{h,k}(t)) \right|^2 dt \leq C \delta^{1/2} \quad \forall \delta: \quad 0 < \delta < T, \quad (67)$$

with $C > 0$ independent of h, k and δ .

Proof: Since $\rho_{h,k}$ and $\mathbf{u}_{h,k}$ are piecewise constant functions, to obtain (67) it suffices to consider δ as a multiple of the time step k , that is, $\delta = rk$ with $r = 0, \dots, N$ and to prove

$$k \sum_{m=0}^{N-r} |\sqrt{[\rho_h^{m+r}]_T} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 \leq C (rk)^{1/2}, \quad \forall r : 0 \leq r \leq N. \quad (68)$$

Firstly, we will write the time derivative to the momentum equation (29) in a conservative form. It is obtained by adding to both sides of (29) the term $\frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right)$:

$$\left\{ \begin{aligned} & \left(\frac{[\rho_h^{n+1}]_T \mathbf{u}_h^{n+1} - [\rho_h^n]_T \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ & + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) \\ & = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right). \end{aligned} \right. \quad (69)$$

Next, multiplying by k and summing for $n = m, \dots, m-1+r$ in (69), we arrive at

$$\left\{ \begin{aligned} & \left([\rho_h^{m+r}]_T \mathbf{u}_h^{m+r} - [\rho_h^m]_T \mathbf{u}_h^m, \bar{\mathbf{u}}_h \right) + k \sum_{n=m}^{m-1+r} a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ & + k \sum_{n=m}^{m-1+r} c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - \sum_{n=m}^{m-1+r} (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) \\ & = k \sum_{n=m}^{m-1+r} \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \frac{k}{2} \sum_{n=m}^{m-1+r} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right). \end{aligned} \right. \quad (70)$$

Taking $\bar{\mathbf{u}}_h = \mathbf{u}_h^{m+r} - \mathbf{u}_h^m$ as a test function and keeping in mind the identity

$$\begin{aligned} \left([\rho_h^{m+r}]_T \mathbf{u}_h^{m+r} - [\rho_h^m]_T \mathbf{u}_h^m, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m \right) &= \left([\rho_h^{m+r}]_T (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m), \mathbf{u}_h^{m+r} - \mathbf{u}_h^m \right) \\ &+ \left([\rho_h^{m+r}]_T - [\rho_h^m]_T, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right), \end{aligned}$$

we get

$$\left\{ \begin{aligned} & |\sqrt{[\rho_h^{m+r}]_T} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 = - \left([\rho_h^m]_T - [\rho_h^{m+r}]_T, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \\ & - k \sum_{n=m}^{m-1+r} a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) - k \sum_{n=m}^{m-1+r} c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \\ & + k \sum_{n=m}^{m-1+r} \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m \right) + k \sum_{n=m}^{m-1+r} \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right). \end{aligned} \right. \quad (71)$$

On the other hand, multiplying by k , summing for $n = m, \dots, m-1+r$ and taking as a test function $\bar{\rho}_h = \rho_h^m - \rho_h^{m+r}$ in the density equation (31)_a, we find the equality

$$|\rho_h^m - \rho_h^{m+r}|^2 = -k \sum_{n=m}^{m-1+r} \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n + \lambda \omega_h^{n+1}, \rho_h^m - \rho_h^{m+r} \right). \quad (72)$$

Now, estimating the right-hand side of (72) as

$$|\rho_h^m - \rho_h^{m+r}|^2 \leq k \sum_{n=m}^{m-1+r} (\|\mathbf{u}_h^n\|_{L^4(\Omega)} \|\nabla \rho_h^n\|_{L^4(\Omega)} + \lambda |\omega_h^{n+1}|) |\rho_h^m - \rho_h^{m+r}|,$$

one gets

$$\begin{aligned} |\rho_h^m - \rho_h^{m+r}| &\leq C k \sum_{n=m}^{m-1+r} (\|\mathbf{u}_h^n\|_{L^4(\Omega)} \|\nabla \rho_h^n\|_{L^4(\Omega)} + |\omega_h^{n+1}|) \\ &\leq C k \left(\sum_{n=m}^{m-1+r} \|\mathbf{u}_h^n\|_{L^4(\Omega)}^2 \|\nabla \rho_h^n\|_{L^4(\Omega)}^2 + |\omega_h^{n+1}|^2 \right)^{1/2} (rk)^{1/2} \\ &\leq C (rk)^{1/2}. \end{aligned}$$

Therefore, we have obtained that $\max_{1 \leq m \leq N} |\rho_h^m - \rho_h^{m+r}| \leq C (rk)^{1/2}$. Consequently, using that $|[\rho_h^m]_T - [\rho_h^{m+r}]_T| \leq |\rho_h^m - \rho_h^{m+r}|$, one also obtains that

$$\max_{1 \leq m \leq N} |[\rho_h^m]_T - [\rho_h^{m+r}]_T| \leq C (rk)^{1/2}. \quad (73)$$

Finally, multiplying by k and summing for $m = 0, \dots, N-r$ in (71) and bounding adequately, we can obtain the required bound (68). For brevity, we only bound the two main terms of (71):

$$-k \sum_{m=0}^{N-r} \left([\rho_h^m]_T - [\rho_h^{m+r}]_T, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \leq Crk \quad (74)$$

$$-k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m, \mathbf{u}_h^{n+1} \right) \leq C (rk)^{1/2}. \quad (75)$$

Indeed, we bound (74) as follows:

$$\begin{aligned} &-k \sum_{m=0}^{N-r} \left([\rho_h^m]_T - [\rho_h^{m+r}]_T, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \\ &\leq k \sum_{m=0}^{N-r} |[\rho_h^m]_T - [\rho_h^{m+r}]_T| \|\mathbf{u}_h^m\|_{L^4(\Omega)} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^4(\Omega)} \\ &\leq \max_{1 \leq m \leq N} |[\rho_h^m]_T - [\rho_h^{m+r}]_T| \left(k \sum_{m=0}^{N-r} \|\mathbf{u}_h^m\|_{L^4(\Omega)}^2 \right)^{1/2} \left(k \sum_{m=0}^{N-r} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^4(\Omega)} \right)^{1/2} \\ &\leq C (rk)^{1/2} \quad (\text{using (73)}). \end{aligned}$$

We bound (75) using (27), as follows:

$$\begin{aligned} &k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m, \mathbf{u}_h^{n+1} \right) \\ &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}\|_{L^3} \|\mathbf{u}_h^{n+1}\| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\| \\ &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\|\rho_h^{n+1}\|_{H^1(\Omega)} \|\mathbf{u}_h^n\| + |\omega_h^{n+1}| \right) \|\mathbf{u}_h^{n+1}\| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|, \end{aligned}$$

where in the last line we have used $\|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq C|\omega_h^{n+1}|$ thanks to the imbedding $L^4(\Omega) \hookrightarrow L^3(\Omega)$, (34) and $|\nabla \rho_h^{n+1}| \leq |\omega_h^{n+1}|$. Interchanging the sum order (Fubini's discrete rule) and using the estimate $\|\rho_h^{n+1}\|_{H^1(\Omega)} \leq C$, we get

$$\begin{aligned} & k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c\left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m, \mathbf{u}_h^{n+1}\right) \\ & \leq C k^2 \sum_{n=0}^{N-1} \left(\|\mathbf{u}_h^n\| + |\omega_h^{n+1}|\right) \|\mathbf{u}_h^{n+1}\| \sum_{m=n-r+1}^{\bar{n}} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|, \end{aligned}$$

where

$$\bar{n} = \begin{cases} 0 & \text{if } n < 0, \\ n & \text{if } 0 \leq n \leq N-r, \\ N-r & \text{if } n > N-r. \end{cases}$$

Next, using the inequality $|\bar{n} - \overline{n-r+1}| \leq r$,

$$\begin{aligned} & k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c\left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m, \mathbf{u}_h^{n+1}\right) \\ & \leq C \sum_{n=0}^{N-1} k \left(\|\mathbf{u}_h^n\| + |\omega_h^{n+1}|\right) \|\mathbf{u}_h^{n+1}\| \left(\sum_{m=\overline{n-r+1}}^{\bar{n}} k \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|^2 \right)^{1/2} \left(\sum_{m=\overline{n-r+1}}^{\bar{n}} k \right)^{1/2} \\ & \leq C (rk)^{1/2} \left(k \sum_{n=0}^{N-1} \left(\|\mathbf{u}_h^n\| + |\omega_h^{n+1}|\right)^2 \right)^{1/2} \left(k \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1}\|^2 \right)^{1/2} \leq C (rk)^{1/2}. \end{aligned}$$

This is finished the proof. \square

Remark 27 From the a priori estimates of $\mathbf{u}_{h,k}$ in $L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega))$ and the fractional in time estimate (67), we can apply a compactness result ([16]) of Aubin-Lions type, obtaining that

$$\mathbf{u}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

Consequently, thanks to (55),

$$\widehat{\mathbf{u}}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

7 Convergence for the momentum system

In order to eliminate the discrete pressure, we are going to consider adequate test functions, thanks to the following:

Lemma 28 Let $\bar{\mathbf{u}} \in \mathbf{C}_c^\infty(\Omega)$. Then, there exists $\bar{\mathbf{u}}_h \in \mathbf{V}_h$ such that:

$$\begin{aligned} \text{i)} \quad & \bar{\mathbf{u}}_h \rightarrow \bar{\mathbf{u}} \text{ in } \mathbf{H}_0^1(\Omega), \\ \text{ii)} \quad & \left(\nabla \cdot \bar{\mathbf{u}}_h, q_h \right) = \left(\nabla \cdot \bar{\mathbf{u}}, q_h \right), \quad \forall q_h \in M_h. \end{aligned}$$

Proof: We consider \mathbf{t}_h as the interpolation of $\bar{\mathbf{u}}$ into \mathbf{V}_h . Then, $\|\bar{\mathbf{u}} - \mathbf{t}_h\| \rightarrow 0$ as $h \rightarrow 0$. We define $(\mathbf{e}_h, r_h) \in \mathbf{V}_h \times M_h$ as the solution of the following ‘‘discrete Stokes’’ problem:

$$\begin{cases} \left(\nabla \mathbf{e}_h, \nabla \mathbf{y}_h \right) - \left(r_h, \nabla \cdot \mathbf{y}_h \right) = \left(\nabla(\bar{\mathbf{u}} - \mathbf{t}_h), \nabla \mathbf{y}_h \right), & \forall \mathbf{y}_h \in \mathbf{V}_h, \\ \left(\nabla \cdot \mathbf{e}_h, \bar{p}_h \right) = \left(\nabla \cdot (\bar{\mathbf{u}} - \mathbf{t}_h), \bar{p}_h \right), & \forall \bar{p}_h \in M_h. \end{cases} \quad (76)$$

It is easy to deduce, using the *inf-sup* condition, that (76) has a unique solution. The estimate

$$\|\mathbf{e}_h\| + |r_h| \leq C \|\bar{\mathbf{u}} - \mathbf{t}_h\|.$$

also holds. Since $\|\bar{\mathbf{u}} - \mathbf{t}_h\| \rightarrow 0$, then $(\mathbf{e}_h, r_h) \rightarrow 0$ in $\mathbf{H}^1 \times L^2$. By defining $\bar{\mathbf{u}}_h = \mathbf{e}_h + \mathbf{t}_h$, one has

$$\|\bar{\mathbf{u}} - \bar{\mathbf{u}}_h\| \leq \|\bar{\mathbf{u}} - \mathbf{t}_h\| + \|\mathbf{e}_h\| \leq \|\bar{\mathbf{u}} - \mathbf{t}_h\|.$$

Therefore, we have proved *i*). The statement *ii*) holds from the definition of $\bar{\mathbf{u}}_h$. \square

Let $\mathbf{v} \in C^1([0, T]; \mathbf{C}_c^\infty(\Omega))$ be a free divergence function such that $\mathbf{v}(T) = 0$. We consider \mathbf{v}_h^n the projection (by a discrete Stokes problem) of $\mathbf{v}(t^n)$ given by Lemma 28. We define $\mathbf{v}_{h,k} \in L^\infty(0, T; \mathbf{V}_h)$ as the piecewise constant function taking the value \mathbf{v}_h^{n+1} on $(t_n, t_{n+1}]$ and $\tilde{\mathbf{v}}_{h,k} \in C^0([0, T]; \mathbf{V}_h)$ the corresponding globally continuous piecewise linear function such that $\tilde{\mathbf{v}}_{h,k}(t_n) = \mathbf{v}_h^n$. Then, as $(h, k) \rightarrow 0$, one has

$$\mathbf{v}_{h,k} \rightarrow \mathbf{v} \quad \text{in } L^\infty(0, T; \mathbf{H}_0^1(\Omega)), \quad (77)$$

$$\tilde{\mathbf{v}}_{h,k} \rightarrow \mathbf{v} \quad \text{in } W^{1,\infty}(0, T; \mathbf{H}_0^1(\Omega)). \quad (78)$$

Taking $\bar{\mathbf{u}}_h = \mathbf{v}_h^{n+1}$ as a test function in (69), multiplying by k , adding over n and using the identity (discrete integration by parts in time)

$$\sum_{n=0}^{N-1} \left(\rho_h^{n+1} \mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n, \mathbf{v}(t_{n+1}) \right) = \left(\rho_h^N \mathbf{u}_h^N, \mathbf{v}_h^N \right) - \sum_{n=0}^{N-1} \left(\rho_h^n \mathbf{u}_h^n, \mathbf{v}_h^{n+1} - \mathbf{v}_h^n \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right)$$

and the fact that $\mathbf{v}_h^N = 0$ (since $\mathbf{v}(T) = 0$), the following statement holds:

$$\begin{cases} - \sum_{n=0}^{N-1} \left(\rho_h^n \mathbf{u}_h^n, \mathbf{v}_h^{n+1} - \mathbf{v}_h^n \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right) \\ + \sum_{n=0}^{N-1} a \left([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \mathbf{v}_h^{n+1} \right) + \sum_{n=0}^{N-1} c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{v}_h^{n+1} \right) \\ = k \sum_{n=0}^{N-1} \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \mathbf{v}_h^{n+1} \right) + k \sum_{n=0}^{N-1} \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \mathbf{v}_h^{n+1} \right). \end{cases}$$

Next, using Definition 16,

$$\left\{ \begin{aligned} & - \int_0^T \left(\widehat{\rho}_{h,k}(t) \widehat{\mathbf{u}}_{h,k}(t), \frac{\partial}{\partial t} \widetilde{\mathbf{v}}_{h,k}(t) \right) dt - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right) \\ & + \int_0^T c \left(\rho_{h,k}(t) \widehat{\mathbf{u}}_{h,k}(t) - \lambda \nabla \rho_{h,k}(t), \mathbf{u}_{h,k}(t), \mathbf{v}_{h,k}(t) \right) dt + \int_0^T a \left(\rho_{h,k}(t), \mathbf{u}_{h,k}(t), \mathbf{v}_{h,k}(t) \right) dt \\ & = \int_0^T \left(\rho_{h,k}^T(t) \mathbf{f}_k(t), \mathbf{v}_{h,k}(t) \right) dt + \frac{k}{2} \int_0^T \left(\frac{\partial}{\partial t} \widetilde{\rho}_{h,k}^T(t), \mathbf{u}_{h,k}(t) \cdot \mathbf{v}_{h,k}(t) \right) dt \end{aligned} \right. \quad (79)$$

where we denote $\rho_{h,k}^T$, $\widetilde{\rho}_{h,k}^T$, \mathbf{f}_k as in the foregoing definitions.

From this weak statement for the discrete momentum system, one can pass to the limit in a standard way thanks to the convergence properties obtained throughout this work. Notice that, to take the limit in the last term, the estimate of Corollary 21 is used.

Then the limit function (ρ, \mathbf{u}) , jointly with an associated pressure p (obtained a posteriori by de Rham's lemma), is the weak solution of the continuous problem. Notice that, thanks to the uniqueness of this weak solution in $2D$ domains, it is easy to obtain the convergence of the whole sequences. Consequently, the proof of Theorem 1 is concluded.

8 Pollution model with mass diffusion

8.1 The continuous model

In this section we will study a variant of the *Kazhikhov-Smagulov* model where the main difference with the previous one is the appearance of the nonlinear diffusion, changing $-\mu \nabla \cdot (\nabla \mathbf{u})$ by $-\lambda \nabla \cdot (\rho \nabla \mathbf{u})$ in the momentum system, which remains

$$\left\{ \begin{aligned} & \rho \mathbf{u}_t + (\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla \mathbf{u} - \lambda \nabla \cdot (\rho \nabla \mathbf{u} - \rho (\nabla \mathbf{u})^t) + \nabla p = \mathbf{f} \quad \text{en } Q, \\ & \nabla \cdot \mathbf{u} = 0 \quad \text{en } Q, \quad \rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0 \quad \text{en } Q. \end{aligned} \right. \quad (80)$$

with the boundary and initial conditions:

$$\mathbf{u}(\mathbf{x}, t) = 0, \quad \frac{\partial \rho}{\partial \mathbf{n}} = 0, \quad \mathbf{x} \in \Gamma, \quad t \in (0, T), \quad (81)$$

$$\rho(\mathbf{x}, 0) = \rho_0, \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0, \quad \mathbf{x} \in \Omega. \quad (82)$$

This problem can be rewritten such as the previous model in Section 2, arriving at an analogous definition of weak solution.

The existence and uniqueness of a weak solution of (8), (9)-(10) was established in [3, 4], without the restrictive hypothesis (14).

Theorem 29 *Let $\mathbf{u}_0 \in \mathbf{H}$ and $\rho_0 \in H^1(\Omega)$ satisfying (13) and $\mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega))$ with $p > 1$. Then, there exists a (unique) weak solution of (8), (9)-(10) in $(0, T)$.*

We give an outline of the proof for the reader's convenience.

Proof. Suppose that we have (\mathbf{u}, ρ, q) a sufficiently regular solution of (8), (9)-(10). From the maximum principle of the parabolic density equation (8)_c and since $0 < m \leq \rho_0(x) \leq M < +\infty$, one gets $0 < m \leq \rho(x, t) \leq M < +\infty$ in Q .

Multiplying the momentum system (8)_a by \mathbf{u} , the density equation (8)_c by $\frac{1}{2}\mathbf{u} \cdot \mathbf{u}$, integrating over Ω and using the so-called vorticity tensor $W = \nabla \mathbf{u} - \nabla \mathbf{u}^t$, we arrive at

$$\int_{\Omega} \rho (|\nabla \mathbf{u}|^2 - (\nabla \mathbf{u})^t : \nabla \mathbf{u}) \, d\mathbf{x} = \int_{\Omega} \rho W : \nabla \mathbf{u} \, d\mathbf{x} = \int_{\Omega} \rho |\mathbf{rot} \mathbf{u}|^2 \, d\mathbf{x}. \quad (83)$$

Since $W = \mathbf{rot} \mathbf{u} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, one has

$$\frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2 \, d\mathbf{x} + 2\lambda \int_{\Omega} \rho |\mathbf{rot} \mathbf{u}|^2 \, d\mathbf{x} = 2 \int_{\Omega} \rho \mathbf{f} \cdot \mathbf{u} \, d\mathbf{x}.$$

Using $\Delta = \nabla \operatorname{div} - \mathbf{rot} \mathbf{rot}$, one has

$$\int_{\Omega} |\nabla \mathbf{u}|^2 \, d\mathbf{x} = \int_{\Omega} (|\mathbf{rot} \mathbf{u}|^2 + |\nabla \cdot \mathbf{u}|^2) \, d\mathbf{x}; \quad (84)$$

hence since $\nabla \cdot \mathbf{u} = 0$, we get

$$\int_{\Omega} |\nabla \mathbf{u}|^2 \, d\mathbf{x} = \int_{\Omega} |\mathbf{rot} \mathbf{u}|^2 \, d\mathbf{x}. \quad (85)$$

Next, applying the lower bound for the density to $\int_{\Omega} \rho |\mathbf{rot} \mathbf{u}|^2 \, d\mathbf{x} \geq m \int_{\Omega} |\mathbf{rot} \mathbf{u}|^2 \, d\mathbf{x}$ and identity (85), one arrives at

$$\frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2 \, d\mathbf{x} + 2\lambda m \int_{\Omega} |\nabla \mathbf{u}|^2 \, d\mathbf{x} \leq 2(\rho \mathbf{f}, \mathbf{u}) \leq \varepsilon \|\mathbf{u}\|^2 + C_{\varepsilon} \|\mathbf{f}\|_{L^p(\Omega)}^2, \quad (86)$$

with $p > 1$. Therefore, integrating (86) over $(0, t) \forall t \leq T$ and applying the lower estimate for the density to the first term, one arrives at

$$\max_{0 \leq t \leq T} |\mathbf{u}(t)|^2 + \int_0^T \|\mathbf{u}(t)\|^2 \, dt \leq C.$$

The bounds in $L^\infty(H^1) \cap L^2(H^2)$ for the density are obtained as in Theorem 5. \square

8.2 Numerical scheme

We design a numerical scheme for problem (8), (9)-(10), following the same ideas of the numerical scheme given in Section 2, where we will replace the stabilization term of the momentum system

$$-\lambda \int_{\Omega} \frac{M+m}{2} (\nabla \mathbf{u}_h^{n+1})^t : \nabla \bar{\mathbf{u}}_h \, d\mathbf{x}$$

by the term $\lambda m (\nabla \cdot \mathbf{u}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h)$. As well, the density entering into the diffusion term in the momentum system has been truncated. Thus, we arrive at the following numerical scheme:

Given $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

1. Find $\rho_h^{n+1} \in W_h$ such that for each $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (87)$$

2. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + \tilde{a}([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h), \end{array} \right. \quad (88)$$

$$(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h) = 0. \quad (89)$$

where

$$\tilde{a}(\rho, \mathbf{u}, \mathbf{v}) = \lambda (\rho (\nabla \mathbf{u} - (\nabla \mathbf{u})^t), \nabla \mathbf{v}) + \lambda m (\nabla \cdot \mathbf{u}, \nabla \cdot \mathbf{v})$$

and $c(\cdot, \cdot, \cdot)$ is defined as in Section 2. Taking into account equality (83) in (90) and the lower estimate for the truncated density, it follows that

$$\tilde{a}([\rho]_T, \mathbf{u}, \mathbf{u}) \geq \lambda m \int_{\Omega} (|\mathbf{rot} \mathbf{u}|^2 + |\nabla \cdot \mathbf{u}|^2) dx. \quad (90)$$

Observing that $\int_{\Omega} (|\mathbf{rot} \mathbf{u}|^2 + |\nabla \cdot \mathbf{u}|^2) dx = \int_{\Omega} |\nabla \mathbf{u}|^2 dx$ for any $\mathbf{u} \in \mathbf{H}_0^1(\Omega)$ thanks to equality (84) (see Theorem 29), we arrive at

$$\tilde{a}([\rho]_T, \mathbf{u}, \mathbf{u}) \geq \lambda m \|\mathbf{u}\|^2 \quad \forall \mathbf{u} \in \mathbf{H}_0^1(\Omega).$$

Accordingly, following the same arguments developed for the model of linear diffusion, one can arrive at exactly the same conclusions. Notice that the passage to the limit in the new diffusion term $([\rho_{h,k}]_T (\nabla \mathbf{u}_{h,k} - \nabla \mathbf{u}_{h,k}^t), \nabla \mathbf{v}_{h,k})$ is controlled thanks to the convergences, $[\rho_{h,k}]_T \rightarrow \rho$ in $L^2(Q)$ -strong and in $L^\infty(Q)$ -weak and $\nabla \mathbf{u}_{h,k} \rightarrow \nabla \mathbf{u}$ in $L^2(Q)$ -weak and $\nabla \mathbf{v}_{h,k} \rightarrow \nabla \mathbf{v}$ in $L^2(Q)$ -strong.

9 A generalization of the pollution model

The pollution model (8) is a particular case of a general model derived in [3, 4]. For this general model, we will define a numerical scheme (using the main ideas of the previous schemes) which will be unconditionally stable, but the convergence remains as an open problem.

Such a model again begins from the compressible model (1) assuming this time the following decomposition:

$$\rho \mathbf{v} = \rho \mathbf{u} - \lambda \nabla \Psi(\rho) \quad \text{with} \quad \nabla \cdot \mathbf{u} = 0.$$

Then, imposing $\mu = \lambda$ the compressible model (1) reads ([3, 4]):

$$\begin{cases} (\rho \mathbf{u})_t + \nabla \cdot \left((\rho \mathbf{u} - \lambda \nabla \Psi(\rho)) \otimes \mathbf{u} - \lambda \mathbf{u} \otimes \nabla \Psi(\rho) \right) - \lambda \nabla \cdot (\Psi(\rho) \nabla \mathbf{u}) + \nabla P = \rho \mathbf{f} & \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0 & \text{in } Q, \quad \rho_t + \nabla \cdot (\rho \mathbf{u} - \lambda \nabla \Psi(\rho)) = 0 & \text{in } Q, \end{cases} \quad (91)$$

where $P = q - (\mu + \tilde{\lambda}) \nabla \cdot \left(\mathbf{u} - \frac{\lambda}{\rho} \nabla \Psi(\rho) \right) - \lambda \Psi(\rho)_t - \lambda^2 \left(\Psi(\rho) \nabla \cdot \left(\frac{1}{\rho} \nabla \Psi(\rho) \right) + \frac{|\nabla \Psi(\rho)|^2}{\rho} \right)$. Now observe that the λ^2 -terms which are not canceled are all of potential type (using an auxiliary function φ such that $\nabla \varphi(\rho) = \frac{1}{\rho} \nabla \Psi(\rho)$) and they are included into the modified pressure P .

Note that when $\Psi(\rho) = \rho$ (then $\varphi(\rho) = \log \rho$), we arrive at the pollution model (8).

The weak definition for the general model (91) remains as follows (now, equality (5) is again used, replacing ρ by $\Psi(\rho)$):

Definition 30 A pair (ρ, \mathbf{u}) is called a weak solution of (91), (9)-(10) in $(0, T)$ if it satisfies:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$,

$$\rho \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)), \quad 0 < m \leq \rho(\mathbf{x}, t) \leq M, \quad \text{a.e. } (\mathbf{x}, t) \in Q.$$

b) $\forall \phi \in C^1([0, T]; \mathbf{V})$ such that $\phi(T) = 0$,

$$\begin{aligned} & \int_0^T \left\{ - \left(\mathbf{u}, \rho \phi_t + (\rho \mathbf{u} - \lambda \nabla \Psi(\rho)) \cdot \nabla \phi \right) + \lambda \left(\Psi(\rho) (\nabla \mathbf{u} - (\nabla \mathbf{u})^t), \nabla \phi \right) \right\} dt \\ &= \int_0^T \left(\rho \mathbf{f}, \phi \right) dt + \left(\rho_0 \mathbf{u}_0, \phi(0) \right). \end{aligned}$$

c) $\forall \eta \in C^1([0, T]; H^1(\Omega))$ such that $\eta(T) = 0$,

$$\int_0^T \left\{ - \left(\rho, \eta_t \right) - \left(\rho \mathbf{u}, \nabla \eta \right) + \left(\lambda \nabla \Psi(\rho), \nabla \eta \right) \right\} dt = \left(\rho_0 \mathbf{u}_0, \eta(0) \right).$$

Remark 31 Observe that the density solution for this general model $\rho \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$; therefore it loses one regularity order in space in comparison with the two earlier models (7) and (8) for which $\rho \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega))$. This regularity implies $\rho_t \in L^2(0, T; L^2(\Omega))$. Now, only $\rho_t \in L^2(0, T; H^1(\Omega)')$ holds.

The existence of weak solutions for this general model (91) is established in ([3, 4]).

Theorem 32 Let $\mathbf{u}_0 \in \mathbf{H}$, $\rho_0 \in H^1(\Omega)$ satisfying (13), $\mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega))$ with $p > 1$ and $\Psi \in C^1([m, M])$ is a real function such that $0 < \alpha \leq \Psi$ and $0 < \beta \leq \Psi'$ in $[m, M]$. Then, there exists at least a weak solution of (91), (9)-(10) in $(0, T)$.

In order to approximate numerically the general model (91), we propose the following scheme inspired in the foregoing ideas for models (7) and (8):

Initialization: Let $(\mathbf{u}_h^0, \rho_h^0) \in (\mathbf{V}_h, W_h)$ be suitable approximations of (\mathbf{u}_0, ρ_0) as $h \rightarrow 0$.

Time step $n + 1$: Given $(\mathbf{u}_h^n, \rho_h^n, \Psi_h^n) \in \mathbf{V}_h \times W_h \times W_h$.

1. Find $\rho_h^{n+1} \in W_h$ such that for each $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + c(\mathbf{u}_h^n, \rho_h^{n+1}, \bar{\rho}_h) + \lambda \left(\Psi'([\rho_h^n]_T) \nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0, \quad (92)$$

2. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a(\Psi([\rho_h^{n+1}]_T), \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \Psi'([\rho_h^{n+1}]_T) \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h), \end{array} \right. \quad (93)$$

$$(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h) = 0, \quad (94)$$

where the trilinear forms $a(\cdot, \cdot, \cdot)$ and $c(\cdot, \cdot, \cdot)$ and the discrete truncating operator $[\cdot]_T$ are defined as before.

The convective term for ρ_h^{n+1} has been approximated by $c(\mathbf{u}_h^n, \rho_h^{n+1}, \bar{\rho}_h)$ instead of $(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h)$ in order to obtain unconditional stability, since the control of the explicit form introduces constraints between the discretization parameters because the estimates for the density are now satisfied only in weak norms.

In fact, using the techniques developed for the foregoing schemes there are no additional difficulties in obtaining the following unconditional stability estimates:

Lemma 33 *Suppose $\mathbf{u}_0 \in \mathbf{H}$, $\rho_0 \in L^2(\Omega)$ satisfying (13), $\mathbf{f} \in L^2(0, T; \mathbf{L}^p(\Omega))$ with $p > 1$ and $\Psi \in C^1([m, M])$ is a real function such that $0 < \alpha \leq \Psi$ and $0 < \beta \leq \Psi'$ in $[m, M]$. Then, the solution of the discrete scheme (92)-(94) satisfies the following estimates:*

$$\begin{array}{lll} \text{i)} \max_{0 \leq n \leq N} |\mathbf{u}_h^n| \leq C, & \text{ii)} k \sum_{n=0}^N \|\mathbf{u}_h^n\|^2 \leq C, & \text{iii)} \sum_{n=0}^{N-1} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 \leq C, \\ \text{iv)} \max_{0 \leq n \leq N} |\rho_h^n| \leq C, & \text{v)} k \sum_{n=1}^N |\nabla \rho_h^n|^2 \leq C, & \text{vi)} \sum_{n=0}^{N-1} |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 \leq C, \end{array}$$

with $C > 0$ depending only on $(\rho_0, \mathbf{u}_0, \mathbf{f})$.

For the convergence of scheme (92)-(94), the main difficulty lies in the compactness argument of the approximate velocity in $\mathbf{L}^2(Q)$ based on a fractional estimate (see Proposition 26), for which it was essential to control the terms

$$\frac{k^2}{2} \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \mathbf{u}_h^{m+r} - \mathbf{u}_h^m \right) \quad (95)$$

and

$$k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \Psi'([\rho_h^{n+1}]_T) \nabla \rho_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m, \mathbf{u}_h^{n+1}) \quad (96)$$

by $C(rk)^\gamma$ with $0 < \gamma \leq 1$. Now, because of the loss of regularity of the discrete density with respect to models (7) and (8), the estimate for the discrete time derivative of the approximate density in $L^2(Q)$ changes by an estimate in $L^2(0, T; H^1(\Omega)')$, which is not enough to bound (95). Obviously this weak regularity of the density is not enough to bound (96) either.

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Capítulo 2

Conditional stability and
convergence of a fully discrete
scheme for $3D$ Navier-Stokes
equations with mass diffusion

Conditional stability and convergence of a fully discrete scheme for 3D Navier-Stokes equations with mass diffusion

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Abstract

We construct a fully discrete numerical scheme for three-dimensional incompressible fluids with mass diffusion (in density-velocity-pressure formulation), also called the Kazhikhov-Smagulov model. We will prove conditional stability and convergence, by using at most C^0 -finite elements, although the density of the limit problem will have H^2 -regularity.

The key idea of our argument is first to obtain pointwise estimates for the discrete density by imposing the constraint $\lim_{(h,k) \rightarrow 0} h/k = 0$ on the time and space parameters (k, h) . Afterwards, under the same constraint on the parameters, strong estimates for the discrete density in $l^\infty(H^1)$ and for the discrete Laplacian of the density in $l^2(L^2)$ are obtained. From here, the compactness and convergence of the scheme can be concluded with similar arguments as we used in [12], where a different scheme is studied for two-dimensional domains which is unconditionally stable and convergent.

Moreover, we study the asymptotic behavior of the numerical scheme as the diffusion parameter λ goes to zero, obtaining convergence as $(k, h, \lambda) \rightarrow 0$ towards a weak solution of the density-dependent Navier-Stokes system provided that the constraint $\lim_{(\lambda, h, k) \rightarrow 0} h/(\lambda^2 k) = 0$ on (h, k, λ) is satisfied.

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1 Introduction

1.1 The model

Let $\Omega \subset \mathbb{R}^3$ be an open bounded set with boundary Γ . We denote by $[0, T]$ ($0 < T < +\infty$) the time interval of observation. We will use the notation $Q = \Omega \times (0, T)$, $\Sigma = \Gamma \times (0, T)$, and $\mathbf{n}(\mathbf{x})$ the outwards unit normal vector to Γ at the point $\mathbf{x} \in \Gamma$.

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We consider the Navier-Stokes system with mass diffusion (the so-called Kazhikhov-Smagulov model) in Q :

$$\begin{cases} \rho \mathbf{u}_t + ((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla) \mathbf{u} - \nabla \cdot (\mu \nabla \mathbf{u} - \lambda \rho (\nabla \mathbf{u})^t) + \nabla p = \rho \mathbf{f}, \\ \nabla \cdot \mathbf{u} = 0, \\ \rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0. \end{cases} \quad (1)$$

The unknowns for this model are $\rho : Q \rightarrow \mathbb{R}^+$, the density of the fluid, $\mathbf{u} : Q \rightarrow \mathbb{R}^3$, the incompressible (averaged) velocity vector field, and $p : Q \rightarrow \mathbb{R}$, a potential function (modified pressure).

Model (1) can be derived from the compressible Navier-Stokes system, by imposing that the velocity \mathbf{v} can be decomposed as $\mathbf{v} = \mathbf{u} - \lambda \nabla \log \rho$, with $\nabla \cdot \mathbf{u} = 0$ (it decomposes into an incompressible part \mathbf{u} and a potential part $-\lambda \nabla \log \rho$), and eliminating the λ^2 -terms (see [12]).

We complete (1) with the boundary conditions on Σ :

$$\mathbf{u}|_{\Sigma} = 0, \quad \frac{\partial \rho}{\partial \mathbf{n}} \Big|_{\Sigma} = 0 \quad (2)$$

and the initial conditions in Ω :

$$\rho|_{t=0} = \rho_0, \quad \mathbf{u}|_{t=0} = \mathbf{u}_0, \quad (3)$$

where $\rho_0 : \Omega \rightarrow \mathbb{R}^+$ and $\mathbf{u}_0 : \Omega \rightarrow \mathbb{R}^d$ are given functions.

Throughout this work, we assume the hypothesis on the initial density:

$$0 < m \leq \rho_0(\mathbf{x}) \leq M \quad \text{in } \Omega. \quad (4)$$

1.2 Known results

Concerning the simplified model (1), Kazhikhov and Smagulov [13] proved, via a semi-Galerkin method, the existence of global weak solutions, under the following hypothesis:

$$\lambda < 2\mu/(M - m) \quad (5)$$

and the existence of local strong solutions (which is global in the two-dimensional case). Salvi [15] proved the existence of weak solutions for non-cylindrical domains. On the other hand, Secchi [17] studied the problem for $\Omega = \mathbb{R}^3$, proving the local existence and uniqueness of strong solutions, by using a fixed point argument.

For the complete model (including the λ^2 -terms), Beirão da Veiga [2] and Secchi [16] established the local existence of strong solutions by using linearization and a fixed point argument. In [16], global existence and uniqueness are shown for two-dimensional (2D) domains by imposing that λ/μ is small enough as well as the asymptotic behavior as $\lambda \rightarrow 0$ towards a weak solution of the Navier-Stokes system with variable density. In the case of positive initial density

for the 3D case, Guillén-González [10] proved the global existence of weak solutions and the behavior, as $\lambda \rightarrow 0$, towards the Navier-Stokes system with variable density. Recently, in [11] by means of an iterative method, the existence and regularity of strong solutions (and some error estimates) have been proved.

A time-space numerical scheme has been recently developed by using C^0 -finite elements for density and velocity in [12] for model (1) in the 2D case, which is unconditionally stable and convergent towards the (unique) weak solution of the continuous problem. This scheme is of the backward Euler type, where in each time step the computation of the discrete density and the discrete velocity-pressure are decoupled, by means of linear problems.

Concerning the numerical analysis for the density-dependent Navier-Stokes problem, a stable, convergent scheme is proposed in [14], by using in particular a discontinuous Galerkin finite element method to approximate the density transport equation.

1.3 Main results of the paper

Our main objective is to design a linear scheme by using finite elements to approximate all unknowns (density, velocity, and pressure) of problem (1)-(3). To this end, we consider for simplicity a uniform partition of $[0, T]$, $(t_n = nk)_{n=0}^N$, with $k = T/N$ being the time step, and propose a backward Euler time scheme which is implicit with respect to the diffusion terms and semi-implicit with respect to the convection terms. Specific properties of the finite element spaces associated to the parameter h are described in Section 3.1.

In what follows we consider the notation (\cdot, \cdot) and $|\cdot|$ for the $L^2(\Omega)$ -inner product and the $L^2(\Omega)$ -norm, respectively. Also, we denote $\|\mathbf{u}\| = |\nabla \mathbf{u}|$, which is an equivalent norm to the usual one in $H_0^1(\Omega)$.

The scheme is described as follows:

Initialization: Let $(\mathbf{u}_h^0, \rho_h^0) \in \mathbf{V}_h \times W_h$ be an approximation of (\mathbf{u}_0, ρ_0) as $h \rightarrow 0$.

Time step $n + 1$: Given $(\rho_h^n, \mathbf{u}_h^n, p_h^n) \in W_h \times \mathbf{V}_h \times M_h$,

1. find $(\mathbf{w}_h^n, q_h^n) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$ such that, for each $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$,

$$\begin{cases} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0; \end{cases} \quad (6)$$

2. find $\rho_h^{n+1} \in W_h$ such that, for each $\bar{\rho}_h \in W_h$,

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0; \quad (7)$$

3. find $(\mathbf{w}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that, for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$,

$$\begin{cases} \left(\rho_h^n \frac{\mathbf{w}_h^{n+1} - \mathbf{w}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k} \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) + a(\rho_h^{n+1}, \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1} \mathbf{w}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h) = (\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h), \end{cases} \quad (8)$$

$$(\nabla \cdot \mathbf{w}_h^{n+1}, q_h) = 0, \quad (9)$$

where

$$\mathbf{f}^{n+1} = \frac{1}{k} \int_{t_n}^{t_{n+1}} \mathbf{f}(t) dt,$$

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu (\nabla \mathbf{u}, \nabla \mathbf{v}) + \lambda \int_{\Omega} \left(\frac{\widetilde{M} + \widetilde{m}}{2} - \rho \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} dx,$$

with $\widetilde{M} > M$, $0 < \widetilde{m} < m$ such that $\lambda \frac{\widetilde{M} - \widetilde{m}}{2} < \mu$ (here (5) is imposed), and

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) = \frac{1}{2} \left[((\mathbf{w} \cdot \nabla) \mathbf{u}, \mathbf{v}) - ((\mathbf{w} \cdot \nabla) \mathbf{v}, \mathbf{u}) \right].$$

The following properties of continuity and coercivity hold:

$$a(\rho, \mathbf{u}, \mathbf{u}) \geq \frac{\mu_1}{2} \|\mathbf{u}\|^2 \quad \text{if } \widetilde{m} \leq \rho \leq \widetilde{M}, \quad \text{with } \frac{\mu_1}{2} = \mu - \lambda \frac{\widetilde{M} - \widetilde{m}}{2} (> 0),$$

$$a(\rho, \mathbf{u}, \mathbf{v}) \leq C_{\lambda} \|\mathbf{u}\| \|\mathbf{v}\| \quad (\text{if } \|\rho\|_{L^{\infty}(\Omega)} \leq C),$$

$$c(\mathbf{w}, \mathbf{u}, \mathbf{u}) = 0,$$

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) \leq C \|\mathbf{w}\|_{L^3} \|\mathbf{u}\| \|\mathbf{v}\|. \quad (10)$$

Here and in what follows, we denote by C_{λ} and C different positive constants independent of (h, k) and (h, k, λ) , respectively.

From the computational point of view, scheme (6)-(9) decouples the calculation between ρ_h^{n+1} and $(\mathbf{w}_h^{n+1}, p_h^{n+1})$ where \mathbf{w}_h^n is an intermediate velocity, which is obtained as the H^1 orthogonal projection of \mathbf{u}_h^n onto a discrete free-divergence space. We will see that scheme (6)-(9) is conditionally stable and convergent. As the diffusion parameter is close to zero in many practical situations; we will prove that when the diffusion parameter λ goes to zero together with the space and time parameters (h, k) , scheme (6)-(9) approximates to a weak solution of the Navier-Stokes with variable density system, under a constraint involving the parameters h , k , and λ . In fact, to our knowledge, it is the first convergent scheme to (55) based on C^0 -finite elements for the discrete density, avoiding to perform directly an algorithm for (55) which presents important difficulties by itself, mainly for the approximation of the density transport equation. Recall that in [14] a convergent scheme is given based on a discontinuous Galerkin method for the density.

The corresponding study for the complete model, with λ^2 -terms, will be the subject of a forthcoming paper.

By defining in $[0, T]$ piecewise constant functions $\mathbf{u}_{h,k}, \rho_{h,k}$ such that $\mathbf{u}_{h,k}, \rho_{h,k}|_{(t_{n-1}, t_n]} = \mathbf{u}_h^n, \rho_h^n$, respectively, that we will denote by $\mathbf{u}_{h,k,\lambda}, \rho_{h,k,\lambda}$ when the diffusion parameter $\lambda \rightarrow 0$ is considered, we present the following main results of this paper.

Theorem 1 *Assuming hypotheses (H0)-(H5) given in Section 3.1 jointly with the constraint on the parameters*

$$(S) \quad \lim_{(h,k) \rightarrow 0} \frac{h}{k} = 0,$$

then there exists a convergent subsequence of $(\mathbf{u}_{h,k}, \rho_{h,k})$ (denoted in the same way) as $(h, k) \rightarrow 0$ towards a weak solution (\mathbf{u}, ρ) of problem (1), (2)-(3) (see Definition 3), in the following sense: $(\mathbf{u}_{h,k}, \rho_{h,k}) \rightarrow (\mathbf{u}, \rho)$ in $L^2(0, T; \mathbf{L}^2(\Omega)) \times L^2(0, T; H^1(\Omega))$ -strong, in $L^\infty(0, T; \mathbf{L}^2(\Omega)) \times (H^1(\Omega) \cap L^\infty(\Omega))$ -weak*, and in $L^2(0, T; \mathbf{H}_0^1(\Omega)) \times L^4(0, T; W^{1,3}(\Omega))$ -weak. Moreover, $\tilde{m} \leq \rho_{h,k} \leq \tilde{M}$.

Theorem 2 *Under the hypotheses of Theorem 1 and by extending (H2) by (H2') (given in Section 8.1), and changing (S) by the more restrictive constraint*

$$(S') \quad \lim_{(\lambda, h, k) \rightarrow 0} \frac{1}{\lambda} \sqrt{\frac{h}{k}} = 0,$$

then there exists a convergent subsequence of $(\mathbf{u}_{h,k,\lambda}, \rho_{h,k,\lambda})$ as $(h, k, \lambda) \rightarrow 0$ towards a weak solution (\mathbf{u}, ρ) of the Navier-Stokes with variable density problem (see Definition 23) in the following sense: $\mathbf{u}_{h,k,\lambda} \rightarrow \mathbf{u}$ in $L^2(0, T; \mathbf{L}^2(\Omega))$ -strong, in $L^\infty(0, T; \mathbf{L}^2(\Omega))$ -weak* and in $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -weak, and $\rho_{h,k,\lambda} \rightarrow \rho$ in $L^\infty(Q)$ -weak*.

The idea for the derivation of this scheme can be found in [12], where the following scheme has been studied:

Time step $(n+1)$: Given $(\rho_h^n, \mathbf{u}_h^n, p_h^n) \in W_h \times \mathbf{V}_h \times M_h$,

1. Find $\rho_h^{n+1} \in W_h$ such that, for each $\bar{\rho}_h \in W_h$,

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h \right); \quad (11)$$

2. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that, for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$,

$$\begin{cases} \left([\rho_h^n]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) + a([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) = ([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h), \end{cases} \quad (12)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{\rho}_h\right) = 0, \quad (13)$$

where

$$[w_h]_T(\mathbf{x}_i) = \begin{cases} w_h(\mathbf{x}_i) & \text{if } w_h(\mathbf{x}_i) \in [m, M], \\ m & \text{if } w_h(\mathbf{x}_i) < m, \\ M & \text{if } w_h(\mathbf{x}_i) > M, \end{cases}$$

with \mathbf{x}_i the nodes of the mesh \mathcal{T}_h of Ω .

Comparing both schemes we can observe the following differences: the discrete densities involved in the mixed variational problem for velocity-pressure (12)-(13) which require the property of the maximum principle are truncated, whereas this truncation is not necessary for scheme (6)-(9). Moreover, in (11) the convective term for the density scheme is considered in the explicit form $\left(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h\right)$ and it is now taken in semi-implicit form $\left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h\right)$ where \mathbf{w}_h^n is a projection of \mathbf{u}_h^n onto a discrete zero-divergence space. This space is chosen to hold $\left(\nabla \cdot \mathbf{w}_h^n, \bar{\rho}_h^2\right) = 0$ for all $\bar{\rho}_h \in W_h$.

Concerning the numerical analysis we remark on the following three main differences between both schemes:

1. The argument to obtain pointwise estimates for the discrete density under some constraints on the discrete parameters done in subsection 3.4 is completely new. Moreover, the extension of this argument to the scheme in [12] is not clear even assuming some constraints on the discrete parameters. This justifies the presence of the truncation operator in the discrete momentum system (12). On the other hand, the scheme in [12] is unconditionally stable, and now the obtention of a maximum principle is subject to a constraint between the discretization parameters.
2. Strong estimates for the discrete density are obtained in two different ways in [12] and in the present paper. In [12], we used a discrete version of the *Gagliardo-Nirenberg* interpolation $\|\nabla \rho\|_{L^4}^2 \leq C \|\rho\|_{H^1} \|\Delta \rho\|_{L^2}$ which does not need pointwise estimates for the discrete density. Since this interpolation is exclusive for two-dimensional domains, we cannot use it for three-dimensional domains. Accordingly, we change the *Gagliardo-Nirenberg* interpolation by a discrete version of the interpolation $\|\nabla \rho\|_{L^4}^2 \leq C \|\rho\|_{L^\infty} \|\Delta \rho\|_{L^2}$ and make a discrete integration by parts (which mimics the argument of the exact problem to obtain strong estimates of the density). Observe that we have to assure a maximum principle or at least pointwise estimates for the discrete density in order for this other interpolation to work.
3. Another difference is the asymptotic behavior with respect to the diffusion parameter λ (jointly with the discretization parameters). Due to the fact that the convective term of the discrete density equation is handled in different ways as has been explained in point 2, we find that the strong estimates of the discrete density provided in [12] degenerate

when $\lambda \rightarrow 0$, and we cannot pass to the limit towards a weak solution of the Navier-Stokes problem with variable density. However, now the dependence of λ is improved, and the scheme (13)-(9) gives a numerical approximation for the Navier-Stokes problem with variable density using continuous finite elements.

The rest of the paper can be described as follows. The main ideas for the mathematical analysis of problem (1)-(3) are provided in Section 2. In Section 3, by using appropriate auxiliary schemes, we establish conditional stability estimates, energy estimates for the velocity, and pointwise estimates for the density. In Section 4, strong estimates for the discrete density are obtained, by using the discrete Laplacian of the density. In Sections 5, 6, and 7, weak and strong convergences and the passage to the limit are shown, respectively, concluding the proof of Theorem 1. In Section 8, we study the asymptotic behavior as the diffusion parameter goes to zero, proving Theorem 2.

2 Analysis of the continuous model

To define the concept of a weak solution of problem (1)-(3), we introduce the following function spaces:

$$\begin{aligned} \mathbf{H} &= \{ \mathbf{u} : \mathbf{u} \in \mathbf{L}^2(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \Gamma \}, \\ \mathbf{V} &= \{ \mathbf{u} : \mathbf{u} \in \mathbf{H}_0^1(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega \}, \\ L_0^2(\Omega) &= \left\{ p : p \in L^2(\Omega), \int_{\Omega} p(\mathbf{x}) d\mathbf{x} = 0 \right\}, \\ H_N^2(\Omega) &= \left\{ \rho \in H^2(\Omega) : \frac{\partial \rho}{\partial \mathbf{n}} = 0 \text{ on } \Gamma, \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x} \right\}. \end{aligned}$$

In \mathbf{V} the $\|\mathbf{u}\|_{H^1(\Omega)}$ -norm is equivalent to $|\nabla \mathbf{u}|$ (which will be denoted by $\|\mathbf{u}\|$). $H_N^2(\Omega)$ is an affine space: $H_N^2(\Omega) = \frac{1}{|\Omega|} \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x} + H_{N,0}^2(\Omega)$, and in $H_{N,0}^2(\Omega)$ (zero-average function space) the norm $\|\rho\|_{H^1(\Omega)}$ is equivalent to $|\nabla \rho|$ and the norm $\|\rho\|_{H^2(\Omega)}$ is equivalent to $|\Delta \rho|$. In particular, in $H_N^2(\Omega)$ the following norms are equivalents: $\|\rho - \frac{1}{|\Omega|} \int_{\Omega} \rho_0\|_{H^1(\Omega)} \sim |\nabla \rho|$ and $\|\nabla \rho\|_{H^1(\Omega)} \sim |\Delta \rho|$.

Definition 3 A pair (ρ, \mathbf{u}) is called a weak solution of (1)-(3) in $(0, T)$ if it verifies:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$, $\rho \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H_N^2(\Omega))$, with $0 < m \leq \rho(\mathbf{x}, t) \leq M$, a. e. $(\mathbf{x}, t) \in Q$.

b) $\forall \phi \in C^1([0, T]; \mathbf{V})$ such that $\phi(T) = 0$,

$$\begin{aligned} & \int_0^T \left\{ -\left(\mathbf{u}, \rho \phi_t + (\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla \phi \right) + \left(\mu \nabla \mathbf{u} - \lambda \rho (\nabla \mathbf{u})^t, \nabla \phi \right) \right\} dt \\ &= \int_0^T \left(\rho \mathbf{f}, \phi \right) dt + \left(\rho_0 \mathbf{u}_0, \phi(0) \right). \end{aligned}$$

c) The equation of mass diffusion (1)_c is verified almost everywhere in Q .

Remark 4 As usual, the pressure p can be obtained by using b) and De Rham's lemma [19].

We state the existence of (global in time) weak solution of problem (1), (2)-(3) (see [13, 1]).

Theorem 5 Let $\mathbf{u}_0 \in \mathbf{H}$, $\rho_0 \in H^1(\Omega)$ satisfying (4), and $\mathbf{f} \in L^2(0, T; \mathbf{L}^{6/5}(\Omega))$. Suppose that the constants λ , μ , m , and M satisfy (5). Then there exists at least a weak solution of (1)-(3) in $(0, T)$.

Proof (Outline of proof). The proof is divided into the following steps:

a) Pointwise estimates for the density. From the maximum principle applied to the density equation (1)_c and hypothesis (4), one gets

$$0 < m \leq \rho(\mathbf{x}, t) \leq M \quad \text{in} \quad Q.$$

b) Weak estimates for the velocity. Adding the momentum system (1)_a by \mathbf{u} to the density equation (1)_c by $\frac{1}{2}\mathbf{u} \cdot \mathbf{u}$, one arrives at the following energy equality:

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{u}|^2 dx + \mu \|\mathbf{u}\|^2 = \lambda \int_{\Omega} \rho (\nabla \mathbf{u})^t : \nabla \mathbf{u} dx + (\rho \mathbf{f}, \mathbf{u}). \quad (14)$$

The first term on the right-hand side of (14) can be rewritten as

$$\int_{\Omega} \rho (\nabla \mathbf{u})^t : \nabla \mathbf{u} dx = \int_{\Omega} \left(\rho - \frac{M+m}{2} \right) (\nabla \mathbf{u})^t : \nabla \mathbf{u} dx \leq \lambda \frac{M-m}{2} \|\mathbf{u}\|^2,$$

where we have used the pointwise inequality $|\rho - (M+m)/2| \leq (M-m)/2$ (obtained from $m \leq \rho \leq M$). By imposing the constraint on the coefficients (5), one arrives at the estimate

$$\max_{0 \leq t \leq T} |\mathbf{u}(t)|^2 + \int_0^T \|\mathbf{u}(t)\|^2 dt \leq C.$$

c) Strong estimates for the density. By multiplying the density equation (1)_c by $-\Delta \rho$ and bounding the convective term (previously integrated by parts) thanks to the interpolation inequality

$$\|\nabla \rho\|_{L^4(\Omega)} \leq C \|\rho\|_{\infty}^{1/2} |\Delta \rho|^{1/2} \leq C |\Delta \rho|^{1/2}, \quad (15)$$

as

$$\int_{\Omega} \mathbf{u} \cdot \nabla \rho \Delta \rho \leq C \int_{\Omega} |\nabla \mathbf{u}| |\nabla \rho|^2 \leq C \|\nabla \mathbf{u}\| \|\nabla \rho\|_{L^4}^2 \leq C \|\nabla \mathbf{u}\| |\Delta \rho|,$$

the following estimate holds:

$$\max_{0 \leq t \leq T} |\nabla \rho(t)|^2 + \int_0^T |\Delta \rho(t)|^2 dt \leq C \lambda.$$

d) Compactness for the velocity. By using a rather technical argument [1], one can get the following estimate of the “time fractional derivative”:

$$\int_0^{T-\delta} |\mathbf{u}(t+\delta) - \mathbf{u}(t)|^2 dt \leq C_\lambda \delta^{1/2} \quad \forall \delta \in (0, T),$$

which implies [18] compactness for the velocity \mathbf{u} in $L^2(0, T; \mathbf{L}^2(\Omega))$.

From here, it is rather standard to obtain the existence of weak solutions, by using, for instance, the *semi-Galerkin* method [1]. \square

3 Weak and pointwise estimates

Since (6), (7), and (8)-(9) can be reduced to three independent algebraic linear systems, it suffices to check the uniqueness of the solution to guarantee that these problems are well-posed. In particular, the uniqueness will be a consequence of the weak and pointwise estimates that we will obtain in this section.

3.1 Hypotheses

Throughout this work we will assume the following hypotheses:

(H0) Hypotheses for the data: Assume (5), and let $\widetilde{M} > M$ and $0 < \widetilde{m} < m$ such that $\lambda \frac{\widetilde{M} - \widetilde{m}}{2} < \mu$ and $\mathbf{u}_0 \in \mathbf{V}$, $\rho_0 \in H^1(\Omega)$, with $0 < m \leq \rho_0 \leq M$ in Ω , and $\mathbf{f} \in L^2(0, T; \mathbf{L}^{6/5}(\Omega))$.

(H1) Assume that Ω is an open, bounded set of \mathbb{R}^3 whose boundary is polyhedral and such that the continuous dependencies in the H^2 -norm of the *Poisson-Neumann* problem and in the $\mathbf{H}^2 \times H^1$ -norm of the *Stokes* hold (see (33) and (21), respectively). This is verified, for example, if Ω is convex [9].

(H2) The triangulation of Ω and the discrete spaces verify:

- the inverse inequalities:

$$\begin{aligned} |\nabla \bar{\rho}_h| &\leq C h^{-1} |\bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h, \\ \|\nabla \bar{\rho}_h\|_{L^3(\Omega)} &\leq C h^{-1/2} |\bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h, \\ \|\bar{\rho}_h\|_{L^\infty(\Omega)} &\leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)} \quad \forall \bar{\rho}_h \in W_h. \end{aligned}$$

- and the interpolation errors:

$$\|\bar{\mathbf{u}} - \widetilde{J}_h \bar{\mathbf{u}}\|_{H^1(\Omega)} + \|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{H^1(\Omega)} \leq C h \|\bar{\mathbf{u}}\|_{H^2(\Omega)} \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$|\bar{p} - \tilde{K}_h \bar{p}| + |\bar{p} - K_h \bar{p}| \leq C h \|\bar{p}\|_{H^1(\Omega)} \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\|\bar{\rho} - I_h \bar{\rho}\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{1/2} \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),$$

$$|\bar{\rho} - I_h \bar{\rho}| + h \|\bar{\rho} - I_h \bar{\rho}\|_{H^1(\Omega)} \leq C h^2 \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),$$

where $J_h, \tilde{J}_h, K_h, \tilde{K}_h,$ and I_h are interpolation operators from $\mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ into $\mathbf{V}_h, \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ into $\tilde{\mathbf{V}}_h, H^1(\Omega) \cap L_0^2(\Omega)$ into $M_h, H^1(\Omega) \cap L_0^2(\Omega)$ into $\tilde{M}_h,$ and $H^2(\Omega)$ into $W_h,$ respectively. Here and in what follows, we denote by $|v|_{H^k(\Omega)} = \sum_{|\alpha|=k} |D^\alpha v|$ the standard seminorm of higher order derivatives.

(H3) Inf-sup conditions. There exist $\beta > 0$ and $\tilde{\beta} > 0$ (independent of h) such that, $\forall \bar{p}_h \in M_h$ and $\forall \bar{q}_h \in \tilde{M}_h,$

$$\|\bar{p}_h\|_{L_0^2(\Omega)} \leq \beta \sup_{\bar{\mathbf{u}}_h \in \mathbf{V}_h \setminus \{0\}} \frac{(\bar{p}_h, \nabla \cdot \bar{\mathbf{u}}_h)}{\|\bar{\mathbf{u}}_h\|},$$

$$\|\bar{q}_h\|_{L_0^2(\Omega)} \leq \tilde{\beta} \sup_{\bar{\mathbf{w}}_h \in \tilde{\mathbf{V}}_h \setminus \{0\}} \frac{(\bar{q}_h, \nabla \cdot \bar{\mathbf{w}}_h)}{\|\bar{\mathbf{w}}_h\|}.$$

(H4) Compatibility condition between \tilde{M}_h and W_h :

$$(W_h \cdot W_h) \cap L_0^2(\Omega) \subset \tilde{M}_h,$$

that is,

$$\forall \bar{\rho}_h^1, \bar{\rho}_h^2 \in W_h, \quad \bar{\rho}_h^1 \bar{\rho}_h^2 - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h^1(\mathbf{x}) \bar{\rho}_h^2(\mathbf{x}) d\mathbf{x} \in \tilde{M}_h.$$

(H5) Compatibility condition between (M_h, \tilde{M}_h) :

$$M_h \subset \tilde{M}_h.$$

For instance, a way of defining the discrete spaces $(W_h, \mathbf{V}_h, M_h, \tilde{\mathbf{V}}_h, \tilde{M}_h)$ verifying (H2)-(H5) is the following: Let $\{\mathcal{T}_h\}_{h>0}$ be a regular, quasi-uniform family of triangulations of $\Omega,$ with $h = \max_{K \in \mathcal{T}_h} h_K$ ($h_K = \text{diameter of } K$), and

$$X_h^l = \{x_h \in C^0(\bar{\Omega}) \text{ such that } x_h|_K \in \mathbb{P}_l(K) \forall K \in \mathcal{T}_h\}.$$

Then we define $W_h = X_h^1.$ There are several possibilities for (\mathbf{V}_h, M_h) [9], by using the *Taylor-Hood* element $(\mathbb{P}_2 \times \mathbb{P}_1)$ or the minielement $(\mathbb{P}_1 + \text{bubble} \times \mathbb{P}_1),$ for instance. For the spaces $(\tilde{\mathbf{V}}_h, \tilde{M}_h)$ we choose $\tilde{\mathbf{V}}_h = \mathbf{X}_h^3 \cap \mathbf{H}_0^1(\Omega)$ and $\tilde{M}_h = X_h^2 \cap L_0^2(\Omega).$

Note that if $\mathbf{V}_h = \tilde{\mathbf{V}}_h$ and $M_h = \tilde{M}_h$ we need not consider the projection problem (6).

Remark 6 Hypothesis (H5) says us that $(\nabla \cdot \mathbf{w}_h^n, \bar{\rho}_h^1 \bar{\rho}_h^2) = 0$ for all $\bar{\rho}_h^1, \bar{\rho}_h^2 \in W_h$ which will play an important role in our analysis. Indeed, we shall write

$$\begin{aligned} 0 &= \left(\nabla \cdot \mathbf{w}_h^n, \bar{\rho}_h^1, \bar{\rho}_h^2 - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h^1 \bar{\rho}_h^2 \right) = \left(\nabla \cdot \mathbf{w}_h^n, \bar{\rho}_h^1 \bar{\rho}_h^2 \right) - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h^1 \bar{\rho}_h^2 \int_{\Omega} \nabla \cdot \mathbf{w}_h^n \\ &= \left(\nabla \cdot \mathbf{w}_h^n, \bar{\rho}_h^1 \bar{\rho}_h^2 \right), \end{aligned}$$

where we have used $\mathbf{u}_h^n = 0$ on Γ .

As a consequence, by taking $\bar{\rho}_h = 1$ in (7) we have that $\int_{\Omega} \rho_h^n = \int_{\Omega} \rho_h^0$, for each n . This property is the discrete version of the continuous one $\int_{\Omega} \rho(\mathbf{x}, t_1) d\mathbf{x} = \int_{\Omega} \rho(\mathbf{x}, t_2) d\mathbf{x}$ for any $t_1, t_2 \in [0, T]$, whose physical meaning is the conservation of mass.

3.2 Auxiliary truncate scheme

To prove a priori estimates for scheme (6)-(9), we will introduce an auxiliary scheme in which some of the densities appearing in the discrete problem of the momentum system are truncated between \tilde{m} and \tilde{M} as follows:

Initialization: Let \mathbf{u}_h^0 and ρ_h^0 be given as in scheme (6)-(9).

Time step $n + 1$: Given $(\rho_h^n, \mathbf{u}_h^n, p_h^n) \in W_h \times \mathbf{V}_h \times M_h$.

1. find $(\mathbf{w}_h^n, q_h^n) \in \tilde{\mathbf{V}}_h \times \tilde{M}_h$ such that, for each $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \tilde{\mathbf{V}}_h \times \tilde{M}_h$,

$$\begin{cases} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0; \end{cases} \quad (16)$$

2. find $\rho_h^{n+1} \in W_h$ such that, for each $\bar{\rho}_h \in W_h$,

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0; \quad (17)$$

3. find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that, for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$,

$$\begin{cases} \left(\left[\rho_h^n \right]_T \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k} \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + a \left([\rho_h^{n+1}]_T, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{cases} \quad (18)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, q_h \right) = 0. \quad (19)$$

Here the truncation $[\cdot]_T$ is defined as follows: given $w_h \in W_h$, then

$$[w_h]_T(\mathbf{x}) = \begin{cases} w_h(\mathbf{x}) & \text{if } w_h(\mathbf{x}) \in [\tilde{m}, \tilde{M}], \\ \tilde{m} & \text{if } w_h(\mathbf{x}) < \tilde{m}, \\ \tilde{M} & \text{if } w_h(\mathbf{x}) > \tilde{M}. \end{cases}$$

The idea was to truncate in those density terms which required to hold L^∞ estimates or to be positivity in order to obtain weak energy estimates (see the proof of Theorem 5).

We may again deduce that (16), (17), and (18)-(19) are well-posed problems, obtaining a priori estimates.

3.3 Weak estimates for the truncate scheme

Lemma 7 *The discrete solution of scheme (16)-(19) verifies the following estimates:*

$$\begin{aligned} \text{i)} \max_{0 \leq n \leq N} |\mathbf{u}_h^n| \leq C, \quad \text{ii)} k \sum_{n=0}^N \|\mathbf{u}_h^n\|^2 \leq C, \quad \text{iii)} \sum_{n=0}^{N-1} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 \leq C, \\ \text{iv)} \max_{0 \leq n \leq N} |\rho_h^n| \leq C, \quad \text{v)} \lambda k \sum_{n=0}^{N-1} |\nabla \rho_h^{n+1}|^2 \leq C \quad \text{vi)} \sum_{n=0}^{N-1} |\rho_h^{n+1} - \rho_h^n|^2 \leq C, \end{aligned}$$

where $C > 0$ depends on the data $(\rho_0, \mathbf{u}_0, \mathbf{f})$, but is independent of k, h , and λ .

Proof. To obtain a priori estimates for the velocity (\mathbf{u}_h^n) , we take $\bar{\mathbf{u}}_h = 2k\mathbf{u}_h^{n+1}$ and $\bar{q}_h = p_h^{n+1}$ as test functions in (18)-(19), resulting in [12]:

$$\begin{aligned} & |\sqrt{[\rho_h^{n+1}]_T} \mathbf{u}_h^{n+1}|^2 - |\sqrt{[\rho_h^n]_T} \mathbf{u}_h^n|^2 + |\sqrt{[\rho_h^n]_T} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 + \mu_1 k \|\mathbf{u}_h^{n+1}\|^2 \\ & \leq 2k \left([\rho_h^{n+1}]_T \mathbf{f}^{n+1}, \mathbf{u}_h^{n+1} \right) \leq 2k \|[\rho_h^{n+1}]_T\|_{L^\infty(\Omega)} \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)} \|\mathbf{u}_h^{n+1}\|_{L^6(\Omega)} \\ & \leq \frac{\mu_1 k}{2} \|\mathbf{u}_h^{n+1}\|^2 + C k \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2. \end{aligned}$$

Consequently,

$$\begin{aligned} & |\sqrt{[\rho_h^{n+1}]_T} \mathbf{u}_h^{n+1}|^2 - |\sqrt{[\rho_h^n]_T} \mathbf{u}_h^n|^2 + |\sqrt{[\rho_h^n]_T} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 \\ & + \frac{\mu_1}{2} k \|\mathbf{u}_h^{n+1}\|^2 \leq C k \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2. \end{aligned} \tag{20}$$

By adding (20) for $n = 0, \dots, r$ with any $r < N$, estimates **i)**, **ii)**, and **iii)** hold.

On the other hand, to obtain weak energy estimates for the density (ρ_h^n) , we take $\bar{\rho}_h = 2k\rho_h^{n+1}$ in (17) and use the fact that $(\nabla \cdot \mathbf{w}_h^n, (\rho_h^{n+1})^2) = 0$ thanks to Remark 6:

$$|\rho_h^{n+1}|^2 - |\rho_h^n|^2 + |\rho_h^{n+1} - \rho_h^n|^2 + 2\lambda k |\nabla \rho_h^{n+1}|^2 = 0.$$

By adding over n , one deduces estimates **iv)**, **v)** and **vi)**. □

Corollary 8 *The following estimates hold:*

$$\text{vii)} \max_{0 \leq n \leq N} |\mathbf{w}_h^n| \leq C, \quad \text{viii)} k \sum_{n=0}^N \|\mathbf{w}_h^n\|^2 \leq C,$$

where $C > 0$ is independent of k, h , and λ .

Proof. By taking $\bar{w}_h = \mathbf{w}_h^n$ in (6) and using (H5), $(\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n), \nabla \mathbf{w}_h^n) = 0$ and hence one has $|\nabla \mathbf{w}_h^n| \leq |\nabla \mathbf{u}_h^n|$. So from **ii)** we get **viii)**. Now we are going to get estimate **vii)** using a duality technique and the constraint (S). Indeed, let $(\mathbf{z}, \xi) \in (\mathbf{V} \cap \mathbf{H}^2(\Omega)) \times (L_0^2(\Omega) \cap H^1(\Omega))$ be the strong solution of the Stokes problem

$$-\Delta \mathbf{z} + \nabla \xi = \mathbf{w}_h^n - \mathbf{u}_h^n, \quad \nabla \cdot \mathbf{z} = 0 \text{ in } \Omega, \quad \mathbf{z} = 0 \text{ on } \Gamma. \quad (21)$$

By taking $\mathbf{w}_h^n - \mathbf{u}_h^n$ as a test function in the variational formulation of (21), we get

$$|\mathbf{w}_h^n - \mathbf{u}_h^n|^2 = \left(\nabla \mathbf{z}, \nabla(\mathbf{w}_h^n - \mathbf{u}_h^n) \right) + \left(\xi, \nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n) \right). \quad (22)$$

Let $(\mathbf{z}_h, \xi_h) \in \widetilde{V}_h \times \widetilde{M}_h$ be the discrete approximation of (21) defined as

$$\begin{cases} \left(\nabla \mathbf{z}_h, \nabla \bar{w}_h \right) - \left(\xi_h, \nabla \cdot \bar{w}_h \right) = \left(\mathbf{w}_h^n - \mathbf{u}_h^n, \bar{w}_h \right), & \forall \bar{w}_h \in \widetilde{V}_h, \\ \left(\nabla \cdot \mathbf{z}_h, \bar{q}_h \right) = 0, & \forall \bar{q}_h \in \widetilde{M}_h. \end{cases}$$

In view of hypothesis (H5), $(K_h \xi, \nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n)) = 0$, and hence we write (22) as follows:

$$|\mathbf{w}_h^n - \mathbf{u}_h^n|^2 = \left(\nabla \mathbf{z} - \nabla \mathbf{z}_h, \nabla(\mathbf{w}_h^n - \mathbf{u}_h^n) \right) + \left(\nabla \mathbf{z}_h, \nabla(\mathbf{w}_h^n - \mathbf{u}_h^n) \right) + \left(\xi - K_h \xi, \nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n) \right),$$

where K_h is the interpolation operator defined in hypothesis (H2). From (6), it follows that $(\nabla \mathbf{z}_h, \nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)) = 0$. Thus, we find

$$\begin{aligned} |\mathbf{w}_h^n - \mathbf{u}_h^n|^2 &\leq |\nabla \mathbf{z} - \nabla \mathbf{z}_h| |\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)| + |\xi - K_h \xi| |\nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n)| \\ &\leq Ch \left(\|\mathbf{z}\|_{H^2(\Omega)} + \|\xi\|_{H^1(\Omega)} \right) |\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)| \leq Ch |\mathbf{w}_h^n - \mathbf{u}_h^n| |\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)|, \end{aligned}$$

where in the second line we have used the approximation property (see [9]) $|\nabla \mathbf{z} - \nabla \mathbf{z}_h| \leq Ch(\|\mathbf{z}\|_{H^2} + \|\xi\|_{H^1})$, the interpolation error $|\xi - K_h \xi| \leq Ch\|\xi\|_{H^1(\Omega)}$ assumed in (H2), and the $H^2 \times H^1$ continuous dependency of the Stokes problem (21) $\|\mathbf{z}\|_{H^2(\Omega)} + \|\xi\|_{H^1(\Omega)} \leq C|\mathbf{w}_h^n - \mathbf{u}_h^n|$ assumed in (H1).

Therefore, we have

$$|\mathbf{w}_h^n - \mathbf{u}_h^n| \leq Ch |\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)|. \quad (23)$$

Now, in view of (S), we may get $h \leq Ck$ for (h, k) small enough. Then, since $k^{1/2} |\nabla \mathbf{w}_h^n| \leq k^{1/2} |\nabla \mathbf{u}_h^n| \leq C$ (thanks to the estimate $|\nabla \mathbf{w}_h^n| \leq |\nabla \mathbf{u}_h^n|$ and estimate **ii)** of Lemma 7), it is easy to see that $|\mathbf{w}_h^n| \leq Ck^{1/2} + |\mathbf{u}_h^n| \leq C$, and we get estimate **vii)**. \square

3.4 Discrete maximum principle (of the truncate scheme)

In this subsection we prove that the discrete density of scheme (17) has pointwise estimates by excess and defect with respect to the upper and lower bounds of the initial density ρ_0 , respectively. Namely, we will see that $\tilde{m} \leq \rho_h^n \leq \widetilde{M}$ in Ω for all k and h small enough and satisfying constraint (S).

3.4.1 Study of an auxiliary time discrete scheme

We define a sequence (ρ^n) associated to (\mathbf{w}_h^n) by means of the following time discrete scheme:

Initialization: Let $\rho^0 = \rho_0$.

Time step $n + 1$: Given ρ^n , we compute $\rho^{n+1} \in H^2(\Omega)$, verifying the elliptic problem

$$\begin{cases} \frac{\rho^{n+1} - \rho^n}{k} + \mathbf{w}_h^n \cdot \nabla \rho^{n+1} - \lambda \Delta \rho^{n+1} = 0 & \text{in } \Omega, \\ \frac{\partial \rho^{n+1}}{\partial \mathbf{n}} = 0 & \text{on } \Gamma. \end{cases} \quad (24)$$

Lemma 9 *Let $\{\mathbf{w}_h^n\}_{n=0}^N \subset \mathbf{H}_0^1(\Omega)$ such that $k \sum_{n=0}^N \|\mathbf{w}_h^n\|^2 \leq C$. Then there exists a unique solution $\rho^{n+1} \in H^2(\Omega)$ of (24), which also verifies:*

$$\begin{aligned} 0 < m \leq \rho^{n+1}(\mathbf{x}) \leq M, \quad \forall \mathbf{x} \in \Omega \quad \forall n = 0, \dots, N-1, \\ \lambda^2 k \sum_{n=0}^{N-1} \|\rho^{n+1}\|_{H^2(\Omega)}^2 \leq C, \end{aligned} \quad (25)$$

where $C > 0$ is a constant independent of k, h , and λ .

Proof. The proof of this lemma can be found in Appendix A. □

3.4.2 Error estimates between ρ^{n+1} and ρ_h^{n+1}

Denote by $e_\rho^{n+1} = \rho^{n+1} - \rho_h^{n+1}$ the difference between the solutions of problems (24) and (17).

Our intention now is to state the following error estimate:

$$\|e_\rho^{n+1}\|_{H^1(\Omega)} \leq C \left(\frac{h^2}{\lambda \sqrt{\lambda} k} + \frac{h \sqrt{h}}{\lambda^2 k} + \frac{h h^{1/4}}{\lambda^{3/2} k^{3/4}} + \frac{h}{\lambda \sqrt{k}} \right). \quad (26)$$

Indeed, by subtracting (24) multiplied by $\bar{\rho}_h \in W_h$ and (17), one has

$$\left(\frac{e_\rho^{n+1} - e_\rho^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla e_\rho^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla e_\rho^{n+1}, \nabla \bar{\rho}_h \right) = 0$$

for each $\bar{\rho}_h \in W_h$. By decomposing the convective term as

$$\left(\mathbf{w}_h^n \cdot \nabla e_\rho^{n+1}, \bar{\rho}_h \right) = \left(\mathbf{w}_h^n \cdot \nabla (\rho^{n+1} - I_h \rho^{n+1}), \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla (I_h \rho^{n+1} - \rho_h^{n+1}), \bar{\rho}_h \right),$$

taking $\bar{\rho}_h = 2k(e_\rho^{n+1} - \rho^{n+1} + I_h \rho^{n+1}) = 2k(I_h \rho^{n+1} - \rho_h^{n+1})$, with $I_h \rho^{n+1} \in W_h$, and using the fact that $(\nabla \cdot \mathbf{w}_h^n, \bar{\rho}_h^2) = 0$ for all $\bar{\rho}_h \in W_h$ (see Remark 6), we get

$$\begin{aligned} & |e_\rho^{n+1}|^2 - |e_\rho^n|^2 + |e_\rho^{n+1} - e_\rho^n|^2 + 2\lambda k |\nabla e_\rho^{n+1}|^2 \\ & \leq 2 \left(e_\rho^{n+1} - e_\rho^n, \rho^{n+1} - I_h \rho^{n+1} \right) - 2k \left(\mathbf{w}_h^n \cdot \nabla (\rho^{n+1} - I_h \rho^{n+1}), e_\rho^{n+1} \right) \\ & \quad - k \left(\nabla \cdot \mathbf{w}_h^n, (\rho^{n+1} - I_h \rho^{n+1})^2 \right) + 2\lambda k \left(\nabla e_\rho^{n+1}, \nabla (\rho^{n+1} - I_h \rho^{n+1}) \right). \end{aligned}$$

Next, by integrating by parts the second term on the right-hand side and bounding adequately, we infer that

$$\begin{aligned}
& |e_\rho^{n+1}|^2 - |e_\rho^n|^2 + |e_\rho^{n+1} - e_\rho^n|^2 + 2\lambda k |\nabla e_\rho^{n+1}|^2 \\
& \leq 2|e_\rho^{n+1} - e_\rho^n| |\rho^{n+1} - I_h \rho^{n+1}| + Ck \|\mathbf{w}_h^n\| \|e_\rho^{n+1}\|_{H^1(\Omega)} \|\rho^{n+1} - I_h \rho^{n+1}\|_{L^3(\Omega)} \\
& + k \|\mathbf{w}_h^n\| \|\rho^{n+1} - I_h \rho^{n+1}\|_{L^4(\Omega)}^2 + 2\lambda k |\nabla e_\rho^{n+1}| |\nabla(\rho^{n+1} - I_h \rho^{n+1})| \\
& \leq \frac{1}{2} |e_\rho^{n+1} - e_\rho^n|^2 + C |\rho^{n+1} - I_h \rho^{n+1}|^2 + C\lambda k |\nabla(\rho^{n+1} - I_h \rho^{n+1})|^2 \\
& + \frac{C}{\lambda} k \|\mathbf{w}_h^n\|^2 \|\rho^{n+1} - I_h \rho^{n+1}\|_{L^3(\Omega)}^2 + k \|\mathbf{w}_h^n\| \|\rho^{n+1} - I_h \rho^{n+1}\|_{L^4(\Omega)}^2 + \lambda k |e_\rho^{n+1}|^2 + \lambda k |\nabla e_\rho^{n+1}|^2,
\end{aligned}$$

and then, by taking into account the interpolation errors:

$$|\rho^{n+1} - I_h \rho^{n+1}| + h |\nabla(\rho^{n+1} - I_h \rho^{n+1})| \leq C h^2 \|\rho^{n+1}\|_{H^2(\Omega)},$$

and

$$\begin{aligned}
\|\rho^{n+1} - I_h \rho^{n+1}\|_{L^3(\Omega)} & \leq C h^{3/2} \|\rho^{n+1}\|_{H^2(\Omega)}, \\
\|\rho^{n+1} - I_h \rho^{n+1}\|_{L^4(\Omega)} & \leq C h^{5/4} \|\rho^{n+1}\|_{H^2(\Omega)}
\end{aligned}$$

(the last two are a consequence of the previous one and the 3D interpolation inequalities $\|\rho\|_{L^3(\Omega)} \leq C |\rho|^{1/2} \|\rho\|_{H^1(\Omega)}^{1/2}$ and $\|\rho\|_{L^4(\Omega)} \leq C |\rho|^{1/4} \|\rho\|_{H^1(\Omega)}^{3/4}$), and the estimate $k \|\mathbf{w}_h^n\|^2 \leq C$ thanks to estimate *vii*) of Corollary 8, one arrives at

$$|e_\rho^{n+1}|^2 - |e_\rho^n|^2 + \lambda k |\nabla e_\rho^{n+1}|^2 \leq C \left(h^4 + \frac{h^3}{\lambda} + k^{1/2} h^{5/2} + \lambda k h^2 \right) \|\rho^{n+1}\|_{H^2(\Omega)}^2 + \lambda k |e_\rho^{n+1}|^2.$$

By adding up for $n = 0, \dots, l$ and using the fact that $\lambda^2 k \sum_{n=0}^l \|\rho^{n+1}\|_{H^2}^2 \leq C$ and by virtue of the generalized discrete Gronwall lemma, we infer that for all (k, λ) , with $\lambda k < 1$ (for instance, $\lambda k \leq 1/2$), there exists $C > 0$ independent of λ such that

$$|e_\rho^{l+1}|^2 + \lambda k \sum_{n=0}^l |\nabla e_\rho^{n+1}|^2 \leq C \left(\frac{h^4}{\lambda^2 k} + \frac{h^3}{\lambda^3 k} + \frac{h^{5/2}}{\lambda^2 k^{1/2}} + \frac{h^2}{\lambda} + |e_\rho^0|^2 \right).$$

By taking $|e_\rho^0|^2 = |\rho^0 - \rho_h^0|^2 \leq C h^2$, we deduce the bound

$$|e_\rho^{n+1}|^2 + \lambda k \sum_{n=0}^l |\nabla e_\rho^{n+1}|^2 \leq C \left(\frac{h^4}{\lambda^2 k} + \frac{h^3}{\lambda^3 k} + \frac{h^{5/2}}{\lambda^2 k^{1/2}} + \frac{h^2}{\lambda} \right),$$

whence, in particular, (26) holds.

3.4.3 Pointwise estimates of the truncate scheme

Here we will prove the following pointwise estimates [7]:

$$m-C h^{-1/2} \left(\frac{h^2}{\lambda^{3/2}k} + \frac{h\sqrt{h}}{\lambda^2k} + \frac{hh^{1/4}}{\lambda^2k^{3/4}} + \frac{h}{\lambda\sqrt{k}} \right) \leq \rho_h^{n+1} \leq M+C h^{-1/2} \left(\frac{h^2}{\lambda^{3/2}k} + \frac{h\sqrt{h}}{\lambda^2k} + \frac{hh^{1/4}}{\lambda^2k^{3/4}} + \frac{h}{\lambda\sqrt{k}} \right). \quad (27)$$

To prove (27) it suffices to prove that

$$\|\rho_h^{n+1} - \rho^{n+1}\|_{L^\infty(\Omega)} \leq C h^{-1/2} \left(\frac{h^2}{\lambda^{3/2}k} + \frac{h\sqrt{h}}{\lambda^2k} + \frac{hh^{1/4}}{\lambda^2k^{3/4}} + \frac{h}{\lambda\sqrt{k}} \right).$$

For this, from the triangle inequality

$$\begin{aligned} \|\rho_h^{n+1} - \rho^{n+1}\|_{L^\infty(\Omega)} &\leq \|\rho_h^{n+1} - I_h\rho^{n+1}\|_{L^\infty(\Omega)} + \|I_h\rho^{n+1} - \rho^{n+1}\|_{L^\infty(\Omega)} \\ &\leq \|\rho_h^{n+1} - I_h\rho^{n+1}\|_{L^\infty(\Omega)} + C \frac{h^{1/2}}{\lambda k^{1/2}}, \end{aligned}$$

where in the last line we have used the approximation inequality $\|\rho^{n+1} - I_h\rho^{n+1}\|_{L^\infty(\Omega)} \leq C h^{1/2} \|\rho^{n+1}\|_{H^2(\Omega)}$ and the estimate $\|\rho^{n+1}\|_{H^2(\Omega)} \leq \frac{C}{\lambda k^{1/2}}$ (see (25)). Hence, it suffices to obtain the inequality

$$\|\rho_h^{n+1} - I_h\rho^{n+1}\|_{H^1(\Omega)} \leq C \left(\frac{h^2}{\lambda^{3/2}k} + \frac{h\sqrt{h}}{\lambda^2k} + \frac{hh^{1/4}}{\lambda^2k^{3/4}} + \frac{h}{\lambda\sqrt{k}} \right) \quad (28)$$

and to use the inverse inequality (see [3])

$$\|\bar{\rho}_h\|_{L^\infty(\Omega)} \leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)}, \quad \forall \bar{\rho}_h \in W_h.$$

Let us prove (28). From the triangle inequality,

$$\|\rho_h^{n+1} - I_h\rho^{n+1}\|_{H^1(\Omega)} \leq \|\rho_h^{n+1} - \rho^{n+1}\|_{H^1(\Omega)} + \|\rho^{n+1} - I_h\rho^{n+1}\|_{H^1(\Omega)},$$

and by using the error estimate (26) and the interpolation error $\|w - I_h w\|_{H^1(\Omega)} \leq h \|w\|_{H^2(\Omega)}$ for $w = \rho^{n+1}$ jointly with the estimate $h \|\rho^{n+1}\|_{H^2} \leq C h / \lambda \sqrt{k}$ (thanks to (25)), one easily deduces (28).

Now, by taking into account hypothesis (S), one has

$$\lim_{(h,k) \rightarrow 0} \frac{\frac{h^2}{k} + \frac{h\sqrt{h}}{k} + \frac{hh^{1/4}}{k^{3/4}}}{\frac{h}{\sqrt{k}}} = 0,$$

and consequently, for each (h, k) small enough,

$$C h^{-1/2} \left(\frac{h^2}{\lambda^{3/2}k} + \frac{h\sqrt{h}}{\lambda^2k} + \frac{h}{\lambda\sqrt{k}} \right) \leq C h^{-1/2} \frac{h}{\sqrt{k}} = C \sqrt{\frac{h}{k}}.$$

In particular, thanks to (27), by imposing $h \leq h_0$, $k \leq k_0$ such that

$$C\sqrt{\frac{h}{k}} \leq \min\{m - \tilde{m}, \tilde{M} - M\}, \quad (29)$$

one gets

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M}.$$

3.4.4 Identification between the truncated and nontruncated schemes

Now it is clear that if ρ_h^{n+1} is the solution of the truncate scheme, then $[\rho_h^{n+1}]_T = \rho_h^{n+1}$, and consequently the truncated scheme and the nontruncated scheme coincide, arriving at the following result.

Theorem 10 *Assume that $h \leq h_0$, $k \leq k_0$ satisfying (29) and $\lambda k \leq 1/2$; then scheme (6)-(9) is well-posed and verifies the weak estimates **i)**-**vi)** of Lemma 7, estimates **vii)**-**viii)** of Corollary 8, and the pointwise estimates*

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M} \quad \text{in } \Omega.$$

4 Strong estimates for the density

Let $-\Delta_h : W_h \rightarrow W_h$ be the linear operator defined as follows:

$$-\left(\Delta_h \rho_h, \bar{\rho}_h\right) = \left(\nabla \rho_h, \nabla \bar{\rho}_h\right) \quad \forall \bar{\rho}_h \in W_h. \quad (30)$$

Then the discrete density equation (7) can be rewritten as

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h\right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h\right) - \lambda \left(\Delta_h \rho_h^{n+1}, \bar{\rho}_h\right) = 0. \quad (31)$$

Theorem 11 *Under the hypotheses of Theorem 10, the solution ρ_h^{n+1} of scheme (7) verifies the following estimates, for h and k small enough:*

$$\mathbf{ix}) \lambda \max_{0 \leq n \leq N} |\nabla \rho_h^n|^2 \leq C, \quad \mathbf{x}) \lambda^2 k \sum_{n=0}^N |\Delta_h \rho_h^{n+1}|^2 \leq C, \quad \mathbf{xi}) \lambda \sum_{n=0}^{N-1} |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 \leq C,$$

where $C > 0$ is independent of h , k , and λ .

Proof. By taking $\bar{\rho}_h = -2k\Delta_h \rho_h^{n+1}$ in (31), we arrive at:

$$|\nabla \rho_h^{n+1}|^2 - |\nabla \rho_h^n|^2 + |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 + 2\lambda k |\Delta_h \rho_h^{n+1}|^2 = 2k \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \Delta_h \rho_h^{n+1}\right) := I. \quad (32)$$

To bound I , we use an idea given in [12], where a regular function associated to the discrete Laplacian function $-\Delta_h \rho_h^{n+1}$ is considered. But here, the type of estimates used in [12] must be

changed, making use of the pointwise estimates of ρ_h^{n+1} . We define $\rho(h) \in H^2(\Omega)$ as the solution of the problem:

$$-\Delta\rho(h) = -\Delta_h\rho_h^{n+1} \quad \text{in } \Omega, \quad \frac{\partial\rho(h)}{\partial\mathbf{n}}\Big|_{\partial\Omega} = 0, \quad \int_{\Omega}\rho(h) = \int_{\Omega}\rho_h^0. \quad (33)$$

From the H^2 -regularity of the previous problem $\|\rho(h) - \frac{1}{|\Omega|} \int \rho_h^0\|_{H^2(\Omega)} \leq C |\Delta_h\rho_h^{n+1}|$, and hence one has in particular

$$|\rho(h)|_{H^2(\Omega)} \leq C |\Delta_h\rho_h^{n+1}|. \quad (34)$$

We write I as $I = 2k\left(\mathbf{w}_h^n \cdot \nabla\rho(h), \Delta\rho(h)\right) + 2k\left(\mathbf{w}_h^n \cdot \nabla(\rho_h^{n+1} - \rho(h)), \Delta_h\rho_h^{n+1}\right)$. By integrating by parts the first term on the right-hand side, and using (15),

$$\begin{aligned} 2k\left(\mathbf{w}_h^n \cdot \nabla\rho(h), \Delta\rho(h)\right) &= -2k\left(\nabla\mathbf{w}_h^n, \nabla\rho(h) \otimes \nabla\rho(h)\right) - 2k\left((\mathbf{w}_h^n \cdot \nabla)\nabla\rho(h), \nabla\rho(h)\right) \\ &= -2k\left(\nabla\mathbf{w}_h^n, \nabla\rho(h) \otimes \nabla\rho(h)\right) + k\left(\nabla \cdot \mathbf{w}_h^n, |\nabla\rho(h)|^2\right) \\ &\leq Ck\|\mathbf{w}_h^n\| \|\nabla\rho(h)\|_{L^4(\Omega)}^2 \leq Ck\|\mathbf{w}_h^n\| \|\rho(h)\|_{L^\infty(\Omega)} |\Delta\rho(h)| \\ &\leq Ck\|\mathbf{w}_h^n\| \|\rho(h)\|_{L^\infty(\Omega)} |\Delta_h\rho_h^{n+1}|, \end{aligned}$$

where $\mathbf{a} \otimes \mathbf{b}$ denotes the tensorial product matrix of two vectors $\mathbf{a} = (a_i)_{i=1}^2$, $\mathbf{b} = (b_i)_{i=1}^2$, with coefficients $(\mathbf{a} \otimes \mathbf{b})_{i,j} = a_i b_j$. Accordingly,

$$I \leq Ck\|\mathbf{w}_h^n\| \left(\|\rho(h)\|_{L^\infty(\Omega)} + \|\nabla(\rho_h^{n+1} - \rho(h))\|_{L^3(\Omega)} \right) |\Delta_h\rho_h^{n+1}|. \quad (35)$$

Now we will prove the inequality:

$$\|\nabla(\rho_h^{n+1} - \rho(h))\|_{L^3(\Omega)} \leq Ch^{1/2} |\rho(h)|_{H^2(\Omega)}. \quad (36)$$

For this, we write

$$\|\nabla(\rho_h^{n+1} - \rho(h))\|_{L^3} \leq \|\nabla(\rho_h^{n+1} - I_h\rho(h))\|_{L^3} + \|\nabla(I_h\rho(h) - \rho(h))\|_{L^3}. \quad (37)$$

By multiplying (33) by $\bar{\rho}_h \in W_h$ and subtracting to (30), one gets

$$\left(\nabla\rho_h^{n+1} - \nabla\rho(h), \nabla\bar{\rho}_h\right) = 0 \quad \forall \bar{\rho}_h \in W_h.$$

By adding and subtracting $\nabla I_h\rho(h)$, and considering $\bar{\rho}_h = \rho_h^{n+1} - I_h\rho(h) \in W_h$, we obtain

$$\begin{aligned} |\nabla\rho_h^{n+1} - \nabla I_h\rho(h)|^2 &= -\left(\nabla I_h\rho(h) - \nabla\rho(h), \nabla\rho_h^{n+1} - \nabla I_h\rho(h)\right) \\ &\leq |\nabla I_h\rho(h) - \nabla\rho(h)| |\nabla\rho_h^{n+1} - \nabla I_h\rho(h)|, \end{aligned}$$

whence

$$|\nabla\rho_h^{n+1} - \nabla I_h\rho(h)| \leq |\nabla I_h\rho(h) - \nabla\rho(h)| \leq Ch |\rho(h)|_{H^2(\Omega)}, \quad (38)$$

$$|\nabla\rho_h^{n+1} - \nabla\rho(h)| \leq Ch |\rho(h)|_{H^2(\Omega)}. \quad (39)$$

Thus, by using the inverse inequality [8]

$$\|\nabla \rho_h^{n+1} - \nabla I_h \rho(h)\|_{L^3(\Omega)} \leq C h^{-1/2} |\nabla \rho_h^{n+1} - \nabla I_h \rho(h)|$$

and (38), we arrive at

$$\|\nabla \rho_h^{n+1} - \nabla I_h \rho(h)\|_{L^3(\Omega)} \leq C h^{1/2} |\rho(h)|_{H^2(\Omega)}. \quad (40)$$

So, from (37) and (40) one gets (36) by taking into account the interpolation error $\|\nabla(\rho(h) - I_h \rho(h))\|_{L^3(\Omega)} \leq C h^{1/2} |\rho(h)|_{H^2(\Omega)}$.

By getting back to (35) and using (36), we bound

$$I \leq C k \|\mathbf{w}_h^n\| \left(\|\rho(h) - \rho_h^{n+1}\|_{L^\infty} + \|\rho_h^{n+1}\|_{L^\infty} + h^{1/2} |\rho(h)|_{H^2} \right) |\Delta_h \rho_h^{n+1}|. \quad (41)$$

Now we write

$$\|\rho_h^{n+1} - \rho(h)\|_{L^\infty(\Omega)} \leq \|\rho_h^{n+1} - I_h \rho(h)\|_{L^\infty(\Omega)} + \|I_h \rho(h) - \rho(h)\|_{L^\infty(\Omega)}.$$

By using the interpolation error $\|\rho(h) - I_h \rho(h)\|_{L^\infty(\Omega)} \leq C h^{1/2} |\rho(h)|_{H^2(\Omega)}$, the inverse inequality in 3D

$$\begin{aligned} \|\rho_h^{n+1} - I_h \rho(h)\|_{L^\infty(\Omega)} &\leq C h^{-1/2} \|\rho_h^{n+1} - I_h \rho(h)\|_{H^1(\Omega)} \\ &\leq C h^{-1/2} (\|\rho_h^{n+1} - \rho(h)\|_{H^1(\Omega)} + \|\rho(h) - I_h \rho(h)\|_{H^1(\Omega)}) \\ &\leq C h^{-1/2} (|\nabla(\rho_h^{n+1} - \rho(h))| + h |\rho(h)|_{H^2(\Omega)}), \end{aligned}$$

where the generalized Poincare inequality has been used in the last line, since $\int_\Omega \rho_h^{n+1} = \int_\Omega \rho_h^0$ (see Remark 6) and $\int_\Omega \rho_h^0 = \int_\Omega \rho(h)$ (see (33)). By using (39) and (34),

$$\|\rho_h^{n+1} - \rho(h)\|_{L^\infty(\Omega)} \leq C h^{1/2} |\rho(h)|_{H^2(\Omega)} \leq C h^{1/2} |\Delta_h \rho_h^{n+1}|.$$

By applying the above estimate in (41), we bound

$$\begin{aligned} I &\leq C k \|\mathbf{w}_h^n\| \left(h^{1/2} |\Delta_h \rho_h^{n+1}| + \widetilde{M} \right) |\Delta_h \rho_h^{n+1}| \\ &\leq C k \|\mathbf{w}_h^n\| h^{1/2} |\Delta_h \rho_h^{n+1}|^2 + \frac{C}{\lambda} k \|\mathbf{w}_h^n\|^2 + \frac{\lambda}{2} k |\Delta_h \rho_h^{n+1}|^2. \end{aligned}$$

By Corollary 8 we infer the bound $\|\mathbf{w}_h^n\| \leq C/k^{1/2}$ (with C independent of λ, h, k), and by choosing h and k small enough such that

$$C \sqrt{\frac{h}{k}} \leq \frac{1}{2} \lambda,$$

we get

$$I \leq \frac{C}{\lambda} k \|\mathbf{w}_h^n\|^2 + \lambda k |\Delta_h \rho_h^{n+1}|^2.$$

Therefore, from (32) we get the inequality

$$|\nabla \rho_h^{n+1}|^2 - |\nabla \rho_h^n|^2 + |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 + \lambda k |\Delta_h \rho_h^{n+1}|^2 \leq C \frac{k}{\lambda} \|\mathbf{w}_h^n\|^2. \quad (42)$$

By adding (42) for $n = 0, \dots, r$, with $r < N$, we arrive at

$$\lambda |\nabla \rho_h^{r+1}|^2 + \lambda \sum_{n=0}^r |\nabla(\rho_h^{n+1} - \rho_h^n)|^2 + \lambda^2 k \sum_{n=0}^r |\Delta_h \rho_h^{n+1}|^2 \leq C k \sum_{n=0}^r \|\mathbf{w}_h^n\|^2 + \lambda |\nabla \rho_h^0|^2$$

Finally, from estimate **ii)** of Lemma 7, one gets the desired estimates **ix)-xi)**. \square

Corollary 12 *The following inequality holds:*

$$\|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq C |\nabla \rho_h^{n+1}|^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2}. \quad (43)$$

Consequently, under the hypotheses of Theorem 11, one has the estimate

$$\lambda^3 k \sum_{n=0}^{N-1} \|\rho_h^{n+1}\|_{W^{1,3}(\Omega)}^4 \leq C,$$

where $C > 0$ is independent of h, k , and λ .

Proof. Thanks to estimates **ix)** for (ρ_h^n) and **x)** for $(\Delta_h \rho_h^n)$, it suffices to prove (43). For this, by considering $\rho(h)$ the solution of problem (33), we have

$$\|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq \|\nabla(\rho_h^{n+1} - \rho(h))\|_{L^3(\Omega)} + \|\nabla \rho(h)\|_{L^3(\Omega)}.$$

By using inequality (36) and the interpolation inequality $\|\nabla \rho(h)\|_{L^3(\Omega)} \leq C |\nabla \rho(h)|^{1/2} \|\rho(h)\|_{H^2(\Omega)}^{1/2}$, we arrive at

$$\|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq C h^{1/2} |\Delta_h \rho_h^{n+1}| + C |\nabla \rho(h)|^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2}.$$

Next, we bound the term $|\nabla \rho(h)|$ by using (38) as follows:

$$|\nabla \rho(h)| \leq |\nabla(\rho(h) - \rho_h^{n+1})| + |\nabla \rho_h^{n+1}| \leq C h |\Delta_h \rho_h^{n+1}| + |\nabla \rho_h^{n+1}|.$$

Therefore, using (34)

$$\|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq C h^{1/2} |\Delta_h \rho_h^{n+1}| + C |\nabla \rho_h^{n+1}|^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2}.$$

On the other hand, by considering $\bar{\rho}_h = -\Delta_h \rho_h^{n+1}$ in (30), we get

$$|\Delta_h \rho_h^{n+1}|^2 \leq |\nabla \rho_h^{n+1}| |\nabla \Delta_h \rho_h^{n+1}| \leq \frac{C}{h} |\nabla \rho_h^{n+1}| |\Delta_h \rho_h^{n+1}|,$$

where we have used the inverse inequality between L^2 and H^1 . The last two estimates imply (43). \square

5 Weak convergence

To study the convergence of scheme (7)-(9) towards a solution of (1)-(3), we define the following functions.

Definition 13 *One defines $\mathbf{u}_{h,k}$ (respectively, $\widehat{\mathbf{u}}_{h,k}$, $\widehat{\mathbf{w}}_{h,k}$, and $p_{h,k}$) as the piecewise constant functions taking values \mathbf{u}_h^{n+1} on $(t_n, t_{n+1}]$ (respectively \mathbf{u}_h^n , \mathbf{w}_h^n , and p_h^{n+1}). Analogously, we define $\rho_{h,k}$ and $\widehat{\rho}_{h,k}$. Moreover, one defines $\widetilde{\rho}_{h,k} \in C^0([0, T]; \mathbf{V}_h)$ as the piecewise linear functions such that $\widetilde{\rho}_{h,k}(t_n) = \rho_h^n$.*

Now let us pass to the limit in both (9) and (16)₂. Consider $q \in C^0([0, T]; C^\infty(\Omega))$ such that $\int_{\Omega} q(\mathbf{x}) d\mathbf{x} = 0$, $q_h^n = K_h q(t_n) \in M_h$, and $\bar{q}_h^n = \widetilde{K}_h(t_n) \in \widetilde{M}_h$. Define $q_{h,k}$ and $\bar{q}_{h,k}$ as $p_{h,k}$ in Definition 13. On the other hand, we know that there exist two limit functions \mathbf{w} and \mathbf{u} belonging to $\mathbf{H}_0^1(\Omega)$ such that $\mathbf{u}_{h,k} \rightarrow \mathbf{u}$ and $\mathbf{w}_{h,k} \rightarrow \mathbf{w}$ weakly in $L^2(0, T; \mathbf{H}_0^1(\Omega))$ as $(h, k) \rightarrow 0$. Thus, we write from (9)

$$0 = \sum_{n=0}^{N-1} \left(\nabla \cdot \mathbf{u}_h^n, q_h^n \right) = \int_{\Omega} \left(\nabla \cdot \mathbf{u}_{h,k}, q_{h,k} \right) d\mathbf{x} \rightarrow \int_{\Omega} \left(\nabla \cdot \mathbf{u}, q \right) d\mathbf{x} = 0$$

for all $q \in C^0([0, T]; C^\infty(\Omega))$, with $\int_{\Omega} q(\mathbf{x}) d\mathbf{x} = 0$. A density argument says us that we can replace the space $C^\infty(Q)$ with $\int_{\Omega} q(\mathbf{x}) d\mathbf{x} = 0$ by the less regular space $L_0^2(\Omega)$. Therefore, we have that $\mathbf{u} \in \mathbf{V}$. In an analogous way, we can prove that $\mathbf{w} \in \mathbf{V}$ as well.

Next, we wish to derive a test function for (6), a discrete zero-divergence approximation of a function $\mathbf{v} \in \mathbf{C}_c^\infty(\Omega)$, with $\nabla \cdot \mathbf{v} = 0$.

Lemma 14 *Let $\bar{\mathbf{w}} \in \mathbf{C}_c^\infty(\Omega)$. Then there exists $\bar{\mathbf{w}}_h \in \widetilde{\mathbf{V}}_h$ such that:*

$$\bar{\mathbf{w}}_h \rightarrow \bar{\mathbf{w}} \text{ in } \mathbf{H}_0^1(\Omega) \quad \text{and} \quad \left(\nabla \cdot \bar{\mathbf{w}}_h, \bar{q}_h \right) = \left(\nabla \cdot \bar{\mathbf{w}}, \bar{q}_h \right) \quad \forall \bar{q}_h \in \widetilde{M}_h.$$

A proof of this result can be found in [12].

Then, thanks to the estimates of Lemma 7, Corollary 8, Theorem 11 and Corollary 12, it is easy to deduce the following result.

Lemma 15 *Under the hypotheses of Theorem 11, the following estimates (independent of h and k , but some of them depend on λ) hold:*

$$\begin{aligned} \{\mathbf{u}_{h,k}\}_{h,k}, \{\widehat{\mathbf{u}}_{h,k}\}_{h,k}, \{\widehat{\mathbf{w}}_{h,k}\}_{h,k} & \text{ are bounded in } L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)), \\ \{\widetilde{\rho}_{h,k}\}_{h,k}, \{\rho_{h,k}\}_{h,k}, \{\widehat{\rho}_{h,k}\}_{h,k} & \text{ are bounded in } L^\infty(0, T; H^1(\Omega)) \cap L^\infty(Q), \\ \{\rho_{h,k}\}_{h,k} & \text{ is bounded in } L^4(0, T; W^{1,3}(\Omega)). \end{aligned}$$

In addition, there exist subsequences of $\{\mathbf{u}_{h,k}\}_{h,k}$, $\{\widehat{\mathbf{u}}_{h,k}\}_{h,k}$, $\{\widehat{\mathbf{w}}_{h,k}\}_{h,k}$, $\{\rho_{h,k}\}_{h,k,\lambda}$, $\{\widehat{\rho}_{h,k}\}_{h,k}$ and $\{\widetilde{\rho}_{h,k}\}_{h,k}$ (denoted in the same way) and limit functions \mathbf{u} , ρ verifying the following weak convergences as $(h, k) \rightarrow 0$:

$$\begin{aligned} \mathbf{u}_{h,k} \rightharpoonup \mathbf{u}, \quad \widehat{\mathbf{u}}_{h,k} \rightharpoonup \mathbf{u}, \quad \widehat{\mathbf{w}}_{h,k} \rightharpoonup \mathbf{u} \quad \text{in} \quad & \begin{cases} L^2(0, T; \mathbf{H}_0^1(\Omega))\text{-weak}, \\ L^\infty(0, T; \mathbf{L}^2(\Omega))\text{-weak*}, \end{cases} \\ \rho_{h,k} \rightharpoonup \rho, \quad \widehat{\rho}_{h,k} \rightharpoonup \rho, \quad \widetilde{\rho}_{h,k} \rightharpoonup \rho \quad \text{in} \quad & \begin{cases} L^\infty(Q)\text{-weak*}, \\ L^\infty(0, T; H^1(\Omega))\text{-weak*}, \end{cases} \\ \widehat{\rho}_{h,k} \rightharpoonup \rho \quad \text{in} \quad & L^4(0, T; W^{1,3}(\Omega))\text{-weak}. \end{aligned}$$

Proof. Let us prove only that $\widehat{\mathbf{w}}_{h,k} \rightharpoonup \mathbf{u}$ in $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -weak. Consider $\mathbf{v} \in C^0([0, T]; \mathbf{C}_c^\infty(\Omega))$, with $\nabla \cdot \mathbf{v} = 0$ and $\mathbf{v}_h^n \in \widetilde{\mathbf{V}}_h$ an approximation of $\mathbf{v}(t_n)$ given by Lemma 14. Define $\mathbf{v}_{h,k} \in L^\infty(0, T; \widetilde{\mathbf{V}}_h)$ as the piecewise constant functions taking values \mathbf{v}_h^{n+1} on $(t_n, t_{n+1}]$ which verifies the convergence

$$\mathbf{v}_{h,k} \rightarrow \mathbf{v} \quad \text{in } L^\infty(0, T; \mathbf{H}_0^1(\Omega)).$$

Next, by testing (6) by the test function \mathbf{v}_h^n , we have

$$\left(\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n), \nabla \mathbf{v}_h^n \right) = 0,$$

since the pressure term vanishes. By multiplying by the time step k , summing over n , and passing to limit as (h, k) tend to zero, we infer that

$$\int_0^T \left(\nabla(\mathbf{w} - \mathbf{u}), \nabla \mathbf{v} \right) = 0 \quad \forall \mathbf{v} \in C^0([0, T]; \mathbf{C}_c^\infty(\Omega)), \quad \text{with } \nabla \cdot \mathbf{v} = 0.$$

A density argument provides that this equality holds for any $\mathbf{v} \in L^2(0, T; \mathbf{V})$. Therefore, we can choose $\mathbf{v} = \mathbf{w} - \mathbf{u}$ (since $\nabla \cdot \mathbf{u} = 0$ and $\nabla \cdot \mathbf{w} = 0$); then $\mathbf{w} = \mathbf{u}$. \square

6 Strong convergence

As usual for nonlinear systems, strong convergence in some suitable space is necessary to identify the limit of the nonlinear terms.

6.1 Strong convergence for the density in $L^2(\Omega)$

Lemma 16 *Under the hypotheses of Theorem 11, one has:*

$$k \sum_{n=0}^N \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^{4/3} \leq C_\lambda,$$

where $C_\lambda > 0$ is independent of h and k (but depends on λ).

Proof. We consider $P_h : L^2(\Omega) \rightarrow W_h$ the orthogonal projector, defined as $(P_h w - w, w_h) = 0$ for any $w_h \in W_h$. Let $w \in L^2(\Omega)$. By taking in (7) as a test function $w_h = P_h w$, we arrive at

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, w \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, P_h w \right) - \lambda \left(\Delta_h \rho_h^{n+1}, w \right) = 0,$$

where we have used the definition of P_h in the first and last terms. By taking into account the stability of the projector operator $|P_h w| \leq |w|$, we get

$$\left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right| \leq \|\mathbf{w}_h^n\|_{L^6(\Omega)} \|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} + \lambda |\Delta_h \rho_h^{n+1}|.$$

By summing up over n and using the estimates of $\{\widehat{\mathbf{w}}_{h,k}\}_{h,k}$ in $L^2(0, T; \mathbf{L}^6(\Omega))$ (due to the estimates in $L^2(0, T; \mathbf{H}^1(\Omega))$), of $\{\lambda \Delta_h \rho_{h,k}\}_{h,k}$ in $L^2(0, T; L^2(\Omega))$, and of $\{\nabla \rho_{h,k}\}_{h,k}$ in $L^4(0, T; \mathbf{L}^3(\Omega))$ (this last estimate depends on λ), we can conclude the result. \square

Remark 17 *As a consequence of the previous lemma, the estimate holds:*

$$\left\| \frac{d}{dt} \widetilde{\rho}_{h,k} \right\|_{L^{4/3}(0, T; L^2(\Omega))} \leq C_\lambda.$$

On the other hand, from Lemma 7, we get $\|\widetilde{\rho}_{h,k}\|_{L^\infty(0, T; H^1(\Omega))} \leq C_\lambda$. Then, thanks to Aubin-Lions' Compactness Theorem in $L^p(0, T; X)$ space with X a Banach spaces, one has

$$\widetilde{\rho}_{h,k} \rightarrow \rho \text{ in } L^\infty(0, T; L^p(\Omega)) \text{ as } (h, k) \rightarrow 0,$$

with $p < 6$. From this convergence, we deduce that

$$\rho_{h,k}, \widehat{\rho}_{h,k} \rightarrow \rho \text{ in } L^2(0, T; L^2(\Omega)) \text{ as } (h, k) \rightarrow 0,$$

since $\|\widetilde{\rho}_{h,k} - \rho_{k,h}\|_{L^2(0, T; L^2(\Omega))}^2 \leq \|\widehat{\rho}_{h,k} - \rho_{k,h}\|_{L^2(0, T; L^2(\Omega))}^2 = k \sum_{n=0}^{N-1} |\rho_h^{n+1} - \rho_h^n|^2 \leq C k$.

6.2 Strong convergence for the velocity

Proposition 18 *Under the hypotheses of Theorem 11, the following estimate holds:*

$$\int_0^{T-\delta} \left| \sqrt{\rho_{h,k}(t+\delta)} (\mathbf{u}_{h,k}(t+\delta) - \mathbf{u}_{h,k}(t)) \right|^2 dt \leq C_\lambda \delta^{1/4} \quad \forall \delta : 0 < \delta < T, \quad (44)$$

where $C_\lambda > 0$ is independent of h, k , and δ (but depends on λ).

Proof. Throughout the proof we will keep in mind Lemmas 7 and 11 and Remark 8. As $\rho_{h,k}$ and $\mathbf{u}_{h,k}$ are piecewise constant functions, it suffices to suppose that δ is proportional to the time step k , i.e., $\delta = r k$ for any $r = 0, \dots, N$. Then, to obtain (44), it suffices to prove that

$$k \sum_{m=0}^{N-r} \left| \sqrt{\rho_h^{m+r}} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right|^2 \leq C_\lambda (r k)^{1/4} \quad \forall r : 0 \leq r \leq N. \quad (45)$$

Let us write the time derivative of the discrete momentum system (8) in conservative form. By adding at the right- and left-hand sides of (8) the term $\frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right)$:

$$\left\{ \begin{aligned} & \left(\frac{\rho_h^{n+1} \mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) \\ & + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) = (\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right). \end{aligned} \right. \quad (46)$$

By multiplying (46) by k and summing for $n = m, \dots, m-1+r$, we have

$$\left\{ \begin{aligned} & \left(\rho_h^{m+r} \mathbf{u}_h^{m+r} - \rho_h^m \mathbf{u}_h^m, \bar{\mathbf{u}}_h \right) + k \sum_{n=m}^{m-1+r} a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - \sum_{n=m}^{m-1+r} (p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) \\ & + k \sum_{n=m}^{m-1+r} c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ & = k \sum_{n=m}^{m-1+r} (\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h) + \frac{k}{2} \sum_{n=m}^{m-1+r} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right). \end{aligned} \right.$$

By taking $\bar{\mathbf{u}}_h = \mathbf{u}_h^{m+r} - \mathbf{u}_h^m$ and making use of the identity

$$\rho_h^{m+r} \mathbf{u}_h^{m+r} - \rho_h^m \mathbf{u}_h^m = \rho_h^{m+r} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) + (\rho_h^{m+r} - \rho_h^m) \mathbf{u}_h^m \quad (47)$$

we get

$$\left\{ \begin{aligned} & |\sqrt{\rho_h^{m+r}} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 = -(\rho_h^{m+r} - \rho_h^m, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) \\ & -k \sum_{n=m}^{m-1+r} \left\{ a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right\} \\ & +k \sum_{n=m}^{m-1+r} \left\{ (\rho_h^{n+1} \mathbf{f}^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \right\}. \end{aligned} \right. \quad (48)$$

On the other hand, by taking $\bar{\rho}_h = \rho_h^{m+r} - \rho_h^m$ as a test function in the density scheme (31), multiplying by k , and summing for $n = m, \dots, m-1+r$, we obtain

$$\begin{aligned} |\rho_h^{m+r} - \rho_h^m|^2 &= -k \sum_{n=m}^{m-1+r} \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1} - \lambda \Delta_h \rho_h^{n+1}, \rho_h^m - \rho_h^{m+r} \right) \\ &\leq k \sum_{n=m}^{m-1+r} (\|\mathbf{w}_h^n\|_{\mathbf{L}^6(\Omega)} \|\nabla \rho_h^n\|_{\mathbf{L}^3(\Omega)} + \lambda |\Delta_h \rho_h^{n+1}|) |\rho_h^m - \rho_h^{m+r}|. \end{aligned}$$

Therefore,

$$\begin{aligned} |\rho_h^m - \rho_h^{m+r}| &\leq C \left(k \sum_{n=m}^{m-1+r} \|\mathbf{w}_h^n\|_{\mathbf{L}^6(\Omega)}^2 \right)^{1/2} \left(k \sum_{n=m}^{m-1+r} \|\nabla \rho_h^n\|_{\mathbf{L}^3(\Omega)}^4 \right)^{1/4} (rk)^{1/4} \\ &\quad + C \left(k \sum_{n=m}^{m-1+r} \lambda |\Delta_h \rho_h^{n+1}|^2 \right)^{1/2} (rk)^{1/2} \\ &\leq C_\lambda (rk)^{1/4} + C(rk)^{1/2}, \end{aligned}$$

where $C_\lambda > 0$ is a constant independent of h and k (and depending on λ). Then we have

$$\max_{1 \leq m \leq N} |\rho_h^m - \rho_h^{m+r}| \leq C_\lambda (rk)^{1/4}. \quad (49)$$

By multiplying (48) by k and summing for $m = 0, \dots, N - r$, we are going to get the desired bound (45) using (49). Indeed, from (49), one can obtain (with a similar argument as in [12])

$$-k \sum_{m=0}^{N-r} \left(\rho_h^m - \rho_h^{m+r}, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \leq C_\lambda (rk)^{1/4}.$$

We analyze only the two terms whose estimates will be different from the ones done in ([12]):

$$J_1 := -k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m \right),$$

$$J_2 := \frac{k^2}{2} \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right).$$

To estimate J_1 , we use (10) as follows:

$$\begin{aligned} J_1 &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}\|_{\mathbf{L}^3(\Omega)} \|\mathbf{u}_h^{n+1}\| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\| \\ &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\|\rho_h^{n+1}\|_{L^\infty(\Omega)} \|\mathbf{u}_h^n\|_{\mathbf{L}^3(\Omega)} + \lambda \|\nabla \rho_h^{n+1}\|_{\mathbf{L}^3(\Omega)} \right) \|\mathbf{u}_h^{n+1}\| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|. \end{aligned}$$

By interchanging the sum order (Fubini's discrete rule) and using the estimate $\|\rho_h^{n+1}\|_{L^\infty(\Omega)} \leq C$,

$$J_1 \leq C k^2 \sum_{n=0}^{N-1} \left(\|\mathbf{u}_h^n\|_{\mathbf{L}^3(\Omega)} + \lambda \|\nabla \rho_h^{n+1}\|_{\mathbf{L}^3(\Omega)} \right) \|\mathbf{u}_h^{n+1}\| \sum_{m=\overline{n-r+1}}^{\overline{n}} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|,$$

where

$$\overline{n} = \begin{cases} 0 & \text{si } n < 0, \\ n & \text{si } 0 \leq n \leq N - r, \\ N - r & \text{si } n > N - r. \end{cases}$$

Next, by taking into account that $|\overline{n} - \overline{n - r + 1}| \leq r$ and Corollary 12, we get

$$\begin{aligned} J_1 &\leq C k \sum_{n=0}^{N-1} \left(\|\mathbf{u}_h^n\|_{\mathbf{L}^3(\Omega)} + \lambda \|\nabla \rho_h^{n+1}\|_{\mathbf{L}^3(\Omega)} \right) \|\mathbf{u}_h^{n+1}\| \\ &\quad \left(\sum_{m=\overline{n-r+1}}^{\overline{n}} k \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|^2 \right)^{1/2} \left(\sum_{m=\overline{n-r+1}}^{\overline{n}} k \right)^{1/2} \\ &\leq C (rk)^{1/2} \left(k \sum_{n=0}^{N-1} \left(\|\mathbf{u}_h^n\|_{\mathbf{L}^3(\Omega)} + \lambda \|\nabla \rho_h^{n+1}\|_{\mathbf{L}^3(\Omega)} \right)^2 \right)^{1/2} \left(k \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1}\|^2 \right)^{1/2} \\ &\leq C (rk)^{1/2}. \end{aligned}$$

In the same way, we can bound the term $k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m)$.

We bound J_2 as follows:

$$\begin{aligned}
J_2 &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right| \|\mathbf{u}_h^{n+1}\|_{L^3(\Omega)} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\| \\
(\text{Fubini}) &\leq C k^2 \sum_{n=0}^{N-1} \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right| \|\mathbf{u}_h^{n+1}\|^{1/2} |\mathbf{u}_h^{n+1}|^{1/2} \sum_{m=n-r+1}^{\bar{n}} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\| \\
&\leq C k \sum_{n=0}^{N-1} \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right| \|\mathbf{u}_h^{n+1}\|^{1/2} \left(k \sum_{m=n-r+1}^{\bar{n}} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|^2 \right)^{1/2} (rk)^{1/2} \\
&\leq C (rk)^{1/2} \left(k \sum_{n=0}^{N-1} \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^{4/3} \right)^{3/4} \left(k \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1}\|^2 \right)^{1/4} \leq C_\lambda (rk)^{1/2}.
\end{aligned}$$

□

Remark 19 From the weak estimates of the discrete velocity $\mathbf{u}_{h,k}$ in $L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega))$ and the fractional in time estimate of $\mathbf{u}_{h,k}$ given in (44), we can apply a compactness result [18] and obtain

$$\mathbf{u}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

Consequently, thanks to estimate **iii**),

$$\widehat{\mathbf{u}}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

As $\{\mathbf{u}_{h,k}\}_{h,k}$ is bounded in $L^\infty(0, T; \mathbf{L}^2(\Omega))$ we improve the compactness of $\{\mathbf{u}_{h,k}\}_{h,k}$ to $L^p(0, T; \mathbf{L}^2(\Omega))$, with $p < \infty$.

Remark 20 From (23), we infer the inequality

$$|\mathbf{w}_h^n - \mathbf{u}| \leq C k |\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)| + |\mathbf{u}_h^n - \mathbf{u}| \leq C k^{1/2} + |\mathbf{u}_h^n - \mathbf{u}|.$$

Therefore, it holds

$$\widehat{\mathbf{w}}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

6.3 Strong convergence for the density in $H^1(\Omega)$

By using the compactness of the discrete density in $L^2(0, T; \mathbf{L}^2(\Omega))$ and comparing the equation for the discrete Laplacian and its limit (see [12]), one can obtain the convergence of the $L^2(0, T; \mathbf{L}^2(\Omega))$ -norm of $\nabla \rho_{h,k}$ towards the same norm of $\nabla \rho$. Consequently, one has

$$\|\rho_{h,k} - \rho\|_{L^2(0, T; H^1(\Omega))} \rightarrow 0 \text{ as } (h, k) \rightarrow 0.$$

7 Passing to the limit

7.1 Convergence for the density scheme

Thanks to the previous convergences, we can prove [12] the convergence of the density scheme as $(h, k) \rightarrow 0$, obtaining

$$\rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0 \text{ in } Q, \quad \frac{\partial \rho}{\partial \mathbf{n}} \Big|_{\Sigma} = 0, \quad \rho(0) = \rho_0 \text{ in } \Omega. \quad (50)$$

7.2 Convergence for the momentum scheme

We use the following convergence result, which is similar to Lemma 14.

Lemma 21 *Let $\bar{\mathbf{u}} \in \mathbf{C}_c^\infty(\Omega)$. Then there exists $\bar{\mathbf{u}}_h \in \mathbf{V}_h$ such that:*

$$\bar{\mathbf{u}}_h \rightarrow \bar{\mathbf{u}} \text{ in } \mathbf{H}_0^1(\Omega) \text{ and } \left(\nabla \cdot \bar{\mathbf{u}}_h, q_h \right) = \left(\nabla \cdot \bar{\mathbf{u}}, q_h \right) \forall q_h \in M_h.$$

To pass to the limit in the discrete momentum system, we consider $\mathbf{v} \in C^1([0, T]; \mathbf{C}_c^\infty(\Omega))$, with $\nabla \cdot \mathbf{v} = 0$ and $\mathbf{v}(T) = 0$. We define \mathbf{v}_h^n as the projection of $\mathbf{v}(t^n)$ furnished by Lemma 21. We define $\mathbf{v}_{h,k} \in L^\infty(0, T; \mathbf{V}_h)$ as the piecewise constant functions taking values \mathbf{v}_h^{n+1} on $(t_n, t_{n+1}]$ and let $\tilde{\mathbf{v}}_{h,k} \in C^0([0, T]; \mathbf{V}_h)$ be the piecewise linear, globally continuous functions and such that $\tilde{\mathbf{v}}_{h,k}(t_n) = \mathbf{v}_h^n$. It is known that, as $(h, k) \rightarrow 0$,

$$\mathbf{v}_{h,k} \rightarrow \mathbf{v} \text{ in } L^\infty(0, T; \mathbf{H}_0^1(\Omega)),$$

$$\tilde{\mathbf{v}}_{h,k} \rightarrow \mathbf{v} \text{ in } W^{1,\infty}(0, T; \mathbf{H}_0^1(\Omega)).$$

By taking $\bar{\mathbf{u}}_h = \mathbf{v}_h^{n+1}$ as a test function in (46), multiplying by k , summing over n , and using the expression (discrete integration by parts in time)

$$\sum_{n=0}^{N-1} \left(\rho_h^{n+1} \mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n, \mathbf{v}_h^{n+1} \right) = \left(\rho_h^N \mathbf{u}_h^N, \mathbf{v}_h^N \right) - \sum_{n=0}^{N-1} \left(\rho_h^n \mathbf{u}_h^n, \mathbf{v}_h^{n+1} - \mathbf{v}_h^n \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right)$$

and the fact that $\mathbf{v}_h^N = 0$ (since $\mathbf{v}(T) = 0$), the following formulation holds:

$$\left\{ \begin{array}{l} -k \sum_{n=0}^{N-1} \left(\rho_h^n \mathbf{u}_h^n, \frac{\mathbf{v}_h^{n+1} - \mathbf{v}_h^n}{k} \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right) \\ +k \sum_{n=0}^{N-1} c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{v}_h^{n+1}) + k \sum_{n=0}^{N-1} a(\mathbf{u}_h^{n+1}, \mathbf{v}_h^{n+1}) \\ = k \sum_{n=0}^{N-1} \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \mathbf{v}_h^{n+1} \right) + k \sum_{n=0}^{N-1} \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \mathbf{v}_h^{n+1} \right). \end{array} \right.$$

Next, by taking into account Definition 13,

$$\left\{ \begin{array}{l} - \int_0^T \left(\widehat{\rho}_{h,k} \widehat{\mathbf{u}}_{h,k}, \frac{\partial}{\partial t} \widetilde{\mathbf{v}}_{h,k} \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right) \\ + \int_0^T c \left(\rho_{h,k} \widehat{\mathbf{u}}_{h,k} - \lambda \nabla \rho_{h,k}, \mathbf{u}_{h,k}, \mathbf{v}_{h,k} \right) + \sum_{n=0}^{N-1} a \left(\rho_{h,k}, \mathbf{u}_{h,k}, \mathbf{v}_{h,k} \right) \\ = \int_0^T \left(\rho_{h,k} \mathbf{f}_k, \mathbf{v}_{h,k} \right) + \frac{1}{2} \int_0^T \left(\frac{\partial}{\partial t} \widetilde{\rho}_{h,k}, \mathbf{u}_{h,k} \cdot \mathbf{v}_{h,k} \right) \end{array} \right.$$

This variational formulation of the discrete momentum system allows us to pass to the limit in a standard way. We pass to the limit only in the last term on the right-hand side since this term does not appear in the theoretical analysis. We know that $\frac{\partial}{\partial t} \widetilde{\rho}_{h,k} \rightharpoonup \frac{\partial}{\partial t} \rho$ weakly in $L^{4/3}(0, T; L^2(\Omega))$ and $\mathbf{u}_{h,k} \rightarrow \mathbf{u}$ strongly in $L^p(0, T; L^2(\Omega))$, with $p < \infty$, and is bounded in $L^4(0, T; \mathbf{L}^3(\Omega))$, and hence $\frac{\partial}{\partial t} \widetilde{\rho}_{h,k} \mathbf{u}_{h,k} \rightharpoonup \frac{\partial}{\partial t} \rho \mathbf{u}$ weakly in $L^1(0, T; \mathbf{L}^{6/5}(\Omega))$. As $\mathbf{v}_{h,k} \rightarrow \mathbf{v}$ in $L^\infty(0, T; \mathbf{H}_0^1(\Omega))$, we have

$$\int_0^T \left(\frac{\partial}{\partial t} \widetilde{\rho}_{h,k}, \mathbf{u}_{h,k} \cdot \mathbf{v}_{h,k} \right) \rightarrow \int_0^T \left(\frac{\partial}{\partial t} \rho, \mathbf{u} \cdot \mathbf{v} \right) \text{ as } (h, k) \rightarrow 0.$$

This concludes the proof of Theorem 1.

Remark 22 A variant of the Kazhikhov-Smagulov model is obtained by replacing the linear diffusion term $-\nabla \cdot (\mu \nabla \mathbf{u})$ in (1) by a nonlinear diffusion term $-\lambda \nabla \cdot (\rho \nabla \mathbf{u})$ (i.e., by taking $\mu = \lambda \rho$). It is a model of pollution studied by D. Bresch, E.H. Essoufi, and M. Sy in [4, 5], where they prove the existence of a global in time weak solution, without imposing the restrictive hypothesis (5) on the coefficients.

The scheme that we design for this model is obtained by replacing the stabilizing term of the momentum system

$$-\lambda \int_{\Omega} \frac{M+m}{2} (\nabla \mathbf{u}_h^{n+1})^t : \nabla \bar{\mathbf{u}}_h \, d\mathbf{x}$$

by the term $\frac{\lambda m}{2} (\nabla \cdot \mathbf{u}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h)$ and the remainder with the following scheme:

Given $(\rho_h^n, \mathbf{u}_h^n, p_h^n) \in W_h \times \mathbf{V}_h \times M_h$,

1. find $(\mathbf{w}_h^n, q_h^n) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$ such that, for each $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$,

$$\left\{ \begin{array}{l} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0; \end{array} \right. \quad (51)$$

2. find $\rho_h^{n+1} \in W_h$ such that, for each $\bar{\rho}_h \in W_h$,

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0; \quad (52)$$

3. Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that, for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$,

$$\begin{cases} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) \\ + c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + \lambda \left(\rho_h^{n+1} (\nabla \mathbf{u}_h^{n+1} - (\nabla \mathbf{u}_h^{n+1})^t), \nabla \bar{\mathbf{u}}_h \right) + \frac{\lambda m}{2} (\nabla \cdot \mathbf{u}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) \\ = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{cases} \quad (53)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0. \quad (54)$$

By following arguments of this paper, one may establish the same conclusions of Theorem 1 for this scheme.

8 Asymptotic behavior when $\lambda \rightarrow 0$

In this section we are interested in the asymptotic behavior of scheme (7)-(9) when the diffusion parameter λ goes to zero. More precisely, we will see that, by imposing the stability condition

$$(S') \quad \lim_{(\lambda, h, k) \rightarrow 0} \frac{1}{\lambda} \sqrt{\frac{h}{k}} = 0$$

and completing (H2) with the additional approximation property

$$(H2') \quad |\bar{\rho} - I_h \bar{\rho}| \leq C h^{2/3} \|\bar{\rho}\|_{W^{1,3/2}(\Omega)}, \quad \forall \bar{\rho} \in W^{1,3/2}(\Omega),$$

then scheme (7)-(9) approximates, as $(h, k, \lambda) \rightarrow 0$, to a weak solution of the density-dependent Navier-Stokes problem:

$$\begin{cases} \rho [\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}] - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{f} & \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0, \quad \rho_t + \mathbf{u} \cdot \nabla \rho = 0 & \text{in } Q, \\ \mathbf{u} = 0 & \text{on } \Sigma, \\ \mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \rho|_{t=0} = \rho_0 & \text{in } \Omega, \end{cases} \quad (55)$$

which is defined as follows.

Definition 23 A pair (ρ, \mathbf{u}) is said to be a weak solution of (55) in $(0, T)$ if it verifies:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{V})$, $\rho \in L^\infty(Q)$ with $0 < m \leq \rho(\mathbf{x}, t) \leq M$ a.e. $(\mathbf{x}, t) \in Q$.

b) For all $\phi \in C^1([0, T]; \mathbf{V})$, with $\phi(T) = 0$,

$$\int_0^T \left\{ -(\rho \mathbf{u}, \phi_t + (\mathbf{u} \cdot \nabla) \phi) + \mu (\nabla \mathbf{u}, \nabla \phi) \right\} dt = \int_0^T (\rho \mathbf{f}, \phi) dt + (\rho_0 \mathbf{u}_0, \phi(0));$$

c) for all $\varphi \in C^1([0, T]; \mathbf{H}^1(\Omega))$, with $\varphi(T) = 0$,

$$- \int_0^T (\rho, \varphi_t) dt - \int_0^T (\rho \mathbf{u}, \nabla \varphi) dt = (\rho_0, \varphi(0));$$

The rest of this section is devoted to the proof of Theorem 2.

8.1 Uniform estimates with respect to (h, k, λ) .

By following arguments of the previous sections, assuming (S') , and (h, k, λ) small enough, we can obtain the following estimates independent of h, k , and λ (now we denote piecewise functions associated to the scheme also with the parameter λ explicitly):

$$\begin{aligned} \{\mathbf{u}_{h,k,\lambda}\}_{h,k,\lambda}, \{\widehat{\mathbf{u}}_{h,k,\lambda}\}_{h,k,\lambda}, \{\widehat{\mathbf{w}}_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in } L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)), \\ \{\widetilde{\rho}_{h,k,\lambda}\}_{h,k,\lambda}, \{\rho_{h,k,\lambda}\}_{h,k,\lambda}, \{\widehat{\rho}_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in } L^\infty(Q), \\ \lambda^{1/2}\{\rho_{h,k,\lambda}\}_{h,k,\lambda}, \lambda^{1/2}\{\widehat{\rho}_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in } L^\infty(0, T; H^1(\Omega)), \\ \lambda^{3/4}\{\rho_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in } L^4(0, T; W^{1,3}(\Omega)), \\ \lambda^{3/4}\left\{\frac{\partial}{\partial t}\widetilde{\rho}_{h,k,\lambda}\right\}_{h,k,\lambda} & \text{ in } L^{4/3}(0, T; L^2(\Omega)). \end{aligned}$$

In addition, $0 < \widetilde{m} \leq \rho_{h,k,\lambda}, \widehat{\rho}_{h,k,\lambda}, \widetilde{\rho}_{h,k,\lambda} \leq \widetilde{M}$ in Q ,

$$\begin{aligned} \|\widetilde{\rho}_{h,k,\lambda} - \rho_{h,k,\lambda}\|_{L^2(0,T;L^2(\Omega))} & \leq \|\rho_{h,k,\lambda} - \widehat{\rho}_{h,k,\lambda}\|_{L^2(0,T;L^2(\Omega))} \leq C\sqrt{k}, \\ \|\mathbf{u}_{h,k,\lambda} - \widehat{\mathbf{u}}_{h,k,\lambda}\|_{L^2(0,T;\mathbf{H}_0^1(\Omega))} & \leq C\sqrt{k}. \end{aligned}$$

In fact, we have the following result.

Lemma 24 *By assuming (S') and (h, k, λ) small enough, there exist subsequences of $\{\mathbf{u}_{h,k,\lambda}\}_{h,k}$, $\{\widehat{\mathbf{u}}_{h,k,\lambda}\}_{h,k}$, $\{\rho_{h,k,\lambda}\}_{h,k,\lambda}$, $\{\widehat{\rho}_{h,k,\lambda}\}_{h,k}$, and $\{\widetilde{\rho}_{h,k,\lambda}\}_{h,k}$ (denoted in the same way) and limit functions \mathbf{u} and ρ such that $\nabla \cdot \mathbf{u} = 0$ a.e. in Ω , and the following weak convergences hold as $(h, k, \lambda) \rightarrow 0$:*

$$\begin{aligned} \mathbf{u}_{h,k,\lambda} \rightarrow \mathbf{u}, \quad \widehat{\mathbf{u}}_{h,k,\lambda} \rightarrow \mathbf{u}, \quad \widehat{\mathbf{w}}_{h,k,\lambda} \rightarrow \mathbf{u} & \text{ in } \begin{cases} L^2(0, T; \mathbf{H}_0^1(\Omega))\text{-weak} , \\ L^\infty(0, T; \mathbf{L}^2(\Omega))\text{-weak*}, \end{cases} \\ \widetilde{\rho}_{h,k,\lambda} \rightarrow \rho, \quad \rho_{h,k,\lambda} \rightarrow \rho, \quad \widehat{\rho}_{h,k,\lambda} \rightarrow \rho & \text{ in } L^\infty(Q)\text{-weak*}. \end{aligned}$$

8.2 Compactness

Proposition 25 *Under the hypotheses of Lemma 24, the estimate*

$$\int_0^{T-\delta} \left| \sqrt{\rho_{h,k,\lambda}(t+\delta)} (\mathbf{u}_{h,k,\lambda}(t+\delta) - \mathbf{u}_{h,k,\lambda}(t)) \right|^2 dt \leq C \delta^{1/2} \quad \forall \delta : \quad 0 < \delta < T, \quad (56)$$

holds, with $C > 0$ independent of h, k, δ , and λ .

In particular, since $\rho_{h,k,\lambda} \geq \widetilde{m}$, then

$$\mathbf{u}_{h,k,\lambda} \rightarrow \mathbf{u}, \quad \mathbf{w}_{h,k,\lambda} \rightarrow \mathbf{u} \quad \text{in } L^2(0, T; \mathbf{L}^2(\Omega)) \quad \text{as } (h, k, \lambda) \rightarrow 0.$$

Proof. Again, since $\rho_{h,k,\lambda}$ and $\mathbf{u}_{h,k,\lambda}$ are piecewise constant functions, (56) is equivalent to

$$k \sum_{m=0}^{N-r} |\sqrt{\rho_h^{m+r}}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 \leq C (rk)^{1/2}, \quad \forall r : 0 \leq r \leq N. \quad (57)$$

By following the proof of Proposition 18, one observes that the terms which are not necessarily bounded independent of λ are

$$T_1 := k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right)$$

and

$$T_2 := -k \sum_{m=0}^{N-r} \left(\rho_h^{m+r} - \rho_h^m, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right).$$

Here we are going to bound these terms.

We consider the projection operator on W_h with respect to $L^2(\Omega)$ -inner product:

$$P_h : L^2(\Omega) \rightarrow W_h \quad \text{such that} \quad (P_h v, w) = (v, w) \quad \forall w \in W_h.$$

We take $\bar{\rho}_h = P_h(\mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) \in W_h$ in (31), arriving at

$$\begin{aligned} & \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, P_h(\mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) \right) \\ & - \lambda \left(\Delta_h \rho_h^{n+1}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) = 0, \end{aligned} \quad (58)$$

where we have used the definition of projection operator in $L^2(\Omega)$ in the first and the last term.

Thus, we decompose $T_1 = T_{1,1} + T_{1,2}$, where:

$$T_{1,1} = -k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, P_h(\mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) \right),$$

$$T_{1,2} = \lambda k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\Delta_h \rho_h^{n+1}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right).$$

By writing $T_{1,1}$ as follows:

$$\begin{aligned} T_{1,1} &= -k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, P_h(\mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) - \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \\ &- k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) := T_{1,1}^1 + T_{1,1}^2, \end{aligned}$$

we bound it as

$$T_{1,1}^1 \leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\mathbf{w}_h^n\|_{L^6(\Omega)} \|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} h^{2/3} \|\mathbf{u}_h^{n+1}\| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|,$$

where we have used the interpolation error $|\bar{\rho} - P_h \bar{\rho}| \leq C h^{2/3} \|\bar{\rho}\|_{W^{1,3/2}(\Omega)}$ thanks to $(H2)'$ and the inequality $\|\mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{W^{1,3/2}(\Omega)} \leq \|\mathbf{u}_h^{n+1}\| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|$. Next, by taking (λ, h, k) small enough and such that

$$h^{2/3} \leq C \lambda^{3/4} k^{1/2}, \quad (59)$$

using the fact that $\lambda^{3/4} k^{1/2} \|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq C$ (with C independent of λ, h, k), and applying the discrete Fubini rule, we arrive at the estimate $T_{1,1}^1 \leq C (rk)^{1/2}$.

The bound $T_{1,1}^2 \leq C (rk)^{1/2}$ is obtained easily by integrating by parts and using the pointwise bound $\|\rho_h^{n+1}\|_{L^\infty(\Omega)} \leq C$ (where C is independent of λ):

$$\begin{aligned} T_{1,1}^2 &\leq k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(|\nabla \cdot \mathbf{w}_h^n| |\mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)| + \|\mathbf{w}_h^n\|_{L^6(\Omega)} |\nabla \mathbf{u}_h^{n+1}| \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^3(\Omega)} \right) \\ &+ k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\mathbf{w}_h^n\|_{L^6(\Omega)} \|\mathbf{u}_h^{n+1}\|_{L^3(\Omega)} |\nabla(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)| \\ &\leq C k^2 \sum_{n=0}^{N-1} \|\mathbf{w}_h^n\| \|\mathbf{u}_h^{n+1}\| \sum_{m=\bar{n}-r+1}^{\bar{n}} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\| \leq C (rk)^{1/2}. \end{aligned}$$

The bound $T_{1,2} \leq C (rk)^{1/2}$ is obtained using the fact that $\lambda^2 k \sum_{n=0}^{N-1} |\Delta_h \rho_h^{n+1}|^2 \leq C$ and Fubini's rule.

By summing up (58) multiplied by k^2 for $n = m, \dots, m+r-1$ and then summing up for $m = 0, \dots, N-r$ we can write T_2 as:

$$\begin{aligned} T_2 &= -k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m+r-1} (\mathbf{w}_h^n \cdot \nabla \rho_h^n, P_h(\mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m))) \\ &+ k^2 \lambda \sum_{m=0}^{N-r} \sum_{n=m}^{m+r-1} (\Delta_h \rho_h^{n+1}, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)). \end{aligned}$$

These new terms are bounded in an analogous manner (now, without using Fubini's rule), resulting in

$$T_2 \leq C (rk)^{1/2}.$$

Note that the restriction on the parameters (59) imposed to get the bound of $T_{1,1}^1$ is included in the constraint (S') imposed to obtain a priori estimates. Indeed, (59) is equivalent to $\frac{1}{\lambda^{3/4}} \frac{h^{2/3}}{k^{1/4}} \leq C$. But as

$$\lim_{(h,k,\lambda) \rightarrow 0} \frac{\frac{1}{\lambda} \sqrt{\frac{h}{k}}}{\frac{1}{\lambda^{3/4}} \frac{h^{2/3}}{k^{1/4}}} = \lim_{(h,k,\lambda) \rightarrow 0} \frac{1}{\lambda^{1/4} k^{1/2} h^{1/6}} = \infty,$$

then $\frac{1}{\lambda^{3/4}} \frac{h^{2/3}}{k^{1/4}} \leq C \frac{1}{\lambda} \sqrt{\frac{h}{k}} \rightarrow 0$ (thanks to (S')). \square

Remark 26 *By comparing the fractional in time estimates for the discrete velocity in the case of λ fixed (done in Proposition 18) with respect to the case of $\lambda \rightarrow 0$ (done now in Proposition 25), one can observe that condition (59) on the parameters h and k imposed now in the proof of Proposition 25 is not necessary in the case of λ fixed; however, in this case only order $(rk)^{1/4}$ is obtained. Now, in the case $\lambda \rightarrow 0$, we have to impose constraint (59) and the estimate order is improved from $(rk)^{1/4}$ to $(rk)^{1/2}$.*

8.3 Passing to the limit.

8.3.1 Density equation

Let $\eta \in C^1([0, T]; C_c^\infty(\Omega))$ such that $\eta(T) = 0$. We define η_h^n as the interpolation in W_h of $\eta(t_n)$ and $\eta_{h,k} \in L^\infty(0, T; W_h)$ as the piecewise constant function taking values η_h^{n+1} in $(t_n, t_{n+1}]$ and let $\tilde{\eta}_{h,k} \in C^0([0, T]; W_h)$ be the piecewise linear, globally continuous function such that $\tilde{\eta}_{h,k}(t_n) = \eta_h^n$. One has, as $(h, k) \rightarrow 0$,

$$\eta_{k,h} \rightarrow \eta \quad \text{in } L^\infty(0, T; H^1(\Omega)) \quad \text{and} \quad \tilde{\eta}_{k,h} \rightarrow \eta \quad \text{in } W^{1,\infty}(0, T; H^1(\Omega)).$$

By using these discrete test functions in the discrete density formulation (7), together with an integration by parts in time, we arrive [12] at the formulation

$$\begin{aligned} & - \int_0^T \left(\hat{\rho}_{h,k,\lambda}, \frac{d}{dt} \tilde{\eta}_{h,k} \right) dt + \lambda \int_0^T \left(\nabla \rho_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt \\ & + \int_0^T \left(\hat{\mathbf{w}}_{h,k,\lambda} \cdot \nabla \rho_{h,k,\lambda}, \eta_{h,k} \right) dt = \left(\rho_{0h}, \eta_h^0 \right). \end{aligned} \tag{60}$$

Before taking a limit in (60), we rewrite the convective term in the following form:

$$\begin{aligned} \int_0^T \left(\hat{\mathbf{w}}_{h,k,\lambda} \cdot \nabla \rho_{h,k,\lambda}, \eta_{h,k} \right) dt &= - \int_0^T \left(\nabla \cdot \hat{\mathbf{w}}_{h,k,\lambda} \rho_{h,k,\lambda}, \eta_{h,k} \right) dt - \int_0^T \left(\rho_{h,k,\lambda} \hat{\mathbf{w}}_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt \\ &= - \int_0^T \left(\rho_{h,k,\lambda} \hat{\mathbf{w}}_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt, \end{aligned}$$

where we have used Remark 6. Therefore, (60) remains as

$$\begin{aligned} & - \int_0^T \left(\hat{\rho}_{h,k,\lambda}, \frac{d}{dt} \tilde{\eta}_{h,k} \right) dt + \lambda \int_0^T \left(\nabla \rho_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt \\ & - \int_0^T \left(\hat{\mathbf{w}}_{h,k,\lambda} \rho_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt = \left(\rho_{0h}, \eta_h^0 \right). \end{aligned}$$

By taking into account the weak and strong convergences obtained in previous subsections, it is possible to pass to the limit. Notice that, by arguing as in [10], one can prove that

$$\lambda \int_0^T \left(\nabla \rho_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt \rightarrow 0 \quad \text{as } (h, k, \lambda) \rightarrow 0.$$

8.3.2 Velocity system

Before taking a limit in the discrete momentum system (8), we will write (8) in a completely conservative form. For this, summing to both side of (8) the terms

$$\frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right)$$

provides that, for each $\bar{\mathbf{u}}_h \in \mathbf{V}_h$,

$$\left\{ \begin{array}{l} \left(\frac{\rho_h^{n+1} \mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) - \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \otimes \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ + a \left(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right), \end{array} \right. \quad (61)$$

On the other hand, we consider Q_h the projector operator onto W_h respect to the H^1 -norm:

$$Q_h : H^1(\Omega) \rightarrow W_h \text{ such that } (Q_h v, w)_{H^1(\Omega)} = (v, w)_{H^1(\Omega)} \quad \forall w \in W_h,$$

where $(\cdot, \cdot)_{H^1(\Omega)}$ denotes the usual H^1 -inner product.

By subtracting from the second member of (61) the result of taking $\bar{\rho}_h = \frac{1}{2} Q_h(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h)$ as a test function in (7) and integrating by parts the convective term, one has

$$\left\{ \begin{array}{l} \left(\frac{\rho_h^{n+1} \mathbf{u}_h^{n+1} - \rho_h^n \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) - \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \otimes \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ + a \left(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h - Q_h(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right) \\ - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n, \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h - Q_h(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h)) \right) \\ - \frac{1}{2} \left(\rho_h^{n+1} (\mathbf{u}_h^n - \mathbf{w}_h^n), \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right) \\ + \frac{1}{2} \left(\nabla \cdot \mathbf{w}_h^n \rho_h^{n+1}, Q_h(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right) \\ - \frac{\lambda}{2} \left(\rho_h^{n+1}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h - Q_h(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right), \end{array} \right.$$

where we have used the definition of Q_h in the last term on the right-hand side. Note that the term $\left(\nabla \cdot \mathbf{w}_h^n \rho_h^{n+1}, Q_h(\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right) = 0$ thanks to Remark 6.

In a similar way to Section 7, we arrive at

$$\left\{ \begin{array}{l} - \int_0^T \left(\widehat{\rho}_{h,k,\lambda} \widehat{\mathbf{u}}_{h,k,\lambda}, \frac{\partial}{\partial t} \widetilde{\mathbf{v}}_{h,k} \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right) \\ - \int_0^T \left(\rho_{h,k,\lambda} \widehat{\mathbf{u}}_{h,k} - \lambda \nabla \rho_{h,k,\lambda} \otimes \mathbf{u}_{h,k,\lambda}, \nabla \mathbf{v}_{h,k} \right) + a \left(\rho_{h,k,\lambda}, \mathbf{u}_{h,k,\lambda}, \mathbf{v}_{h,k} \right) \\ = \int_0^T \left(\rho_{h,k,\lambda} \mathbf{f}_k, \mathbf{v}_{h,k} \right) + \frac{1}{2} \int_0^T \left(\frac{\partial}{\partial t} \widetilde{\rho}_{h,k}, \mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}) \right) \\ - \frac{1}{2} \int_0^T \left(\rho_{h,k,\lambda} \widehat{\mathbf{w}}_{h,k,\lambda}, \nabla(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k})) \right) \\ - \frac{1}{2} \int_0^T \left(\rho_{h,k,\lambda} (\widehat{\mathbf{u}}_{h,k,\lambda} - \widehat{\mathbf{w}}_{h,k,\lambda}), \nabla(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k})) \right) \\ - \frac{\lambda}{2} k \int_0^T \left(\rho_{h,k,\lambda}, \mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}) \right) \\ := \int_0^T \left(\rho_{h,k,\lambda} \mathbf{f}_k, \mathbf{v}_{h,k} \right) + R_1 + R_2 + R_3 + R_4, \end{array} \right.$$

where $\mathbf{v}_{h,k}$ and $\widetilde{\mathbf{v}}_{h,k}$ are suitable approximations of a test function $\mathbf{v} \in C^1([0, T]; \mathbf{C}_c^\infty(\Omega))$.

Again, by using the estimates independent of λ and arguing as in the continuous case [10], one can prove that

$$\begin{aligned} \lambda \int_0^T \left(\nabla \rho_{h,k,\lambda} \otimes \mathbf{u}_{h,k,\lambda}, \nabla \mathbf{v}_{h,k} \right) &\rightarrow 0 \quad \text{as } (h, k, \lambda) \rightarrow 0, \\ \lambda \int_0^T \left(\rho_{h,k,\lambda} - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{u}_{h,k,\lambda})^t, \nabla \mathbf{v}_{h,k} &\rightarrow 0 \quad \text{as } (h, k, \lambda) \rightarrow 0. \end{aligned}$$

To finish the passage to the limit, we show only that the residual terms R_i vanish as $(h, k, \lambda) \rightarrow 0$. For this, we impose that the sequence of test functions $\mathbf{v}_{h,k}$ is bounded in $L^\infty(0, T; \mathbf{W}^{1,3}(\Omega) \cap \mathbf{L}^\infty(\Omega))$.

We bound R_1 , thanks to estimates *ii)* and *vi)* of Lemma 7, as follows;

$$R_1 \leq C \sum_{n=0}^{N-1} |\rho_h^{n+1} - \rho_h^n| h \|\mathbf{u}_h^{n+1}\| \|\mathbf{v}_h^n\|_{\mathbf{W}^{1,3} \cap \mathbf{L}^\infty} \leq C \frac{h}{k} \rightarrow 0 \quad (\text{thanks to } (S')).$$

by integrating by parts R_2 ,

$$\begin{aligned} R_2 &= - \int_0^T \left(\widehat{\mathbf{u}}_{h,k,\lambda} \cdot \nabla \rho_{h,k,\lambda}, \mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}) \right) \\ &\quad - \int_0^T \left(\nabla \cdot \widehat{\mathbf{u}}_{h,k,\lambda} \rho_{h,k,\lambda}, \mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}) \right) := R_2^1 + R_2^2. \end{aligned}$$

By using the (duality) result of the Aubin-Nitsche type $|u - Q_h u| \leq C h \|u\|_{H^1(\Omega)}$, the first term of R_2 can be estimated as follows:

$$\begin{aligned} R_2^1 &\leq \int_0^T \|\widehat{\mathbf{u}}_{h,k,\lambda}\| \|\nabla \rho_{h,k,\lambda}\|_{L^3(\Omega)} h \|\mathbf{u}_{h,k,\lambda}\| \|\mathbf{v}_{h,k}\|_{\mathbf{W}^{1,\infty}(\Omega)} \\ &\leq C \frac{h}{k^{1/4} \lambda^{3/4}} \|\widehat{\mathbf{u}}_{h,k,\lambda}\|_{L^2(0,T;H_0^1(\Omega))} \lambda^{3/4} k^{1/4} \|\nabla \rho_{h,k,\lambda}\|_{L^\infty(0,T;L^3(\Omega))} \|\mathbf{u}_{h,k,\lambda}\|_{L^2(0,T;H_0^1(\Omega))} \\ &\leq C \frac{h}{k^{1/4} \lambda^{3/4}} \lambda^{3/4} \|\nabla \rho_{h,k,\lambda}\|_{L^4(0,T;L^3(\Omega))} \leq C \frac{h}{k^{1/4} \lambda^{3/4}} \rightarrow 0 \quad (\text{thanks to } (S')). \end{aligned}$$

The convergence to zero of the other term R_2^2 can be made in a similar way.

The term R_3 is handled as follows:

$$\begin{aligned} R_3 &\leq \int_0^T \|\rho_{h,k,\lambda}\|_{L^\infty(\Omega)} |\widehat{\mathbf{u}}_{h,k,\lambda} - \widehat{\mathbf{w}}_{h,k,\lambda}| |\nabla(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}))| \\ &\leq C h \int_0^T \|\widehat{\mathbf{u}}_{h,k,\lambda} - \widehat{\mathbf{w}}_{h,k,\lambda}\| \|\mathbf{u}_{h,k,\lambda}\| \|\mathbf{v}_{h,k}\|_{W^{1,3}(\Omega) \cap L^\infty(\Omega)} \leq C h \rightarrow 0, \end{aligned}$$

where we have used (23) and the stability property of Q_h in the H^1 -norm.

Finally, the convergence to zero of R_4 is easy to deduce. This concludes the proof of Theorem 2.

Remark 27 *The asymptotic behavior as λ goes to zero of the scheme (51)-(54) (see Remark 22), associated to a problem with density-dependent diffusion, remains as an open problem. In fact, when $\lambda \rightarrow 0$, both diffusion coefficients (viscosity and mass diffusion) vanish. Therefore, we find a viscosity-vanishing problem, which is an open problem even in the continuous case.*

A Proof of Lemma 9

We consider the following auxiliary semi-discrete scheme.

Find $\rho^{n+1} \in H^2(\Omega)$ as the solution of the problem:

$$\begin{cases} \frac{\rho^{n+1} - \rho^n}{k} + \mathbf{w}_h^n \cdot \nabla T_m^M \rho^{n+1} - \lambda \Delta \rho^{n+1} = 0 & \text{in } \Omega, \\ \frac{\partial \rho^{n+1}}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0, \end{cases} \quad (62)$$

where

$$T_m^M \rho^{n+1}(\mathbf{x}, t) = \begin{cases} \rho^{n+1} & \text{if } \rho^{n+1}(\mathbf{x}, t) \in [m, M], \\ m & \text{if } \rho^{n+1}(\mathbf{x}, t) < m, \\ M & \text{if } \rho^{n+1}(\mathbf{x}, t) > M. \end{cases}$$

Lemma 28 *Problem (62) has a unique solution.*

Proof Let $R : H^1(\Omega) \rightarrow H^1(\Omega)$ be defined by $Rw = v$, where v is the solution of:

$$\frac{v}{k} - \lambda \Delta v = -\mathbf{w}_h^n \cdot \nabla w + \frac{1}{k} \rho^n \text{ in } \Omega, \quad \frac{\partial v}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0. \quad (63)$$

Notice that $T_m^M w$ is defined a.e. in Q . In addition, as $\frac{1}{2} \nabla \cdot \mathbf{w}_h^n K_m^M w + \frac{1}{k} \rho^n \in L^2(\Omega)$, R is well-defined, that is, there exists a unique $w \in H^2(\Omega)$ such that $Rw = v$.

By using v as a test function in (63) and integrating by parts, we arrive at

$$\frac{1}{k} |v|^2 + \lambda |\nabla v|^2 \leq |\nabla \cdot \mathbf{w}_h^n| \|T_m^M w\|_{L^\infty(\Omega)} |v| + |\mathbf{w}_h^n| \|T_m^M w\|_{L^\infty(\Omega)} |\nabla w| + \frac{1}{k} |\rho^n| |v|.$$

Since $\|T_m^M w\|_{L^\infty(\Omega)} = M$, then $\|v\|_{H^1(\Omega)} \leq C$, with $C > 0$ a constant independent of w . Therefore, by taking any $r \geq C$, one has that if $\|w\|_{H^1(\Omega)} \leq r$, then $\|Rw\|_{H^1(\Omega)} \leq r$. To apply Schauder's fixed point theorem we have to prove that $R : H^1(\Omega) \rightarrow H^1(\Omega)$ is continuous and compact. For this, it suffices to demonstrate that

$$\text{if } w_l \rightharpoonup w \text{ in } H^1(\Omega) \text{ then } Rw_l \rightarrow Rw \text{ in } H^1(\Omega) \text{ as } l \rightarrow \infty.$$

Indeed, from $w_l \rightharpoonup w$ in $H^1(\Omega)$, it holds by compactness that $w_l \rightarrow w$ in $L^2(\Omega)$. Therefore, there exists a subsequence, that to simplify notation is denoted in the same way, such that $w_l \rightarrow w$ a.e. in Ω . By virtue of dominated convergence theorem, we have

$$\mathbf{w}_h^n \cdot \nabla T_m^M w_l + \frac{1}{k} \rho^n \longrightarrow \mathbf{w}_h^n \cdot \nabla T_m^M w + \frac{1}{k} \rho^n \text{ in } H^1(\Omega)', \text{ as } l \rightarrow \infty. \quad (64)$$

On the other hand, the mapping $h \in H^1(\Omega)' \rightarrow z \in H^1(\Omega)$, where z is the solution

$$\frac{1}{k} (z, \bar{z}) - \lambda (\nabla z, \nabla \bar{z}) = \langle h, \bar{z} \rangle_{H^1(\Omega)' H^1(\Omega)} \quad \forall \bar{z} \in H^1(\Omega),$$

is linear and continuous (by Lax-Milgram's theorem). Then, from (64) we have $Rw_l \rightarrow Rw$ in $H^1(\Omega)$.

In conclusion, $R|_{\overline{B}(0,r)} : \overline{B}(0,r) \rightarrow \overline{B}(0,r)$ is continuous and compact. By Schauder's fixed point theorem, we have the desired result after a regularity result for elliptic equations. \square

Theorem 29 *The solution of problem (62) verifies the maximum principle; i.e., if $m \leq \rho^0 \leq M$, then $m \leq \rho^n \leq M$ for each $n \geq 1$.*

Proof Let us first see that if $\rho^n \leq M$, then $\rho^{n+1} \leq M$. By multiplying (62) by $(\rho^{n+1} - M)_+$ and integrating over Ω (we denote $f(x)_+ = \begin{cases} f(x) & \text{si } f(x) > 0, \\ 0 & \text{si } f(x) \leq 0, \end{cases}$) this gives us

$$\left(\frac{\rho^{n+1} - \rho^n}{k}, (\rho^{n+1} - M)_+ \right) + \left(\mathbf{w}_h^n \cdot \nabla T_m^M \rho^{n+1}, (\rho^{n+1} - M)_+ \right) + \lambda (\nabla \rho^{n+1}, \nabla (\rho^{n+1} - M)_+) = 0.$$

By using properties of the positive part function and the fact that $T_m^M \rho^{n+1} = M$ as $(\rho^{n+1} - M)_+ \neq 0$, we rewrite it as

$$\left(\frac{\rho^{n+1} - \rho^n}{k}, (\rho^{n+1} - M)_+ \right) + \lambda (\nabla (\rho^{n+1} - M)_+, \nabla (\rho^{n+1} - M)_+) = 0. \quad (65)$$

Therefore, we deduce from (65) that

$$\left(\rho^{n+1} - \rho^n, (\rho^{n+1} - M)_+ \right) \leq 0.$$

By adding and subtracting M , one arrives at

$$\left((\rho^{n+1} - M) - (\rho^n - M), (\rho^{n+1} - M)_+ \right) \leq 0.$$

Again, by the properties of the positive part function, we obtain

$$\left((\rho^{n+1} - M), (\rho^{n+1} - M)_+ \right) = \left((\rho^{n+1} - M)_+, (\rho^{n+1} - M)_+ \right) = |(\rho^{n+1} - M)_+|^2$$

On the other hand, by the induction hypothesis $\rho^n - M \leq 0$, and then

$$\left(\rho^n - M, (\rho^{n+1} - M)_+ \right) \leq 0$$

Consequently,

$$|(\rho^{n+1} - M)_+|^2 \leq \left(\rho^n - M, (\rho^{n+1} - M)_+ \right) \leq 0,$$

and then $\rho^{n+1} \leq M$ holds.

The proof of the other bound – if $\rho^n \geq m$ then $\rho^{n+1} \geq m$ – can be obtained in the same way. \square

Corollary 30 *Problem (62) is equivalent to problem (24).*

Proof Since ρ^{n+1} the solution of problem (62) verifies the maximum principle, $m \leq \rho^{n+1} \leq M$, then, in particular from the definition of truncating operator T_m^M , one has $T_m^M \rho^{n+1} = \rho^{n+1}$, and problem (62) is rewritten as problem (24). \square

From the uniqueness of the solution of problem (24), we have, in particular, that problem (24) verifies the maximum principle

$$0 < m \leq \rho^n(\mathbf{x}) \leq M, \quad \forall \mathbf{x} \in \Omega \quad \forall n.$$

Therefore, to finish the proof of Lemma 9, it remains to prove strong estimates (independent of λ, h, k) for the ρ^{n+1} solution of (24). For this, it will be fundamental to use the pointwise estimates $m \leq \rho^{n+1} \leq M$ in Q .

We define $\eta^{n+1} = \rho^{n+1} - \oint_{\Omega} \rho^{n+1}$, and hence $\oint_{\Omega} \eta^{n+1} = 0$. Then, the $\|\eta^{n+1}\|_{H^1}$ -norm is equivalent to $|\nabla \eta^{n+1}|$ and the $\|\eta^{n+1}\|_{H^2}$ -norm is equivalent to $|\Delta \eta^{n+1}|$. Since $m \leq \oint_{\Omega} \rho^{n+1} \leq M$, the estimates for $\|\eta^{n+1}\|_{H^1}$ and $\|\eta^{n+1}\|_{H^2}$ imply estimates for $\|\rho^{n+1}\|_{H^1}$ and $\|\rho^{n+1}\|_{H^2}$, respectively.

With this definition of η^{n+1} , problem (24) can be rewritten as:

$$\frac{\eta^{n+1} - (\rho^n - \oint_{\Omega} \rho^{n+1})}{k} + \mathbf{w}_h^n \cdot \nabla \eta^{n+1} - \lambda \Delta \eta^{n+1} = \text{in } \Omega, \quad \frac{\partial \eta^{n+1}}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0.$$

By multiplying by $-2k \Delta \eta^{n+1}$, we arrive at

$$\begin{aligned} & |\nabla \eta^{n+1}|^2 - |\nabla(\rho^n - \oint_{\Omega} \rho^{n+1})|^2 + |\nabla(\rho^{n+1} - \rho^n)|^2 + 2\lambda k |\Delta \eta^{n+1}|^2 \\ & \leq 2k \left(\mathbf{w}_h^n \cdot \nabla \eta^{n+1}, \Delta \eta^{n+1} \right) := K_1. \end{aligned}$$

By integrating by parts in K_1 ,

$$K_1 = -2k \left(\nabla \mathbf{w}_h^n, \nabla \eta^{n+1} \otimes \nabla \eta^{n+1} \right) + k \left(\nabla \cdot \mathbf{w}_h^n, |\nabla \eta^{n+1}|^2 \right).$$

By using the interpolation inequality $\|\nabla \eta^{n+1}\|_{L^4(\Omega)} \leq C \|\eta^{n+1}\|_{L^\infty}^{1/2} |\Delta \eta^{n+1}|^{1/2} \leq C |\Delta \eta^{n+1}|^{1/2}$, we get

$$\begin{aligned} K_1 & \leq Ck \|\mathbf{w}_h^n\| \|\nabla \eta^{n+1}\|_{L^4(\Omega)}^2 \\ & \leq Ck \|\mathbf{w}_h^n\| |\Delta \eta^{n+1}| \leq \frac{C_\varepsilon}{\lambda} k \|\mathbf{w}_h^n\|^2 + \varepsilon \lambda k |\Delta \eta^{n+1}|^2. \end{aligned}$$

Therefore,

$$|\nabla \eta^{n+1}|^2 - |\nabla(\rho^n - \oint_{\Omega} \rho^{n+1})|^2 + \lambda k |\Delta \eta^{n+1}|^2 \leq \frac{C}{\lambda} k \|\mathbf{w}_h^n\|^2.$$

By using that $\nabla(\rho^n - \oint \rho^{n+1}) = \nabla \rho^n = \nabla \eta^n$, we have

$$\lambda \|\eta^{n+1}\|_{H^1}^2 - \lambda \|\eta^n\|_{H^1}^2 + \lambda \|\rho^{n+1} - \rho^n\|_{H^1}^2 + \lambda^2 k \|\eta^{n+1}\|_{H^2}^2 \leq Ck \|\mathbf{w}_h^n\|^2.$$

By summing over n and applying $k \sum_{n=1}^N \|\mathbf{w}_h^n\|^2 \leq C$, we get the following bounds:

$$\lambda \max_{0 \leq n \leq N} \|\rho^n\|_{H^1(\Omega)}^2 \leq C, \quad \lambda^2 k \sum_{n=1}^N \|\rho^n\|_{H^2(\Omega)}^2 \leq C,$$

where $C > 0$ a constant independent of λ, h, k . This concludes the proof of Lemma 9.

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Capítulo 3

Stability and convergence for a complete model of mass diffusion

Stability and convergence for a complete model of mass diffusion

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Abstract

We study a fully discrete scheme for a three-dimensional strongly nonlinear model of mass diffusion, also called the complete Kakhikhov-Smagulov model. This scheme is based on continuous (at most) finite elements for approximating all unknowns (density, velocity and pressure) although the limit density solution of the continuous problem has H^2 -regularity.

The goal is to extend to the complete model, the results already obtained in [7] for a simplified model where λ^2 -terms are not considered, λ being the mass diffusion coefficient.

An approximate discrete maximum principle for the discrete density, weak estimates for the discrete velocity and strong ones for the density are deduced. For this, different arguments to [7] must be introduced, based mainly on an induction process with respect to the time step. From those estimates, compactness and convergence are showed by extending the ideas in [7].

Finally, convergence towards a weak solution of the density-dependent Navier-Stokes problem is also obtained as the diffusion parameter λ goes to zero (jointly with the space and time parameters).

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1 Introduction

1.1 The model

Let $\Omega \subseteq \mathbb{R}^3$ be a bounded domain with boundary Γ that is sufficiently regular. We denote by $[0, T]$ ($0 < T < \infty$) the time interval of observation. We will use the notation $Q = \Omega \times (0, T)$, $\Sigma = \Gamma \times (0, T)$, and $\mathbf{n}(\mathbf{x})$ the outwards unit normal vector to Ω at the point $\mathbf{x} \in \Gamma$.

We consider the (fully nonlinear) equations for viscous fluids with mass diffusion in Q (in

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conservative form):

$$\left\{ \begin{array}{l} (\rho \mathbf{u})_t + \nabla \cdot ((\rho \mathbf{u} - \lambda \nabla \rho) \otimes \mathbf{u} - \lambda \mathbf{u} \otimes \nabla \rho) - \mu \Delta \mathbf{u} \\ \quad + \lambda^2 \nabla \cdot \left(\frac{1}{\rho} \nabla \rho \otimes \nabla \rho \right) + \nabla P = \rho \mathbf{f} \quad \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0 \quad \text{in } Q, \\ \rho_t + \nabla \cdot (\rho \mathbf{u} - \lambda \nabla \rho) = 0 \quad \text{in } Q. \end{array} \right. \quad (1)$$

where the unknowns are $\rho : Q \rightarrow \mathbb{R}^+$, the fluid density, $\mathbf{u} : Q \rightarrow \mathbb{R}^3$, the average velocity field, and $P : Q \rightarrow \mathbb{R}$, the fluid pressure. The data are \mathbf{f} , the external force, and the constants $\mu > 0$ and $\lambda > 0$, viscosity and diffusion coefficients, respectively.

The difference with the model studied in [7] is the presence of the strongly nonlinear term $\lambda^2 \nabla \cdot \left(\frac{1}{\rho} \nabla \rho \otimes \nabla \rho \right)$ in (1)₁.

Here and in what follows, $\mathbf{a} \otimes \mathbf{b}$ denotes the (tensorial product) matrix of two vectors $\mathbf{a} = (a_i)_{i=1}^n$, $\mathbf{b} = (b_i)_{i=1}^n$, with coefficients $(\mathbf{a} \otimes \mathbf{b})_{i,j} = a_i b_j$. Bold-face letters will denote vectorial elements.

Using in (1) the equalities

$$(\rho \mathbf{u})_t + \nabla \cdot ((\rho \mathbf{u} - \lambda \nabla \rho) \otimes \mathbf{u}) = \rho \mathbf{u}_t + ((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla) \mathbf{u},$$

and

$$-\lambda \nabla \cdot (\mathbf{u} \otimes \nabla \rho) = -\lambda (\mathbf{u} \cdot \nabla) \nabla \rho = -\lambda \nabla (\mathbf{u} \cdot \nabla \rho) + \lambda \nabla \cdot (\rho (\nabla \mathbf{u})^t),$$

one arrives at the following (non-conservative) formulation:

$$\left\{ \begin{array}{l} \rho \mathbf{u}_t + ((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla) \mathbf{u} + \nabla \cdot (\lambda \rho (\nabla \mathbf{u})^t - \mu \nabla \mathbf{u}) \\ \quad + \lambda^2 \nabla \cdot \left(\frac{1}{\rho} \nabla \rho \otimes \nabla \rho \right) + \nabla p = \rho \mathbf{f} \quad \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0 \quad \text{in } Q, \\ \rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0 \quad \text{in } Q, \end{array} \right. \quad (2)$$

where $p = P - \lambda \mathbf{u} \cdot \nabla \rho$ is a new potential function.

We complete the model with the boundary conditions

$$\mathbf{u}|_{\Sigma} = 0, \quad \frac{\partial \rho}{\partial \mathbf{n}} \Big|_{\Sigma} = 0, \quad (3)$$

and the initial conditions

$$\rho(0) = \rho_0, \quad \mathbf{u}(0) = \mathbf{u}_0, \quad \text{in } \Omega. \quad (4)$$

Throughout this paper, the initial density will be assumed to satisfy:

$$0 < m \leq \rho_0(\mathbf{x}) \leq M \quad \text{in } \Omega. \quad (5)$$

1.2 Known results

With respect to the mathematical analysis of the model without the λ^2 -term, Kazhikhov and Smagulov ([8]) proved, via a semi-Galerkin method, the existence of global weak solutions under the hypothesis on the coefficients: $\lambda < 2\mu/(M - m)$, and the local existence in time of strong solutions (global for the two-dimensional case).

For the mathematical analysis of the complete model (1), Beirão da Veiga ([2]) and Secchi([9]) established the local existence of strong solutions using linearization and fixed point argument. In ([9]) the existence and uniqueness of global weak solutions in two-dimensional domains are showed by imposing λ/μ small enough, and the asymptotic behavior as $\lambda \rightarrow 0$ towards weak solutions of the density-dependent Navier-Stokes problem. In the case of a positive initial density and 3D domains, Guillén-González ([4]) proved the global existence of weak solutions, and the asymptotic behavior, as $\lambda \rightarrow 0$, towards the density-dependent Navier-Stokes problem. Recently, in ([5]) an iterative method is used to prove the existence and regularity of strong solutions of(1) and some error estimates are also obtained.

In [6], an unconditionally stable, convergent, linear numerical scheme for the 2D model without the λ^2 -term is studied. This scheme is of the backward Euler type (decoupling the computation of the discrete density from the velocity-pressure pair) and approximate with C^0 -finite elements.

For the 3D case and without the λ^2 -term, a conditionally stable, convergent fully discrete scheme is studied in [7]. The main differences given in [7] with respect to [6] are to prove an approximate discrete maximum principle for the discrete density and the asymptotic behavior as $\lambda \rightarrow 0$ towards a weak solution of the density-dependent Navier-Stokes problem.

1.3 Main results of the paper

For simplicity, we consider a uniform partition of $[0, T]$ with time step $k = T/N$: $(t_n = nk)_{n=0}^{n=N}$. We propose a backward Euler type scheme in time which is implicit in diffusion terms, linear and decoupled with respect to the problems for (\mathbf{u}, p) and ρ , jointly with an approximation in space furnished by at most C^0 finite elements for the density, velocity, and pressure.

Throughout this work we consider the notation (\cdot, \cdot) and $|\cdot|$ for the L^2 -inner product and L^2 -norm, respectively.

We present the following scheme:

Initialization: Let $(\mathbf{u}_h^0, \rho_h^0) \in \mathbf{V}_h \times W_h$ be approximations of (\mathbf{u}_0, ρ_0) as $h \rightarrow 0$.

Time step $n + 1$: Given $(\mathbf{u}_h^n, p_h^n, \rho_h^n) \in \mathbf{V}_h \times M_h \times W_h$.

- Find $(\mathbf{w}_h^n, q_h^n) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$ such that, for each $(\bar{\mathbf{w}}_h, \bar{q}_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{M}_h$,

$$\begin{cases} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) &= \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) &= 0. \end{cases} \quad (6)$$

- Find $\rho_h^{n+1} \in W_h$ such that, for each $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (7)$$

- Find $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ such that, for each $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\begin{cases} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k} \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ + c \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) + a \left(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ - \lambda^2 \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^n, \nabla \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{cases} \quad (8)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, q_h \right) = 0, \quad (9)$$

where

$$\mathbf{f}^{n+1} = \frac{1}{k} \int_{t_n}^{t_{n+1}} \mathbf{f}(t) dt,$$

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu \left(\nabla \mathbf{u}, \nabla \mathbf{v} \right) + \lambda \int_{\Omega} \left(\frac{\widetilde{M} + \widetilde{m}}{2} - \rho \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} dx,$$

with $\widetilde{M} > M$ and $0 < \widetilde{m} < m$, and

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) = \frac{1}{2} \left[\left((\mathbf{w} \cdot \nabla) \mathbf{u}, \mathbf{v} \right) - \left((\mathbf{w} \cdot \nabla) \mathbf{v}, \mathbf{u} \right) \right].$$

The following coercivity and continuity properties hold:

$$a(\rho, \mathbf{u}, \mathbf{u}) \geq \left(\mu - \lambda \frac{\widetilde{M} - \widetilde{m}}{2} \right) |\nabla \mathbf{u}|^2 \quad \text{if } \widetilde{m} \leq \rho \leq \widetilde{M}, \quad (10)$$

$$a(\rho, \mathbf{u}, \mathbf{v}) \leq C \|\mathbf{u}\|_{H^1} \|\mathbf{v}\|_{H^1} \quad \text{if } \|\rho\|_{L^\infty(\Omega)} \leq C$$

$$c(\mathbf{w}, \mathbf{u}, \mathbf{u}) = 0, \quad (11)$$

$$c(\mathbf{w}, \mathbf{u}, \mathbf{v}) \leq C \|\mathbf{w}\|_{L^3} \|\mathbf{u}\|_{H^1} \|\mathbf{v}\|_{H^1}. \quad (12)$$

Here and below, we denote by K and C , with or without subscripts, different positive constants, always independent of the discrete parameters (k, h) and, eventually, depending on the diffusion parameter λ . In this last case, we will denote them by C_λ .

In [7], a similar numerical scheme is studied, but for model (1) without the λ^2 -term, i.e. eliminating the term $\lambda^2 \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^n, \nabla \bar{\mathbf{u}}_h \right)$ in (8). We now treat to extend the results

in [7] for the case of the complete model, including the λ^2 -term. The incorporation of this term introduces new difficulties, obligating to change the strategy of main proofs.

In [7], firstly weak estimates for the velocity and pointwise ones for the density are obtained, comparing with an auxiliary scheme where some density terms are truncated. Afterwards, strong estimates for the density are deduced. Finally, convergence is established with compactness arguments.

Now, the relation with a truncate scheme does not work due to the weak estimates for the velocity and strong estimates for the density are not obtained in an independent way. Then, one needs to change the technique developed in [7], obtaining now by an induction process with respect to each time step, firstly pointwise estimates for the density and afterwards the weak estimates for the velocity and strong estimates for the density at the same time. We will see that scheme (6)-(9) is conditionally stable and convergent (imposing the same relation between the space and time parameters as in [7], see (S) below).

We will also obtain, as in [7], convergence towards a weak solution of the density-dependent Navier-Stokes equations, as the diffusion parameter goes to zero jointly with the space and time parameters according to a certain constraint (see (S') below).

Defining in $[0, T]$ the piecewise constant functions $\mathbf{u}_{h,k}, \rho_{h,k}$, such that $\mathbf{u}_{h,k}, \rho_{h,k}|_{(t_{n-1}, t_n]} = \mathbf{u}_h^n, \rho_h^n$, respectively (which we will denote $\mathbf{u}_{h,k,\lambda}, \rho_{h,k,\lambda}$ when studied the asymptotic behavior respect to λ), we arrive at the following results.

Theorem 1 *Assuming hypotheses (H0)-(H5) given in Section 3.1, and the constraint*

$$(S) \quad \lim_{(h,k) \rightarrow 0} \frac{h}{k} = 0,$$

then there exists a convergent subsequence of $(\mathbf{u}_{h,k}, \rho_{h,k})$ (denoted in the same way) as $(h, k) \rightarrow 0$ towards a weak solution (\mathbf{u}, ρ) of problem (1), (3)-(4) (see Definition 3), in the following sense: $(\mathbf{u}_{h,k}, \rho_{h,k}) \rightarrow (\mathbf{u}, \rho)$ in $L^2(0, T; \mathbf{L}^2(\Omega)) \times L^2(0, T; H^1(\Omega))$ -strong, in $L^\infty(0, T; \mathbf{L}^2(\Omega) \times (H^1(\Omega) \cap L^\infty(\Omega)))$ -weak \star , and in $L^2(0, T; \mathbf{H}_0^1(\Omega)) \times L^4(0, T; W^{1,3}(\Omega))$ -weak. Moreover, $\tilde{m} \leq \rho_{h,k} \leq \tilde{M}$.

Theorem 2 *Under the hypotheses of Theorem 1, and extending (H2) by hypothesis (H2') (given in Section 6.1) and changing (S) by*

$$(S') \quad \lim_{(\lambda, h, k) \rightarrow 0} \frac{1}{\lambda} \sqrt{\frac{h}{k}} = 0,$$

then there exists a convergent subsequence of $(\mathbf{u}_{h,k,\lambda}, \rho_{h,k,\lambda})$ as $(h, k, \lambda) \rightarrow 0$ towards a weak solution (\mathbf{u}, ρ) of the density-dependent Navier-Stokes problem (see Definition 19) in the following sense: $\mathbf{u}_{h,k,\lambda} \rightarrow \mathbf{u}$ in $L^2(0, T; \mathbf{L}^2(\Omega))$ -strong, $L^\infty(0, T; \mathbf{L}^2(\Omega))$ -weak \star , in $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -weak, and $\rho_{h,k,\lambda} \rightarrow \rho$ in $L^\infty(Q)$ -weak \star .

The rest of the paper is divided as follows. In Section 2, we give the main ideas for the mathematical analysis of problem (1), (3)-(4). In Section 3, by means of an induction argument, we first prove pointwise estimates for the density, and then energy estimates for the velocity and strong estimates for the density are obtained, using the discrete Laplacian of the density. In Sections 4 and 5, we show compactness for the density and velocity, and the passage to the limit, concluding the proof of Theorem 1. In Section 6, we study the asymptotic behavior as the diffusion parameter goes to zero, proving Theorem 2.

2 Mathematical analysis of the complete Kazhikhov-Smagulov model

To define the concept of weak solutions, we introduce the following space of functions:

$$\begin{aligned}\mathbf{H} &= \{\mathbf{u} \in \mathbf{L}^2(\Omega) : \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \Gamma\}, \\ \mathbf{V} &= \{\mathbf{u} \in \mathbf{H}_0^1(\Omega) : \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega\}, \\ L_0^2(\Omega) &= \left\{ p \in L^2(\Omega) : \int_{\Omega} p(\mathbf{x}) d\mathbf{x} = 0 \right\}, \\ H_N^2(\Omega) &= \left\{ \rho \in H^2(\Omega) : \frac{\partial \rho}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega, \int_{\Omega} \rho(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x} \right\}.\end{aligned}$$

In $\mathbf{H}_0^1(\Omega)$, the $\|\mathbf{u}\|_{H^1(\Omega)}$ -norm is equivalent to $\|\nabla \mathbf{u}\|_{L^2}$, that we denote by $|\nabla \mathbf{u}|$ in the sequel. On the other hand, $H_N^2(\Omega)$ is a affine space, $H_N^2(\Omega) = \frac{1}{|\Omega|} \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x} + H_{N,0}^2(\Omega)$, and $\|\nabla \rho\|_{H^1(\Omega)}$ and $|\Delta \rho|$ are equivalent semi-norms in $H_N^2(\Omega)$.

Definition 3 A pair (ρ, \mathbf{u}) is said to be a weak solution of (1), (3)-(4) in $(0, T)$ if it verifies:

a)

$$\begin{aligned}\mathbf{u} &\in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V}), \\ \rho &\in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H_N^2(\Omega)), \\ 0 &< m \leq \rho(\mathbf{x}, t) \leq M, \quad \forall (\mathbf{x}, t) \in Q.\end{aligned}$$

b) $\forall \phi \in C^1([0, T]; \mathbf{V})$ such that $\phi(T) = 0$,

$$\begin{aligned}&\int_0^T \left\{ -\left(\mathbf{u}, \rho \phi_t + (\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla \phi \right) + \left(\mu \nabla \mathbf{u} - \lambda \rho (\nabla \mathbf{u})^t, \nabla \phi \right) \right\} dt \\ &- \lambda^2 \int_0^T \left(\frac{1}{\rho} \nabla \rho \otimes \nabla \rho, \nabla \phi \right) dt = \int_0^T \left(\rho \mathbf{f}, \phi \right) dt + \left(\rho_0 \mathbf{u}_0, \phi(0) \right).\end{aligned}$$

c) The equation of mass diffusion (1)_c is satisfied almost everywhere in Q .

Theorem 4 ([9]) Let $\mathbf{u}_0 \in \mathbf{H}$, $\rho_0 \in H^1(\Omega)$, and $\mathbf{f} \in L^2(0, T; \mathbf{L}^{6/5}(\Omega))$. If λ/μ is sufficiently small, then there exists a weak solution of problem (1), (3)-(4) in $(0, T)$.

Outline of proof: Here, we only give an outline of the proof for the reader's convenience because some ideas of the proof will be use later. We will only see the manner of getting the estimates assuming (ρ, \mathbf{u}) a sufficiently regular solution of (1), (3)-(4).

Applying the maximum principle to the density parabolic equation (1)_c and from (5),

$$0 < m \leq \rho(\mathbf{x}, t) \leq M \quad \text{in } Q.$$

Multiplying (1)_c by $-\lambda\Delta\rho$, integrating over Ω , integrating by parts in the convective term, and taking into account the interpolation inequality

$$\|\nabla\rho\|_{L^4(\Omega)} \leq C_\Omega\|\rho\|_{L^\infty(\Omega)}|\Delta\rho|^{1/2}, \quad (13)$$

one arrives at

$$\frac{d}{dt}|\nabla\rho|^2 + \lambda^2|\Delta\rho|^2 \leq C_0|\nabla\mathbf{u}|^2. \quad (14)$$

Adding the momentum system (1)_a by \mathbf{u} to the density equation (1)_c by $\frac{1}{2}\mathbf{u} \cdot \mathbf{u}$, integrated over Ω , the following energy equality holds:

$$\frac{1}{2}\frac{d}{dt}\int_\Omega\rho|\mathbf{u}|^2d\mathbf{x} + \mu|\nabla\mathbf{u}|^2 = \lambda\int_\Omega\rho(\nabla\mathbf{u})^t : \nabla\mathbf{u}d\mathbf{x} + \lambda^2\left(\frac{1}{\rho}\nabla\rho \otimes \nabla\rho, \nabla\mathbf{u}\right) + (\rho\mathbf{f}, \mathbf{u}). \quad (15)$$

Reasoning as in the simplified model (see [8]), one has

$$\lambda\int_\Omega\rho(\nabla\mathbf{u})^t : \nabla\mathbf{u}d\mathbf{x} \leq \lambda\frac{M-m}{2}|\nabla\mathbf{u}|^2 = C_1\lambda|\nabla\mathbf{u}|^2. \quad (16)$$

To estimate the second term on the right-hand side of (15), we use the interpolation inequality (13), the pointwise estimate for the density $m \leq \rho \leq M$, and *Young's* inequality, getting

$$\lambda^2\left|\left(\frac{1}{\rho}\nabla\rho \otimes \nabla\rho, \nabla\mathbf{u}\right)\right| \leq \varepsilon_1\mu\lambda^2|\Delta\rho|^2 + \frac{C_2\lambda^2}{\varepsilon_1\mu}|\nabla\mathbf{u}|^2.$$

The last term of (15) is easily bounded by

$$(\rho\mathbf{f}, \mathbf{u}) \leq \frac{\mu}{4}|\nabla\mathbf{u}|^2 + C\|\mathbf{f}\|_{L^{6/5}(\Omega)}^2.$$

Compiling the above estimates into (15), we arrive at

$$\frac{d}{dt}\int_\Omega\rho|\mathbf{u}|^2d\mathbf{x} + \mu|\nabla\mathbf{u}|^2 \leq \left(\frac{1}{4} + C_1\frac{\lambda}{\mu} + \frac{C_2\lambda^2}{\varepsilon_1\mu^2}\right)\mu|\nabla\mathbf{u}|^2 + \varepsilon_1\mu\lambda^2|\Delta\rho|^2 + C\|\mathbf{f}\|_{L^{6/5}(\Omega)}^2. \quad (17)$$

Adding up (17) to (14) multiplied by $\mu\varepsilon_2$ with $\varepsilon_2 > 0$ to be chosen later on, this gives us

$$\begin{aligned} \varepsilon_2\mu\lambda\frac{d}{dt}|\nabla\rho|^2 + \frac{d}{dt}|\sqrt{\rho}\mathbf{u}|^2 + (\varepsilon_2 - \varepsilon_1)\mu\lambda^2|\Delta\rho|^2 \\ + \left(\frac{3}{4} - C_1\frac{\lambda}{\mu} - \frac{C_2\lambda^2}{\varepsilon_1\mu^2} - \varepsilon_2C_0\right)\mu|\nabla\mathbf{u}|^2 \leq C\|\mathbf{f}\|_{L^{6/5}(\Omega)}^2. \end{aligned}$$

Selecting $\varepsilon_1 = \varepsilon_2/2$ and ε_2 and λ/μ small enough such that $C_1 \frac{\lambda}{\mu} + \frac{C_2}{\varepsilon_1} \left(\frac{\lambda}{\mu}\right)^2 + \varepsilon_2 C_0 \leq 1/4$, we get

$$\varepsilon_2 \mu \lambda \frac{d}{dt} |\nabla \rho|^2 + \frac{d}{dt} |\sqrt{\rho} \mathbf{u}|^2 + \frac{\varepsilon_2}{2} \lambda^2 \mu |\Delta \rho|^2 + \frac{\mu}{2} |\nabla \mathbf{u}|^2 \leq C \|\mathbf{f}\|_{L^{6/5}(\Omega)}^2.$$

Integrating for $t \in (0, T)$ and bounding from below the density, we obtain

$$\max_{0 \leq t \leq T} \left(\varepsilon_2 \mu \lambda |\nabla \rho(t)|^2 + m |\mathbf{u}|^2 \right) + \frac{1}{2} \int_0^T \left(\varepsilon_2 \mu \lambda^2 |\Delta \rho(t)|^2 + \mu |\nabla \mathbf{u}(t)|^2 \right) dt \leq C.$$

On the other hand, the following ‘‘fractional in time estimate’’ holds ([1]):

$$\int_0^{T-\delta} |\mathbf{u}(t+\delta) - \mathbf{u}(t)|^2 dt \leq C \delta^{1/2} \quad \forall \delta \in (0, T).$$

This estimate implies compactness for the velocity \mathbf{u} in $L^2(0, T; \mathbf{L}^2(\Omega))$ ([10]). Then, existence of weak solutions can be deduced in a standard form ([1]), using the *Faedo-Galerkin* method.

3 A priori estimates for the scheme

Since (6)-(9) are algebraic linear systems, they will be well-posed (that is, there exists a unique solution) as a consequence of the weak estimates of scheme (7)-(9) given in this section.

3.1 Hypotheses

Throughout this work we will suppose the following hypotheses:

(H0) Regularity for the data:

$$\mathbf{u}_0 \in \mathbf{V}, \rho_0 \in H_N^2(\Omega) \text{ with } 0 < m \leq \rho_0 \leq M \text{ in } \Omega, \text{ and } \mathbf{f} \in L^2(0, T; \mathbf{L}^{6/5}(\Omega)).$$

Assume λ/μ sufficiently small.

(H1) Assume Ω an open, bounded set of \mathbb{R}^3 , whose boundary is polyhedral and such that the continuous dependencies in the H^2 -norm of the *Poisson-Neumann* problem and in the $\mathbf{H}^2 \times H^1$ -norm of the *Stokes* hold (see (23) and (31) respectively). This is satisfied, for example, if Ω is convex ([3]).

(H2) The triangulation of Ω and the discrete spaces verify:

- the inverse inequality:

$$\begin{aligned} |\nabla \bar{\rho}_h| &\leq C h^{-1} |\bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h, \\ \|\bar{\rho}_h\|_{L^\infty(\Omega)} + \|\nabla \bar{\rho}_h\|_{L^3(\Omega)} &\leq C h^{-1/2} |\nabla \bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h, \\ \|\nabla \bar{\rho}_h\|_{L^4(\Omega)} &\leq C h^{-3/4} |\nabla \bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h, \end{aligned}$$

- and the interpolation errors:

$$\begin{aligned}
\|\bar{\mathbf{u}} - \tilde{J}_h \bar{\mathbf{u}}\|_{H^1(\Omega)} + \|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{H^1(\Omega)} &\leq C h \|\bar{\mathbf{u}}\|_{H^2(\Omega)} \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega), \\
|\bar{p} - \tilde{K}_h \bar{p}| + |\bar{p} - K_h \bar{p}| &\leq C h \|\bar{p}\|_{H^1(\Omega)} \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega), \\
|\bar{\rho} - I_h \bar{\rho}| + h \|\bar{\rho} - I_h \bar{\rho}\|_{H^1(\Omega)} &\leq C h^2 \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega), \\
\|\bar{\rho} - I_h \bar{\rho}\|_{W^{1,3}(\Omega) \cap L^\infty(\Omega)} &\leq C h^{1/2} \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega), \\
\|\bar{\rho} - I_h \bar{\rho}\|_{W^{1,4}(\Omega)} &\leq C h^{1/4} \|\bar{\rho}\|_{H^2(\Omega)} \quad \forall \bar{\rho} \in H^2(\Omega),
\end{aligned}$$

where $J_h, \tilde{J}_h, K_h, \tilde{K}_h$ and I_h are interpolation operators from $\mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ into $\mathbf{V}_h, \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$ into $\tilde{\mathbf{V}}_h, H^1(\Omega) \cap L_0^2(\Omega)$ into $M_h, H^1(\Omega) \cap L_0^2(\Omega)$ into $\tilde{M}_h,$ and $H^2(\Omega)$ into $W_h,$ respectively.

- (H3) Inf-sup conditions. There exists $\beta > 0$ (independent of h) such that, $\forall \bar{p}_h \in M_h$ and $\forall \bar{q}_h \in \tilde{M}_h,$

$$\begin{aligned}
\|\bar{p}_h\|_{L_0^2(\Omega)} &\leq \beta \sup_{\bar{\mathbf{u}}_h \in \mathbf{V}_h \setminus \{0\}} \frac{(\bar{p}_h, \nabla \cdot \bar{\mathbf{u}}_h)}{|\nabla \bar{\mathbf{u}}_h|}, \\
\|\bar{q}_h\|_{L_0^2(\Omega)} &\leq \beta \sup_{\bar{\mathbf{w}}_h \in \tilde{\mathbf{V}}_h \setminus \{0\}} \frac{(\bar{q}_h, \nabla \cdot \bar{\mathbf{w}}_h)}{|\nabla \bar{\mathbf{w}}_h|}.
\end{aligned}$$

- (H4) Compatibility condition between \tilde{M}_h and W_h :

$$(W_h \cdot W_h) \cap L_0^2(\Omega) \subset \tilde{M}_h,$$

that is,

$$\forall \bar{\rho}_h^1, \bar{\rho}_h^2 \in W_h, \quad \bar{\rho}_h^1 \bar{\rho}_h^2 - \frac{1}{|\Omega|} \int_{\Omega} \bar{\rho}_h^1(\mathbf{x}) \bar{\rho}_h^2(\mathbf{x}) d\mathbf{x} \in \tilde{M}_h.$$

- (H5) Compatibility condition between (M_h, \tilde{M}_h) :

$$M_h \subset \tilde{M}_h.$$

For instance, a way of defining the discrete spaces $(W_h, \mathbf{V}_h, M_h, \tilde{\mathbf{V}}_h, \tilde{M}_h)$ satisfying (H2)-(H5) is the following: Let $\{\mathcal{T}_h\}_{h>0}$ be a regular, quasi-uniform family of triangulations of $\Omega,$ with $h = \max_{K \in \mathcal{T}_h} h_K$ (h_K =diameter of K), and

$$X_h^l = \{x_h \in C^0(\bar{\Omega}) \text{ such that } x_h|_K \in \mathbb{P}_l(K) \forall K \in \mathcal{T}_h\}.$$

Then, we define $W_h = X_h^1$. There are several possibilities for (\mathbf{V}_h, M_h) ([3]), by using the *Taylor-Hood* element $(\mathbb{P}_2 \times \mathbb{P}_1)$ or the mini-element $(\mathbb{P}_1 + \text{bubble} \times \mathbb{P}_1),$ for instance. For the spaces $(\tilde{\mathbf{V}}_h, \tilde{M}_h)$ we choose $\tilde{\mathbf{V}}_h = \mathbf{X}_h^3 \cap \mathbf{H}_0^1(\Omega)$ and $\tilde{M}_h = X_h^2 \cap L_0^2(\Omega).$

Note that if $\mathbf{V}_h = \tilde{\mathbf{V}}_h$ and $M_h = \tilde{M}_h$ we need not consider the projection problem (6).

3.2 Discrete maximum principle

The proof of the following lemma can be found in [7].

Lemma 5 *Fixed $n : 0 \leq n \leq N - 1$, if the discrete velocities $(\mathbf{w}_h^l)_{l=0}^n$ satisfy $k \sum_{l=0}^n |\nabla \mathbf{w}_h^l|^2 \leq C_d$ with $C_d > 0$ independent of h, k, n , and λ , then there exist h_0 and k_0 (independent of n) such that for any $h \leq h_0, k \leq k_0$ satisfying (S), there exists a unique solution ρ_h^{n+1} of (7), which also satisfies the pointwise estimates*

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M} \quad \text{in } \Omega.$$

3.3 Weak estimates for the velocity and strong ones for the density

Consider the linear operator $\Delta_h : W_h \rightarrow W_h$ defined as

$$-\left(\Delta_h \rho_h, \bar{\rho}_h\right) = \left(\nabla \rho_h, \nabla \bar{\rho}_h\right) \quad \forall \bar{\rho}_h \in W_h. \quad (18)$$

Then, the discrete density equation (7) can be rewritten as

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h\right) + \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h\right) - \lambda \left(\Delta_h \rho_h^{n+1}, \bar{\rho}_h\right) = 0. \quad (19)$$

In the following result of discrete interpolations, in particular we will see a discrete version of (13).

Lemma 6 *There exists $C = C(\Omega) > 0$ such that*

$$\|\nabla \rho_h^{n+1}\|_{L^3(\Omega)} \leq C |\nabla \rho_h^{n+1}|^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2}, \quad (20)$$

$$\|\nabla \rho_h^{n+1}\|_{L^4(\Omega)} \leq C \left(h^{1/4} |\Delta_h \rho_h^{n+1}| + \|\rho_h^{n+1}\|_{L^\infty(\Omega)}^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2} \right). \quad (21)$$

Proof: Estimate (20) is obtained in [7].

To prove (21), one obtains firstly

$$\|\nabla \rho_h^{n+1}\|_{L^4(\Omega)} \leq C \left(h^{1/4} |\Delta_h \rho_h^{n+1}| + \|\rho^{n+1}(h)\|_{L^\infty(\Omega)}^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2} \right), \quad (22)$$

based on the inverse inequality $\|\nabla \bar{\rho}_h\|_{L^4(\Omega)} \leq C_\Omega h^{-3/4} |\nabla \bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h$, the approximation inequality $\|\nabla \rho - \nabla I_h \rho\|_{L^4(\Omega)} \leq C_\Omega h^{1/4} \|\rho\|_{H^2(\Omega)}$, and the interpolation inequality (13), where $\rho^{n+1}(h) \in H^2(\Omega)$ is the solution of the following elliptic problem

$$-\Delta \rho^{n+1}(h) = -\Delta_h \rho_h^{n+1} \quad \text{in } \Omega, \quad \frac{\partial \rho^{n+1}(h)}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0, \quad \int_{\Omega} \rho^{n+1}(h)(\mathbf{x}) d\mathbf{x} = 0. \quad (23)$$

To obtain (21) from (22), it is necessary to reason as in [7] comparing $\rho^{n+1}(h)$ with ρ_h^{n+1} , using the inverse inequality $\|\bar{\rho}_h\|_{L^\infty(\Omega)} \leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1} \quad \forall \bar{\rho}_h \in W_h$ and the interpolation error $\|\rho - I_h \rho\|_{L^\infty(\Omega)} \leq C_\Omega h^{1/2} \|\rho\|_{H^2(\Omega)} \quad \forall \rho \in H^2(\Omega)$. \square

Lemma 7 Fixed $n : 0 \leq n \leq N - 1$, assume

$$0 < \tilde{m} \leq \rho_h^n, \rho_h^{n+1} \leq \tilde{M} \quad \text{in } \Omega$$

and

$$\frac{1}{16C_2} \lambda^2 \mu k |\Delta_h \rho_h^n|^2 + \frac{1}{2} \mu k |\nabla \mathbf{u}_h^n|^2 \leq C_d,$$

with $C_d > 0$ independent of h, k, n and λ . Then there exist h_0 and k_0 so that for any $h \leq h_0$, $k \leq k_0$ satisfying (S), there exists a unique solution $(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1})$ of scheme (6)-(9), and the following estimates hold:

$$\begin{cases} |\sqrt{\rho_h^{n+1}} \mathbf{u}_h^{n+1}|^2 - |\sqrt{\rho_h^n} \mathbf{u}_h^n|^2 + |\sqrt{\rho_h^n} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 + \frac{3\mu}{4} k |\nabla \mathbf{u}_h^{n+1}|^2 \\ \leq k C_1 \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 + \varepsilon \mu \lambda^2 k \left(|\Delta_h \rho_h^{n+1}|^2 + |\Delta_h \rho_h^n|^2 \right), \end{cases} \quad (24)$$

$$\lambda |\nabla \rho_h^{n+1}|^2 - \lambda |\nabla \rho_h^n|^2 + \lambda |\nabla (\rho_h^{n+1} - \rho_h^n)|^2 + \frac{\lambda^2}{2} k |\Delta_h \rho_h^{n+1}|^2 \leq C_2 k |\nabla \mathbf{u}_h^n|^2, \quad (25)$$

with $C_1, C_2 > 0$ independent of h, k, n , and λ , and $\varepsilon > 0$ arbitrarily small (also independent of h, k and λ).

Proof: Taking $\bar{\mathbf{u}}_h = 2k \mathbf{u}_h^{n+1}$ and $\bar{p}_h = p_h^{n+1}$ in (8)-(9), using the identity $(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2$ and properties (10) and (11), one has

$$\begin{cases} \left(|\sqrt{\rho_h^{n+1}} \mathbf{u}_h^{n+1}|^2 - |\sqrt{\rho_h^n} \mathbf{u}_h^n|^2 + |\sqrt{\rho_h^n} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 \right) + \left(\mu - \lambda(\tilde{M} - \tilde{m}) \right) k |\nabla \mathbf{u}_h^{n+1}|^2 \\ \leq k C_1 \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 + A, \end{cases} \quad (26)$$

where $A = 2k \frac{\lambda^2}{\tilde{m}} \|\nabla \rho_h^{n+1}\|_{L^4(\Omega)} \|\nabla \rho_h^n\|_{L^4(\Omega)} |\nabla \mathbf{u}_h^{n+1}|$ and $C_1 = C_1(\mu) > 0$ a constant independent of (h, k, λ) , and n .

In view of inequality (21), the term A can be bounded by

$$\begin{aligned} A &\leq C k \lambda^2 \left(h^{1/2} |\Delta_h \rho_h^{n+1}| |\Delta_h \rho_h^n| \right. \\ &\quad \left. + \tilde{M}^{1/2} h^{1/4} \left(|\Delta_h \rho_h^{n+1}| |\Delta_h \rho_h^n|^{1/2} + |\Delta_h \rho_h^n| |\Delta_h \rho_h^{n+1}|^{1/2} \right) \right. \\ &\quad \left. + \tilde{M} |\Delta_h \rho_h^{n+1}|^{1/2} |\Delta_h \rho_h^n|^{1/2} \right) |\nabla \mathbf{u}_h^{n+1}| \\ &:= A_1 + A_2 + A_3 + A_4. \end{aligned}$$

By hypothesis $|\Delta_h \rho_h^n| \leq C_d^{1/2} / (\lambda \mu^{1/2} k^{1/2})$, then the term A_1 is bounded as follows:

$$\begin{aligned} A_1 &\leq \frac{C C_d^{1/2}}{\mu^{1/2}} h^{1/2} k^{1/2} \lambda |\Delta_h \rho_h^{n+1}| |\nabla \mathbf{u}_h^{n+1}| \\ &\leq k \frac{C_0}{\varepsilon_1} \frac{h}{k} \lambda^2 \mu |\Delta_h \rho_h^{n+1}|^2 + \varepsilon_1 \mu k |\nabla \mathbf{u}_h^{n+1}|^2, \end{aligned}$$

for any $\varepsilon_1 > 0$ and $C_0 = C_0(\mu)$. Thus, taking $h \leq h_0$ and $k \leq k_0$ such that $\frac{C_0 h}{\varepsilon_1 k} \leq \varepsilon_2$ with $\varepsilon_2 > 0$ sufficiently small (thanks to hypothesis (S)), we arrive at

$$A_1 \leq \varepsilon_2 \lambda^2 \mu k |\Delta_h \rho_h^{n+1}|^2 + \varepsilon_1 \mu k |\nabla \mathbf{u}_h^{n+1}|^2.$$

The term A_2 has a similar treatment as A_1 ,

$$\begin{aligned} A_2 &\leq C k \lambda^2 h^{1/4} \frac{C_d^{1/4}}{\lambda^{1/2} \mu^{1/4} k^{1/4}} |\Delta_h \rho_h^{n+1}| |\nabla \mathbf{u}_h^{n+1}| \\ &\leq \varepsilon_2 \lambda^2 \mu k |\Delta_h \rho_h^{n+1}|^2 + \varepsilon_1 \mu k |\nabla \mathbf{u}_h^{n+1}|^2, \end{aligned}$$

taking $h \leq h_0$ and $k \leq k_0$ such that $\frac{C}{\varepsilon_1} \lambda \left(\frac{h}{k}\right)^{1/2} \leq \varepsilon_2$, where $C = C(\tilde{m}, \tilde{M}, \Omega, \mu)$.

Analogously, we estimate the term A_3 by

$$\begin{aligned} A_3 &\leq 2C k \lambda^2 h^{1/4} \frac{C_d^{1/4}}{\lambda^{1/2} \mu^{1/4} k^{1/4}} |\Delta_h \rho_h^n|^{1/2} |\Delta_h \rho_h^{n+1}|^{1/2} |\nabla \mathbf{u}_h^{n+1}| \\ &\leq \varepsilon_2 \mu \lambda^2 k \left(|\Delta_h \rho_h^n|^2 + |\Delta_h \rho_h^{n+1}|^2 \right) + \varepsilon_1 \mu k |\nabla \mathbf{u}_h^{n+1}|^2 \end{aligned}$$

selecting $h \leq h_0$ and $k \leq k_0$ such that $\frac{C}{\varepsilon_1} \lambda \left(\frac{h}{k}\right)^{1/2} \leq \varepsilon_2$, where $C = C(\tilde{m}, \tilde{M}, \Omega, \mu)$.

For A_4 , we bound as follows:

$$A_4 \leq \varepsilon_2 \mu \lambda^2 k \left(|\Delta_h \rho_h^{n+1}|^2 + |\Delta_h \rho_h^n|^2 \right) + k C \frac{\lambda^2}{\mu} |\nabla \mathbf{u}_h^{n+1}|^2,$$

where $C = C(\tilde{m}, \tilde{M}, \Omega, \varepsilon_3)$.

Using the previous estimates for the A_i terms in (26), we get

$$\begin{aligned} &|\sqrt{\rho_h^{n+1}} \mathbf{u}_h^{n+1}|^2 - |\sqrt{\rho_h^n} \mathbf{u}_h^n|^2 + |\sqrt{\rho_h^n} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 \\ &+ \left(1 - \frac{\lambda}{\mu} (\tilde{M} - \tilde{m}) - C \frac{\lambda^2}{\mu^2} - 4\varepsilon_1 \right) \mu k |\nabla \mathbf{u}_h^{n+1}|^2 \\ &\leq k C_1 \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 + \varepsilon_2 \mu \lambda^2 k \left(4|\Delta_h \rho_h^{n+1}|^2 + 2|\Delta_h \rho_h^n|^2 \right). \end{aligned} \quad (27)$$

Accordingly, choosing $\varepsilon_1, \varepsilon_2$ and λ/μ sufficiently small, one arrives at (24).

To obtain (25) we write the scheme for the density (7) as (19). Taking $\bar{\rho}_h = \lambda k \Delta_h \rho_h^{n+1}$ as a test function in (19), $\bar{\rho}_h = \lambda(\rho_h^{n+1} - \rho_h^n)$ in (18) for $\rho_h = \rho_h^{n+1}$, and using the identity $(a - b, a) = \frac{1}{2} (|a|^2 - |b|^2 + |a - b|^2)$, we arrive at:

$$\begin{aligned} &\frac{\lambda}{2} \left(|\nabla \rho_h^{n+1}|^2 - \lambda |\nabla \rho_h^n|^2 + \lambda |\nabla (\rho_h^{n+1} - \rho_h^n)|^2 \right) + \lambda^2 k |\Delta_h \rho_h^{n+1}|^2 \\ &= \lambda k \left(\mathbf{w}_h^n \cdot \nabla \rho_h^{n+1}, \Delta_h \rho_h^{n+1} \right) := I. \end{aligned} \quad (28)$$

As $-\Delta \rho^{n+1}(h) = -\Delta_h \rho_h^{n+1}$, where $\rho^{n+1}(h)$ is defined in (23) we may write the term I_1 of (28) as

$$I = \lambda k \left(\mathbf{w}_h^n \cdot \nabla \rho(h), \Delta \rho(h) \right) + \lambda k \left(\mathbf{w}_h^n \cdot \nabla (\rho_h^{n+1} - \rho(h)), \Delta_h \rho_h^{n+1} \right).$$

We estimate I as in [7]:

$$\begin{aligned} I &\leq C \lambda k |\nabla \mathbf{u}_h^n| \left(h^{1/2} |\Delta \rho_h^{n+1}| + \widetilde{M} \right) |\Delta_h \rho_h^{n+1}| \\ &\leq C \lambda k |\nabla \mathbf{u}_h^n| h^{1/2} |\Delta_h \rho_h^{n+1}|^2 + C_2 k |\nabla \mathbf{u}_h^n|^2 + \frac{1}{4} \lambda^2 k |\Delta_h \rho_h^{n+1}|^2, \end{aligned}$$

where we have used the stability property $|\nabla \mathbf{w}_h^n| \leq |\nabla \mathbf{u}_h^n|$ of problem (6) (see the proof of Corollary 10 below).

Making use of the hypothesis $\frac{1}{2} \mu k |\nabla \mathbf{u}_h^n|^2 \leq C_d$, and selecting $h \leq h_0$ and $k \leq k_0$ such that $\frac{C}{\lambda} \sqrt{\frac{h}{k}} \leq \frac{1}{4}$, we get (25). \square

To prove stability of the scheme, we consider that the approximations of the data $(\rho_0, \mathbf{u}_0, \mathbf{f})$ satisfying the following properties:

$$\begin{aligned} 0 &< \tilde{m} \leq \rho_h^0 \leq \widetilde{M}, \\ \frac{1}{C_2} \mu \lambda |\nabla \rho_h^0|^2 &\leq K_1, \quad |\sqrt{\rho_h^0} \mathbf{u}_h^0|^2 \leq K_2, \\ \frac{1}{2} \mu k |\nabla \mathbf{u}_h^0|^2 &\leq K_3, \quad \frac{1}{16 C_2} \lambda^2 \mu k |\Delta_h \rho_h^0|^2 \leq K_4, \\ C_1 k \sum_{n=0}^{N-1} \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 &\leq K_5, \end{aligned}$$

where $K_i > 0$ are constants independent of h , k , and λ .

These properties can be guaranteed thanks to hypotheses (H0) and (H2), considering $\rho_h^0 = I_h \rho_0$ and $\mathbf{u}_h^0 = J_h \mathbf{u}_0$. Indeed, the pointwise estimates for ρ_h^0 are deduced from $0 < m \leq \rho_0 \leq M < \infty$ and from the error estimate $\|\rho_0 - I_h \rho_0\|_{L^\infty(\Omega)} \leq C h^{1/2} \|\rho_0\|_{H^2(\Omega)}$. In view of the stability of the interpolation operators, $\|\rho_h^0\|_{H^1(\Omega)} \leq C \|\rho_0\|_{H^1(\Omega)}$ and $|\nabla \mathbf{u}_h^0| \leq C |\nabla \mathbf{u}_0|$, there exist $K_1 > 0$, $K_2 > 0$ and $K_3 > 0$ such that $\frac{1}{C_2} \mu \lambda |\nabla \rho_h^0|^2 \leq K_1$, $|\sqrt{\rho_h^0} \mathbf{u}_h^0|^2 \leq K_2$, and $\mu k |\nabla \mathbf{u}_h^0|^2 \leq K_3$. To prove $\lambda^2 \mu k |\Delta_h \rho_h^0|^2 \leq K_4$, we take $\rho_h = \rho_h^0$ and $\bar{\rho}_h = -\Delta_h \rho_h^0$ into (18), arriving at

$$\begin{aligned} |\Delta_h \rho_h^0|^2 &\leq -\left(\nabla \rho_h^0, \nabla \Delta_h \rho_h^0 \right) = \left(\nabla \rho_0 - \nabla \rho_h^0, \nabla \Delta_h \rho_h^0 \right) - \left(\nabla \rho_0, \nabla \Delta_h \rho_h^0 \right) \\ &\leq \frac{C}{h} |\nabla(\rho_0 - \nabla I_h \rho_0)| |\Delta_h \rho_h^0| + |\Delta \rho_0| |\Delta_h \rho_h^0| \\ &\leq C \|\rho_0\|_{H^2(\Omega)} |\Delta_h \rho_h^0|, \end{aligned}$$

where we have used the inverse inequality $\|\bar{\rho}_h\|_{H^1(\Omega)} \leq \frac{C}{h} |\bar{\rho}_h| \quad \forall \bar{\rho}_h \in W_h$ and the interpolation error $|\nabla \bar{\rho} - I_h \bar{\rho}| \leq C h \|\bar{\rho}\|_{H^2(\Omega)}$. Therefore, we may find a constant $K_4 > 0$ such that $\lambda^2 \mu k |\Delta_h \rho_h^0|^2 \leq K_4$. Finally, $C_1 k \sum_{n=0}^{N-1} \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 \leq K_5$ is easily deduced from the regularity $\mathbf{f} \in L^2(0, T, \mathbf{L}^{6/5}(\Omega))$.

Theorem 8 Assume (S) and (H0) – (H5). Then, there exist $h_0 > 0$ and $k_0 > 0$ (depending on λ) so that for any $h \leq h_0$, $k \leq k_0$, and for each $n = 0, \dots, N - 1$, the discrete problem (7)-(9) has a unique solution $(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, p_h^{n+1})$ which verifies the following estimates:

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M} \quad \text{in } \Omega \quad (29)$$

and

$$\begin{aligned} & \frac{1}{4C_2} \mu \lambda |\nabla \rho_h^{n+1}|^2 + |\sqrt{\rho_h^{n+1}} \mathbf{u}_h^{n+1}|^2 - \left(\frac{1}{4C_2} \mu \lambda |\nabla \rho_h^n|^2 + |\sqrt{\rho_h^n} \mathbf{u}_h^n|^2 \right) \\ & + |\sqrt{\rho_h^n} (\mathbf{u}_h^{n+1} - \mathbf{u}_h^n)|^2 + \frac{1}{4C_2} \mu \lambda |\nabla (\rho_h^{n+1} - \rho_h^n)|^2 + \frac{3\mu}{4} k |\nabla \mathbf{u}_h^{n+1}|^2 \\ & + \frac{1}{8C_2} \mu \lambda^2 k |\Delta_h \rho_h^{n+1}|^2 \leq C_1 k \|\mathbf{f}^{n+1}\|_{L^{6/5}(\Omega)}^2 + \varepsilon \mu \lambda^2 k |\Delta_h \rho_h^n|^2 + \frac{1}{4} \mu k |\nabla \mathbf{u}_h^n|^2. \end{aligned} \quad (30)$$

where $C_1 > 0$ and $C_2 > 0$ are constants independent of h , k , n , and λ , and $\varepsilon > 0$ is sufficiently small (which appears in Lemma 7).

Proof: We proceed by induction on n . Let us define $C_d = K_1 + K_2 + K_3 + K_4 + K_5$. With such a constant C_d , the hypotheses of Lemma 5 are satisfied when $n = 0$, then $0 < \tilde{m} \leq \rho_h^1 \leq \tilde{M}$ holds. In virtue of Lemma 7 (since $\mu \lambda^2 k |\Delta_h \rho_h^0|^2 \leq C_d$ and the discrete maximum principle for ρ_h^0 and ρ_h^1 hold, that is, $\tilde{m} \leq \rho_h^0, \rho_h^1 \leq \tilde{M}$), we get (24) and (25) for $n = 0$. Next, multiplying (25) by $\frac{\mu}{4C_4}$ for $n = 0$ and adding it to (24) for $n = 0$, we arrive at (30) for $n = 0$.

We now assume that the induction hypothesis is true for $l = 0, \dots, n - 1$. Adding (30) for $l = 0, \dots, n - 1$, we obtain $\mu k \sum_{l=1}^n |\nabla \mathbf{u}_h^l|^2 \leq C_d$; hence thanks to $|\nabla \mathbf{w}_h^n| \leq |\nabla \mathbf{u}_h^n|$, one has

$\mu k \sum_{l=1}^n |\nabla \mathbf{w}_h^l|^2 \leq C_d$. Thus, we are in the situation of Lemma 5 for n , then $\tilde{m} \leq \rho_h^{n+1} \leq \tilde{M}$ holds. Accordingly, by Lemma 7 we get estimates (24) and (25). Balancing both estimates (as in case $n = 0$) we arrive at (30). \square

From this theorem, it is easy to obtain the following estimates:

Corollary 9 Under the assumptions of Theorem 8, the solution $(\rho_h^{n+1}, \mathbf{u}_h^{n+1})$ of the discrete problem (7)-(9) verifies the following estimates:

$$\begin{aligned} \text{i)} \quad & \max_{0 \leq n \leq N} |\mathbf{u}_h^n| \leq C, & \text{ii)} \quad & k \sum_{n=0}^N |\nabla \mathbf{u}_h^n|^2 \leq C, & \text{iii)} \quad & \sum_{n=0}^{N-1} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 \leq C, \\ \text{iv)} \quad & \max_{0 \leq n \leq N} \left(\|\rho_h^n\|_{L^\infty}^2 + \lambda |\nabla \rho_h^n|^2 \right) \leq C, & \text{v)} \quad & k \lambda^2 \sum_{n=0}^{N-1} |\Delta_h \rho_h^{n+1}|^2 \leq C, & \text{vi)} \quad & \lambda \sum_{n=0}^{N-1} |\nabla (\rho_h^{n+1} - \rho_h^n)|^2 \leq C, \end{aligned}$$

where $C > 0$ is a constant depending only on the data $(\mathbf{f}, \mathbf{u}_0, \rho_0, \mu)$, and independent of k , h , and λ .

Corollary 10 The following estimates hold:

$$\text{vii)} \quad \max_{0 \leq n \leq N} |\mathbf{w}_h^n| \leq C, \quad \text{viii)} \quad k \sum_{n=0}^N |\nabla \mathbf{w}_h^n|^2 \leq C$$

where $C > 0$ is independent of k , h , and λ .

Proof: Taking $\bar{\mathbf{w}}_h = \mathbf{w}_h^n$ in (6), we have

$$|\nabla \mathbf{w}_h^n| \leq |\nabla \mathbf{u}_h^n|.$$

So, we get the stability estimate **viii**). Now, we are going to get estimate **vii**) using a duality technique and constraint (S). Indeed, let $(\mathbf{z}, \xi) \in (\mathbf{V} \cap \mathbf{H}^2) \times (L_0^2(\Omega) \cap H^1(\Omega))$ be the solution of the Stokes problem

$$\begin{aligned} -\Delta \mathbf{z} + \nabla \xi &= \mathbf{w}_h^n - \mathbf{u}_h^n & \text{in } \Omega, \\ \nabla \cdot \mathbf{z} &= 0 & \text{in } \Omega, \\ \mathbf{z} &= 0 & \text{on } \Gamma. \end{aligned} \tag{31}$$

Taking $\mathbf{w}_h^n - \mathbf{u}_h^n$ as a test function in the variational formulation of (31), we get

$$|\mathbf{w}_h^n - \mathbf{u}_h^n|^2 = \left(\nabla \mathbf{z}, \nabla (\mathbf{w}_h^n - \mathbf{u}_h^n) \right) + \left(\xi, \nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n) \right).$$

Let $(\mathbf{z}_h, \xi_h) \in \widetilde{\mathbf{V}}_h \times \widetilde{\mathbf{M}}_h$ be the discrete solution of (31) defined as

$$\begin{cases} \left(\nabla \mathbf{z}_h, \nabla \bar{\mathbf{w}}_h \right) - \left(\xi_h, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\mathbf{w}_h^n - \mathbf{u}_h^n, \bar{\mathbf{w}}_h \right) & \forall \bar{\mathbf{w}}_h \in \widetilde{\mathbf{V}}_h, \\ \left(\nabla \cdot \mathbf{z}_h, \bar{q}_h \right) = 0 & \forall \bar{q}_h \in \widetilde{\mathbf{M}}_h. \end{cases}$$

In view of hypothesis (H5), we write

$$|\mathbf{w}_h^n - \mathbf{u}_h^n|^2 = \left(\nabla \mathbf{z} - \nabla \mathbf{z}_h, \nabla (\mathbf{w}_h^n - \mathbf{u}_h^n) \right) + \left(\nabla \mathbf{z}_h, \nabla (\mathbf{w}_h^n - \mathbf{u}_h^n) \right) + \left(\xi - K_h \xi, \nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n) \right),$$

where K_h is the interpolation operator defined in hypothesis (H2). From (6), it follows that $\left(\nabla \mathbf{z}_h, \nabla (\mathbf{w}_h^n - \mathbf{u}_h^n) \right) = 0$. Thus, we find

$$\begin{aligned} |\mathbf{w}_h^n - \mathbf{u}_h^n|^2 &\leq |\nabla \mathbf{z} - \nabla \mathbf{z}_h| |\nabla (\mathbf{w}_h^n - \mathbf{u}_h^n)| + |\xi - K_h \xi| |\nabla \cdot (\mathbf{w}_h^n - \mathbf{u}_h^n)| \\ &\leq Ch \left(\|\mathbf{z}\|_{H^2(\Omega)} + \|\xi\|_{H^1(\Omega)} \right) |\nabla (\mathbf{w}_h^n - \mathbf{u}_h^n)| \\ &\leq Ch |\mathbf{w}_h^n - \mathbf{u}_h^n| |\nabla (\mathbf{w}_h^n - \mathbf{u}_h^n)|, \end{aligned}$$

where in the second line we have used that $|\nabla \mathbf{z} - \nabla \mathbf{z}_h| \leq Ch \|\mathbf{z}\|_{H^2}$ resulting from the regularity $\mathbf{z} \in \mathbf{V} \cap \mathbf{H}_0^1(\Omega)$ and the interpolations errors $\|\bar{\mathbf{u}} - \tilde{\mathcal{J}}_h \bar{\mathbf{u}}\|_{H^1(\Omega)} \leq Ch \|\bar{\mathbf{u}}\|_{H^2(\Omega)}$, $\forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega)$, $|\bar{p} - K_h \bar{p}| \leq Ch \|\bar{p}\|_{H^1(\Omega)}$, and $\forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega)$ given in hypotheses (H1) and (H2), respectively.

Therefore, we have

$$|\mathbf{w}_h^n - \mathbf{u}_h^n| \leq Ch |\nabla (\mathbf{w}_h^n - \mathbf{u}_h^n)|. \tag{32}$$

Now, in view of (S) we may get that $h \leq Ck$ for (h, k) small enough. Then, since $k^{1/2} |\nabla \mathbf{w}_h^n| \leq k^{1/2} |\nabla \mathbf{u}_h^n| \leq C$ thanks to estimate **ii**) of Corollary 9 and estimate **viii**), it is easy to see that

$$|\mathbf{w}_h^n| \leq Ck^{1/2} + |\mathbf{u}_h^n| \leq C.$$

So, we get that

$$\max_{0 \leq n \leq N} |\mathbf{w}_h^n| \leq C.$$

□

To study the convergence of scheme (6)-(9) towards a solution of (1), (3)-(4), let us define the following auxiliary functions.

Definition 11 *One defines $\mathbf{u}_{h,k}$, $\widehat{\mathbf{u}}_{h,k}$, $\widehat{\mathbf{w}}_{h,k}$, $\rho_{h,k}$, $\widehat{\rho}_{h,k}$, and $p_{h,k}$ as the piecewise constant functions, taking values \mathbf{u}_h^{n+1} , \mathbf{u}_h^n , \mathbf{w}_h^n , ρ_h^{n+1} , ρ_h^n y p_h^{n+1} on $(t_n, t_{n+1}]$, respectively. In addition, we define $\widetilde{\rho}_{h,k} \in C^0([0, T]; \mathbf{V}_h)$ as the continuous piecewise linear function that such $\widetilde{\rho}_{h,k}(t_n) = \rho_h^n$.*

Then, thanks to the estimates of Lemma 5, Corollaries 9 and 10 and inequality (20), the following result holds.

Lemma 12 *Under the hypotheses of Theorem 8, the following estimates (independent of h and k) hold:*

$$\begin{aligned} \{\mathbf{u}_{h,k}\}_{h,k}, \{\widehat{\mathbf{u}}_{h,k}\}_{h,k}, \{\widehat{\mathbf{w}}_{h,k}\}_{h,k} & \text{ bounded in } L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)), \\ \{\rho_{h,k}\}_{h,k}, \{\widehat{\rho}_{h,k}\}_{h,k}, \{\widetilde{\rho}_{h,k}\}_{h,k} & \text{ bounded in } L^\infty(0, T; H^1(\Omega) \cap L^\infty(\Omega)), \\ \{\rho_{h,k}\}_{h,k} & \text{ bounded in } L^4(0, T; W^{1,3}(\Omega)). \end{aligned}$$

Furthermore, there exists a subsequence of $\{\mathbf{u}_{h,k}\}_{h,k}$, $\{\widehat{\mathbf{u}}_{h,k}\}_{h,k}$, $\{\widehat{\mathbf{w}}_{h,k}\}_{h,k}$, $\{\rho_{h,k}\}_{h,k}$, $\{\widehat{\rho}_{h,k}\}_{h,k}$, $\{\widetilde{\rho}_{h,k}\}_{h,k}$ (denoted in the same way), and limit functions \mathbf{u} , ρ satisfying the following weak convergence, as $(h, k) \rightarrow 0$:

$$\begin{aligned} \mathbf{u}_{h,k} \rightharpoonup \mathbf{u}, \quad \widehat{\mathbf{u}}_{h,k} \rightarrow \mathbf{u}, \quad \widehat{\mathbf{w}}_{h,k} \rightarrow \mathbf{u} & \text{ in } \begin{cases} L^2(0, T; \mathbf{H}_0^1(\Omega))\text{-weak}, \\ L^\infty(0, T; \mathbf{L}^2(\Omega))\text{-weak*}, \end{cases} \\ \rho_{h,k} \rightharpoonup \rho, \quad \widehat{\rho}_{h,k} \rightarrow \rho, \quad \widetilde{\rho}_{h,k} \rightarrow \rho & \text{ in } \begin{cases} L^\infty(Q)\text{-weak*}, \\ L^\infty(0, T; H^1(\Omega))\text{-weak*}, \end{cases} \\ \widehat{\rho}_{h,k} \rightarrow \rho & \text{ in } L^4(0, T; W^{1,3}(\Omega))\text{-weak}. \end{aligned}$$

A proof of this lemma can be found in [7].

4 Compactness

To establish the convergence of scheme (6)-(9) we need compactness for the discrete velocity and density. The proof of the following result can be found in [7].

Lemma 13 *In the assumptions of Theorem 8, one has*

$$k \sum_{n=0}^N \left| \frac{\rho_h^{n+1} - \rho_h^n}{k} \right|^{4/3} \leq C_\lambda,$$

where $C_\lambda > 0$ depends only on the data $(\rho_0, \mathbf{u}_0, \mathbf{f}, \mu, \lambda)$, but is independent of h and k .

Remark 14 *As a consequence of the previous Lemma, one has $\|\frac{d}{dt} \tilde{\rho}_{h,k}\|_{L^{4/3}(0,T;L^2(\Omega))} \leq C_\lambda$. On the other hand, by Lemma 9 one has $\|\tilde{\rho}_{h,k}\|_{L^\infty(0,T;H^1(\Omega))} \leq C$. Then, in virtue of an Aubin-Lions type compactness theorem for $L^p(0,T;X)$ spaces (X being a Banach space), we have*

$$\tilde{\rho}_{h,k} \rightarrow \rho \text{ in } L^\infty(0,T;L^p(\Omega))\text{-strong as } (h,k) \rightarrow 0,$$

where $p < 6$. In particular, we deduce

$$\rho_{h,k}, \hat{\rho}_{h,k} \rightarrow \rho \text{ in } L^2(0,T;L^2(\Omega))\text{-strong as } (h,k) \rightarrow 0,$$

since $\|\tilde{\rho}_{h,k} - \rho_{k,h}\|_{L^2(0,T;L^2(\Omega))}^2 \leq \|\hat{\rho}_{h,k} - \rho_{k,h}\|_{L^2(0,T;L^2(\Omega))}^2 = k \sum_{n=0}^{N-1} |\rho_h^{n+1} - \rho_h^n|^2 \leq Ck$.

Finally, since the discrete density is bounded in $L^\infty(Q)$, one gets the strong convergence in $L^p(Q)$ for any $p < \infty$.

By using the compactness of the discrete density in $L^2(0,T;L^2(\Omega))$ and comparing the equation for the discrete Laplacian and its limit (see [6]), one can obtain the convergence of the norm $L^2(0,T;L^2(\Omega))$ of $\nabla \rho_{h,k}$ towards the same norm of $\nabla \rho$. Consequently, one has

$$\|\rho_{h,k} - \rho\|_{L^2(0,T;H^1(\Omega))} \rightarrow 0 \text{ as } (h,k) \rightarrow 0.$$

Proposition 15 *In the hypotheses of Theorem 8, the following estimate holds:*

$$\int_0^{T-\delta} \left| \sqrt{\rho_{h,k}(t+\delta)} (\mathbf{u}_{h,k}(t+\delta) - \mathbf{u}_{h,k}(t)) \right|^2 dt \leq C_\lambda \delta^{1/4} \quad \forall \delta : 0 < \delta < T, \quad (33)$$

with $C > 0$ independent of h, k and δ (but depends on λ).

Proof: Since $\rho_{h,k}$ and $\mathbf{u}_{h,k}$ are piecewise constant functions, it suffices to suppose that δ is a multiple of time step k , that is, $\delta = rk$, for $r = 0, \dots, N$, and to demonstrate

$$k \sum_{m=0}^{N-r} |\sqrt{\rho_h^{m+r}} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 \leq C_\lambda (rk)^{1/4}, \quad \forall r : 0 \leq r \leq N. \quad (34)$$

A proof of (34), eliminating the λ^2 -term, has been done in [7]. Then, we only focus on the λ^2 -term.

Adding to both sides of (8) the term $\frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right)$, multiplying by k , summing for $n = m, \dots, m-1+r$, taking $\bar{\mathbf{u}}_h = \mathbf{u}_h^{m+r} - \mathbf{u}_h^m$ and using the equality

$$\rho_h^{m+r} \mathbf{u}_h^{m+r} - \rho_h^m \mathbf{u}_h^m = \rho_h^{m+r} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) + (\rho_h^{m+r} - \rho_h^m) \mathbf{u}_h^m,$$

we get (see [7]):

$$\left\{ \begin{array}{l} |\sqrt{\rho_h^{m+r}} (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 = -(\rho_h^{m+r} - \rho_h^m, \mathbf{u}_h^m \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) \\ -k \sum_{n=m}^{m-1+r} \left\{ a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) + c(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \mathbf{u}_h^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right\} \\ +k \sum_{n=m}^{m-1+r} \left\{ (\rho_h^{n+1} \mathbf{f}^{n+1}, \mathbf{u}_h^{m+r} - \mathbf{u}_h^m) + \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \right\} \\ -\lambda^2 k \sum_{n=m}^{m-1+r} \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^n, \nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right). \end{array} \right. \quad (35)$$

Multiplying by k , summing for $m = 0, \dots, N-r$ in (35), and bounding adequately on the right-hand side, we are going to get the desired estimate (34). Indeed,

$$\begin{aligned} I &:= \left| \lambda^2 k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^n, \nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \right| \\ &\leq \frac{\lambda^2 k^2}{\tilde{m}} \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\nabla \rho_h^{n+1}\|_{L^4(\Omega)} \|\nabla \rho_h^n\|_{L^4(\Omega)} |\nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)| \\ (\text{Fubini}) &= \frac{\lambda^2 k^2}{\tilde{m}} \sum_{n=0}^{N-1} \sum_{m=n-r+1}^{\bar{n}} \|\nabla \rho_h^{n+1}\|_{L^4(\Omega)} \|\nabla \rho_h^n\|_{L^4(\Omega)} |\nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|, \end{aligned}$$

where

$$\bar{n} = \begin{cases} 0 & \text{if } n < 0, \\ n & \text{if } 0 \leq n \leq N-r, \\ N-r & \text{if } n > N-r. \end{cases}$$

Using the discrete interpolation inequality (21), we obtain

$$\begin{aligned} I &\leq C \lambda^2 k^2 \sum_{n=0}^{N-1} \sum_{m=n-r+1}^{\bar{n}} \left(|\Delta_h \rho_h^{n+1}| |\Delta_h \rho_h^n| + |\Delta_h \rho_h^{n+1}| |\Delta_h \rho_h^n|^{1/2} \right) |\nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)| \\ &\quad + C \lambda^2 k^2 \sum_{n=0}^{N-1} \sum_{m=n-r+1}^{\bar{n}} \left(|\Delta_h \rho_h^n| |\Delta_h \rho_h^{n+1}|^{1/2} + |\Delta_h \rho_h^{n+1}|^{1/2} |\Delta_h \rho_h^n|^{1/2} \right) |\nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)| \\ &:= I_1 + I_2 + I_3 + I_4. \end{aligned}$$

We estimate I_1 as follows:

$$\begin{aligned} I_1 &\leq C \frac{\lambda^2 k}{\tilde{m}} \sum_{n=0}^{N-1} |\Delta_h \rho_h^{n+1}| |\Delta_h \rho_h^n| \left(k \sum_{m=n-r+1}^{\bar{n}} |\nabla (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 \right)^{1/2} \left(\sum_{m=n-r+1}^{\bar{n}} k \right)^{1/2} \\ &\leq C (rk)^{1/2} \left(\lambda^2 k \sum_{n=0}^{N-1} |\Delta_h \rho_h^{n+1}|^2 \right)^{1/2} \left(\lambda^2 k \sum_{n=0}^{N-1} |\Delta_h \rho_h^n|^2 \right)^{1/2} \leq C (rk)^{1/2} \end{aligned}$$

The rest of the I_i terms can be bounded in a similar way, and to conclude the proof. \square

Remark 16 *In view of the weak estimates for the discrete velocity $\mathbf{u}_{h,k}$ in $L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega))$ and the fractional derivative type estimate of $\mathbf{u}_{h,k}$ given in (33), a compactness result [10] can be applied to obtain that*

$$\mathbf{u}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

As a consequence, thanks to estimate **iii**) of Corollary 9,

$$\widehat{\mathbf{u}}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

As $\{\mathbf{u}_{h,k}\}_{h,k}$ is bounded in $L^\infty(0, T; \mathbf{L}^2(\Omega))$ we can improve the compactness of $\{\mathbf{u}_{h,k}\}_{h,k}$ to $L^p(0, T; \mathbf{L}^2(\Omega))$ with any $p < \infty$.

Remark 17 *From (32) and (S), we infer the inequality*

$$|\mathbf{w}_h^n - \mathbf{u}| \leq Ck |\nabla(\mathbf{w}_h^n - \mathbf{u}_h^n)| + |\mathbf{u}_h^n - \mathbf{u}| \leq Ck^{1/2} + |\mathbf{u}_h^n - \mathbf{u}|.$$

Therefore, it holds

$$\widehat{\mathbf{w}}_{h,k} \rightarrow \mathbf{u} \text{ in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (h, k) \rightarrow 0.$$

5 Passing to the limit in the momentum system

Consider $\mathbf{v} \in C^1([0, T]; \mathbf{C}_c^\infty(\Omega))$ with $\nabla \cdot \mathbf{v} = 0$ and $\mathbf{v}(T) = 0$. We define \mathbf{v}_h^n as the Stokes projection of $\mathbf{v}(t^n)$ which provides the following result.

Lemma 18 *Let $\bar{\mathbf{u}} \in \mathbf{C}_c^\infty(\Omega)$. Then there exists $\bar{\mathbf{u}}_h \in \mathbf{V}_h$ such that*

$$\bar{\mathbf{u}}_h \rightarrow \bar{\mathbf{u}} \text{ in } \mathbf{H}_0^1(\Omega) \text{ and } (\nabla \cdot \bar{\mathbf{u}}_h, q_h) = (\nabla \cdot \bar{\mathbf{u}}, q_h) \quad \forall q_h \in M_h.$$

A proof of this Lemma can be seen in [6].

Let $\mathbf{v}_{h,k} \in L^\infty(0, T; \mathbf{V}_h)$ be the piecewise constant function taking values \mathbf{v}_h^{n+1} on $(t_n, t_{n+1}]$ and let $\tilde{\mathbf{v}}_{h,k} \in C^0([0, T]; \mathbf{V}_h)$ be the continuous piecewise linear function such that $\tilde{\mathbf{v}}_{h,k}(t_n) = \mathbf{v}_h^n$. It holds that as $(h, k) \rightarrow 0$,

$$\mathbf{v}_{h,k} \rightarrow \mathbf{v} \text{ in } L^\infty(0, T; \mathbf{H}_0^1(\Omega)) \text{ and } \tilde{\mathbf{v}}_{h,k} \rightarrow \mathbf{v} \text{ in } W^{1,\infty}(0, T; \mathbf{H}_0^1(\Omega)).$$

Taking $\bar{\mathbf{u}}_h = \mathbf{v}_h^{n+1}$ as a test function in (8) and using Definition 11, we arrive at the variational formulation ([7]):

$$\left\{ \begin{array}{l} - \int_0^T \left(\widehat{\rho}_{h,k} \widehat{\mathbf{u}}_{h,k}, \frac{\partial}{\partial t} \tilde{\mathbf{v}}_{h,k} \right) - \left(\rho_{0h} \mathbf{u}_{0h}, \mathbf{v}_h^0 \right) + \int_0^T a \left(\rho_{h,k}, \mathbf{u}_{h,k}, \mathbf{v}_{h,k} \right) \\ + \int_0^T c \left(\rho_{h,k} \widehat{\mathbf{u}}_{h,k} - \lambda \nabla \rho_{h,k}, \mathbf{u}_{h,k}, \mathbf{v}_{h,k} \right) + \lambda^2 \int_0^T \left(\frac{1}{\rho_{h,k}} \nabla \rho_{h,k} \otimes \nabla \widehat{\rho}_{h,k}, \nabla \mathbf{v}_{h,k} \right) \\ = \int_0^T \left(\rho_{h,k} \mathbf{f}_k, \mathbf{v}_{h,k} \right) + \frac{1}{2} \int_0^T \left(\frac{\partial}{\partial t} \tilde{\rho}_{h,k}, \mathbf{u}_{h,k} \cdot \mathbf{v}_{h,k} \right) \end{array} \right.$$

We just analyze the passage to the limit of the term $\lambda^2 \int_0^T \left(\frac{1}{\rho_{h,k}} \nabla \rho_{h,k} \otimes \nabla \widehat{\rho}_{h,k}, \nabla \mathbf{v}_{h,k} \right)$. As $\rho_0 \in H_N^2(\Omega)$ the same statements for $\rho_{h,k}$ can be assured to $\widehat{\rho}_{h,k}$. On one hand, taking $\bar{\rho} = -\Delta_h \rho_h^{n+1}$ and $\bar{\rho}_h = -\Delta_h \rho_h^{n+1}$ into (18), we get

$$|\Delta_h \rho_h^{n+1}|^2 \leq |\nabla \rho_h^{n+1}| |\nabla \Delta_h \rho_h^{n+1}| \leq \frac{C}{h} |\nabla \bar{\rho}_h| |\Delta_h \rho_h^{n+1}|.$$

Therefore, $|\Delta_h \rho_h^{n+1}| \leq \frac{C}{h} |\nabla \rho_h^{n+1}|$. In view of the discrete interpolation (21), we infer

$$\|\nabla \rho_h^{n+1}\|_{L^4(\Omega)} \leq C |\nabla \rho_h^{n+1}|^{1/4} |\Delta_h \rho_h^{n+1}|^{3/4} + C |\Delta_h \rho_h^{n+1}|^{1/2},$$

which shows that $\{\nabla \rho_{h,k}\}_{h,k}$ is bounded in $L^{8/3}(0, T; \mathbf{L}^4(\Omega))$. On the other hand, $\nabla \rho_{h,k}$ is compact in $L^2(0, T; \mathbf{L}^2(\Omega))$ and is bounded in $L^\infty(0, T; L^2(\Omega))$, then $\nabla \rho_{h,k}$ is compact in $L^p(0, T; \mathbf{L}^2(\Omega))$ for any $p < \infty$. Therefore, the convergence $\nabla \rho_{h,k} \otimes \nabla \widehat{\rho}_{h,k} \rightarrow \nabla \rho \otimes \nabla \rho$ in $L^{4/3}(0, T; L^2(\Omega))$ -weak as $(h, k) \rightarrow 0$ holds. Now, as $1/\rho_{h,k} \rightarrow \frac{1}{\rho}$ weakly- \star in $L^\infty(Q)$ and strongly in $L^2(Q)$, then $1/\rho_{h,k} \rightarrow \frac{1}{\rho}$ strongly in $L^p(Q)$ for any $p < \infty$. Thus, we have $\frac{1}{\rho_{h,k}} \nabla \rho_{h,k} \otimes \nabla \widehat{\rho}_{h,k} \rightarrow \frac{1}{\rho} \nabla \rho \otimes \nabla \rho$ in $L^{4/3}(0, T; L^2(\Omega))$ -weak. Finally, using that $\mathbf{v}_{h,k} \rightarrow \mathbf{v}$ in $L^\infty(0, T; \mathbf{H}_0^1(\Omega))$ -strong, one gets the desired convergence:

$$\int_0^T \left(\frac{1}{\rho_{h,k}} \nabla \rho_{h,k} \otimes \nabla \widehat{\rho}_{h,k}, \nabla \mathbf{v}_{h,k} \right) \rightarrow \int_0^T \left(\frac{1}{\rho} \nabla \rho \otimes \nabla \rho, \nabla \mathbf{v} \right).$$

The convergence of the rest of terms follows as in [6] and [7]. Then, the proof of Theorem 1 is finished.

6 Asymptotic behavior $\lambda \rightarrow 0$

We will see that if we impose the stability condition (see [7])

$$(S') \quad \lim_{(\lambda, h, k) \rightarrow 0} \frac{1}{\lambda} \sqrt{\frac{h}{k}} = 0,$$

and we complete (H2) with the additional property of approximation:

$$(H2') \quad |\bar{\rho} - I_h \bar{\rho}| \leq C h^{2/3} \|\bar{\rho}\|_{W^{1,3/2}(\Omega)}, \quad \forall \bar{\rho} \in W^{1,3/2}(\Omega),$$

then scheme (6)-(9) is convergent, as $(h, k, \lambda) \rightarrow 0$, towards a weak solution of the Navier-Stokes problem with variable density:

$$\left\{ \begin{array}{l} \rho [\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u}] - \mu \Delta \mathbf{u} + \nabla p = \rho \mathbf{f} \quad \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0, \quad \rho_t + \mathbf{u} \cdot \nabla \rho = 0 \quad \text{in } Q, \\ \mathbf{u} = 0 \quad \text{on } \Sigma, \\ \mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \rho|_{t=0} = \rho_0 \quad \text{in } \Omega, \end{array} \right. \quad (36)$$

which is define as follows:

Definition 19 A pair (ρ, \mathbf{u}) is said to be a weak solution of (36) in $(0, T)$ if it verifies:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{V})$, $\rho \in L^\infty(Q)$ with $0 < m \leq \rho(\mathbf{x}, t) \leq M$ a.e. $(\mathbf{x}, t) \in Q$.

b) For all $\phi \in C^1([0, T]; \mathbf{V})$ with $\phi(T) = 0$,

$$\int_0^T \left\{ -(\rho \mathbf{u}, \phi_t + (\mathbf{u} \cdot \nabla) \phi) + \mu(\nabla \mathbf{u}, \nabla \phi) \right\} dt = \int_0^T (\rho \mathbf{f}, \phi) dt + (\rho_0 \mathbf{u}_0, \phi(0)).$$

c) For all $\varphi \in C^1([0, T]; H^1(\Omega))$ with $\varphi(T) = 0$,

$$-\int_0^T (\rho, \varphi_t) dt - \int_0^T (\rho \mathbf{u}, \nabla \varphi) dt = (\rho_0, \varphi(0)).$$

The rest of this section is devoted to the proof of Theorem 2.

6.1 Uniform estimates with respect to (h, k, λ) .

If observe the more restrictive constraint for (h, k, λ) going to zero is $\frac{C}{\lambda} \sqrt{\frac{h}{k}}$ sufficiently small which is due to estimate (25) and in proving the pointwise estimates of Lemma 5 (see [7]). That is the reason that we say that k_0 and h_0 provided by Lemma 7 depend on λ for fixed λ .

From Section 3, the following estimates (independent of h, k and λ) can be deduced:

$$\begin{aligned} \{\mathbf{u}_{h,k,\lambda}\}_{h,k,\lambda}, \{\widehat{\mathbf{u}}_{h,k,\lambda}\}_{h,k,\lambda}, \{\widehat{\mathbf{w}}_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in bounded } L^\infty(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T; \mathbf{H}_0^1(\Omega)), \\ \{\rho_{h,k,\lambda}\}_{h,k,\lambda}, \{\widehat{\rho}_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in bounded } L^\infty(Q), \\ \lambda^{1/2} \{\rho_{h,k,\lambda}\}_{h,k,\lambda}, \lambda^{1/2} \{\widehat{\rho}_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in bounded } L^\infty(0, T; H^1(\Omega)), \\ \lambda^{3/4} \{\rho_{h,k,\lambda}\}_{h,k,\lambda} & \text{ in bounded } L^4(0, T; W^{1,3}(\Omega)), \\ \lambda^{3/4} \left\{ \frac{\partial}{\partial t} \widetilde{\rho}_{h,k,\lambda} \right\}_{h,k,\lambda} & \text{ in bounded } L^{4/3}(0, T; L^2(\Omega)), \end{aligned}$$

whereas $h \leq h_0$, $k \leq k_0$ and $\lambda \leq \lambda_0$ satisfying (S') . In addition, $0 < \widetilde{m} \leq \rho_{h,k,\lambda} \leq \widetilde{M}$,

$$\|\widetilde{\rho}_{h,k,\lambda} - \rho_{h,k,\lambda}\|_{L^2(0,T;L^2(\Omega))} \leq \|\rho_{h,k,\lambda} - \widehat{\rho}_{h,k,\lambda}\|_{L^2(0,T;L^2(\Omega))} \leq C\sqrt{k},$$

$$\|\mathbf{u}_{h,k,\lambda} - \widehat{\mathbf{u}}_{h,k,\lambda}\|_{L^2(0,T;\mathbf{H}_0^1(\Omega))} \leq C\sqrt{k}.$$

Now, considering the piecewise functions associated to the scheme, which will be denoted explicitly by the subscripts h, k and λ , we have

Lemma 20 Assume (S') , $(H0)$, $(H1)$, $(H2) + (H2')$, $(H3)$ - $(H5)$. Then, whereas $h \leq h_0$, $k \leq k_0$ and $\lambda \leq \lambda_0$, there exist subsequences of $\{\mathbf{u}_{h,k,\lambda}\}_{h,k,\lambda}$, $\{\widehat{\mathbf{u}}_{h,k,\lambda}\}_{h,k,\lambda}$, $\{\rho_{h,k,\lambda}\}_{h,k,\lambda}$, $\{\widehat{\rho}_{h,k,\lambda}\}_{h,k,\lambda}$ (denoted in the same manner), and limit functions \mathbf{u}, ρ such that the following weak convergences hold as $(h, k, \lambda) \rightarrow 0$:

$$\begin{aligned} \mathbf{u}_{h,k,\lambda} \rightharpoonup \mathbf{u}, \quad \widehat{\mathbf{u}}_{h,k,\lambda} \rightharpoonup \mathbf{u}, \quad \widehat{\mathbf{w}}_{h,k,\lambda} \rightharpoonup \mathbf{u} & \text{ in } \begin{cases} L^2(0, T; \mathbf{H}_0^1(\Omega))\text{-weak}, \\ L^\infty(0, T; \mathbf{L}^2(\Omega))\text{-weak*}, \end{cases} \\ \rho_{h,k,\lambda} \rightarrow \rho, \quad \widehat{\rho}_{h,k,\lambda} \rightarrow \rho, \quad \widetilde{\rho}_{h,k,\lambda} \rightarrow \rho & \text{ in } L^\infty(Q)\text{-weak*}. \end{aligned}$$

6.2 Compactness

The following estimate holds:

$$\int_0^{T-\delta} \left| \sqrt{\rho_{h,k,\lambda}(t+\delta)} (\mathbf{u}_{h,k,\lambda}(t+\delta) - \mathbf{u}_{h,k,\lambda}(t)) \right|^2 dt \leq C \delta^{1/4} \quad \forall \delta: \quad 0 < \delta < T,$$

with $C > 0$ independent of h, k, δ , and λ . Indeed, a proof of this inequality has been done in [7], where the λ^2 -term is not considered, but this λ^2 -term has been estimated independent of λ in the proof of Proposition 15.

In particular, since $\rho_{h,k,\lambda} \geq \tilde{m}$, one deduces the compactness result:

$$\mathbf{u}_{h,k,\lambda} \rightharpoonup \mathbf{u} \quad \text{and} \quad \widehat{\mathbf{w}}_{h,k,\lambda} \rightarrow \mathbf{u} \quad \text{in } L^2(0, T; \mathbf{L}^2(\Omega)) \quad \text{as } (h, k, \lambda) \rightarrow 0.$$

6.3 Passing to the limit

We write the scheme in the following conservative form ([7]):

$$\left\{ \begin{aligned} & - \int_0^T \left(\widehat{\rho}_{h,k,\lambda} \widehat{\mathbf{u}}_{h,k,\lambda}, \frac{\partial}{\partial t} \widetilde{\mathbf{v}}_{h,k} \right) - \left(\rho_h^0 \mathbf{u}_h^0, \widetilde{\mathbf{v}}_{h,k}(0) \right) + \int_0^T a(\rho_{h,k,\lambda}, \mathbf{u}_{h,k,\lambda}, \mathbf{v}_{h,k}) \\ & - \int_0^T \left(\rho_{h,k,\lambda} \widehat{\mathbf{u}}_{h,k} - \lambda \nabla \rho_{h,k,\lambda} \otimes \mathbf{u}_{h,k,\lambda}, \nabla \mathbf{v}_{h,k} \right) + \lambda^2 \int_0^T \left(\frac{1}{\rho_{h,k,\lambda}} \nabla \rho_{h,k,\lambda} \otimes \nabla \widehat{\rho}_{h,k,\lambda}, \nabla \mathbf{v}_{h,k} \right) \\ & = \int_0^T \left(\rho_{h,k,\lambda} \mathbf{f}_k, \mathbf{v}_{h,k} \right) + \frac{1}{2} \int_0^T \left(\frac{\partial}{\partial t} \widetilde{\rho}_{h,k}, \mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}) \right) \\ & - \frac{1}{2} \int_0^T \left(\rho_{h,k,\lambda} \widehat{\mathbf{u}}_{h,k}, \nabla(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k})) \right) \\ & - \frac{\lambda}{2} k \int_0^T \left(\rho_{h,k,\lambda}, \mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k} - Q_h(\mathbf{u}_{h,k,\lambda} \cdot \mathbf{v}_{h,k}) \right). \end{aligned} \right. \quad (37)$$

$$\left\{ \begin{aligned} & - \int_0^T \left(\widehat{\rho}_{h,k,\lambda}, \frac{d}{dt} \widetilde{\eta}_{h,k} \right) dt + \lambda \int_0^T \left(\nabla \rho_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt \\ & - \int_0^T \left(\widehat{\mathbf{w}}_{h,k,\lambda} \rho_{h,k,\lambda}, \nabla \eta_{h,k} \right) dt = \left(\rho_{0h}, \eta_h^0 \right). \end{aligned} \right.$$

where $\mathbf{v}_{h,k}, \widetilde{\mathbf{v}}_{h,k}$ ($\eta_{h,k}, \widetilde{\eta}_{h,k}$, respectively) are suitable approximations of a free-divergence test functions $\mathbf{v} \in C^1([0, T]; \mathbf{C}_c^\infty(\Omega))$ ($C^1([0, T]; C_c^\infty(\Omega))$, respectively) with $\mathbf{v}(T) = 0$ ($\eta(T) = 0$, respectively) such that the sequence $\{\mathbf{v}_{h,k,\lambda}\}_{h,k,\lambda}$ is bounded in $L^\infty(0, T; \mathbf{W}^{1,3}(\Omega) \cap \mathbf{L}^\infty(\Omega))$.

Here, we only pass to the limit in the λ^2 -term, because the convergence of the rest of terms has been done in [7]. We must prove that

$$J := \lambda^2 \int_0^T \left(\frac{1}{\rho_{h,k,\lambda}} \nabla \rho_{h,k,\lambda} \otimes \nabla \widehat{\rho}_{h,k,\lambda}, \nabla \mathbf{v}_{h,k} \right) \rightarrow 0 \quad \text{as } (h, k, \lambda) \rightarrow 0.$$

Indeed, since in particular $\mathbf{v}_{h,k}$ is bounded in $L^2(0, T; \mathbf{W}^{1,3}(\Omega))$, one has

$$\begin{aligned} J & \leq C \lambda^{1/2} \left(\lambda^3 \int_0^T \|\nabla \rho_{h,k,\lambda}\|_{L^3(\Omega)}^4 \right)^{1/4} \left(\lambda^3 \int_0^T \|\nabla \widehat{\rho}_{h,k,\lambda}\|_{L^3(\Omega)}^4 \right)^{1/4} \left(\int_0^T \|\nabla \mathbf{v}_{h,k}\|_{L^3(\Omega)}^2 \right)^{1/2} \\ & \leq C \lambda^{1/2} \rightarrow 0. \end{aligned}$$

Therefore, the proof of Theorem 2 is concluded.

Remark 21 Replacing the semi-implicit approximation of the λ^2 -term

$$\lambda^2 \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^n, \nabla \bar{\mathbf{u}}_h \right)$$

by the fully explicit approximation

$$\lambda^2 \left(\frac{1}{\rho_h^n} \nabla \rho_h^n \otimes \nabla \rho_h^n, \nabla \bar{\mathbf{u}}_h \right),$$

one can establish the same stability, compactness and convergence results obtained previously in this work.

On the contrary, if we consider the fully implicit approximation

$$\lambda^2 \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right),$$

then the term $\lambda^2 \left(\frac{1}{\rho_h^{n+1}} \nabla \rho_h^{n+1} \otimes \nabla \rho_h^{n+1}, \nabla \mathbf{u}_h^{n+1} \right)$ is estimated using the discrete interpolation (21) by

$$C_\Omega k \frac{\lambda^2}{\tilde{m}} \left(h^{1/2} |\Delta_h \rho_h^{n+1}|^2 + 2\tilde{M}^{1/2} h^{1/4} |\Delta_h \rho_h^{n+1}|^{3/2} + \tilde{M} |\Delta_h \rho_h^{n+1}| \right) |\nabla \mathbf{u}_h^{n+1}|.$$

Then, it is not clear how to control the terms

$$C_\Omega k \frac{\lambda^2}{\tilde{m}} \left(h^{1/2} |\Delta_h \rho_h^{n+1}|^2 + 2\tilde{M}^{1/2} h^{1/4} |\Delta_h \rho_h^{n+1}|^{3/2} \right) |\nabla \mathbf{u}_h^{n+1}|$$

in order to obtain stability estimates.

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Capítulo 4

Estimaciones de error para un modelo de difusión de masa tridimensional

Estimaciones de error para un modelo de difusión de masa tridimensional

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Abstract

Se presentan estimaciones de error de un esquema de tipo diferencias finitas en tiempo y elementos finitos a lo más globalmente continuos en espacio para aproximar las incógnitas densidad y velocidad-presión para el modelo tridimensional de Kazhikhov-Smagulov (o de Navier-Stokes con difusión de masa).

Bajo ciertas hipótesis de regularidad de la solución continua que no exigen condiciones implícitas de compatibilidad, obtenemos orden de convergencia para las normas débiles de $O(h + k^{1/2})$, que resulta ser no optimal en tiempo, siendo h y k los parámetros de discretización de espacio y tiempo, respectivamente. Además, mostramos tasas de error de $O(h + k^{1/2})$ para la densidad en normas más fuertes. Todas las estimaciones anteriores resultan ser optimales, de $O(h + k)$, imponiendo regularidad sobre la solución exacta que exigen condiciones de compatibilidad no local para la presión en $t = 0$.

Aunque el esquema resulta ser lineal y desacopla la densidad del par velocidad-presión, también se analizan y proponen sendos métodos iterativos convergentes hacia cada uno de estos problemas en cada etapa de tiempo, que mantienen constantes las matrices en cada iteración.

1 Introducción

1.1 Modelo

Consideramos $\Omega \subseteq \mathbb{R}^d$ ($d = 2$ ó 3) abierto, acotado y de frontera Γ suficientemente regular. Denotamos por $[0, T]$ el intervalo de observación, para $T > 0$. Usaremos la notación $Q = \Omega \times (0, T)$, $\Sigma = \Gamma \times (0, T)$ y $\mathbf{n}(\mathbf{x})$ la normal unitaria exterior a Ω en el punto $\mathbf{x} \in \Gamma$.

Consideramos el sistema de ecuaciones que gobierna la mezcla de dos fluidos con difusión de masa ([1]), llamado modelo de *Navier-Stokes* con difusión de masa o modelo de *Kazhikhov-Smagulov* ([17]). Las incógnitas para este modelo son: $\mathbf{u} : Q \rightarrow \mathbb{R}^d$ el campo incompresible de

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velocidades del fluido, $q : Q \rightarrow \mathbb{R}$ una función potencial (relacionada con la presión) y $\rho : Q \rightarrow \mathbb{R}$ concentración de masa del fluido, que verifican el siguiente problema en derivadas parciales:

$$\begin{cases} \rho \mathbf{u}_t + ((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla) \mathbf{u} - \mu \Delta \mathbf{u} - \lambda (\mathbf{u} \cdot \nabla) \nabla \rho + \nabla q = \rho \mathbf{f} & \text{en } Q, \\ \nabla \cdot \mathbf{u} = 0 & \text{en } Q, \quad \rho_t + \mathbf{u} \cdot \nabla \rho - \lambda \Delta \rho = 0 & \text{en } Q, \end{cases} \quad (1)$$

donde \mathbf{f} es la fuerza externa y $\mu > 0$, $\lambda > 0$ son los coeficientes de viscosidad y de difusión de masa, respectivamente.

Una manera de obtener (1) es suponer que la velocidad \mathbf{v} del sistema de Navier-Stokes compresible puede descomponerse en $\mathbf{v} = \mathbf{u} - \lambda \nabla \log \rho$ con $\nabla \cdot \mathbf{u} = 0$ (i.e. es suma de una parte incompresible \mathbf{u} y una parte potencial $-\lambda \nabla \log \rho$) despreciando los términos de $O(\lambda^2)$ (see [14]).

Descomponiendo el término que involucra orden 2 de derivabilidad para la densidad como

$$-\lambda (\mathbf{u} \cdot \nabla) \nabla \rho = -\lambda \nabla (\mathbf{u} \cdot \nabla \rho) + \lambda \nabla \cdot (\rho (\nabla \mathbf{u})^t), \quad (2)$$

y definiendo $p = q - \lambda \mathbf{u} \cdot \nabla \rho$ una función potencial modificada, el sistema de momentos (1)₁ es escrito como

$$\rho \mathbf{u}_t + ((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla) \mathbf{u} - \mu \Delta \mathbf{u} + \lambda \nabla \cdot (\rho (\nabla \mathbf{u})^t) + \nabla p = \rho \mathbf{f} \quad \text{en } Q.$$

Completamos (1) con condiciones fronteras

$$\mathbf{u}|_{\Sigma} = 0, \quad \frac{\partial \rho}{\partial \mathbf{n}} \Big|_{\Sigma} = 0 \quad (3)$$

y condiciones iniciales

$$\rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad (4)$$

donde $\rho_0 : \Omega \rightarrow \mathbb{R}^+$ y $\mathbf{u}_0 : \Omega \rightarrow \mathbb{R}^d$ son funciones dadas.

En todo el trabajo, asumimos la hipótesis sobre la densidad inicial:

$$0 < m \leq \rho_0(\mathbf{x}) \leq M \quad \text{en } \Omega. \quad (5)$$

1.2 Notación

En esta sección describimos los espacios de funciones usados a lo largos de este trabajo.

Como es usual $L^p(\Omega)$ denota el espacio de las funciones p-integrables de Ω en \mathbb{R} , y por $\|\cdot\|_{L^p(\Omega)}$ su norma. Denotamos el producto escalar en L^2 por (\cdot, \cdot) y por $\|\cdot\|_{L^2(\Omega)} = |\cdot|$ su norma. Por $H^k(\Omega)$ y $H_0^k(\Omega)$ denotamos los espacios clásicos de Sobolev y por $\|\cdot\|_{H^k(\Omega)}$ su norma. Usaremos letras negritas para hacer referencias a los elementos vectoriales y a los espacios vectoriales.

A continuación, describiremos brevemente los espacios de funciones habituales en el marco de la mecánica de fluidos:

$$\mathbf{H} = \{\mathbf{u} : \mathbf{u} \in \mathbf{L}^2(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ en } \Omega, \mathbf{u} \cdot \mathbf{n} = 0 \text{ sobre } \Gamma\},$$

$$\mathbf{V} = \{ \mathbf{u} : \mathbf{u} \in \mathbf{H}_0^1(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ en } \Omega \},$$

$$L_0^2(\Omega) = \left\{ p : p \in L^2(\Omega), \int_{\Omega} p(\mathbf{x}) d\mathbf{x} = 0 \right\}$$

Por otra parte, para la densidad consideremos el espacio afín ($k \geq 2$)

$$H_N^k(\Omega) = \left\{ \rho \in H^k(\Omega) : \frac{\partial \rho}{\partial \mathbf{n}} = 0 \text{ sobre } \partial\Omega, \int_{\Omega} \rho(\mathbf{x}) = \int_{\Omega} \rho_0(\mathbf{x}) \right\}.$$

Obviamente, $H_N^k(\Omega) = \bar{\rho}_0 + H_{N,0}^k(\Omega)$, donde $\bar{\rho}_0 = \frac{1}{|\Omega|} \int_{\Omega} \rho_0(\mathbf{x}) d\mathbf{x}$ y

$$H_{N,0}^k(\Omega) = \left\{ \rho \in H^k(\Omega) : \frac{\partial \rho}{\partial \mathbf{n}} = 0 \text{ sobre } \partial\Omega, \int_{\Omega} \rho(\mathbf{x}) = 0 \right\}.$$

Por lo tanto, $H_N^k(\Omega)$ es un espacio afín asociado a $H_{N,0}^k$. Como consecuencia, gracias a la regularidad H^2 del problema *Poisson-Neumann*, las seminormas $\|\nabla \rho\|_{H^1}$ y $\|\Delta \rho\|_{L^2}$ son equivalentes en $H_N^2(\Omega)$.

1.3 Resultados conocidos

Respecto al modelo simplificado (1), Kazhikhov y Smagulov ([17]) probaron, vía un método de semi-Galerkin, la existencia de solución débil global bajo la hipótesis sobre los coeficientes:

$$\lambda < 2\mu/(M - m) \tag{6}$$

y la existencia local en tiempo de solución fuerte (global para el caso bidimensional). Salvi ([19]) probó la existencia de solución débil para un dominio no cilíndrico. Por otro lado, Secchi ([21]) estudio el caso $\Omega = \mathbb{R}^3$, probando la existencia local y unicidad de solución fuerte, usando un argumento de punto fijo.

Para el modelo completo (con los términos de $O(\lambda^2)$), Beirão da Veiga ([2]) y Secchi ([20]) establecieron la existencia local de solución fuerte usando un argumento de linealización y punto fijo. En [20] se muestra la existencia y unicidad global en dimensión 2 imponiendo pequeñez sobre λ/μ y el comportamiento asintótico cuando $\lambda \rightarrow 0$ hacia una solución débil de Navier-Stokes con densidad variable. En el caso de densidad inicial positiva para el caso 3D, Guillén-González ([12]) probó la existencia global de solución débil y el comportamiento asintótico, cuando $\lambda \rightarrow 0$, hacia el problema de Navier-Stokes con densidad variable. Recientemente, en [13] se ha probado usando un método iterativo la existencia de solución fuerte y algunas estimaciones de error entre la aproximación y la solución exacta en diversas normas.

No existen muchos resultados concernientes al análisis numérico para (1). Usando un método de elementos finitos, ha sido recientemente desarrollado en [14] y [15] dos esquemas numéricos para el modelo (1) en el caso 2D y 3D, respectivamente. Para el caso 2D se construye un esquema numérico incondicionalmente estable y convergente hacia la (única) solución débil del

problema continuo. Para ello es necesario aplicar un operador de truncamiento en los términos que dependen de la densidad discreta que requieran positividad y cotas puntuales. Para el caso $3D$, se construye un esquema numérico para el cual se demuestra la existencia de un principio del máximo aproximado por exceso y por defecto respecto de las cotas máxima y mínima de la densidad inicial, gracias a que la velocidad del término convectivo de la ecuación discreta de la densidad es proyectada en espacio de divergencia discreta nula relacionada con el espacio de la densidad. Se prueba estabilidad condicional y convergencia hacia una solución débil del problema continuo.

Ambos esquemas se basan en métodos iterativos en tiempo de tipo Euler retrógrado, donde en cada etapa se desacopla el cálculo de la densidad discreta del par velocidad-presión, quedando dos problemas lineales.

En [7] se desarrolla un algoritmo numérico usando el método de las características para la discretización en tiempo y elementos finitos en espacio. Los autores dan cotas de error optimas bajo ciertas restricciones sobre los parámetros de discretización y asumiendo hipótesis de regularidad sobre la solución continua, como por ejemplo $\mathbf{u} \in L^\infty(0, T; \mathbf{H}^3(\Omega))$, que resultan ser más exigentes de las que impondremos en este trabajo. En particular, dicha regularidad exige la condición de compatibilidad no local para los datos en $t = 0$.

1.4 Formulación del esquema numérico

El método de aproximación que estudiamos en este trabajo está fundamentado en la siguiente formulación débil mixta del problema (1), (3), (4):

$$\left\{ \begin{array}{l} \left(\rho \mathbf{u}_t, \bar{\mathbf{u}} \right) + \left((\rho \mathbf{u} - \lambda \nabla \rho) \cdot \nabla \mathbf{u}, \bar{\mathbf{u}} \right) + \left(\mu \nabla \mathbf{u} - \lambda \rho (\nabla \mathbf{u})^t, \nabla \bar{\mathbf{u}} \right) \\ \quad - \left(p, \nabla \cdot \bar{\mathbf{u}} \right) = \left(\rho \mathbf{f}, \bar{\mathbf{u}} \right), \quad \forall \bar{\mathbf{u}} \in \mathbf{H}_0^1(\Omega), \\ \left(\nabla \cdot \mathbf{u}, \bar{p} \right) = 0, \quad \forall \bar{p} \in L_0^2(\Omega), \\ \left(\rho_t, \bar{\rho} \right) + \left(\mathbf{u} \cdot \nabla \rho, \bar{\rho} \right) + \lambda \left(\nabla \rho, \nabla \bar{\rho} \right) = 0, \quad \forall \bar{\rho} \in H^1(\Omega). \end{array} \right. \quad (7)$$

Se trata de la formulación variacional mixta de (1) usando la reescritura (2).

Consideramos un esquema de diferencias finitas en tiempo sobre una partición, que suponemos por simplicidad, uniforme de $[0, T]$ de paso $k = T/N$: $(t_n = nk)_{n=0}^{n=N}$. Para aproximar las incógnitas densidad, velocidad y presión, fijamos espacios de elementos finitos (W_h, \mathbf{V}_h, M_h) aproximaciones internas de $(H^1, \mathbf{H}_0^1, L_0^2)$, verificando las hipótesis (H0)-(H4) descritas en la Sección 2.

Proponemos el siguiente esquema numérico:

Inicialización: Se define $(\mathbf{u}_h^0, \rho_h^0) \in \mathbf{V}_h \times W_h$ aproximaciones de (\mathbf{u}_0, ρ_0) , cuando $h \rightarrow 0$.

Etapa $n + 1$: Dados $\rho_h^n \in W_h$ y $\mathbf{u}_h^n \in \mathbf{V}_h$, hallar $\rho_h^{n+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) - \lambda \left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h \right) = 0. \quad (8)$$

Dados $\rho_h^n, \rho_h^{n+1} \in W_h$ y $\mathbf{u}_h^n \in \mathbf{V}_h$, hallar $(\mathbf{u}_h^{n+1}, p_h^{n+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla, \bar{\mathbf{u}}_h \right) + a(\rho_h^{n+1}, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) \\ + \frac{1}{2} \left((\nabla \cdot \mathbf{u}_h^n) \rho_h^{n+1}, \bar{\mathbf{u}}_h \right) = \left(\rho_h^{n+1} \mathbf{f}(t_{n+1}), \bar{\mathbf{u}}_h \right) + \left(p_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right), \end{array} \right. \quad (9)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1}, \bar{p}_h \right) = 0, \quad (10)$$

donde

$$a(\rho, \mathbf{u}, \mathbf{v}) = \mu \left(\nabla \mathbf{u}, \nabla \mathbf{v} \right) - \lambda \int_{\Omega} \left(\rho - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{u})^t : \nabla \mathbf{v} \, dx$$

con

$$\widetilde{M} > M, \quad 0 < \widetilde{m} < m \quad \text{tales que} \quad \lambda \frac{\widetilde{M} - \widetilde{m}}{2} < \mu.$$

Notar que esta elección de \widetilde{M} y \widetilde{m} es posible gracias a la hipótesis (6).

La forma trilineal $a(\cdot, \cdot, \cdot)$ verifica las siguientes propiedades: si $0 < \widetilde{m} \leq \rho \leq \widetilde{M}$, se tiene:

$$a(\rho, \mathbf{u}, \mathbf{u}) \geq \frac{\mu_1}{2} |\nabla \mathbf{u}|^2 \quad \text{donde} \quad \frac{\mu_1}{2} = \mu - \lambda \frac{\widetilde{M} - \widetilde{m}}{2} (> 0), \quad (\text{coercitividad}) \quad (11)$$

$$a(\rho, \mathbf{u}, \mathbf{v}) \leq C |\nabla \mathbf{u}| |\nabla \mathbf{v}|. \quad (\text{continuidad}) \quad (12)$$

Nótese que el esquema numérico presentado es lineal y desacoplado respecto de los problemas para calcular ρ_h^{n+1} y $(\mathbf{u}_h^{n+1}, p_h^{n+1})$.

Comparando los esquemas desarrollados en [14] y [15] con el esquema (8)-(10) encontramos las siguientes semejanzas y diferencias:

En el esquema de [15] se reemplaza la velocidad \mathbf{u}_h^n del término convectivo del esquema (8) por la velocidad proyectada \mathbf{w}_h^n sobre un espacio de velocidad de divergencia discreta nula, i.e., \mathbf{w}_h^n es tal que

$$\left\{ \begin{array}{l} \left(\nabla \mathbf{w}_h^n, \nabla \bar{\mathbf{w}}_h \right) - \left(q_h^n, \nabla \cdot \bar{\mathbf{w}}_h \right) = \left(\nabla \mathbf{u}_h^n, \nabla \bar{\mathbf{w}}_h \right), \quad \forall \bar{\mathbf{w}}_h \in \widetilde{\mathbf{V}}_h, \\ \left(\nabla \cdot \mathbf{w}_h^n, \bar{q}_h \right) = 0, \quad \forall \bar{q}_h \in \widetilde{M}_h, \end{array} \right. \quad (13)$$

donde $(\widetilde{\mathbf{V}}_h, \widetilde{M}_h)$ verifican la condición *inf-sup*, $(W_h)^2 \cap L_0^2(\Omega) \subset \widetilde{M}_h$ y $M_h \subset \widetilde{M}_h$. Obviamente, tal proyección se puede evitar eligiendo $\mathbf{V}_h = \widetilde{\mathbf{V}}_h$ y $M_h = \widetilde{M}_h$. Además, en el sistema de momentos discreto (9) se reemplaza el término estabilizador $\frac{1}{2} \left((\nabla \cdot \mathbf{u}_h^n) \rho_h^{n+1}, \bar{\mathbf{u}}_h \right)$ por los términos estabilizadores

$$\frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right).$$

Resulta fácil observar que si admitimos (H4) nos encontramos que

$$\frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right) = \frac{1}{2} \left((\nabla \cdot \mathbf{u}_h^n) \rho_h^{n+1} \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right),$$

sin más que tomar $\bar{\rho}_h = \frac{1}{2} \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h$ en (8) e integrar por partes en el término convectivo. Por lo tanto, (9) coincide con el sistema de momentos discreto de [15]. Pero la hipótesis $(\mathbf{V}_h \cdot \mathbf{V}_h) \subset M_h$ que imponemos en (H4) y la hipótesis $(W_h \cdot W_h) \cap L_0^2(\Omega) \subset \widetilde{M}_h$ impuesta en [15] son opuestas, ya que si por simplificar suponemos $\mathbf{V}_h = \widetilde{\mathbf{V}}_h$ y $M_h = \widetilde{M}_h$, llegamos a las siguientes inclusiones desde el punto de vista de los grados de libertad de los espacios:

$$(\mathbf{V}_h \cdot \mathbf{V}_h \cdot \mathbf{V}_h \cdot \mathbf{V}_h) \subset (W_h \cdot W_h) \subset M_h \subset \mathbf{V}_h$$

(la última inclusión es debido a la condición *inf-sup* entre (\mathbf{V}_h, M_h)) las cuales son contradictorias.

En el esquema dado en [14] para dominios $2D$, se reemplaza el término convectivo semi-implícito $(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h)$ de (8) por el término totalmente explícito $(\mathbf{u}_h^n \cdot \nabla \rho_h^n, \bar{\rho}_h)$, se introducen los términos estabilizadores

$$\frac{1}{2} \left(\frac{[\rho_h^{n+1}]_T - [\rho_h^n]_T}{k}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla (\mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h) \right),$$

en lugar de $\frac{1}{2} \left((\nabla \cdot \mathbf{u}_h^n) \rho_h^{n+1} \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right)$ del sistema de momentos (9), donde $[\cdot]_T$ es un operador de truncamiento por nodos entre las cotas máxima y mínima de la densidad inicial, y se considera en el sistema de momentos este mismo truncamiento en los términos que dependen de la densidad discreta que requieran positividad y cotas puntuales de dicha densidad. En consecuencia, (9) no es equivalente al sistema de momentos discreto desarrollado en [14].

Una observación importante sobre el esquema (8)-(10) que aquí se presenta, es que no está claro como obtener estimaciones a priori de estabilidad de dicho esquema sin imponer hipótesis de regularidad sobre la solución del problema límite, a diferencia de los esquemas desarrollados en [14, 15] que sí son estables (y convergentes).

Es importante reseñar, que el estudio del análisis de error de los esquemas estables de [14, 15], introduce dificultades importantes, respecto al esquema que estudiamos en este trabajo.

El buen planteamiento de (8) se tiene de forma estándar, ya que es un problema elíptico lineal de convección difusión. Para obtener que el problema mixto lineal (9)-(10) está bien planteado, además de imponer la condición de estabilidad de *Brezzi-Babuska* o de tipo *Inf-Sup*, hay que obtener $\rho_h^n > 0$, lo que vamos a conseguir más adelante (ver Lemma 8) imponiendo h/k suficientemente pequeño.

Nota 1 La elección de aproximar la densidad en el término de derivada temporal de las velocidades de forma explícita como $\left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h\right)$ queda justificada con la siguiente igualdad:

$$\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k} \cdot \mathbf{u}_h^{n+1} + \frac{1}{2} \frac{\rho_h^{n+1} - \rho_h^n}{k} \cdot \mathbf{u}_h^{n+1} \cdot \mathbf{u}_h^{n+1} = \frac{1}{2} \left(\frac{\rho_h^{n+1} |\mathbf{u}_h^{n+1}|^2 - \rho_h^n |\mathbf{u}_h^n|^2}{k} + \rho_h^n |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 \right).$$

Se trata de una versión discreta de la siguiente igualdad en continuo:

$$\left(\rho \frac{d}{dt} \mathbf{u}, \mathbf{u}\right) + \frac{1}{2} \left(\frac{d}{dt} \rho, \mathbf{u} \cdot \mathbf{u}\right) = \frac{1}{2} \int_{\Omega} \frac{d}{dt} (\rho |\mathbf{u}|^2).$$

1.5 Resultados principales del trabajo

En adelante, por C vamos a denotar distintas constantes positivas, independientes de los parámetros de discretización h y k .

Definiendo los errores entre la solución continua y la discreta en tiempo para $t = t_n$ como:

$$e_u^n = \mathbf{u}_h^n - \mathbf{u}(t_n), \quad e_p^n = p_h^n - p(t_n), \quad e_\rho^n = \rho_h^n - \rho(t_n),$$

obtendremos los siguientes resultados:

Teorema 2 Asumimos las hipótesis (H0)-(H4) (ver Sección 2.1 más adelante) e imponemos la restricción

$$(S) \quad \lim_{(h,k) \rightarrow 0} \frac{h}{k} = 0.$$

Entonces, se tienen las siguientes estimaciones de error, para h y k suficientemente pequeño:

$$\left\{ \begin{array}{l} \max_{0 \leq n \leq N-1} \left(\tilde{m} |\mathbf{e}_u^{n+1}|^2 + A |e_\rho^{n+1}|^2 \right) + \sum_{n=0}^{N-1} \left(\frac{\tilde{m}}{2} |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + \frac{A}{2} |e_\rho^{n+1} - e_\rho^n|^2 \right) \\ + k \sum_{n=0}^{N-1} \left(\frac{\mu_1}{2} |\nabla \mathbf{e}_u^{n+1}|^2 + A \lambda |\nabla e_\rho^{n+1}|^2 \right) \leq C (k + h^2), \end{array} \right.$$

donde $A > 0$ es una constante dependiente de la solución exacta.

Teorema 3 En las condiciones del Teorema 2, se tienen las siguientes estimaciones de error, para h suficientemente pequeño:

$$\max_{0 \leq n \leq N} |\nabla e_\rho^{n+1}|^2 + \sum_{n=0}^{N-1} |\nabla (e_\rho^{n+1} - e_\rho^n)|^2 + k \sum_{n=0}^{N-1} |e_\Delta^{n+1}|^2 \leq C (k + h^2),$$

donde $e_\Delta^{n+1} := \Delta \rho(t_{n+1}) - \Delta_h \rho_h^{n+1}$ y $\Delta_h \rho_h^{n+1}$ es el laplaciano discreto de ρ_h^{n+1} definido en (44).

Razonando de manera análoga a la demostración del Teorema 2 y Teorema 3, pero imponiendo la regularidad $\mathbf{u}_{tt} \in L^2(0, T; \mathbf{H}^{-1}(\Omega))$ en lugar de $\sigma^{1/2}\mathbf{u}_{tt} \in L^2(0, T, \mathbf{H}^{-1}(\Omega))$ (ver hipótesis (H1)), se consigue orden de convergencia optimal en tiempo, es decir $O(h+k)$ en los Teoremas 2 y 3. Sin embargo, esta mejora en la regularidad de \mathbf{u}_{tt} sólo se asegura imponiendo una condición de compatibilidad no local para la presión en el tiempo inicial $t=0$, dependiente de los datos \mathbf{u}_0, ρ_0 y $\mathbf{f}(0)$, y que no se puede comprobar en la práctica ([16]).

Además, en este trabajo, para aproximar en cada etapa de tiempo los problemas (8) y (10), analizamos y proponemos sendos métodos iterativos, en donde las matrices en cada iteración son constantes. Estos esquemas se describen como sigue:

Método iterativo para el problema (8). Conocidos $(\rho_h^n, \mathbf{u}_h^n)$, se aproxima ρ_h^{n+1} solución de (8) por la sucesión $(\rho_h^{n+1,i})_i$ definida como:

Inicialización: Sean $\rho_h^{n+1,0} = \rho_h^n$.

Etapas $i+1$: Conocido $\rho_h^{n+1,i}$, hallar $\rho_h^{n+1,i+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1,i+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1,i+1}, \nabla \bar{\rho}_h \right) = - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1,i}, \bar{\rho}_h \right). \quad (14)$$

Método iterativo para el problema (9). Conocidos $(\rho_h^n, \rho_h^{n+1}, \mathbf{u}_h^n)$, se aproxima \mathbf{u}_h^{n+1} solución de (8) por la sucesión $(\mathbf{u}_h^{n+1,i})_i$ definida como:

Inicialización: Sea $\mathbf{u}_h^{n+1,0} = \mathbf{u}_h^n$.

Etapas $i+1$: Conocido $\mathbf{u}_h^{n+1,i}$, hallar $(\mathbf{u}_h^{n+1,i+1}, p_h^{n+1,i+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\left\{ \begin{array}{l} \left(\rho_{\tilde{m}}^{\tilde{M}} \frac{\mathbf{u}_h^{n+1,i+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \mu \left(\nabla \mathbf{u}_h^{n+1,i+1}, \nabla \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1,i+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ = - \left(\left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \mathbf{u}_h^{n+1,i}, \bar{\mathbf{u}}_h \right) - \lambda \int_0^T \left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) \left(\nabla \mathbf{u}_h^{n+1,i} \right)^t : \nabla \bar{\mathbf{u}}_h \\ - \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1} \mathbf{u}_h^{n+1,i}, \bar{\mathbf{u}}_h \right) + \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(\left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^n \right) \frac{\mathbf{u}_h^{n+1,i} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right), \end{array} \right. \quad (15)$$

$$\left(\nabla \cdot \mathbf{u}_h^{n+1,i}, \bar{p}_h \right) = 0, \quad (16)$$

donde $\rho_{\tilde{m}}^{\tilde{M}} = \frac{\tilde{M} + \tilde{m}}{2}$. Veremos la convergencia de las aproximaciones $(\mathbf{u}_h^{n+1,i+1}, p_h^{n+1,i+1}, \rho_h^{n+1,i+1})$ hacia $(\mathbf{u}_h^{n+1}, p_h^{n+1}, \rho_h^{n+1})$ cuando $i \rightarrow \infty$, para k suficientemente pequeño.

El resto del trabajo está organizado como sigue. En la Sección 2 describimos las hipótesis sobre el dominio, los datos iniciales y las aproximaciones de elementos finitos, y definimos adecuados operadores de interpolación. En la Sección 3 obtenemos la expresión del error de consistencia en tiempo de la solución continua y las ecuaciones que verifica el error en densidad y en velocidad-presión. En la Sección 4 probamos, mediante un proceso de inducción en la etapa de tiempo, estimaciones puntuales para la densidad discreta que nos permitirán obtener las tasas de

convergencia en normas débiles. La Sección 5 está dedicada a las estimaciones de error fuertes para la densidad. Finalmente, en la Sección 6 vemos que los métodos iterativos (14) y (15) están bien planteados y son convergentes.

2 Preliminares

En lo que sigue, consideramos Ω un abierto acotado de \mathbb{R}^d ($d = 2$ ó 3) con frontera poliédrica y una familia de triangulaciones $\{\mathcal{T}_h\}_{h>0}$ tal que $\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K$, siendo h el diámetro máximo de los elementos de \mathcal{T}_h .

2.1 Hipótesis

(H0) *Regularidad para los datos:* Supongamos $\lambda \frac{M-m}{2} < \mu$ y sean $\widetilde{M} > M$ y $0 < \widetilde{m} < m$ tal que $\lambda \frac{\widetilde{M} - \widetilde{m}}{2} < \mu$.

Sea $\mathbf{u}_0 \in \mathbf{V} \cap \mathbf{H}^2(\Omega)$, $\rho_0 \in H_N^3(\Omega)$ con $0 < m \leq \rho_0 \leq M$ en Ω , $\mathbf{f} \in L^2(0, T; \mathbf{H}^1(\Omega))$ y $\mathbf{f}_t \in L^2(0, T; \mathbf{L}^{6/5}(\Omega))$.

Regularidad para la solución: Supongamos que (ρ, \mathbf{u}) es la única solución del problema (1)-(4) en $(0, T)$ con la siguiente regularidad:

$$(\rho, \mathbf{u}) \in L^\infty(0, T; H_N^3(\Omega) \times \mathbf{H}^2(\Omega)), \quad p \in L^\infty(0, T, H^1(\Omega))$$

$$(\rho_t, \mathbf{u}_t) \in (L^\infty(0, T; H^1) \cap L^2(0, T; H^2)) \times L^\infty(0, T; \mathbf{L}^2(\Omega)),$$

$$(\rho_{tt}, \sigma^{1/2} \mathbf{u}_{tt}) \in L^2(0, T; L^2(\Omega) \times \mathbf{H}^{-1}(\Omega)),$$

donde $\sigma(t) = \min\{1, t\}$.

Suponemos aproximaciones $(\rho_h^0, \mathbf{u}_h^0)$ de los datos iniciales (ρ_0, \mathbf{u}_0) tales que

$$|\mathbf{u}_0 - \mathbf{u}_h^0| + h|\nabla(\mathbf{u}_0 - \mathbf{u}_h^0)| \leq G_1 h^2,$$

$$|\nabla \mathbf{u}_h^0| \leq G_2,$$

$$|\rho_0 - \rho_h^0| + h\|\rho_0 - \rho_h^0\|_{H^1(\Omega)} \leq G_3 h^2,$$

$$0 < \widetilde{m} \leq \rho_h^0(\mathbf{x}) \leq \widetilde{M}.$$

para G_i constantes positivas que dependen de \mathbf{u}_0, ρ_0 y Ω .

(H1) La frontera de Ω es poligonal y tal que se tiene la dependencia continua en norma H^2 del problema *Poisson-Neumann* (ver (54)). Esto es verdad, por ejemplo, si Ω es convexo ([11]).

(H2) La tringulación de Ω y los espacios discretos satisfacen:

- Desigualdades inversas:

$$\|\bar{\rho}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)}, \quad \forall \bar{\rho}_h \in W_h$$

- Errores de interpolación:

$$\inf_{\bar{\mathbf{u}}_h \in \mathbf{V}_h} \{|\bar{\mathbf{u}} - \bar{\mathbf{u}}_h| + h \|\bar{\mathbf{u}} - \bar{\mathbf{u}}_h\|_{H^1(\Omega)}\} \leq C h^2 \|\bar{\mathbf{u}}\|_{H^2(\Omega)}, \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^2(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$\inf_{\bar{p}_h \in M_h} |\bar{p} - \bar{p}_h| \leq C h \|\bar{p}\|_{H^1(\Omega)}, \quad \forall \bar{p} \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\inf_{\bar{\rho}_h \in W_h} \{|\bar{\rho} - \bar{\rho}_h| + h \|\bar{\rho} - \bar{\rho}_h\|_{H^1(\Omega)}\} \leq C h^2 \|\bar{\rho}\|_{H^2(\Omega)}, \quad \forall \bar{\rho} \in H^2(\Omega),$$

$$\inf_{\bar{\rho}_h \in W_h} \|\bar{\rho} - \bar{\rho}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{1/2} \|\bar{\rho}\|_{H^2(\Omega)}, \quad \forall \bar{\rho} \in H^2(\Omega).$$

- Propiedad de estabilidad:

$$\|P_h \bar{\rho}\|_{L^3} \leq C \|\bar{\rho}\|_{L^3}, \quad \forall \bar{\rho} \in L^3(\Omega),$$

donde P_h es la $L^2(\Omega)$ -proyección sobre W_h .

(H3) Condición inf-sup. Existe $\beta > 0$ (independiente de h) tal que $\forall \bar{p}_h \in M_h$

$$\|\bar{p}_h\|_{L_0^2(\Omega)} \leq \beta \sup_{\bar{\mathbf{u}}_h \in \mathbf{V}_h \setminus \{0\}} \frac{(\bar{p}_h, \nabla \cdot \bar{\mathbf{u}}_h)}{\|\bar{\mathbf{u}}_h\|_{H^1(\Omega)}}.$$

(H4) Los espacios discretos en velocidad y densidad (\mathbf{V}_h, W_h) satisfacen $\mathbf{V}_h \cdot \mathbf{V}_h \subset W_h$, es decir,

$$\forall \bar{\mathbf{u}}_h^1, \bar{\mathbf{u}}_h^2 \in \mathbf{V}_h, \quad \bar{\mathbf{u}}_h^1 \cdot \bar{\mathbf{u}}_h^2 \in W_h.$$

Por ejemplo, una forma de definir los espacios discretos (W_h, \mathbf{V}_h, M_h) para que verifiquen (H2)-(H4) es la siguiente: Sea $\{\mathcal{T}_h\}_{h>0}$ una familia de triangulaciones regulares y quasi-uniforme de Ω . Entonces, se considera W_h como el espacio de las funciones globalmente continuas y localmente \mathbb{P}_4 y (\mathbf{V}_h, M_h) el espacio de *Taylor-Hood* $\mathbb{P}_2 \times \mathbb{P}_1$ ([11]).

2.2 Operadores de interpolación globales

A continuación definimos operadores de interpolación globales, como la solución de los siguientes problemas discretos:

Para cada par $(\mathbf{u}, p) \in \mathbf{V} \times L_0^2(\Omega)$, definimos $(I_h \mathbf{u}, J_h p)$ como la solución del siguiente problema de Stokes discreto: Hallar $(I_h \mathbf{u}, J_h p) \in \mathbf{V}_h \times M_h$ tal que,

$$\begin{cases} \mu \left(\nabla(\mathbf{u} - I_h \mathbf{u}), \nabla \bar{\mathbf{u}}_h \right) - \left(p - J_h p, \nabla \cdot \bar{\mathbf{u}}_h \right) = 0, & \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \\ \left(\nabla \cdot (\mathbf{u} - I_h \mathbf{u}), \bar{p}_h \right) = 0, & \forall \bar{p}_h \in M_h. \end{cases} \quad (17)$$

Para cada $\rho \in H^1(\Omega)$, definimos $K_h\rho \in W_h$ tal que

$$\begin{cases} \left(\nabla(\rho - K_h\rho), \nabla\bar{\rho}_h \right) = 0, & \forall \bar{\rho}_h \in W_h, \\ \int_{\Omega} K_h\rho = \int_{\Omega} \rho. \end{cases} \quad (18)$$

De hecho, $K_h\rho$ se puede obtener como sigue:

a) Consideramos $\eta = \rho - \oint_{\Omega} \rho \in L_0^2(\Omega)$.

b) Hallar $\tilde{\eta}_h \in W_h \cap L_0^2(\Omega)$ la solución del siguiente problema de Neumann discreto,

$$\left(\nabla(\eta - \tilde{\eta}_h), \nabla\bar{\rho}_h \right) = 0, \quad \forall \bar{\rho}_h \in W_h \cap L_0^2(\Omega). \quad (19)$$

c) Calcular $K_h\rho = \tilde{\eta}_h + \oint_{\Omega} \rho$.

La prueba del siguiente resultado se pueden encontrar en Girault-Raviart [11] (Capítulo II, Teoremas 1.1 y 1.2) para la obtención de los errores de aproximación y en Girault-Nochetto-Scott [10] para la parte de estabilidad de los operadores de interpolación:

Lema 4 *Supongamos (H3)-(H4). Para cada $\mathbf{u} \in \mathbf{H}^2(\Omega) \cap \mathbf{V}$ y $p \in H^1(\Omega) \cap L_0^2(\Omega)$,*

$$\begin{aligned} \|\mathbf{u} - I_h\mathbf{u}\| + h\|\mathbf{u} - I_h\mathbf{u}\|_{H^1(\Omega)} &\leq C h^2 \|\mathbf{u}\|_{H^2(\Omega)}, \\ \|p - J_h p\| &\leq C h \|p\|_{H^1(\Omega)}, \\ \|I_h\mathbf{u}\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} &\leq C \|\mathbf{u}\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)}. \end{aligned} \quad (20)$$

Un resultado análogo se tiene para el interpolador K_h (ver [8], [11] para más detalles).

Lema 5 *Supongamos (H3). Para cada $\rho \in \mathbf{H}^2(\Omega)$,*

$$\begin{aligned} \|\rho - K_h\rho\| + h\|\rho - K_h\rho\|_{H^1(\Omega)} &\leq C h^2 \|\rho\|_{H^2(\Omega)}, \\ \|\rho - K_h\rho\| &\leq C h \|\rho\|_{H^1(\Omega)}, \\ \|K_h\rho\|_{L^\infty(\Omega)} &\leq C \|\rho\|_{L^\infty(\Omega)}. \end{aligned} \quad (21)$$

Corolario 6 *En las condiciones del Lema 5, para cada $\rho_t \in L^2(0, T; H^2(\Omega))$,*

$$\left\| \frac{\rho(t+k) - \rho(t)}{k} - \frac{K_h\rho(t+k) - K_h\rho(t)}{k} \right\|_{L^2(0, T; H^1(\Omega))} \leq C h \|\rho_t\|_{L^2(0, T; H^2(\Omega))}.$$

3 Ecuaciones de error

3.1 Errores de consistencia en tiempo

A continuación mostraremos la expresión del error de consistencia que se comete cuando la solución continua es puesta en la discretización temporal del esquema numérico (8)-(10). Usando que (ρ, \mathbf{u}, p) es la solución de (1) en $t = t_{n+1}$, se tiene:

$$\frac{\rho(t_{n+1}) - \rho(t_n)}{k} + \mathbf{u}(t_n) \cdot \nabla \rho(t_{n+1}) - \lambda \Delta \rho(t_{n+1}) = R_\rho^{n+1}, \quad (22)$$

$$\begin{cases} \rho(t_n) \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_n)}{k} + (\rho(t_{n+1}) \mathbf{u}(t_n) - \lambda \nabla \rho(t_{n+1})) \cdot \nabla \mathbf{u}(t_{n+1}) \\ - \nabla \cdot (\mu \nabla \mathbf{u}(t_{n+1}) - \lambda \rho(t_{n+1}) (\nabla \mathbf{u}(t_{n+1}))^t) + \nabla p(t_{n+1}) = \rho(t_{n+1}) \mathbf{f}(t_{n+1}) + R_{\mathbf{u}}^{n+1}, \end{cases} \quad (23)$$

donde los errores de consistencias R_ρ^{n+1} y $R_{\mathbf{u}}^{n+1}$ tienen las expresiones:

$$\begin{aligned} R_\rho^{n+1} &= \frac{1}{k} \int_{t_n}^{t_{n+1}} (s - t_n) \rho_{tt} ds - \nabla \cdot \left(\rho(t_{n+1}) \int_{t_n}^{t_{n+1}} \mathbf{u}_t(s) ds \right), \\ R_{\mathbf{u}}^{n+1} &= \frac{\rho(t_{n+1})}{k} \int_{t_n}^{t_{n+1}} (s - t_n) \mathbf{u}_{tt} ds - \nabla \cdot \left(\rho(t_{n+1}) \int_{t_n}^{t_{n+1}} \mathbf{u}_t(s) ds \right) \mathbf{u}(t_{n+1}) \\ &\quad - \frac{1}{k} \left(\int_{t_n}^{t_{n+1}} \rho_t(s) ds \right) \left(\int_{t_n}^{t_{n+1}} \mathbf{u}_t(s) ds \right). \end{aligned}$$

Definición 7 Consideramos las siguientes definiciones:

$$\begin{aligned} \mathbf{e}_u^n &= \mathbf{e}_{d,\mathbf{u}} + \mathbf{e}_{i,\mathbf{u}}, \text{ donde } \mathbf{e}_{d,\mathbf{u}} = \mathbf{u}_h^n - I_h \mathbf{u}(t_n) \text{ y } \mathbf{e}_{i,\mathbf{u}} = I_h \mathbf{u}(t_n) - \mathbf{u}(t_n), \\ e_p^n &= e_{d,p} + e_{i,p}, \text{ donde } e_{d,p} = p_h^n - J_h p(t_n) \text{ y } e_{i,p} = J_h p(t_n) - p(t_n), \\ e_\rho^n &= e_{d,\rho} + e_{i,\rho}, \text{ donde } e_{d,\rho} = \rho_h^n - K_h \rho(t_n) \text{ y } e_{i,\rho} = K_h \rho(t_n) - \rho(t_n). \end{aligned}$$

Observamos que $e_{d,\cdot}$ son errores completamente discretos y $e_{i,\cdot}$ son errores de interpolación.

3.2 Ecuación de error para la densidad

Restando (22) de (8), llegamos a la formulación variacional del error para la densidad

$$\begin{aligned} \left(\frac{e_\rho^{n+1} - e_\rho^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla e_\rho^{n+1}, \nabla \bar{\rho}_h \right) &= \left(\rho_h^{n+1} \mathbf{e}_u^n + e_\rho^{n+1} \mathbf{u}(t_n), \nabla \bar{\rho}_h \right) \\ &\quad + \left(\nabla \cdot \mathbf{e}_u^n \rho_h^{n+1}, \bar{\rho}_h \right) + \left(R_\rho^{n+1}, \bar{\rho}_h \right). \end{aligned} \quad (24)$$

3.3 Ecuación de error para la velocidad

Restando (23) de (9), se obtiene la siguiente formulación variacional del error en velocidad-presión:

$$\left\{ \begin{array}{l} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) - \left(\rho(t_n) \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_n)}{k}, \bar{\mathbf{u}}_h \right) + \mu \left(\nabla \mathbf{e}_u^{n+1}, \nabla \bar{\mathbf{u}}_h \right) - \left(\mathbf{e}_p^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ + \left(((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \left(((\rho(t_{n+1}) \mathbf{u}(t_n) - \lambda \nabla \rho(t_{n+1})) \cdot \nabla) \mathbf{u}(t_{n+1}), \bar{\mathbf{u}}_h \right) \\ - \lambda \left(\left(\rho_h^{n+1} - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{u}_h^{n+1})^t, \nabla \bar{\mathbf{u}}_h \right) + \lambda \left((\rho(t_{n+1})) (\nabla \mathbf{u}(t_{n+1}))^t, \nabla \bar{\mathbf{u}}_h \right) \\ + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) = \left(\mathbf{e}_\rho^{n+1} \mathbf{f}(t_{n+1}), \bar{\mathbf{u}}_h \right) + \left(R_u^{n+1}, \bar{\mathbf{u}}_h \right), \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \end{array} \right. \quad (25)$$

$$\left(\nabla \cdot \mathbf{e}_p^{n+1}, \bar{p}_h \right) = 0, \quad \forall p_h \in M_h. \quad (26)$$

Teniendo en cuenta la definición de los operadores de interpolación global en velocidad-presión

$$\mu \left(\nabla \mathbf{e}_u^{n+1}, \nabla \bar{\mathbf{u}}_h \right) - \left(\mathbf{e}_p^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = \mu \left(\nabla \mathbf{e}_{d,u}^{n+1}, \nabla \bar{\mathbf{u}}_h \right) - \left(\mathbf{e}_{d,p}^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right)$$

y descomponiendo las no linealidades como sigue:

$$\left\{ \begin{array}{l} \left(\rho_h^n \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) - \left(\rho(t_n) \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_n)}{k}, \bar{\mathbf{u}}_h \right) \\ = \left(\rho_h^n \frac{\mathbf{e}_u^{n+1} - \mathbf{e}_u^n}{k}, \bar{\mathbf{u}}_h \right) + \left(\mathbf{e}_\rho^n \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_n)}{k}, \bar{\mathbf{u}}_h \right), \\ \left(((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla) \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \left(((\rho(t_{n+1}) \mathbf{u}(t_n) - \lambda \nabla \rho(t_{n+1})) \cdot \nabla) \mathbf{u}(t_{n+1}), \bar{\mathbf{u}}_h \right) \\ = \left(((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla) \mathbf{e}_u^{n+1}, \bar{\mathbf{u}}_h \right) + \left(((\rho_h^{n+1} \mathbf{e}_u^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla) \mathbf{u}(t_{n+1}), \bar{\mathbf{u}}_h \right) \\ + \left((\mathbf{e}_\rho^{n+1} \mathbf{u}(t_n) \cdot \nabla) \mathbf{u}(t_{n+1}), \bar{\mathbf{u}}_h \right), \\ \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \mathbf{u}_h^{n+1} \cdot \bar{\mathbf{u}}_h \right) = \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \mathbf{e}_u^{n+1} \cdot \bar{\mathbf{u}}_h \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{e}_u^n \rho_h^{n+1}, \mathbf{u}(t_{n+1}) \cdot \bar{\mathbf{u}}_h \right), \\ - \lambda \left(\left(\rho_h^{n+1} - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{u}_h^{n+1})^t, \nabla \bar{\mathbf{u}}_h \right) + \lambda \left(\left(\rho(t_{n+1}) - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{u}(t_{n+1}))^t, \nabla \bar{\mathbf{u}}_h \right) \\ = - \lambda \left(\left(\rho_h^{n+1} - \frac{\widetilde{M} + \widetilde{m}}{2} \right) (\nabla \mathbf{e}_u^{n+1})^t, \nabla \bar{\mathbf{u}}_h \right) - \lambda \left(\mathbf{e}_\rho^{n+1} (\nabla \mathbf{u}(t_{n+1}))^t, \nabla \bar{\mathbf{u}}_h \right), \end{array} \right.$$

donde hemos usado la igualdad $\int_{\Omega} (\nabla \mathbf{u}(t_{n+1}))^t : \nabla \mathbf{u}(t_{n+1}) dx = 0$, ya que $\nabla \cdot \mathbf{u}(t_{n+1}) = 0$ en Ω y $\mathbf{u}(t_{n+1}) = 0$ on Γ , entonces (25)-(26) se re-escribe

$$\left\{ \begin{array}{l} \left(\rho_h^n \frac{\mathbf{e}_u^{n+1} - \mathbf{e}_u^n}{k}, \bar{\mathbf{u}}_h \right) + \left(((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla) \mathbf{e}_u^{n+1}, \bar{\mathbf{u}}_h \right) + a \left(\rho_h^{n+1}, \mathbf{e}_u^{n+1}, \bar{\mathbf{u}}_h \right) \\ + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \mathbf{e}_u^{n+1} \cdot \bar{\mathbf{u}}_h \right) + \left(\mathbf{e}_{d,p}^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) = \left(A_n, \bar{\mathbf{u}}_h \right), \quad \forall \bar{\mathbf{u}}_h \in \mathbf{V}_h, \end{array} \right. \quad (27)$$

$$\left(\nabla \cdot \mathbf{e}_p^{n+1}, \bar{p}_h \right) = 0, \quad \forall p_h \in M_h, \quad (28)$$

donde A_n se define como:

$$\begin{aligned}
(A_n, \bar{\mathbf{u}}_h) &= -\left((\rho_h^{n+1} \mathbf{e}_u^n + e_\rho^{n+1} \mathbf{u}(t_n) - \lambda \nabla e_\rho^{n+1}) \cdot \nabla \right) \mathbf{u}(t_{n+1}), \bar{\mathbf{u}}_h \\
&\quad - \left(e_\rho^n \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_n)}{k}, \bar{\mathbf{u}}_h \right) + \lambda \left(e_\rho^{n+1} (\nabla \mathbf{u}(t_{n+1}))^t, \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \left(e_\rho^{n+1} \mathbf{f}(t_{n+1}), \bar{\mathbf{u}}_h \right) + \mu \left(\nabla e_{i,u}^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\
&\quad - \frac{1}{2} \left(\nabla \cdot e_u^n \rho_h^{n+1}, \mathbf{u}(t_{n+1}) \cdot \bar{\mathbf{u}}_h \right) + \left(R_u^{n+1}, \bar{\mathbf{u}}_h \right)
\end{aligned}$$

4 Estimaciones de error

4.1 Estimaciones puntuales de la densidad discreta

Comenzamos con una estimación puntual de la densidad discreta bajo la hipótesis (S). La idea para obtener este tipo de estimación ya se ha usado en [15], en la cual se usaba un operador de truncamiento, la estimación $k \sum_{l=0}^n |\nabla \mathbf{u}_h^n|^2 \leq C_s$ y la velocidad del término convectivo es una proyección de \mathbf{u}_h^n en un espacio de elementos finitos de mayor orden. Ahora, suponiendo una mejor acotación de la velocidad discreta $|\nabla \mathbf{u}_h^n| \leq C_s$ podemos evitar proyectar la velocidad, como se ve en el siguiente:

Lema 8 *Para cada $n = 0, \dots, N-1$, supongamos que $|\nabla \mathbf{u}_h^l| \leq C_s$, para cada $l = 0, \dots, n$, siendo $C_s > 0$ una constante independiente de los parámetros de discretización (k, h) y de n . Si imponemos la hipótesis (S), entonces para h/k suficientemente pequeño (independiente de la etapa de tiempo n) la densidad discreta del esquema (8) verifica*

$$0 < \tilde{m} \leq \rho_h^{l+1} \leq \tilde{M}, \quad \forall l : 0 \leq l \leq n. \quad (29)$$

Prueba: Aquí únicamente veremos una idea de la demostración, que se hace por inducción en n (ver [15] para los detalles). Consideramos el siguiente esquema auxiliar sólo discreto en tiempo: Sea $\rho^0 = \rho_0$ y dado $\rho^l \in H^2(\Omega)$, hallar $\rho^{l+1} \in H^2(\Omega)$ solución del problema:

$$\frac{\rho^{l+1} - \rho^l}{k} + \mathbf{u}_h^n \cdot \nabla \rho^{l+1} - \lambda \Delta \rho^{l+1} = 0 \quad \text{en } \Omega, \quad \frac{\partial \rho^{l+1}}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0. \quad (30)$$

Se prueba que existe ρ^{l+1} solución de (30) y verifica: $0 < m \leq \rho^{l+1} \leq M$, para cada $l = 0, \dots, n$. Para ello, resulta fundamental la hipótesis impuesta sobre la cota de tipo $L^\infty(0, T; H^1(\Omega))$ para la velocidad discreta $(\mathbf{u}_h^l)_{l=0}^n$. Además, como $m \leq \rho^{l+1} \leq M$ para $l = 0 \dots, n$, de (30) es fácil deducir las siguientes estimaciones a priori (en normas fuertes):

$$\max_{0 \leq l \leq n} \|\rho^{l+1}\|_{H^1(\Omega)}^2 \leq C, \quad k \sum_{l=0}^n \|\rho^{l+1}\|_{H^2(\Omega)}^2 \leq C.$$

En particular, usando propiedades de aproximación del error de interpolación, tenemos

$$\|\rho^{l+1} - K_h \rho^{l+1}\|_{H^1(\Omega)} \leq C h \|\rho^{l+1}\|_{H^2(\Omega)} \leq C \frac{h}{\sqrt{k}}, \quad \forall l = 0, \dots, n. \quad (31)$$

Por otra parte, comparando (30) con (8) y usando que $|\nabla \mathbf{u}_h^l| \leq C_s$ para $l = 0, \dots, n$, se puede obtener la estimación de error ([15]):

$$\|\rho_h^{l+1} - \rho^{l+1}\|_{H^1(\Omega)} \leq C \frac{h}{\sqrt{k}}. \quad (32)$$

Finalmente, de (31) y (32), deducimos

$$\|\rho_h^{l+1} - K_h \rho^{l+1}\|_{H^1(\Omega)} \leq C \frac{h}{\sqrt{k}}.$$

En consecuencia, usando la desigualdad inversa $\|\bar{\rho}_h\|_{L^\infty(\Omega)} \leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)}$, $\forall \bar{\rho}_h \in W_h$, se tiene $\|\rho_h^{l+1} - K_h \rho^{l+1}\|_{L^\infty(\Omega)} \leq C \sqrt{\frac{h}{k}}$. Luego, usando la estimación del error de interpolación

$$\|\rho^{l+1} - K_h \rho^{l+1}\|_{L^\infty(\Omega)} \leq C h^{1/2} \|\rho^{l+1}\|_{H^2(\Omega)} \leq C \frac{h^{1/2}}{k^{1/2}},$$

se tiene $\|\rho_h^{l+1} - \rho^{l+1}\|_{L^\infty(\Omega)} \leq C \frac{h^{1/2}}{k^{1/2}}$.

Finalmente, se tiene (29) para h/k suficientemente pequeño, gracias a la estimación puntual $m \leq \rho^{l+1} \leq M$, para cada $l = 0, \dots, n$. \square

4.2 Estimaciones de error en normas débiles

El siguiente lema nos proporcionará las estimaciones fundamentales en cada etapa de tiempo, para luego obtener las tasas de convergencias por un proceso de inducción.

Lema 9 *Supongamos $0 < \tilde{m} \leq \rho_h^n, \rho_h^{n+1} \leq \tilde{M}$ en Ω . Entonces, para k y h suficientemente pequeño y $h \leq C k$ (gracias a la hipótesis (S)), existe una constante $A > 0$ (dependiente de la solución exacta) tal que se verifica la desigualdad*

$$\left\{ \begin{array}{l} \left(|\sqrt{\rho_h^{n+1}} \mathbf{e}_u^{n+1}|^2 + A |e_\rho^{n+1}|^2 \right) - \left(|\sqrt{\rho_h^n} \mathbf{e}_u^n|^2 + A |e_\rho^n|^2 \right) \\ + \left(\frac{\tilde{m}}{2} |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + \frac{A}{2} |e_\rho^{n+1} - e_\rho^n|^2 \right) + k \frac{3}{4} \left(\mu_1 |\nabla \mathbf{e}_u^{n+1}|^2 + A \lambda |\nabla e_\rho^{n+1}|^2 \right) \\ \leq C_1 k \left(\tilde{m} |\mathbf{e}_u^n|^2 + A |e_\rho^n|^2 \right) + k \frac{1}{4} \left(\mu_1 |\nabla \mathbf{e}_u^n|^2 + A \lambda |\nabla e_\rho^n|^2 \right) + C k \left(\|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 + \|e_{i,\rho}^{n+1}\|_{H^1(\Omega)}^2 \right) \\ + C \left(|\mathbf{e}_{i,u}^{n+1}|^2 + |e_{i,\rho}^{n+1}|^2 \right) + C k^2 \int_{t_n}^{t_{n+1}} \left(\|\rho_{tt}(s)\|_{H^1(\Omega)'}^2 + \|\rho_{tt}(s)\|_{L^{6/5}(\Omega)}^2 + |\mathbf{u}_t(s)|^2 \right) ds \\ + C k \int_{t_n}^{t_{n+1}} (s - t_n) \|\mathbf{u}_{tt}(s)\|_{L^{6/5}(\Omega)}^2 ds, \end{array} \right. \quad (33)$$

donde C y C_1 son constantes positivas independientes de los parámetros de discretización (h, k) y dependientes de la solución exacta.

Prueba: Tomando como función test $\bar{\rho}_h = 2k e_{d,\rho}^{n+1} = 2k(e_\rho^{n+1} - e_{i,\rho}^{n+1})$ en (24) y usando la identidad $(a - b, 2a) = a^2 - b^2 + (a - b)^2$, obtenemos

$$\left\{ \begin{array}{l} |e_\rho^{n+1}|^2 - |e_\rho^n|^2 + |e_\rho^{n+1} - e_\rho^n|^2 + 2\lambda k |\nabla e_\rho^{n+1}|^2 = 2k \left(\frac{e_\rho^{n+1} - e_\rho^n}{k}, e_{i,\rho}^{n+1} \right) \\ + 2\lambda k \left(\nabla e_\rho^{n+1}, \nabla e_{i,\rho}^{n+1} \right) + 2k \left(\rho_h^{n+1} \mathbf{e}_u^n + e_\rho^{n+1} \mathbf{u}(t_n), \nabla (e_\rho^{n+1} - e_{i,\rho}^{n+1}) \right) \\ + 2k \left(\nabla \cdot \mathbf{e}_u^n \rho_h^{n+1}, e_\rho^{n+1} - e_{i,\rho}^{n+1} \right) + 2k \left(R_\rho^{n+1}, e_\rho^{n+1} - e_{i,\rho}^{n+1} \right) := L_1 + L_2 + L_3 + L_4 + L_5. \end{array} \right.$$

Acotamos el lado derecho como:

$$\begin{aligned} L_1 &\leq \varepsilon |e_\rho^{n+1} - e_\rho^n|^2 + C |e_{i,\rho}^{n+1}|^2, \\ L_2 &\leq \varepsilon k |\nabla e_\rho^{n+1}|^2 + C k |\nabla e_{i,\rho}^{n+1}|^2, \\ L_3 &\leq 2k \left(\|\rho_h^{n+1}\|_{L^\infty(\Omega)} |\mathbf{e}_u^n| + \|\mathbf{u}(t_n)\|_{L^\infty(\Omega)} |e_\rho^{n+1}| \right) \left(|\nabla e_\rho^{n+1}| + |\nabla e_{i,\rho}^{n+1}| \right) \\ &\leq C k \left(|\mathbf{e}_u^n|^2 + |e_\rho^{n+1} - e_\rho^n|^2 + |e_\rho^n|^2 \right) + \varepsilon k |\nabla e_\rho^{n+1}|^2 + C k |\nabla e_{i,\rho}^{n+1}|^2, \\ L_4 &\leq 2k |\nabla \mathbf{e}_u^n| \|\rho_h^{n+1}\|_{L^\infty(\Omega)} |e_\rho^{n+1} - e_{i,\rho}^{n+1}| \leq \varepsilon_1 k |\nabla \mathbf{e}_u^n|^2 + C k |e_\rho^{n+1}|^2 + C k |e_{i,\rho}^{n+1}|^2 \\ &\leq \varepsilon_1 k |\nabla \mathbf{e}_u^n|^2 + C k |e_\rho^n|^2 + C k |e_\rho^{n+1} - e_\rho^n|^2 + C k |e_{i,\rho}^{n+1}|^2. \end{aligned}$$

Usando que

$$\|R_\rho^{n+1}\|_{H^1(\Omega)'}^2 \leq C k^2 \int_{t_n}^{t_{n+1}} \left(\|\rho_{tt}(s)\|_{H^1(\Omega)'}^2 + |\mathbf{u}_t(s)|^2 \right) ds,$$

se puede acotar el término L_5 como

$$L_5 \leq \varepsilon k \left(\|e_\rho^{n+1}\|_{H^1(\Omega)}^2 + \|e_{i,\rho}^{n+1}\|_{H^1(\Omega)}^2 \right) + C k^2 \int_{t_n}^{t_{n+1}} \left(\|\rho_{tt}(s)\|_{H^1(\Omega)'}^2 + |\mathbf{u}_t(s)|^2 \right) ds.$$

Recopilando las acotaciones anteriores y eligiendo ε y k pequeños, conseguimos

$$\begin{aligned} &|e_\rho^{n+1}|^2 - |e_\rho^n|^2 + \frac{3}{4} |e_\rho^{n+1} - e_\rho^n|^2 + \lambda k |\nabla e_\rho^{n+1}|^2 \\ &\leq C k \left(|e_\rho^n|^2 + |\mathbf{e}_u^n|^2 + \varepsilon_1 |\nabla \mathbf{e}_u^n|^2 + \|e_{i,\rho}^{n+1}\|_{H^1(\Omega)}^2 \right) \\ &+ C k^2 \int_{t_n}^{t_{n+1}} \left(\|\rho_{tt}(s)\|_{H^1(\Omega)'}^2 + |\mathbf{u}_t(s)|^2 \right) + C |e_{i,\rho}^{n+1}|^2. \end{aligned} \quad (34)$$

Por otra parte, tomando en (27) como función test $\bar{\mathbf{u}}_h = \mathbf{e}_{d,u}^{n+1} = \mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1}$, teniendo en cuenta que $(e_{d,\rho}^{n+1}, \nabla \cdot \mathbf{e}_u^{n+1}) = 0$ y la coercitividad de $a(\cdot, \cdot, \cdot)$ dada en (11), obtenemos

$$\left\{ \begin{array}{l} \left(\rho_h^n \frac{\mathbf{e}_u^{n+1} - \mathbf{e}_u^n}{k}, \mathbf{e}_u^{n+1} \right) + \frac{\mu_1}{2} |\nabla \mathbf{e}_u^{n+1}|^2 + \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \mathbf{e}_u^{n+1}, \mathbf{e}_u^{n+1} \\ + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \mathbf{e}_u^{n+1} \cdot \mathbf{e}_u^{n+1} \right) \leq \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \mathbf{e}_u^{n+1}, \mathbf{e}_{i,u}^{n+1} \\ + a \left(\rho_h^{n+1}, \mathbf{e}_u^{n+1}, \mathbf{e}_{i,u}^{n+1} \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \mathbf{e}_u^{n+1} \cdot \mathbf{e}_{i,u}^{n+1} \right) \\ + \left(A_n, \mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1} \right) + \left(\rho_h^n \frac{\mathbf{e}_u^{n+1} - \mathbf{e}_u^n}{k}, \mathbf{e}_{i,u}^{n+1} \right). \end{array} \right. \quad (35)$$

Continuamos transformando aún más (35). Tomamos en el esquema de la densidad (8) como función test

$$\bar{\rho}_h = \frac{1}{2} |e_{d,u}^{n+1}|^2 = \frac{1}{2} \left[|e_u^{n+1}|^2 + (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right] \in W_h,$$

(notar que $\bar{\rho}_h \in W_h$ gracias a la hipótesis $\mathbf{V}_h \cdot \mathbf{V}_h \subseteq W_h$ de (H4)), y obtenemos

$$\begin{cases} \frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, |e_u^{n+1}|^2 \right) - \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla (|e_u^{n+1}|^2) \right) \\ - \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, |e_u^{n+1}|^2 \right) = \left(B_h^n, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right), \end{cases} \quad (36)$$

donde

$$\left(B_h^n, \bar{\rho} \right) := -\frac{1}{2} \left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho} \right) + \frac{1}{2} \left(\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}, \nabla \bar{\rho} \right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}, \bar{\rho} \right), \quad (37)$$

para cada $\bar{\rho} \in H^1(\Omega)$. Por otra parte, de la ecuación del error de consistencia para la densidad (22) multiplicada por $\frac{1}{2} (e_u^{n+1} - 2e_{i,u}^{n+1}) \cdot e_{i,u}^{n+1}$ e integrada sobre Ω , conseguimos

$$\begin{cases} \left(B_h^n, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) \\ := \frac{1}{2} \left(\frac{\rho(t_{n+1}) - \rho(t_n)}{k}, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) \\ - \frac{1}{2} \left(\rho(t_{n+1}) \mathbf{u}(t_n) - \lambda \nabla \rho(t_{n+1}), \nabla ((e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1}) \right) \\ - \frac{1}{2} \left(R_\rho^{n+1}, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) = 0. \end{cases} \quad (38)$$

Luego, teniendo en cuenta la definición (38) podemos escribir (descomponiendo las no linealidades previamente):

$$\begin{cases} \left(B_h^n, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) \\ = \left(B_h^n - B^n, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) \\ = -\frac{1}{2} \left(\frac{e_\rho^{n+1} - e_\rho^n}{k}, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) \\ + \frac{1}{2} \left(\rho_h^{n+1} e_u^n + e_\rho^{n+1} \mathbf{u}(t_n) - \lambda \nabla e_\rho^{n+1}, \nabla ((e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1}) \right) \\ + \frac{1}{2} \left(\nabla \cdot e_u^n \rho_h^{n+1}, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right) - \frac{1}{2} \left(R_\rho^{n+1}, (e_{i,u}^{n+1} - 2e_u^{n+1}) \cdot e_{i,u}^{n+1} \right). \end{cases} \quad (39)$$

Sumando (36) (cambiando la parte derecha según (39)) a (35) y usando la versión de la derivada discreta de la Nota 1, llegamos

$$\begin{aligned} & \left| \sqrt{\rho_h^{n+1}} e_u^{n+1} \right|^2 - \left| \sqrt{\rho_h^n} e_u^n \right|^2 + \left| \sqrt{\rho_h^n} (e_u^{n+1} - e_u^n) \right|^2 + \mu_1 k |\nabla e_u^{n+1}|^2 \\ & \leq 2k \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla e_u^{n+1}, e_{i,u}^{n+1} \right) + 2k \left(A_n, e_u^{n+1} - e_{i,u}^{n+1} \right) \\ & + 2k a \left(\rho_h^{n+1}, e_u^{n+1}, e_{i,u}^{n+1} \right) + 2 \left(\rho_h^n (e_u^{n+1} - e_u^n), e_{i,u}^{n+1} \right) \\ & + 2k \left(B^n - B_h^n, (2e_u^{n+1} - e_{i,u}^{n+1}) \cdot e_{i,u}^{n+1} \right). \end{aligned} \quad (40)$$

Por último, tenemos que acotar adecuadamente el lado derecho de la desigualdad anterior. Por resumir acotamos los términos más significativos

$$\begin{aligned}
& 2k \left(((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla) \mathbf{e}_u^{n+1}, \mathbf{e}_{i,u}^{n+1} \right) \\
&= 2k \left((\rho_h^{n+1} (\mathbf{e}_u^n + \mathbf{u}(t_n)) - \lambda \nabla (e_\rho^{n+1} + \rho(t_{n+1})) \cdot \nabla) \mathbf{e}_u^{n+1}, \mathbf{e}_{i,u}^{n+1} \right) \\
&\leq C k \left(|\mathbf{e}_u^n| + |\nabla e_\rho^{n+1}| \right) |\nabla \mathbf{e}_u^{n+1}| \|\mathbf{e}_{i,u}^{n+1}\|_{L^\infty(\Omega)} \\
&+ C k \left(\|\mathbf{u}(t_n)\|_{L^6(\Omega)} + \|\nabla \rho(t_{n+1})\|_{L^6(\Omega)} \right) |\nabla \mathbf{e}_u^{n+1}| \|\mathbf{e}_{i,u}^{n+1}\|_{L^3(\Omega)} \\
&\leq C k |\nabla e_\rho^{n+1}|^2 + C k |\mathbf{e}_u^n|^2 + \varepsilon_1 k |\nabla \mathbf{e}_u^{n+1}|^2 + C k \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2,
\end{aligned}$$

donde se ha usado (20) en la última estimación.

$$\text{A partir de ahora comenzamos a acotar } 2k \left(A_n, \mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1} \right) := \sum_{i=1}^7 Q_i:$$

$$\begin{aligned}
Q_1 &\leq C |\rho(t_{n+1}) \mathbf{e}_u^n + e_\rho^{n+1} \mathbf{u}(t_n) - \lambda \nabla e_\rho^{n+1}| \|\nabla \mathbf{u}(t_{n+1})\|_{L^3(\Omega)} \|\mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1}\|_{L^6(\Omega)} \\
&\leq C k \left(|\mathbf{e}_u^n|^2 + |e_\rho^{n+1}|^2 + |\nabla e_\rho^{n+1}|^2 \right) + \varepsilon_1 k \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 \right),
\end{aligned}$$

$$\begin{aligned}
Q_2 &\leq C k \|e_\rho^n\|_{L^3(\Omega)} \|\mathbf{u}_t\|_{L^\infty(0,T;L^2(\Omega))} \|\mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1}\|_{L^6(\Omega)} \\
&\leq C k |e_\rho^n|^2 + \varepsilon k |\nabla e_\rho^n|^2 + \varepsilon_1 k \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 \right),
\end{aligned}$$

$$Q_3 \leq C k \|\mathbf{e}_\rho^{n+1}\|_{H^1(\Omega)}^2 + \varepsilon_1 k \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 \right),$$

$$Q_4 \leq C k |e_\rho^{n+1}|^2 \|\mathbf{f}(t_{n+1})\|_{L^3(\Omega)}^2 + \varepsilon_1 k \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 \right),$$

$$Q_5 \leq \varepsilon_1 k |\nabla \mathbf{e}_u^{n+1}|^2 + C k |\nabla \mathbf{e}_{i,u}^{n+1}|^2,$$

$$Q_6 \leq \varepsilon_1 k |\nabla \mathbf{e}_u^n|^2 + C k |\mathbf{e}_u^{n+1}|^2 + C k |\mathbf{e}_{i,u}^{n+1}|^2.$$

Finalmente, acotamos el error de consistencia Q_7 para el sistema de momentos

$$\begin{aligned}
Q_7 &= 2k \left(R_u^{n+1}, \mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1} \right) \leq 2k \|R_u^{n+1}\|_{H^{-1}(\Omega)} \|\mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)} \\
&\leq C k \left\{ \frac{1}{k} \int_{t_n}^{t_{n+1}} (s - t_n) \|\mathbf{u}_{tt}(s)\|_{L^{6/5}(\Omega)} ds + C k \left(\int_{t_n}^{t_{n+1}} |\mathbf{u}_t(s)| ds \right) \|\mathbf{u}(t_{n+1})\|_{W^{1,3}(\Omega) \cap L^\infty(\Omega)} \right. \\
&\quad \left. + \frac{1}{k} \int_{t_n}^{t_{n+1}} \|\rho_t(s)\|_{L^3(\Omega)} \int_{t_n}^{t_{n+1}} |\mathbf{u}_t(s)| ds \right\} \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)} + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)} \right) \\
&\leq C k \int_{t_n}^{t_{n+1}} (s - t_n) \|\mathbf{u}_{tt}(s)\|_{L^{6/5}(\Omega)}^2 ds + C k^3 + \varepsilon_1 k \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 \right).
\end{aligned}$$

Seguimos estimando el término $2k \left(B^n - B_h^n, (2\mathbf{e}_u^{n+1} - \mathbf{e}_{i,u}^{n+1}) \cdot \mathbf{e}_{i,u}^{n+1} \right) := P_1 + P_2 + P_3 + P_4$, donde se usará repetidamente la estabilidad en $W^{1,3}(\Omega) \cap L^\infty(\Omega)$ del operador de interpolación para la velocidad I_h dada en (20) y el error de interpolación $\|\mathbf{u} - I_h \mathbf{u}\|_{L^\infty(\Omega)} \leq C h^{1/2} \|\mathbf{u}\|_{H^2(\Omega)}$:

$$\begin{aligned}
P_1 &\leq \frac{1}{2} |e_\rho^{n+1} - e_\rho^n| \|\mathbf{e}_{i,u}^{n+1} - 2\mathbf{e}_u^{n+1}\| \|\mathbf{e}_{i,u}^{n+1}\|_{L^\infty(\Omega)} \\
&\leq C h^{1/2} |e_\rho^{n+1} - e_\rho^n| \|\mathbf{e}_{i,u}^{n+1} - 2\mathbf{e}_u^{n+1}\| \\
&\leq \varepsilon |e_\rho^{n+1} - e_\rho^n|^2 + C h |\mathbf{e}_u^{n+1}|^2 + C |\mathbf{e}_{i,u}^{n+1}|^2 \\
&\leq \varepsilon |e_\rho^{n+1} - e_\rho^n|^2 + C h |\mathbf{e}_u^n|^2 + C h |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + C |\mathbf{e}_{i,u}^{n+1}|^2,
\end{aligned}$$

$$\begin{aligned}
P_2 &\leq k \frac{1}{2} |\rho_h^{n+1} \mathbf{e}_u^n + e_\rho^{n+1} \mathbf{u}(t_n) - \lambda \nabla e_\rho^{n+1}| |\nabla((2\mathbf{e}_u^{n+1} + \mathbf{e}_{i,u}^{n+1}) \cdot \mathbf{e}_{i,u}^{n+1})| \\
&\leq C k \left(|\mathbf{e}_u^n| + |e_\rho^{n+1}| + |\nabla e_\rho^{n+1}| \right) \|\mathbf{e}_{i,u}^{n+1} - 2\mathbf{e}_u^{n+1}\|_{H^1(\Omega)} \|\mathbf{e}_{i,u}^{n+1}\|_{W^{1,3}(\Omega) \cap L^\infty(\Omega)} \\
&\leq C k |\mathbf{e}_u^n|^2 + C k |\nabla e_\rho^{n+1}|^2 + \varepsilon_1 k \|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + C k \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2, \\
P_3 &\leq k \frac{1}{2} |\nabla \cdot \mathbf{e}_u^n| \|\rho_h^{n+1}\|_{L^\infty(\Omega)} |\mathbf{e}_{i,u}^{n+1} - 2\mathbf{e}_u^{n+1}| \|\mathbf{e}_{i,u}^{n+1}\|_{L^\infty(\Omega)} \\
&\leq \varepsilon_1 k |\nabla \mathbf{e}_u^n|^2 + C k |\mathbf{e}_u^n|^2 + C k |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + C k |\mathbf{e}_{i,u}^{n+1}|^2, \\
P_4 &\leq C k \|R_\rho^{n+1}\|_{L^{6/5}(\Omega)} \|\mathbf{e}_{i,u}^{n+1} - 2\mathbf{e}_u^{n+1}\|_{H^1(\Omega)} \|\mathbf{e}_{i,u}^{n+1}\|_{W^{1,3}(\Omega) \cap L^\infty(\Omega)} \\
&\leq \varepsilon_1 k \left(\|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 \right) + C k^2 \int_{t_n}^{t_{n+1}} \left(\|\rho_{tt}(s)\|_{L^{6/5}(\Omega)}^2 + |\mathbf{u}_t(s)|^2 \right) ds.
\end{aligned}$$

A continuación, tratamos los términos residuales de la derivada discreta de la velocidad:

$$2k \left(\rho_h^n (\mathbf{e}_u^{n+1} - \mathbf{e}_u^n), \mathbf{e}_{i,u}^{n+1} \right) \leq \frac{\tilde{m}}{4} |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + C |\mathbf{e}_{i,u}^{n+1}|^2.$$

Luego, eligiendo ε_1 , k y h suficientemente pequeño y $h \leq Ck$ (gracias a la hipótesis (S)) e incorporando las desigualdades anteriormente obtenidas en (35), se consigue

$$\begin{aligned}
&|\sqrt{\rho_h^{n+1}} \mathbf{e}_u^{n+1}|^2 - |\sqrt{\rho_h^n} \mathbf{e}_u^n|^2 + \frac{\tilde{m}}{2} |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + \frac{3}{4} \mu_1 k |\nabla \mathbf{e}_u^{n+1}|^2 \\
&\leq C k \left(|\mathbf{e}_u^n|^2 + |e_\rho^{n+1}|^2 + |\nabla e_\rho^{n+1}|^2 \right) + \frac{\mu_1}{8} k |\nabla \mathbf{e}_u^n|^2 + \varepsilon k |\nabla e_\rho^n|^2 + C k \|\mathbf{e}_{i,u}^{n+1}\|_{H^1(\Omega)}^2 + C |\mathbf{e}_{i,u}^{n+1}|^2 \\
&+ \varepsilon |e_\rho^{n+1} - e_\rho^n|^2 + C k \left(\int_{t_n}^{t_{n+1}} (s - t_n) |\mathbf{u}_{tt}(s)|^2 ds + k \int_{t_n}^{t_{n+1}} \|\rho_{tt}(s)\|_{L^{6/5}(\Omega)}^2 ds + k^2 \right).
\end{aligned} \tag{41}$$

Finalmente, acotando $|e_\rho^{n+1}|^2 \leq 2(|e_\rho^{n+1} - e_\rho^n|^2 + |e_\rho^n|^2)$ y haciendo un balance adecuado de las desigualdades (41) y (34) para absorber los términos $|e_\rho^{n+1} - e_\rho^n|^2$ y $|\nabla e_\rho^{n+1}|^2$ de la parte derecha de (41), se obtiene (33). \square

Ya estamos en disposición para la prueba del Teorema 2, cuyo resultado repetimos para conveniencia del lector.

Teorema 10 *Asumiendo las hipótesis (H0)-(H4) y la restricción (S), se tienen las siguientes estimaciones de error, para k y h suficientemente pequeño:*

$$0 < \tilde{m} \leq \rho_h^{n+1} \leq \tilde{M}, \quad \forall n : 0 \leq n \leq N - 1, \tag{42}$$

$$\left\{ \begin{array}{l} \max_{0 \leq n \leq N-1} \left(\tilde{m} |\mathbf{e}_u^{n+1}|^2 + A |e_\rho^{n+1}|^2 \right) + \sum_{n=0}^{N-1} \left(\frac{\tilde{m}}{2} |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n|^2 + \frac{A}{2} |e_\rho^{n+1} - e_\rho^n|^2 \right) \\ + k \sum_{n=0}^{N-1} \left(\frac{\mu_1}{2} |\nabla \mathbf{e}_u^{n+1}|^2 + A \lambda |\nabla e_\rho^{n+1}|^2 \right) \leq C (k + h^2). \end{array} \right. \tag{43}$$

Prueba: Supongamos que (29) y (33) se verifican para cada $n = 0, \dots, N - 1$. Entonces, (42) se tiene trivialmente de (29) y, sumando (33) para $n = 0, \dots, N - 1$ y aplicando (42) y el Lema de Gronwall discreto obtenemos (43). Veamos por tanto (29) y (33) por inducción en n .

Para $n = 0$ tenemos por hipótesis que $0 < \tilde{m} \leq \rho_h^0 \leq \tilde{M}$ y $|\nabla \mathbf{u}_h^0| \leq G_2$ (ver (H1)). Elegimos $C_s := \max\{C_3, G_2\}$, siendo C_3 una constante positiva que se determinará más tarde.

En virtud del Lema 8, se tiene la estimación puntual $0 < \tilde{m} \leq \rho_h^1 \leq \tilde{M}$, es decir (29) para $n = 0$. Entonces, del Lema 9 tenemos (33) para $n = 0$.

Supongamos por inducción que se tiene (29) y (33) para $l = 0, \dots, n-1$. Sumando (33) para $l = 0, \dots, n-1$, se tiene:

$$\begin{aligned} & \tilde{m}|\mathbf{e}_u^n|^2 + A|e_\rho^n|^2 + \frac{k}{2} \sum_{l=1}^n \left(\mu_1 |\nabla \mathbf{e}_u^l|^2 + A\lambda |\nabla e_\rho^l|^2 \right) \\ & \leq C_1 k \sum_{l=0}^{n-1} \left(\tilde{m}|\mathbf{e}_u^l|^2 + A|e_\rho^l|^2 \right) + \tilde{M}|\mathbf{e}_u^0|^2 + A|e_\rho^0|^2 \\ & \quad + k \frac{1}{4} \left(\mu_1 |\nabla \mathbf{e}_u^0|^2 + A\lambda |\nabla e_\rho^0|^2 \right) + C(k + h^2 + \frac{h^4}{k}) \\ & \leq C_1 k \sum_{l=0}^{n-1} \left(\tilde{m}|\mathbf{e}_u^l|^2 + A|e_\rho^l|^2 \right) + C(k + h^2), \end{aligned}$$

donde en la última desigualdad hemos aplicado las propiedades de aproximación inicial dadas en (H1) y que $h \leq Ck$ gracias a (S). Aplicando el Lema de Gronwall discreto, obtenemos que

$$\frac{\mu_1}{2} k \sum_{l=1}^n |\nabla \mathbf{e}_u^l|^2 \leq C e^{2C_1 t_n} (k + h^2) \leq C e^{2C_1 T} (k + h^2),$$

de donde es fácil deducir que existe una constante $C_3 > 0$ tal que $|\nabla \mathbf{u}_h^l| \leq C_3 \leq C_s$, para $l = 0, \dots, n$. Por lo tanto, del Lema 8 tenemos (29) para n , es decir $0 < \tilde{m} \leq \rho_h^{l+1} \leq \tilde{M}$ para cada $l = 0, \dots, n$. De lo anterior, se deduce que estamos en las condiciones del Lema 9 y tenemos (33) para n . \square

Nota 11 *El término responsable de que no se obtenga estimaciones de $O(k)$ es el término $\frac{\rho(t_{n+1})}{k} \int_{t_n}^{t_{n+1}} (s - t_n) \mathbf{u}_{tt} ds$ que proviene del error de consistencia en tiempo R_u^{n+1} . En el caso de densidad constante, para obtener $O(k + h)$ basta pedir $\mathbf{u}_{tt} \in L^2(0, T; \mathbf{V}')$ que no requiere una condición de compatibilidad no local para la presión en $t = 0$, mientras que para nuestro modelo para obtener $O(k + h)$ (en vez de $O(k^{1/2} + h)$) tenemos que imponer $\mathbf{u}_{tt} \in L^2(0, T; \mathbf{H}^{-1}(\Omega))$, que requiere dicha condición de compatibilidad.*

Nota 12 *Las estimaciones de error en normas débiles anteriores no se trasladan a la presión. De hecho, de la ecuación de error para la velocidad (27), usando las hipótesis (H1), (H3), el Lema 8 y el interpolador de la presión J_h (ver (17)), obtenemos*

$$|e_{d,p}^{n+1}| \leq C \frac{1}{k} |\mathbf{e}_u^{n+1} - \mathbf{e}_u^n| + C \|e_{i,u}^{n+1}\|_{H^1(\Omega)} + C \|e_u^{n+1}\|_{H^1(\Omega)} + C \|e_\rho^{n+1}\|_{H^1(\Omega)} + \|R_u^{n+1}\|_{L^{6/5}(\Omega)}.$$

Así, elevando al cuadrado, multiplicando por k , sumando para n y teniendo en cuentas las tasas de error conseguidas en el Teorema 10 (en particular, $\sum_{n=0}^{N-1} |e_{\mathbf{u}}^{n+1} - e_{\mathbf{u}}^n|^2 \leq C(k+h^2)$) y los errores de interpolación, sólo conseguimos la siguiente estimación:

$$k \sum_{n=0}^{N-1} |e_{d,p}^{n+1}|^2 \leq C \left(1 + \frac{h^2}{k}\right).$$

Y de aquí fácilmente deducimos la estimación en $L^2(Q)$ para el error de presión

$$k \sum_{n=0}^{N-1} |e_p^{n+1}|^2 \leq C \left(1 + \frac{h^2}{k}\right) \leq C.$$

Con el mismo argumento, en el caso de deducir $O(k+h)$ para la velocidad, se tiene $O(k^{1/2} + \frac{h}{k^{1/2}})$ para la presión en $L^2(Q)$.

4.3 Estimaciones de error de la densidad en normas fuertes

Para obtener el error de la densidad en mejores normas, consideramos el operador laplaciano discreto $-\Delta_h : W_h \rightarrow W_h$ definido para cada $\bar{\rho} \in W_h$ como la solución del problema

$$\Delta_h \rho_h \in W_h \quad \text{tal que} \quad - \left(\Delta_h \rho_h, \bar{\rho}_h \right) = \left(\nabla \rho_h, \nabla \bar{\rho}_h \right), \quad \forall \bar{\rho}_h \in W_h. \quad (44)$$

Luego, la ecuación discreta de la densidad puede re-escribirse en función de este operador como:

$$\left(\frac{\rho_h^{n+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \left(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1}, \bar{\rho}_h \right) - \lambda \left(\Delta_h \rho_h^{n+1}, \bar{\rho}_h \right) = 0, \quad \forall \bar{\rho}_h \in W_h. \quad (45)$$

Restando (22) de (45) nos encontramos con la nueva ecuación de error para la densidad

$$\left(\frac{e_\rho^{n+1} - e_\rho^n}{k}, \bar{\rho}_h \right) + \lambda \left(e_\Delta^{n+1}, \bar{\rho}_h \right) = - \left(e_{\mathbf{u}}^n \cdot \nabla \rho_h^{n+1} + \mathbf{u}(t_n) \cdot \nabla e_\rho^{n+1}, \bar{\rho}_h \right) + \left(R_\rho^{n+1}, \bar{\rho}_h \right), \quad (46)$$

siendo $e_\Delta^{n+1} := -\Delta_h \rho_h^{n+1} + \Delta \rho(t_{n+1})$.

Ahora estamos en disposición de probar el Teorema 3, cuyo enunciado repetimos para conveniencia del lector.

Teorema 13 *En las hipótesis del Teorema 10, se tienen las siguientes estimaciones de error para h suficientemente pequeño:*

$$\max_{0 \leq n \leq N-1} |\nabla e_\rho^{n+1}|^2 + \sum_{n=0}^{N-1} |\nabla (e_\rho^{n+1} - e_\rho^n)|^2 + k \sum_{n=0}^{N-1} |e_\Delta^{n+1}|^2 \leq C(k+h^2). \quad (47)$$

Nota 14 *Para obtener una cota $C(k^2 + h^2)$ en (47) debemos asumir la hipótesis de regularidad $\mathbf{u}_{tt} \in L^2(0, T; \mathbf{H}^{-1}(\Omega))$ que de nuevo está relacionada con una condición de compatibilidad global.*

Prueba: Definimos $e_{i,\Delta}^{n+1} = -\Delta\rho(t_{n+1}) + P_h(-\Delta\rho(t_{n+1}))$ donde P_h es el proyector ortogonal en $L^2(\Omega)$ sobre W_h . Consideramos $\bar{\rho}_h = e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} := e_{d,\Delta}^{n+1}$ como función test en la formulación variacional (46), llegando

$$\begin{aligned} (e_{\rho}^{n+1} - e_{\rho}^n, e_{\Delta}^{n+1}) + \lambda k |e_{\Delta}^{n+1}|^2 &= (e_{\rho}^{n+1} - e_{\rho}^n, e_{i,\Delta}^{n+1}) + \lambda k (e_{\Delta}^{n+1}, e_{i,\Delta}^{n+1}) \\ -k \left(\mathbf{e}_u^n \cdot \nabla \rho_h^{n+1} + \mathbf{u}(t_n) \cdot \nabla e_{\rho}^{n+1}, e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) &+ k \left(R_{\rho}^{n+1}, e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right). \end{aligned} \quad (48)$$

Ahora, “integramos por partes” en el término $(e_{\rho}^{n+1} - e_{\rho}^n, e_{\Delta}^{n+1})$ como sigue: consideramos la ecuación de error para el laplaciano discreto

$$(e_{\Delta}^{n+1}, \bar{\rho}_h) = (\nabla e_{\rho}^{n+1}, \nabla \bar{\rho}_h), \quad \forall \bar{\rho}_h \in W_h \quad (49)$$

y tomamos $\bar{\rho}_h = e_{\rho}^{n+1} - e_{\rho}^n - (e_{i,\rho}^{n+1} - e_{i,\rho}^n) \in W_h$ en (49), llegando

$$(e_{\Delta}^{n+1}, e_{\rho}^{n+1} - e_{\rho}^n) = (\nabla e_{\rho}^{n+1}, \nabla (e_{\rho}^{n+1} - e_{\rho}^n)) - (\nabla e_{\rho}^{n+1}, \nabla (e_{i,\rho}^{n+1} - e_{i,\rho}^n)) + (e_{\Delta}^{n+1}, e_{i,\rho}^{n+1} - e_{i,\rho}^n). \quad (50)$$

Así, incorporando (50) en (48) y usando la identidad $|a|^2 - |b|^2 + |a - b|^2 = (a - b, 2a)$, tenemos

$$\begin{aligned} |\nabla e_{\rho}^{n+1}|^2 - |\nabla e_{\rho}^n|^2 + |\nabla (e_{\rho}^{n+1} - e_{\rho}^n)|^2 + 2\lambda k |e_{\Delta}^{n+1}|^2 &= 2 (e_{\rho}^{n+1} - e_{\rho}^n, e_{i,\Delta}^{n+1}) \\ -2k \left(\mathbf{e}_u^n \cdot \nabla \rho_h^{n+1} + \mathbf{u}(t_n) \cdot \nabla e_{\rho}^{n+1}, e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) &+ 2k \left(R_{\rho}^{n+1}, e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) + \lambda k (e_{\Delta}^{n+1}, e_{i,\Delta}^{n+1}) \\ + 2 \left(\nabla e_{\rho}^{n+1}, \nabla (e_{i,\rho}^{n+1} - e_{i,\rho}^n) \right) - 2 \left(e_{\Delta}^{n+1}, e_{i,\rho}^{n+1} - e_{i,\rho}^n \right) &:= K_1 + K_2 + K_3 + K_4 + K_5 + K_6. \end{aligned} \quad (51)$$

A continuación, estimamos el lado derecho de (51):

$$K_1 \leq \frac{1}{2} |e_{\rho}^{n+1} - e_{\rho}^n|^2 + C |e_{i,\Delta}^{n+1}|^2.$$

Para acotar el término K_2 actuamos como sigue:

$$\begin{aligned} K_2 &= -k \left(\mathbf{e}_u^n \cdot \nabla \rho_h^{n+1} + \mathbf{u}(t_n) \cdot \nabla e_{\rho}^{n+1}, e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) \\ &\leq -k \left(\mathbf{e}_u^n \cdot \nabla \rho_h^{n+1}, e_{d,\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) + C k |\nabla e_{\rho}^{n+1}|^2 + \varepsilon k |e_{\Delta}^{n+1}|^2 + \varepsilon k |e_{i,\Delta}^{n+1}|^2. \end{aligned} \quad (52)$$

El primer término de la derecha de la desigualdad anterior lo re-escribimos como

$$\begin{aligned} -k \left(\mathbf{e}_u^n \cdot \nabla \rho_h^{n+1}, e_{d,\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) &= -k \left(\mathbf{e}_u^n \cdot \nabla e_{\rho}^{n+1}, e_{d,\Delta}^{n+1} \right) \\ &\quad -k \left(\mathbf{e}_u^n \cdot \nabla \rho(t_{n+1}), e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1} \right) := K_2^1 + K_2^2. \end{aligned}$$

Teniendo en cuenta la regularidad impuesta a la densidad continua no es complicado acotar

$$K_2^2 \leq C k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)}^2 + \varepsilon k |e_{\Delta}^{n+1}|^2 + C k |e_{i,\Delta}^{n+1}|^2. \quad (53)$$

Para obtener un cota para K_2^1 , definimos una aproximación continua asociada a $e_{d,\Delta}^{n+1}$: hallar $e^{n+1}(h) \in H^2(\Omega)$ tal que

$$-\Delta e^{n+1}(h) = e_{d,\Delta}^{n+1} \quad \text{en } \Omega, \quad \frac{\partial e^{n+1}(h)}{\partial \mathbf{n}} \Big|_{\partial \Omega} = 0, \quad \int_{\Omega} e^{n+1}(h) = 0. \quad (54)$$

Es fácil ver que este problema de Neumann está bien planteado, ya que $\int_{\Omega} e_{d,\Delta}^{n+1} = 0$. Usando esta aproximación continua $e^{n+1}(h)$ escribimos

$$K_2^1 = k\left(\mathbf{e}_u^n \cdot \nabla(e_\rho^{n+1} - e^{n+1}(h)), e_{d,\Delta}^{n+1}\right) + k\left(\mathbf{e}_u^n \cdot \nabla e^{n+1}(h), \Delta e^{n+1}(h)\right).$$

Integrando por partes en el último término y acotando, conseguimos

$$\begin{aligned} K_2^1 &= k\left(\mathbf{e}_u^n \cdot \nabla(e_\rho^{n+1} - e^{n+1}(h)), e_{d,\Delta}^{n+1}\right) \\ &\quad - k\left(\nabla \mathbf{e}_u^n, \nabla e^{n+1}(h) \otimes \nabla e^{n+1}(h)\right) + k\left(\nabla \cdot \mathbf{e}_u^n, |\nabla e^{n+1}(h)|^2\right) \\ &\leq C k \|\mathbf{e}_u^n\|_{H^1(\Omega)} \|\nabla(e_\rho^{n+1} - e^{n+1}(h))\|_{L^3(\Omega)} |e_{d,\Delta}^{n+1}| \\ &\quad + C k \|\mathbf{e}_u^n\|_{H^1(\Omega)} \|e^{n+1}(h)\|_{L^\infty(\Omega)} |e_{d,\Delta}^{n+1}|, \end{aligned} \quad (55)$$

donde en los dos últimos términos hemos usado la interpolación $\|\nabla \rho\|_{L^4(\Omega)}^2 \leq C \|\rho\|_{L^\infty(\Omega)} |\Delta \rho|$ para cualquier $\rho \in H_{N,0}^2(\Omega)$ y la dependencia continua $|\Delta e^{n+1}(h)| \leq |e_{d,\Delta}^{n+1}|$ de (54). Además, \otimes denota el producto tensorial de dos vectores $\mathbf{a} = (a_i)_{i=1}^2$, $\mathbf{b} = (b_i)_{i=1}^2$, con coeficientes $(\mathbf{a} \otimes \mathbf{b})_{i,j} = a_i b_j$

A continuación, veremos como tratar los términos $\|\nabla(e_\rho^{n+1} - e^{n+1}(h))\|_{L^3(\Omega)}$ y $\|e^{n+1}(h)\|_{L^\infty(\Omega)}^2$ que aparecen en (55). Los descomponemos como sigue:

$$\|\nabla(e_\rho^{n+1} - e^{n+1}(h))\|_{L^3(\Omega)} \leq \|\nabla e_{i,\rho}^{n+1}\|_{L^3(\Omega)} + \|\nabla(e_{d,\rho}^{n+1} - e^{n+1}(h))\|_{L^3(\Omega)}, \quad (56)$$

$$\begin{aligned} \|e^{n+1}(h)\|_{L^\infty(\Omega)} &\leq \|e^{n+1}(h) - e_\rho^{n+1}\|_{L^\infty(\Omega)} + \|e_\rho^{n+1}\|_{L^\infty(\Omega)} \\ &\leq \|e^{n+1}(h) - e_{d,\rho}^{n+1}\|_{L^\infty(\Omega)} + \|e_{i,\rho}^{n+1}\|_{L^\infty(\Omega)} + \|e_\rho^{n+1}\|_{L^\infty(\Omega)} \\ &\leq \|e^{n+1}(h) - e_{d,\rho}^{n+1}\|_{L^\infty(\Omega)} + C, \end{aligned} \quad (57)$$

donde en la última estimación hemos usado la estabilidad L^∞ de K_h dada en (21).

Ahora, veamos que

$$\|\nabla(e_{d,\rho}^{n+1} - e^{n+1}(h))\|_{L^3(\Omega)} + \|e^{n+1}(h) - e_{d,\rho}^{n+1}\|_{L^\infty(\Omega)} \leq C h^{1/2} |e_{d,\Delta}^{n+1}|. \quad (58)$$

En efecto, se tiene

$$\left(\nabla e_{d,\rho}^{n+1}, \nabla \bar{\rho}_h\right) = \left(e_{d,\Delta}^{n+1}, \bar{\rho}_h\right). \quad (59)$$

Pues, por un lado de la definición de $-\Delta_h$ dada en (44),

$$\left(\nabla \rho_h^{n+1}, \nabla \bar{\rho}_h\right) = -\left(\Delta_h \rho_h^{n+1}, \bar{\rho}_h\right).$$

Y por otro, de la definición del interpolador K_h aplicado a $\rho(t_{n+1})$ y de $-\left(\Delta \rho(t_{n+1}), \bar{\rho}_h\right) = \left(P_h(-\Delta(\rho(t_{n+1}))), \bar{\rho}_h\right)$, obtenemos

$$\left(\nabla K_h \rho(t_{n+1}), \nabla \bar{\rho}_h\right) = \left(P_h(-\Delta \rho(t_{n+1})), \bar{\rho}_h\right).$$

Luego, restando ambas igualdades se encuentra (59). Para las tasas de convergencia (58), comparamos (54) y (59) y tomamos como función test $\bar{\rho}_h = e_{d,\rho}^{n+1} - e^{n+1}(h) + e^{n+1}(h) - \bar{\rho}_h$ para cualquier $\bar{\rho}_h \in W_h$, llegando

$$|\nabla(e_{d,\rho}^{n+1} - e^{n+1}(h))| \leq |\nabla(e^{n+1}(h) - \bar{\rho}_h)| \leq h \|e^{n+1}(h)\|_{H^2(\Omega)} \leq C h |e_{d,\Delta}^{n+1}|, \quad (60)$$

donde hemos usado los errores de interpolación (H3) para el espacio W_h y la dependencia continua del problema (54), $\|e^{n+1}(h)\|_{H^2(\Omega)} \leq C |e_{d,\Delta}^{n+1}|$. A continuación, siguiendo las ideas de [15], sumando y restando un elemento cualquiera $\bar{\rho}_h \in W_h$ en la parte izquierda de (60), utilizando las desigualdades inversas $\|\bar{\rho}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{-1/2} \|\bar{\rho}_h\|_{H^1(\Omega)}$ para todo $\bar{\rho}_h \in W_h$ y la aproximación $\inf_{\bar{\rho}_h \in W_h} \|e^{n+1}(h) - \bar{\rho}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} \leq C h^{1/2} \|e^{n+1}(h)\|_{H^2(\Omega)} \leq C h^{1/2} |e_{d,\Delta}^{n+1}|$, llegamos a (58).

Por lo tanto, aplicando en (55) las descomposiciones (56) y (57), y las tasas de convergencia (58, conseguimos la acotación

$$K_2^1 \leq C k h^{1/2} \|e_{\mathbf{u}}^n\|_{H^1(\Omega)} |e_{d,\Delta}^{n+1}|^2 + C k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)} |e_{d,\Delta}^{n+1}|.$$

Usando la desigualdad de Young y que $e_{d,\Delta}^{n+1} = e_{\Delta}^{n+1} - e_{i,\Delta}^{n+1}$, se llega

$$K_2^1 \leq C k h \|e_{\mathbf{u}}^n\|_{H^1(\Omega)} |e_{\Delta}^{n+1}|^2 + C k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)}^2 + \varepsilon k |e_{\Delta}^{n+1}|^2 + \varepsilon k |e_{i,\Delta}^{n+1}|^2.$$

Ahora, teniendo en cuenta la estimación $k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)}^2 \leq C(k+h^2)$ que proporciona el Teorema 10, conseguimos

$$K_2^1 \leq C k h \left(1 + \frac{h}{k^{1/2}}\right) |e_{\Delta}^{n+1}|^2 + C k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)}^2 + \varepsilon k |e_{\Delta}^{n+1}|^2 + C k |e_{i,\Delta}^{n+1}|^2.$$

Luego, de la estimación (53) y la anterior, tenemos que

$$K_2 \leq k \left(C h \left(1 + \frac{h}{k^{1/2}}\right) + 2\varepsilon \right) |e_{\Delta}^{n+1}|^2 + C k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)}^2 + C k |\nabla e_{\rho}^{n+1}|^2 + C k |e_{i,\Delta}^{n+1}|^2.$$

Los términos K_3 y K_4 se acotan como:

$$K_3 \leq \varepsilon k \left(|e_{\Delta}^{n+1}|^2 + |e_{i,\Delta}^{n+1}|^2 \right) + C k^2 \int_{t_n}^{t_{n+1}} \left(|\rho_{tt}(s)|^2 + |\mathbf{u}_t(s)|^2 \right) ds.$$

$$K_4 = \lambda k \left(e_{\Delta}^{n+1}, e_{i,\Delta}^{n+1} \right) \leq \varepsilon k |e_{\Delta}^{n+1}|^2 + C k |e_{i,\Delta}^{n+1}|^2$$

En virtud del Corolario 6, vemos que

$$K_5 \leq k |\nabla e_{\rho}^{n+1}|^2 + C k h^2 \|\rho_t\|_{L^\infty(0,T;H^2(\Omega))}$$

y

$$K_6 \leq \varepsilon k |e_{\Delta}^{n+1}|^2 + C k h^4 \|\rho_t\|_{L^\infty(0,T;H^2(\Omega))}.$$

Por tanto, usando que $h/k^{1/2} \leq C$ gracias a la hipótesis (S) y eligiendo h y ε suficientemente pequeños, nos resulta

$$\begin{aligned} & |\nabla e_\rho^{n+1}|^2 - |\nabla e_\rho^n|^2 + \frac{1}{2} |\nabla(e_\rho^{n+1} - e_\rho^n)|^2 + \lambda k |e_\Delta^{n+1}|^2 \leq C |e_{i,\Delta}^{n+1}|^2 + C k |e_{i,\Delta}^{n+1}|^2 + C k \|e_{\mathbf{u}}^n\|_{H^1(\Omega)}^2 \\ & + C k^2 \int_{t_n}^{t_{n+1}} (|\rho_{tt}(s)|^2 + |\mathbf{u}_t(s)|^2) ds + C k h^2 \|\rho_t\|_{L^\infty(0,T;H^2(\Omega))}^2. \end{aligned} \quad (61)$$

Por último, de las hipótesis de aproximación (H3) y de las restricciones impuestas a los parámetros de discretización (S), tenemos $|e_{i,\Delta}^{n+1}|^2 \leq C h^2 \leq C k^2$. Luego, sumando en n y usando las hipótesis para la solución continua (H1), encontramos el orden de convergencia buscado. \square

5 Estudio de un método iterativo para desacoplar cada etapa de tiempo

Nuestro objetivo en esta sección es desarrollar esquemas iterativos, donde las matrices de los sistemas lineales para calcular la densidad y el par velocidad-presión sean constantes. La idea es aproximar la etapa $n + 1$ del esquema (9)-(10) por los siguientes métodos iterativos:

Método iterativo para el problema (8). Conocidos $(\rho_h^n, \mathbf{u}_h^n)$, se aproxima ρ_h^{n+1} solución de (8) por la sucesión $(\rho_h^{n+1,i})_i$ definida como:

Inicialización: Sean $\rho_h^{n+1,0} = \rho_h^n$.

Etapas $i + 1$: Conocido $\rho_h^{n+1,i}$, hallar $\rho_h^{n+1,i+1} \in W_h$ tal que para cada $\bar{\rho}_h \in W_h$:

$$\left(\frac{\rho_h^{n+1,i+1} - \rho_h^n}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \rho_h^{n+1,i+1}, \nabla \bar{\rho}_h \right) = - \left(\mathbf{u}_h^n \cdot \nabla \rho_h^{n+1,i}, \bar{\rho}_h \right).$$

Método iterativo para el problema (10)-(9). Conocidos $(\rho_h^n, \rho_h^{n+1}, \mathbf{u}_h^n)$, se aproxima $(\mathbf{u}_h^{n+1}, p_h^{n+1})$ solución de (9)-(10) por la sucesión $(\mathbf{u}_h^{n+1,i}, p_h^{n+1,i})_i$ definida como:

Inicialización: Sea $\mathbf{u}_h^{n+1,0} = \mathbf{u}_h^n$.

Etapas $i + 1$: Conocido $\mathbf{u}_h^{n+1,i}$, hallar $(\mathbf{u}_h^{n+1,i+1}, p_h^{n+1,i+1}) \in \mathbf{V}_h \times M_h$ tal que para cada $(\bar{\mathbf{u}}_h, \bar{p}_h) \in \mathbf{V}_h \times M_h$:

$$\begin{cases} \left(\frac{\rho_{\tilde{m}}^{n+1,i+1} \mathbf{u}_h^{n+1,i+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + \mu \left(\nabla \mathbf{u}_h^{n+1,i+1}, \nabla \bar{\mathbf{u}}_h \right) - \left(p_h^{n+1,i+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ = - \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \mathbf{u}_h^{n+1,i}, \bar{\mathbf{u}}_h \right) - \lambda \int_0^T \left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) \left(\nabla \mathbf{u}_h^{n+1,i} \right)^t : \nabla \bar{\mathbf{u}}_h \\ - \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1} \mathbf{u}_h^{n+1,i}, \bar{\mathbf{u}}_h \right) + \left(\rho_h^{n+1} \mathbf{f}^{n+1}, \bar{\mathbf{u}}_h \right) + \left(\left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^n \right) \frac{\mathbf{u}_h^{n+1,i} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right), \\ \left(\nabla \cdot \mathbf{u}_h^{n+1,i}, \bar{p}_h \right) = 0, \end{cases}$$

donde $\rho_{\tilde{m}}^{\tilde{M}} = \frac{\tilde{M} + \tilde{m}}{2}$.

A continuación, probamos que las aproximaciones $(\mathbf{u}_h^{n+1,i+1}, \rho_h^{n+1,i+1})$ convergen a $(\rho_h^{n+1}, \mathbf{u}_h^{n+1})$ cuando $i \rightarrow \infty$. Para ello, definimos $\Phi_{i+1} = \mathbf{u}_h^{n+1,i+1} - \mathbf{u}_h^{n+1,i}$, $\Lambda_{i+1} = p_h^{n+1,i+1} - p_h^{n+1,i}$ y $\Psi_{i+1} = \rho_h^{n+1,i+1} - \rho_h^{n+1,i}$, las cuales verifican:

$$\left(\frac{\Psi_{i+1}}{k}, \bar{\rho}_h \right) + \lambda \left(\nabla \Psi_{i+1}, \nabla \bar{\rho}_h \right) = - \left(\mathbf{u}_h^n \cdot \nabla \Psi_i, \bar{\rho}_h \right). \quad (62)$$

$$\left\{ \begin{array}{l} \left(\rho_{\tilde{m}}^{\tilde{M}} \frac{\Phi_{i+1}}{k}, \bar{\mathbf{u}}_h \right) + \mu \left(\nabla \Phi_{i+1}, \nabla \bar{\mathbf{u}}_h \right) = - \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \Phi_i, \bar{\mathbf{u}}_h \\ - \lambda \int_0^T \left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) (\nabla \Phi_i)^t : \nabla \bar{\mathbf{u}}_h - \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1} \Phi_i, \bar{\mathbf{u}}_h \right) \\ + \left(\Lambda_{i+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) + \left(\left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) \frac{\Phi_i}{k}, \bar{\mathbf{u}}_h \right), \end{array} \right. \quad (63)$$

$$\left(\nabla \cdot \Phi_{i+1}, \bar{p}_h \right) = 0. \quad (64)$$

Tomamos $\bar{\rho}_h = k \Psi_{i+1}$ como función test en (62) e integramos por partes

$$\begin{aligned} |\Psi_{i+1}|^2 + \lambda k |\nabla \Psi_{i+1}|^2 &= k \left(\Psi_i \mathbf{u}_h^n, \nabla \Psi_{i+1} \right) + k \left(\nabla \cdot \mathbf{u}_h^n \Psi_i, \Psi_{i+1} \right) \\ &\leq C k \|\mathbf{u}_h^n\|_{H^1(\Omega)}^2 \|\Psi_i\|_{L^3(\Omega)}^2 + \frac{1}{4} \lambda k |\nabla \Psi_{i+1}|^2 \\ &\quad + C k \|\mathbf{u}_h^n\|_{H^1(\Omega)}^2 \|\Psi_i\|_{L^3(\Omega)}^2 + \frac{1}{4} \lambda k |\nabla \Psi_{i+1}|^2 + \frac{1}{4} \lambda k |\Psi_{i+1}|^2 \\ &\leq C k \|\mathbf{u}_h^n\|_{H^1(\Omega)}^4 |\Psi_i| |\nabla \Psi_i| + \frac{1}{2} k |\nabla \Psi_{i+1}|^2 + \frac{1}{4} \lambda k |\Psi_{i+1}|^2 \\ &\leq C k^{1/2} \left(\frac{1}{2} |\Psi_i|^2 + \frac{\lambda}{2} k |\nabla \Psi_i|^2 \right) + \frac{1}{2} k |\nabla \Psi_{i+1}|^2 + \frac{1}{4} \lambda k |\Psi_{i+1}|^2. \end{aligned}$$

Eligiendo k suficientemente pequeño tal que $\alpha := C k^{1/2} < 1$ y $\lambda k < 2$ y aplicando el teorema de punto fijo de Banach, tenemos que $\{\rho^{n+1,i}\}_i$ es una sucesión de *Cauchy* en $H^1(\Omega)$, luego $\rho_h^{n+1,i}$ converge a ρ_h^{n+1} en $H^1(\Omega)$ con velocidad de convergencia α^i (ver [9] para los detalles).

Por otro lado, tomamos $\bar{\mathbf{u}}_h = \Phi_{i+1}$ en (63) y $\bar{p}_h = \Lambda_{i+1}$ en (64), obtenemos

$$\left\{ \begin{array}{l} \rho_{\tilde{m}}^{\tilde{M}} |\Phi_{i+1}|^2 + \mu k \|\Phi_{i+1}\|_{H^1(\Omega)}^2 = - \left((\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}) \cdot \nabla \right) \Phi_i, \Phi_{i+1} \\ - \lambda k \int_0^T \left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) (\nabla \Phi_i)^t : \nabla \Phi_{i+1} + \left(\left(\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1} \right) \Phi_i, \Phi_{i+1} \right) \\ - \frac{1}{2} \left(\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1} \Phi_i, \Phi_{i+1} \right) := F_1 + F_2 + F_3 + F_4. \end{array} \right. \quad (65)$$

Usando que $|\rho_{\tilde{m}}^{\tilde{M}} - \rho_h^{n+1}| \leq (\tilde{M} - \tilde{m})/2$ en Ω y admitiendo que $\|\rho_h^{n+1} \mathbf{u}_h^n - \lambda \nabla \rho_h^{n+1}\|_{L^6(\Omega)} \leq C$, acotamos

$$\begin{aligned} F_1 &\leq C k \|\Phi_i\|_{H^1(\Omega)} |\Phi_{i+1}|^{1/2} \|\Phi_{i+1}\|_{H^1(\Omega)}^{1/2} \leq C k \|\Phi_i\|_{H^1(\Omega)} \left(\frac{1}{k^{1/4}} |\Phi_{i+1}| + k^{1/4} \|\Phi_{i+1}\|_{H^1(\Omega)} \right) \\ &\leq \frac{\delta}{2} \left(\rho_{\tilde{m}}^{\tilde{M}} |\Phi_{i+1}|^2 + \mu_1 k |\Phi_{i+1}|^2 \right) + C_\delta k^{1/2} \mu_1 k \|\Phi_i\|_{H^1(\Omega)}^2, \end{aligned}$$

siendo $\mu_1 = \mu - \frac{\lambda \widetilde{M} - \widetilde{m}}{2} > 0$,

$$F_2 \leq \lambda \frac{\widetilde{M} - \widetilde{m}}{2} k \|\Phi_i\|_{H^1(\Omega)} \|\Phi_{i+1}\|_{H^1(\Omega)} \leq \lambda \frac{\widetilde{M} - \widetilde{m}}{2} k \left(\frac{1}{2} \|\Phi_i\|_{H^1(\Omega)}^2 + \frac{1}{2} \|\Phi_{i+1}\|_{H^1(\Omega)}^2 \right),$$

$$F_3 \leq \frac{\widetilde{M} - \widetilde{m}}{2} |\Phi_i| |\Phi_{i+1}| \leq \left(\frac{\widetilde{M} - \widetilde{m}}{2} \right)^2 \frac{1}{2\rho_{\widetilde{m}}^{\widetilde{M}}} |\Phi_i|^2 + \frac{\rho_{\widetilde{m}}^{\widetilde{M}}}{2} |\Phi_{i+1}|^2.$$

De nuevo, como $|\nabla \cdot \mathbf{u}_h^n \rho_h^{n+1}| \leq C$ controlamos F_4 como F_1

$$F_4 \leq C \|\Phi_i\|_{L^6(\Omega)} \|\Phi_{i+1}\|_{L^3(\Omega)} \leq \frac{\delta}{2} \left(\frac{\rho_{\widetilde{m}}^{\widetilde{M}}}{2} |\Phi_{i+1}|^2 + \mu_1 k |\Phi_{i+1}|^2 \right) + C_\delta k^{1/2} \mu_1 k \|\Phi_i\|_{H^1(\Omega)}^2$$

Aplicando estas estimaciones a (65), conseguimos

$$(1 - \delta) \left(\frac{\rho_{\widetilde{m}}^{\widetilde{M}}}{2} |\Phi_{i+1}|^2 + \mu_1 k \|\Phi_{i+1}\|_{H^1(\Omega)}^2 \right) \leq \left(\frac{\widetilde{M} - \widetilde{m}}{\widetilde{M} + \widetilde{m}} \right)^2 \frac{\rho_{\widetilde{m}}^{\widetilde{M}}}{2} |\Phi_i|^2 + \left(C_\delta k^{1/2} + \frac{\lambda \widetilde{M} - \widetilde{m}}{2\mu_1} \right) \mu_1 k \|\Phi_i\|_{H^1(\Omega)}^2.$$

Observemos que $\frac{\lambda \widetilde{M} - \widetilde{m}}{2\mu_1} < 1$ o equivalentemente $\frac{\lambda \widetilde{M} - \widetilde{m}}{2} < \mu_1$ por la definición de μ_1 y por la hipótesis (H1). Luego, eligiendo $C_\delta k^{1/2}$ suficientemente pequeño tal que $C_\delta k^{1/2} + \frac{\lambda \widetilde{M} - \widetilde{m}}{2\mu_1} < 1$ y δ de modo que $(1 - \delta) > \max \left\{ \left(\frac{\widetilde{M} - \widetilde{m}}{\widetilde{M} + \widetilde{m}} \right)^2, C_\delta k^{1/2} + \frac{\lambda \widetilde{M} - \widetilde{m}}{2\mu_1} \right\}$, llegamos a la desigualdad recursiva

$$\left(\frac{\rho_{\widetilde{m}}^{\widetilde{M}}}{2} |\Phi_{i+1}|^2 + \mu_1 k \|\Phi_{i+1}\|_{H^1(\Omega)}^2 \right) \leq \tilde{\alpha} \left(\frac{\rho_{\widetilde{m}}^{\widetilde{M}}}{2} |\Phi_i|^2 + \mu_1 k \|\Phi_i\|_{H^1(\Omega)}^2 \right),$$

siendo $\tilde{\alpha} = \frac{1}{1 - \delta} \max \left\{ \left(\frac{\widetilde{M} - \widetilde{m}}{\widetilde{M} + \widetilde{m}} \right)^2, C_\delta k^{1/2} + \frac{\lambda \widetilde{M} - \widetilde{m}}{2\mu_1} \right\}$. Como $\tilde{\alpha} < 1$, se extraen las mismas convergencias que para la densidad cuando $i \rightarrow +\infty$, es decir, $\mathbf{u}^{n+1,i} \rightarrow \mathbf{u}_h^{n+1}$ en $H^1(\Omega)$. Finalmente, usando la condición *inf-sup* se tiene que $p_h^{n+1,i} \rightarrow p_h^{n+1}$ en $L^2(\Omega)$.

Teorema 15 *Admitiendo k suficientemente pequeño y las estimaciones de estabilidad $0 \leq \widetilde{m} \leq \rho_h^{n+1} \leq \widetilde{M}$, $\|\mathbf{u}_h^n\|_{L^6(\Omega)} \leq C$ y $\|\nabla \rho_h^{n+1}\|_{L^6(\Omega)} \leq C$ para $C > 0$ independiente de h y k . Entonces, se tiene que los métodos iterativos de matrices constantes (14) y (15)-(16) convergen hacia la única solución del esquema (8) y (9)-(10) respectivamente. Además, se encuentran las convergencias $\rho_h^{n+1,i} \rightarrow \rho_h^{n+1}$ en $H^1(\Omega)$, $\mathbf{u}^{n+1,i} \rightarrow \mathbf{u}_h^{n+1}$ en $H^1(\Omega)$ y $p_h^{n+1,i} \rightarrow p_h^{n+1}$ en $L^2(\Omega)$ cuando $i \rightarrow 0$.*

Por último, nótese que las acotaciones uniformes impuestas sobre las soluciones discretas en el Teorema 15 se justifican de las estimaciones de error que hemos obtenido en las secciones previas. En efecto, de las estimaciones de error $k \sum_{n=0}^{N-1} \|\mathbf{e}_u^{n+1}\|_{H^1(\Omega)}^2 \leq C(h^2+k)$ y $k \sum_{n=0}^{N-1} |\mathbf{e}_\Delta^{n+1}|^2 \leq C(h^2+k)$ se tienen las estimaciones uniformes $\|\mathbf{u}_h^{n+1}\|_{H^1(\Omega)} \leq C$ y $|\Delta_h \rho_h^{n+1}| \leq C$. Es claro, que $\|\mathbf{u}_h^n\|_{L^6(\Omega)} \leq C \|\mathbf{u}_h^n\|_{H^1(\Omega)}$. Ahora, vemos que $\|\nabla \rho_h^{n+1}\|_{L^6(\Omega)} \leq C |\Delta_h \rho_h^{n+1}|$:

$$\|\nabla \rho_h^{n+1}\|_{L^6(\Omega)} \leq \|\nabla(\rho_h^{n+1} - K_h \rho^{n+1}(h))\|_{L^6(\Omega)} + \|\nabla(K_h \rho^{n+1}(h) - \rho^{n+1}(h))\|_{L^6(\Omega)} + \|\nabla \rho^{n+1}(h)\|_{L^6(\Omega)},$$

donde $\rho^{n+1}(h) \in H_N^2(\Omega)$ es definido como in (54) que por la hipótesis (H2) nos ofrece la estabilidad $\|\rho^{n+1}(h)\|_{H^2(\Omega)} \leq C |\Delta_h \rho_h^{n+1}|$. Usando la desigualdad inversa $\|\nabla \bar{\rho}_h\|_{L^6(\Omega)} \leq C h^{-1} \|\bar{\rho}_h\|_{H^1(\Omega)}$ y la propiedad de aproximación $|\nabla(\rho_h^{n+1} - \rho^{n+1}(h))| \leq C h |\Delta_h \rho_h^{n+1}|$ análoga a (60), acotamos

$$\begin{aligned} \|\nabla(\rho_h^{n+1} - K_h \rho^{n+1}(h))\|_{L^6(\Omega)} &\leq C h^{-1} \|\rho_h^{n+1} - K_h(\rho^{n+1}(h))\|_{H^1(\Omega)} \leq C |\Delta_h \rho_h^{n+1}|, \\ \|\nabla(\rho^{n+1}(h) - K_h(\rho^{n+1}(h)))\|_{L^6(\Omega)} &\leq C \|\rho^{n+1}(h)\|_{H^2(\Omega)} \leq C |\Delta_h \rho_h^{n+1}|, \\ \|\nabla \rho^{n+1}(h)\|_{L^6(\Omega)} &\leq C \|\rho^{n+1}(h)\|_{H^2(\Omega)} \leq C |\Delta_h \rho_h^{n+1}|, \end{aligned}$$

por lo tanto $\|\nabla \rho_h^{n+1}\|_{L^6(\Omega)} \leq C |\Delta_h \rho_h^{n+1}|$.

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Capítulo 5

A mixed finite element formulation for approximating a liquid crystal model

A mixed finite element formulation for approximating a liquid crystal model

F. Guillén-González*, J.V. Gutiérrez-Santacreu*

Abstract

In this work we construct a fully discrete mixed scheme using continuous finite elements for solving a nematic liquid crystal model of *Eriksen-Leslie* type by means of a penalized model of *Ginzburg-Landau* type.

Stability and convergence towards a weak solution of the continuous problem with respect to the discretization parameters and the penalty parameter are shown by assuming some relations between the discrete spaces and some constraints on the discrete and penalty parameters. Moreover, the results are improved in the case of two-dimensional domains eliminating some relations between the discrete spaces and weakening the constraints on the parameters.

Keywords: liquid crystal, Navier-Stokes, stability, convergence, finite elements, penalization.

1 Introduction

1.1 Statement of the problem

Let Ω be a bounded, open subset of \mathbb{R}^3 with boundary $\partial\Omega$ and $T > 0$ the final time of observation. We will use the notation $Q = \Omega \times (0, T)$, $\Sigma = \partial\Omega \times (0, T)$ and \mathbf{n} the unit outwards normal vector on $\partial\Omega$. The unknowns are $\mathbf{u} : Q \rightarrow \mathbb{R}^3$ the incompressible velocity field, $p : Q \rightarrow \mathbb{R}$ the pressure and $\mathbf{d} : Q \rightarrow \mathbb{R}^3$ the orientation vector of the liquid crystal molecules. These variables satisfy the following system of equations:

$$\left\{ \begin{array}{l} |\mathbf{d}| = 1, \quad \partial_t \mathbf{d} + \mathbf{u} \cdot \nabla \mathbf{d} - \gamma \Delta \mathbf{d} - \gamma |\nabla \mathbf{d}|^2 \mathbf{d} = \mathbf{0} \quad \text{in } Q, \\ \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \lambda \nabla \cdot ((\nabla \mathbf{d})^t \nabla \mathbf{d}) = \mathbf{0} \quad \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0 \quad \text{in } Q, \end{array} \right. \quad (1)$$

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where $\nu > 0$ is a constant depending on the viscosity of the fluid, $\lambda > 0$ is an elasticity constant, and $\gamma > 0$ is a relaxation time constant. $(\nabla \mathbf{d})^t$ denotes the transposed matrix of $\nabla \mathbf{d}$ and $|\mathbf{d}| = |\mathbf{d}(\mathbf{x}, t)|$ is the Euclidean norm in \mathbb{R}^3 .

This model is a simplification of the model proposed by *Ericken-Leslie* for governing the dynamic behavior of nematic liquid crystal flows which was introduced by Liu [12].

To these equations we will add homogenous and non-homogenous boundary conditions for the velocity and the orientation vector fields, respectively:

$$\mathbf{u} = 0, \quad \mathbf{d} = \mathbf{l} \quad \text{on } \Sigma, \quad (2)$$

and the initial conditions

$$\mathbf{d}(\mathbf{x}, 0) = \mathbf{d}_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega. \quad (3)$$

Here, $\mathbf{l} : \Sigma \rightarrow \mathbb{R}^3$, $\mathbf{u}_0 : \Omega \rightarrow \mathbb{R}^3$, and $\mathbf{d}_0 : \Omega \rightarrow \mathbb{R}^3$ are given functions, where throughout this work \mathbf{l} is assumed to be independent of time.

To construct the approximations, we will use the penalty *Ginzburg-Landau* model:

$$\begin{cases} |\mathbf{d}| \leq 1, & \partial_t \mathbf{d} + \mathbf{u} \cdot \nabla \mathbf{d} + \gamma(\mathbf{f}_\varepsilon(\mathbf{d}) - \Delta \mathbf{d}) = \mathbf{0} & \text{in } Q, \\ \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \lambda \nabla \cdot ((\nabla \mathbf{d})^t \nabla \mathbf{d}) = \mathbf{0} & \text{in } Q, \\ \nabla \cdot \mathbf{u} = 0 & \text{in } Q, \end{cases} \quad (4)$$

where

$$\mathbf{f}_\varepsilon(\mathbf{d}) = \varepsilon^{-2}(|\mathbf{d}|^2 - 1)\mathbf{d}$$

is the penalty function used to approximate the constraint $|\mathbf{d}| = 1$, and $\varepsilon > 0$ is the penalty parameter. It is important to observe that \mathbf{f}_ε is the gradient of the scalar potential function

$$F_\varepsilon(\mathbf{d}) = \frac{1}{4\varepsilon^2}(|\mathbf{d}|^2 - 1)^2,$$

that is, $\mathbf{f}_\varepsilon(\mathbf{d}) = \nabla_{\mathbf{d}}(F_\varepsilon(\mathbf{d}))$ for all $\mathbf{d} \in \mathbb{R}^3$.

1.2 Notations and concept of solutions

We will assume the following notation throughout this paper. As usual $L^p(\Omega)$ denotes the space of functions defined and p th-summable in Ω and $\|\cdot\|_{L^p(\Omega)}$ its norm. If $p = 2$ we denote the inner-product in $L^2(\Omega)$ by (\cdot, \cdot) and the norm by $|\cdot|$. By $W^{p,s}(\Omega)$ and $W_0^{p,s}(\Omega)$ with $s \geq 0$ and $p \geq 1$ (or $H^s(\Omega)$ and $H_0^s(\Omega)$ for $p = 2$), we note the classical Sobolev spaces. The dual spaces of $H^s(\Omega)$ and $H_0^s(\Omega)$ will be represented by $(H^s(\Omega))'$ and $H^{-s}(\Omega)$, respectively. For a real Banach space X , $L^p(0, T; X)$ denotes the space of X -valued functions f defined in $(0, T)$

such that $\|\cdot\|_{L^p(0,T;X)} = \left(\int_0^T \|f\|_X^p\right)^{1/p} < \infty$. When we consider vectorial elements bold-face letter will be used, but we do not distinguish this aspect in the notation of norms.

Now we will introduce the function spaces in the framework of fluid mechanics.

$$\mathbf{H} = \{\mathbf{u} : \mathbf{u} \in \mathbf{L}^2(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \Gamma\},$$

$$\mathbf{V} = \{\mathbf{u} : \mathbf{u} \in \mathbf{H}_0^1(\Omega), \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega\},$$

$$L_0^2(\Omega) = \left\{ p : p \in L^2(\Omega), \int_{\Omega} p(\mathbf{x}) d\mathbf{x} = 0 \right\}.$$

Let us recall the concept of weak solutions of (1) and (4), both completed with (2) and (3).

Definition 1 A pair (\mathbf{d}, \mathbf{u}) is said to be a weak solution of (1), (2)-(3) in $(0, T)$ if:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$,

$$\mathbf{d} \in L^\infty(0, T; \mathbf{H}^1(\Omega)), \quad |\mathbf{d}(\mathbf{x}, t)| = 1, \text{ a.e. } (\mathbf{x}, t) \in Q, \quad \mathbf{d}(\mathbf{x}, t) = \mathbf{l}(\mathbf{x}, t) \text{ a.e. } (\mathbf{x}, t) \in \Sigma.$$

b) $\forall \phi \in C^1([0, T]; \mathbf{V} \cap \mathbf{W}^{1,\infty}(\Omega))$ such that $\phi(T) = 0$,

$$\int_0^T \left\{ -(\mathbf{u}, \partial_t \phi) + ((\mathbf{u} \cdot \nabla) \mathbf{u}, \phi) + (\nu \nabla \mathbf{u} - \lambda (\nabla \mathbf{d})^t \nabla \mathbf{d}, \nabla \phi) \right\} dt = (\mathbf{u}_0, \phi(0)).$$

c) $\forall \psi \in C^1([0, T]; \mathbf{H}_0^1(\Omega) \cap L^\infty(\Omega))$ such that $\psi(T) = 0$,

$$\int_0^T \left\{ -(\mathbf{d}, \partial_t \psi) + (\mathbf{u} \cdot \nabla \mathbf{d}, \psi) + \gamma (\nabla \mathbf{d}, \nabla \psi) - \gamma (|\nabla \mathbf{d}|^2 \mathbf{d}, \psi) \right\} dt = (\mathbf{d}_0, \psi(0))$$

Definition 2 A pair (\mathbf{d}, \mathbf{u}) is called a weak solution of (4), (2)-(3) in $(0, T)$ if:

a) $\mathbf{u} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{V})$,

$$\mathbf{d} \in L^\infty(0, T; \mathbf{H}^1(\Omega)) \cap L^2(0, T; \mathbf{H}^2(\Omega)),$$

$$|\mathbf{d}(\mathbf{x}, t)| = 1, \text{ a.e. } (\mathbf{x}, t) \in Q, \quad \mathbf{d}(\mathbf{x}, t) = \mathbf{l}(\mathbf{x}, t) \text{ a.e. } (\mathbf{x}, t) \in \Sigma.$$

b) $\forall \phi \in C^1([0, T]; \mathbf{V})$ such that $\phi(T) = 0$,

$$\int_0^T \left\{ -(\mathbf{u}, \partial_t \phi) + ((\mathbf{u} \cdot \nabla) \mathbf{u}, \phi) + (\nu \nabla \mathbf{u} - \lambda (\nabla \mathbf{d})^t \nabla \mathbf{d}, \nabla \phi) \right\} dt = (\mathbf{u}_0, \phi(0)).$$

c) $\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla \mathbf{d} + \gamma (\mathbf{f}_\varepsilon(\mathbf{d}) - \Delta \mathbf{d}) = \mathbf{0}$ a.e. in Q , $\mathbf{d}(0) = \mathbf{d}_0$ a.e. in Ω .

Comparing both definitions, we note that the orientation vector solution of (1) loses the \mathbf{H}^2 -regularity with respect to the orientation vector solution of the penalty model (4), and therefore the \mathbf{d} -system is satisfied only in a weak sense instead of almost everywhere in Q .

1.3 Known results

Considering the boundary condition for the orientation vector \mathbf{d} independent of time (i.e. $\mathbf{l} = \mathbf{l}(\mathbf{x})$) and for any fixed ε , *Lin* and *Lui* proved in [14], the local existence of classical solutions and the global existence of weak solutions by means of a semi-Galerkin method. To prove those results, they used the energy inequality

$$\frac{d}{dt} \left(\frac{1}{2} |\mathbf{u}|^2 + \frac{\lambda}{2} |\nabla \mathbf{d}|^2 + \lambda \int_{\Omega} F_{\varepsilon}(\mathbf{d}) d\mathbf{x} \right) + \nu |\nabla \mathbf{u}|^2 + \lambda \gamma |\mathbf{f}_{\varepsilon}(\mathbf{d}) - \Delta \mathbf{d}|^2 \leq 0, \quad (5)$$

obtained by selecting $\lambda(\mathbf{f}_{\varepsilon}(\mathbf{d}) - \Delta \mathbf{d})$ and \mathbf{u} as test functions in (4)_b and (4)_c, respectively.

Using the same method, but this time tending the penalty parameter ε to zero, *Guillén-González* and *Rojas-Medar* obtained in [11], the global existence of weak solutions of (1) (where the $L^2(0, T; \mathbf{H}^2(\Omega))$ regularity for \mathbf{d} is lost), thanks to a sharp optimization technique to get the compactness of the gradient of \mathbf{d} in $L^2(0, T; \mathbf{L}^2(\Omega))$ which allows to pass to the limit in (4) towards (1).

The authors *Liu* and *Walkington* studied numerically the penalty model in two works. In the first work [16], they proposed a numerical scheme which requires globally C^1 -finite elements for approximating the orientation vector \mathbf{d} . Later, in a second work [17] introducing an auxiliary variable $\nabla \mathbf{d}$, they replaced the C^1 -approximation for \mathbf{d} by the C^0 -approximation. In both works the resulting schemes are totally coupled and nonlinear.

Using the auxiliary variable $-\Delta \mathbf{d}$ a numerical scheme is introduced in [5] which is totally coupled but linear, unconditionally stable and convergent towards (4). Also, error estimates and convergence of iterative methods for decoupling the scheme are obtained.

In [13], two linear numerical algorithms are presented. The first of them uses an implicit backward Euler to discrete the time derivative and the second one uses the characteristic method, but both schemes consider C^0 finite elements in space. Some numerical experiments show that both schemes recover the results obtained in [16].

1.4 Numerical scheme

The numerical scheme under consideration to approximate all unknowns (velocity, pressure and orientation vector) is based on the following mixed weak formulation of problem (4) (see [5] for

more details):

$$\begin{aligned}
(\partial_t \mathbf{u}, \bar{\mathbf{u}}) + \nu (\nabla \mathbf{u}, \nabla \bar{\mathbf{u}}) + ((\mathbf{u} \cdot \nabla) \mathbf{u}, \bar{\mathbf{u}}) - ((\nabla \mathbf{d})^t \mathbf{w}, \bar{\mathbf{u}}) - (p, \nabla \cdot \bar{\mathbf{u}}) &= 0 \quad \forall \bar{\mathbf{u}} \in \mathbf{H}_0^1, \\
(\partial_t \mathbf{d}, \bar{\mathbf{w}}) + ((\mathbf{u} \cdot \nabla) \mathbf{d}, \bar{\mathbf{w}}) + \gamma (\mathbf{f}_\varepsilon(\mathbf{d}), \bar{\mathbf{w}}) + \gamma (\mathbf{w}, \bar{\mathbf{w}}) &= 0 \quad \forall \bar{\mathbf{w}} \in \mathbf{L}^2, \\
(\nabla \cdot \mathbf{u}, \bar{p}) &= 0 \quad \forall \bar{p} \in L_0^2, \\
(\nabla \widehat{\mathbf{d}}, \nabla \bar{\mathbf{d}}) - (\mathbf{w}, \bar{\mathbf{d}}) &= 0 \quad \forall \bar{\mathbf{d}} \in \mathbf{H}_0^1,
\end{aligned} \tag{6}$$

where we have used the identity

$$\nabla \cdot ((\nabla \mathbf{d})^t \nabla \mathbf{d}) = \frac{1}{2} \nabla (|\nabla \mathbf{d}|^2) + (\nabla \mathbf{d})^t \Delta \mathbf{d},$$

modified the pressure p by $p = p + \frac{1}{2} |\nabla \mathbf{d}|^2$, and introduced the notation $\mathbf{w} = -\Delta \mathbf{d}$, $\widehat{\mathbf{d}} = \mathbf{d} - \widetilde{\mathbf{d}}$, with $\widetilde{\mathbf{d}}$ the following lifting of the boundary condition \mathbf{l} for the orientation vector field \mathbf{d} :

$$\widetilde{\mathbf{d}}|_{\partial\Omega} = \mathbf{l}, \quad (\nabla \widetilde{\mathbf{d}}, \nabla \bar{\mathbf{d}}) = 0, \quad \forall \bar{\mathbf{d}} \in \mathbf{H}_0^1(\Omega). \tag{7}$$

Roughly speaking, velocity, pressure, orientation vector and its Laplacian will be approximated in finite element spaces $(\mathbf{X}_h, Q_h, \mathbf{D}_h, \mathbf{W}_h) \subset (\mathbf{H}_0^1(\Omega), L_0^2(\Omega), \mathbf{H}^1(\Omega), \mathbf{L}^2(\Omega))$. Notice that the pressure and the Laplacian of the orientation vector can be approximated by finite element spaces of discontinuous functions.

Computing previously $\widetilde{\mathbf{d}}_h \in \mathbf{D}_h$ as the solution of the discrete elliptic problem with non-homogenous Dirichlet boundary condition (where \mathbf{l}_h is an approximation of \mathbf{l}):

$$\widetilde{\mathbf{d}}_h|_{\partial\Omega} = \mathbf{l}_h \quad \text{and} \quad (\nabla \widetilde{\mathbf{d}}_h, \nabla \bar{\mathbf{d}}_h) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h} := \mathbf{D}_h \cap \mathbf{H}_0^1(\Omega). \tag{8}$$

By construction, $\widetilde{\mathbf{d}}_h \rightarrow \widetilde{\mathbf{d}}$ in $\mathbf{H}^1(\Omega)$ as $h \rightarrow 0$.

The algorithm that we present consists of:

Initialization: Let $(\mathbf{u}_h^0, \mathbf{d}_h^0) \in (\mathbf{X}_h, \mathbf{D}_h)$ be suitable approximations of $(\mathbf{u}_0, \mathbf{d}_0)$. We define $\widehat{\mathbf{d}}_h^0 \in \mathbf{D}_{0h}$ such that $\mathbf{d}_h^0 = \widehat{\mathbf{d}}_h^0 + \widetilde{\mathbf{d}}_h$

Step $n + 1$: Given $(\mathbf{u}_h^n, \widehat{\mathbf{d}}_h^n) \in (\mathbf{X}_h, \mathbf{D}_{0h})$ (and $\mathbf{d}_h^n = \widehat{\mathbf{d}}_h^n + \widetilde{\mathbf{d}}_h \in \mathbf{D}_h$), find $(\mathbf{u}_h^{n+1}, \mathbf{w}_h^{n+1}) \in \mathbf{X}_h \times \mathbf{W}_h$ and $(p_h^{n+1}, \widehat{\mathbf{d}}_h^{n+1}) \in Q_h \times \mathbf{D}_{0h}$ (with $\mathbf{d}_h^{n+1} = \widehat{\mathbf{d}}_h^{n+1} + \widetilde{\mathbf{d}}_h$) solving the algebraic linear system:

$$\left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{k}, \bar{\mathbf{u}}_h \right) + c(\mathbf{u}_h^n, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) + \nu (\nabla \mathbf{u}_h^{n+1}, \nabla \bar{\mathbf{u}}_h) - \lambda ((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h) + \lambda (\nabla \cdot \bar{\mathbf{u}}_h, F_\varepsilon(\mathbf{d}_h^n)) - (\bar{p}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h) = 0 \quad \forall \bar{\mathbf{u}}_h \in \mathbf{X}_h, \tag{9}$$

$$(\bar{p}_h, \nabla \cdot \mathbf{u}_h^{n+1}) = 0 \quad \forall \bar{p}_h \in Q_h, \tag{10}$$

$$\left(\frac{\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n}{k}, \bar{\mathbf{w}}_h \right) + ((\mathbf{u}_h^{n+1} \cdot \nabla) \widehat{\mathbf{d}}_h^n, \bar{\mathbf{w}}_h) + \gamma (\mathbf{f}_\varepsilon(\widehat{\mathbf{d}}_h^n) + \mathbf{w}_h^{n+1}, \bar{\mathbf{w}}_h) = 0 \quad \forall \bar{\mathbf{w}}_h \in \mathbf{W}_h, \tag{11}$$

$$\left(\nabla \widehat{\mathbf{d}}_h^{n+1}, \nabla \bar{\mathbf{d}}_h\right) - \left(\mathbf{w}_h^{n+1}, \bar{\mathbf{d}}_h\right) = 0 \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}, \quad (12)$$

where $\widehat{p}_h^{n+1} = p_h^{n+1} + \lambda F_\varepsilon(\mathbf{d}_h^n)$ is a modified pressure, and we have introduced the trilinear form $c(\cdot, \cdot, \cdot)$ defined by

$$c(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \left((\mathbf{u} \cdot \nabla) \mathbf{v}, \mathbf{w}\right) + \frac{1}{2} \left(\nabla \cdot \mathbf{u} \mathbf{v}, \mathbf{w}\right), \quad \forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbf{H}_0^1(\Omega),$$

which displays the skew-symmetric property $c(\mathbf{u}, \mathbf{v}, \mathbf{v}) = 0$ although the incompressibility condition of \mathbf{u} does not hold pointwise.

Another way of writing scheme (8)-(12) is to eliminate the lifting $\widetilde{\mathbf{d}}_h$. For this, we replace $\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n$ by $\mathbf{d}_h^{n+1} - \mathbf{d}_h^n$ in (11) and add (8) to (12), getting the equation for \mathbf{d}_h^{n+1} :

$$\mathbf{d}_h^{n+1} \in \mathbf{D}_h \quad \text{such that} \quad \begin{cases} \left(\nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{d}}_h\right) = \left(\mathbf{w}_h^{n+1}, \bar{\mathbf{d}}_h\right), & \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}, \\ \mathbf{d}_h^{n+1}|_{\partial\Omega} = \mathbf{l}_h. \end{cases} \quad (13)$$

For practical computations, we can work with this numerical scheme without the lifting, since the two schemes are equivalent. But, from the numerical analysis point of view, we consider the lifting, in order to apply that $|\nabla \widehat{\mathbf{d}}_h^{n+1}|$ and $\|\widehat{\mathbf{d}}_h^{n+1}\|_{H^1}$ are equivalent norms in $\mathbf{H}_0^1(\Omega)$. Afterwards, the bound of $(\widehat{\mathbf{d}}_h^{n+1})$ in $\mathbf{H}_0^1(\Omega)$ imply the bound for (\mathbf{d}_h^{n+1}) in \mathbf{H}^1 , since the lifting function $\widetilde{\mathbf{d}}_h$ (which is independent of the time parameter) is bounded in the \mathbf{H}^1 -norm.

The main difference between scheme (9)-(12) and the scheme introduced in [5] is that now the stabilized term $\lambda \left(\nabla \cdot \bar{\mathbf{u}}_h, F_\varepsilon(\mathbf{d}_h^n)\right)$ is introduced in (9). This term causes that the original pressure p changes by $p + \lambda F_\varepsilon(\mathbf{d})$.

1.5 Hypotheses

Now and below, we will assume that Ω is a bounded domain whose boundary is polyhedral, and there exists a family of triangulations $\{\mathcal{T}_h\}_{h>0}$ of Ω , furnished by tetrahedrons, where h the maximum diameter of the elements of $\{\mathcal{T}_h\}_{h>0}$.

The following properties will be required:

(S) Stability conditions:

$$(S1) \quad \lim_{(h,k,\varepsilon) \rightarrow 0} \frac{k}{h^2 \varepsilon^6} = 0 \quad \text{and} \quad (S2) \quad \lim_{(h,k,\varepsilon) \rightarrow 0} \frac{h}{\varepsilon^4} = 0.$$

(H0) Hypotheses for the data: $\mathbf{u}_0 \in \mathbf{V}$, $\mathbf{d}_0 \in \mathbf{H}^1(\Omega)$ with $|\mathbf{d}_0| = 1$ in Ω , $\mathbf{l} \in \mathbf{H}^{3/2}(\partial\Omega)$ with $|\mathbf{l}| = 1$ on $\partial\Omega \times (0, T)$.

(H1) $\partial\Omega$ is assumed to hold the continuous dependency in the $\mathbf{W}^{2,r} \times W^{1,r}$ -norm of the *Stokes* problem with $r > 3$, and the continuous dependency in H^2 of the non-homogeneous Dirichlet problem.

(H2) The triangulation of Ω and the discrete spaces verify:

- the inverse inequalities:

$$\begin{aligned}\|\nabla \bar{\mathbf{u}}_h\|_{L^\infty(\Omega)} &\leq C h^{-3/2} |\nabla \bar{\mathbf{u}}_h| \quad \forall \bar{\mathbf{u}}_h \in \mathbf{X}_h, \\ \|\bar{\mathbf{d}}_h\|_{L^\infty(\Omega) \cap W^{1,3}(\Omega)} &\leq C h^{-1/2} \|\bar{\mathbf{d}}_h\|_{H^1(\Omega)} \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_h,\end{aligned}$$

- the approximation properties:

$$\begin{aligned}\|\mathbf{u} - J_h \mathbf{u}\|_{H^1(\Omega)} &\leq C h^2 \|\mathbf{u}\|_{H^3(\Omega)} \quad \forall \mathbf{u} \in \mathbf{H}^3(\Omega) \cap \mathbf{H}_0^1(\Omega), \\ \|\mathbf{u} - J_h \mathbf{u}\|_{W^{1,\infty}(\Omega)} &\leq C h^{1/2} \|\mathbf{u}\|_{H^3(\Omega)} \quad \forall \mathbf{u} \in \mathbf{H}^3(\Omega), \\ |p - K_h p| &\leq C h \|p\|_{H^1(\Omega)} \quad \forall p \in H^1(\Omega) \cap L_0^2(\Omega), \\ \|\mathbf{d} - I_h \mathbf{d}\|_{H^1(\Omega)} &\leq C h \|\mathbf{d}\|_{H^2(\Omega)} \quad \forall \mathbf{d} \in \mathbf{H}^2(\Omega), \\ \|\mathbf{d} - I_h \mathbf{d}\| &\leq C h \|\mathbf{d}\|_{H^1(\Omega)} \quad \forall \mathbf{d} \in \mathbf{H}^1(\Omega), \\ \|I_h \mathbf{d} - \mathbf{d}\|_{L^4(\Omega)} &\leq C h^{1/4} \|\mathbf{d}\|_{H^1(\Omega)} \quad \forall \mathbf{d} \in \mathbf{H}^1(\Omega),\end{aligned}$$

where J_h , K_h and I_h are interpolation operators into \mathbf{X}_h , Q_h , and \mathbf{D}_h , respectively.

(H3) *Inf-Sup condition* (Compatibility condition between (\mathbf{X}_h, Q_h)): There exists $\beta > 0$ (independent of h) such that,

$$\|q_h\|_{L_0^2(\Omega)} \leq \beta \sup_{\mathbf{v} \in \mathbf{X}_h \setminus \{0\}} \frac{(q_h, \nabla \cdot \mathbf{v})}{\|\mathbf{v}\|_{H^1(\Omega)}} \quad \forall q_h \in Q_h.$$

(H4) Compatibility conditions between $(\mathbf{X}_h, \mathbf{W}_h, \mathbf{D}_h)$:

$$(\mathbf{X}_h \cdot \nabla) \mathbf{D}_h \subset \mathbf{W}_h \quad \text{and} \quad \mathbf{D}_h \subset \mathbf{W}_h.$$

For instance, the choice P_2/P_1 for (\mathbf{X}_h, Q_h) and P_2 (*discontinuous*)/ P_1 for $(\mathbf{W}_h, \mathbf{D}_h)$, satisfy the previous hypotheses (H2)-(H4) whether the family of triangulations $\{\mathcal{T}_h\}_{h>0}$ of Ω is regular and quasi-uniform.

Concerning the space discretization, in [5] the discrete Laplacian of the orientation vector is approximated by P_0 (piecewise-polynomial functions of degree 0) and now, for instance, P_2 discontinuous functions have to be used whether *Taylor-Hood* element is chosen to approximate the velocity and pressure as indicated above.

1.6 Main results of the paper

In this work we deal with the first existence theorem, under our knowledge, for a nematic cristal liquid model (1) by using a discrete Galerkin approach for the penalty model (4) of the *Ginzburg-Landau* type. That result is not obvious for the previous numerical works of the penalty model (4) since the stability estimates independent of the penalty parameter ε does not seem evident. Through we do not assure the restriction $|\mathbf{d}| \leq 1$ for the numerical approximations of the orientation vector, we will get the following result.

Theorem 3 *Assume hypotheses (S), (H0)-(H4) given in the previous subsection. Then there exists a convergent subsequence of the approximations defined in Definition 6 (denoted in the same way) as $(h, k, \varepsilon) \rightarrow 0$ towards a weak solution (\mathbf{u}, \mathbf{d}) of problem (1), (2)-(3) (see Definition 1), in the following sense: the discrete velocity in $L^2(0, T; \mathbf{L}^2(\Omega))$ -strong, in $L^\infty(0, T; \mathbf{L}^2(\Omega))$ -weak*, and in $L^2(0, T; \mathbf{H}_0^1(\Omega))$ -weak, and the discrete orientation vector in $L^2(0, T; \mathbf{H}^1(\Omega))$ -strong and in $L^\infty(0, T; \mathbf{H}^1(\Omega))$ -weak*.*

After this introduction, this work is organized as follows: In Section 2, we derive stability estimates for scheme (8)-(12) from a discrete version of (5) by means of an induction process in the time step. Section 3 is devoted to the compactness results: for the discrete orientation vector in $\mathbf{L}^2(Q)$ as a consequence of an estimate of the discrete time derivative, and for the discrete velocity in $\mathbf{L}^2(Q)$ due to an estimate by perturbation of a fractional time derivative of the orthogonal projection of the discrete velocity onto \mathbf{V} in the $\mathbf{L}^2(\Omega)$ -norm. In Section 4 we guarantee that the limit orientation vector satisfies the constraint $|\mathbf{d}| = 1$ by passing to limit in the system for the discrete orientation vector. We improve the compactness up to $L^2(0, T; \mathbf{H}^1(\Omega))$ for the discrete orientation characterizing it as a minimum together with limit orientation vector in Section 5. We pass to the limit in the discrete momentum equation in Section 6. Finally, some improvements are made in Section 7 for the 2D case, where the hypothesis $(\mathbf{X}_h \cdot \nabla) \mathbf{D}_h \subset \mathbf{W}_h$ of (H4) can be eliminated and constraints (S) is weakened.

2 A priori estimates and weak convergences

Since scheme (9)-(12) is a linear system, it is easy to check the existence and uniqueness of a solution, once that a priori estimates are obtained.

It is well-know that the solution $\tilde{\mathbf{d}}_h$ of problem (8) satisfies the bound $\|\tilde{\mathbf{d}}_h\|_{H^1(\Omega)}^2 \leq K_{\mathbf{l}}$, where $K_{\mathbf{l}}$ is a positive constant which depends on the boundary data \mathbf{l} . Now, we are going to obtain a recursive inequality, that will be essential for the a priori estimates of scheme (9)-(12).

Lemma 4 Suppose that there exists a constant $C_d > 0$ independent of h , k , and ε such that

$$|\mathbf{u}_h^n|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 \leq C_d.$$

Then there exist $h_0 > 0$, $k_0 > 0$, and $\varepsilon_0 > 0$ such that for all $h \leq h_0$, $k \leq k_0$ and $\varepsilon \leq \varepsilon_0$ satisfying hypothesis (S1), the corresponding solution $(\mathbf{u}_h^{n+1}, \mathbf{d}_h^{n+1}, \mathbf{w}_h^{n+1})$ of the discrete problem (9)-(12) verifies the following inequality:

$$\left\{ \begin{array}{l} (|\mathbf{u}_h^{n+1}|^2 - |\mathbf{u}_h^n|^2 + |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2) + \nu k |\nabla \mathbf{u}_h^{n+1}|^2 \\ + \lambda (|\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 - |\nabla \widehat{\mathbf{d}}_h^n|^2 + |\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2) + \lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \\ + 2\lambda \int_\Omega (F_\varepsilon(\mathbf{d}_h^{n+1}) - F_\varepsilon(\mathbf{d}_h^n)) + \frac{\lambda}{\varepsilon^2} \int_\Omega \left(\frac{1}{4} (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2)^2 + |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 \right) \end{array} \right\} \leq 0, \quad (14)$$

where P_h is the $\mathbf{L}^2(\Omega)$ -projection onto \mathbf{W}_h .

Proof: By taking $\bar{\mathbf{u}}_h = 2k\mathbf{u}_h^{n+1}$ in (9), $\bar{p}_h = \widehat{p}_h^{n+1}$ in (10), the term $(\widehat{p}_h^{n+1}, \nabla \cdot \mathbf{u}_h^{n+1})$ vanishes, and using the identity $(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2$, we arrive at

$$\begin{aligned} & |\mathbf{u}_h^{n+1}|^2 - |\mathbf{u}_h^n|^2 + |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + 2\nu k |\nabla \mathbf{u}_h^{n+1}|^2 \\ & - 2\lambda k \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \mathbf{u}_h^{n+1} \right) + 2\lambda k \left(\nabla \cdot \mathbf{u}_h^{n+1}, F_\varepsilon(\mathbf{d}_h^n) \right) = 0. \end{aligned} \quad (15)$$

On the other hand, we consider $\bar{\mathbf{w}}_h = 2\lambda k (\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)))$ in (11) jointly with $\bar{\mathbf{d}}_h = \widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n = \mathbf{d}_h^{n+1} - \mathbf{d}_h^n \in \mathbf{D}_{0h}$ in (12) and use that $(\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n \in \mathbf{W}_h$ and $\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n \in \mathbf{W}_h$ (thanks to (H4)) to get

$$\begin{aligned} & \lambda \left(|\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 - |\nabla \widehat{\mathbf{d}}_h^n|^2 + |\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 \right) + 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) \\ & + 2\lambda k \left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{w}_h^{n+1} + \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) + 2\lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 = 0. \end{aligned} \quad (16)$$

Now, by adding (15) to (16), and using the identities

$$- \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \mathbf{u}_h^{n+1} \right) + \left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{w}_h^{n+1} \right) = 0$$

and

$$\left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) + \left(\nabla \cdot \mathbf{u}_h^{n+1}, F_\varepsilon(\mathbf{d}_h^n) \right) = 0,$$

one has

$$\begin{aligned} & \left(|\mathbf{u}_h^{n+1}|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 \right) - \left(|\mathbf{u}_h^n|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 \right) + \left(|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + \lambda |\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 \right) \\ & + 2k \left(\nu |\nabla \mathbf{u}_h^{n+1}|^2 + \gamma \lambda |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 \right) + 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) = 0. \end{aligned} \quad (17)$$

Next, we decompose the last term on the left-hand side of (17) as follows:

$$\begin{aligned} 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) &= \frac{2\lambda}{\varepsilon^2} \left(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n, (|\mathbf{d}_h^{n+1}|^2 - 1) \mathbf{d}_h^n \right) \\ &+ \frac{2\lambda}{\varepsilon^2} \left(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n, (|\mathbf{d}_h^n|^2 - |\mathbf{d}_h^{n+1}|^2) \mathbf{d}_h^n \right) := I_1 - I_2. \end{aligned}$$

Rewriting I_1 as

$$\begin{aligned}
I_1 &= \frac{\lambda}{\varepsilon^2} \int_{\Omega} (|\mathbf{d}_h^{n+1}|^2 - 1)(|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2 - |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2) \\
&= \frac{\lambda}{2\varepsilon^2} \int_{\Omega} \left((|\mathbf{d}_h^{n+1}|^2 - 1)^2 - (|\mathbf{d}_h^n|^2 - 1)^2 + (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2)^2 \right) \\
&\quad + \frac{\lambda}{\varepsilon^2} \int_{\Omega} (1 - |\mathbf{d}_h^{n+1}|^2) |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2
\end{aligned}$$

and bounding I_2 as

$$I_2 \leq \frac{C}{\varepsilon^2} \|\mathbf{d}_h^n\|_{L^\infty(\Omega)}^2 |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 + \frac{\lambda}{4\varepsilon^2} \int_{\Omega} (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2)^2,$$

we arrive at

$$\left\{ \begin{aligned}
&\left(|\mathbf{u}_h^{n+1}|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 + 2\lambda \int_{\Omega} F_\varepsilon(\mathbf{d}_h^{n+1}) \right) - \left(|\mathbf{u}_h^n|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 + 2\lambda \int_{\Omega} F_\varepsilon(\mathbf{d}_h^n) \right) \\
&+ |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + \lambda |\nabla(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 + \frac{\lambda}{\varepsilon^2} \int_{\Omega} \left(\frac{1}{4} (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2)^2 + |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 \right) \\
&+ 2\nu k |\nabla \mathbf{u}_h^{n+1}|^2 + 2\lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \\
&\leq \frac{C}{\varepsilon^2} \left(\|\mathbf{d}_h^n\|_{L^\infty(\Omega)}^2 + \|\mathbf{d}_h^{n+1}\|_{L^\infty(\Omega)}^2 \right) |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 := I_3.
\end{aligned} \right. \quad (18)$$

Now, we want to bound the term $|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2$ of I_3 . By taking as a test function $\bar{\mathbf{w}}_h = \mathbf{d}_h^{n+1} - \mathbf{d}_h^n$ into (11), using the fact that $\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n = \mathbf{d}_h^{n+1} - \mathbf{d}_h^n$ (because the boundary data for \mathbf{d} is time-independent) and that $\mathbf{d}_h^{n+1} - \mathbf{d}_h^n \in \mathbf{W}_h$ (because $\mathbf{D}_h \subset \mathbf{W}_h$ imposed in (H4)), one has

$$|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n| \leq k \|\mathbf{u}_h^{n+1}\|_{L^6(\Omega)} \|\nabla \mathbf{d}_h^n\|_{L^3(\Omega)} + \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|.$$

Using the inverse inequality $\|\nabla \mathbf{d}_h^n\|_{L^3(\Omega)} \leq C h^{-1/2} \|\mathbf{d}_h^n\|_{H^1(\Omega)}$, the bound $\|\widetilde{\mathbf{d}}_h\|_{H^1(\Omega)} \leq K_I$ and the hypothesis $\lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 \leq C_d$, we bound

$$\begin{aligned}
\|\nabla \mathbf{d}_h^n\|_{L^3(\Omega)} &\leq C h^{-1/2} \|\mathbf{d}_h^n\|_{H^1(\Omega)} \leq C h^{-1/2} \left(\|\widetilde{\mathbf{d}}_h\|_{H^1(\Omega)} + \|\widehat{\mathbf{d}}_h^n\|_{H_0^1(\Omega)} \right) \\
&\leq C h^{-1/2} \left(K_I + \frac{C_d}{\lambda} \right) \leq C h^{-1/2},
\end{aligned}$$

arriving at

$$|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n| \leq C \frac{k}{h^{1/2}} |\nabla \mathbf{u}_h^{n+1}| + \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|; \quad (19)$$

whence, in particular,

$$|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 \leq C \frac{k}{h} \left(k \nu |\nabla \mathbf{u}_h^{n+1}|^2 + \lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \right). \quad (20)$$

Then the bound of I_3 remains as

$$I_3 \leq C \frac{k}{h\varepsilon^2} \left(\|\mathbf{d}_h^{n+1}\|_{L^\infty(\Omega)}^2 + \|\mathbf{d}_h^n\|_{L^\infty(\Omega)}^2 \right) \left(k \nu |\nabla \mathbf{u}_h^{n+1}|^2 + \lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \right).$$

By using in the previous estimate the inverse inequality $\|\bar{\mathbf{d}}_h\|_{L^\infty(\Omega)} \leq C h^{-1/2} \|\bar{\mathbf{d}}_h\|_{H^1(\Omega)}$ for all $\bar{\mathbf{d}}_h \in \mathbf{D}_h$ applied to $\bar{\mathbf{d}}_h = \mathbf{d}_h^{n+1}$ and $\bar{\mathbf{d}}_h = \mathbf{d}_h^n$, we have

$$I_3 \leq C \frac{k}{h^2 \varepsilon^2} \left(\|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)}^2 + \|\mathbf{d}_h^n\|_{H^1(\Omega)}^2 \right) \left(k \nu |\nabla \mathbf{u}_h^{n+1}|^2 + \lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \right). \quad (21)$$

Our next goal is to bound $\|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)}$ in terms of $\|\mathbf{d}_h^n\|_{H^1(\Omega)}$ and $|\mathbf{u}_h^n|$. We consider (17) rewritten as

$$\begin{aligned} & \left(|\mathbf{u}_h^{n+1}|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 \right) + \left(|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + \lambda |\nabla(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 \right) \\ & + 2k \left(\nu |\nabla \mathbf{u}_h^{n+1}|^2 + \gamma \lambda |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 \right) \\ & = \left(|\mathbf{u}_h^n|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 \right) - 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right). \end{aligned} \quad (22)$$

Since $|\mathbf{f}_\varepsilon(\mathbf{d}_h^n)| \leq \frac{1}{\varepsilon^2} \left(|\mathbf{d}_h^n|^3 + |\mathbf{d}_h^n| \right)$, we can bound the last term of (22), thanks to Sobolev's inequality, as follows

$$\begin{aligned} 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) & \leq 2\lambda \|\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n\|_{L^6(\Omega)} \|\mathbf{f}_\varepsilon(\mathbf{d}_h^n)\|_{L^{6/5}(\Omega)} \\ & \leq \frac{\lambda}{2} |\nabla(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 + \frac{C}{\varepsilon^4} \left(\|\mathbf{d}_h^n\|_{L^{18/5}(\Omega)}^6 + \|\mathbf{d}_h^n\|_{L^{6/5}(\Omega)}^2 \right) \\ & \leq \frac{\lambda}{2} |\nabla(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 + \frac{C}{\varepsilon^4} \left(\|\mathbf{d}_h^n\|_{H^1(\Omega)}^6 + \|\mathbf{d}_h^n\|_{H^1(\Omega)}^2 \right). \end{aligned} \quad (23)$$

Incorporating this bound to (22), one has in particular

$$|\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 \leq C \left(|\nabla \widehat{\mathbf{d}}_h^n|^2 + |\mathbf{u}_h^n|^2 + \frac{1}{\varepsilon^4} \left(\|\mathbf{d}_h^n\|_{H^1(\Omega)}^6 + \|\mathbf{d}_h^n\|_{H^1(\Omega)}^2 \right) \right),$$

and taking into account that $\mathbf{d}_h^{n+1} = \widehat{\mathbf{d}}_h^{n+1} + \widetilde{\mathbf{d}}_h$, we infer

$$\|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)}^2 \leq C \left(|\nabla \widehat{\mathbf{d}}_h^n|^2 + |\mathbf{u}_h^n|^2 + \frac{1}{\varepsilon^4} \left(\|\mathbf{d}_h^n\|_{H^1(\Omega)}^6 + \|\mathbf{d}_h^n\|_{H^1(\Omega)}^2 \right) + \|\widetilde{\mathbf{d}}_h\|_{H^1(\Omega)}^2 \right).$$

Consequently, by using $\|\widetilde{\mathbf{d}}_h\|_{H^1(\Omega)} \leq K_l$ and the hypotheses $|\nabla \widehat{\mathbf{d}}_h^n|^2 \leq \frac{C_d}{\lambda}$ and $|\mathbf{u}_h^n|^2 \leq C_d$, we get the bound

$$\|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)}^2 \leq \frac{C}{\varepsilon^4}. \quad (24)$$

Therefore, using (24) and that $\|\mathbf{d}_h^n\|_{H^1(\Omega)}^2 \leq C(|\nabla \widehat{\mathbf{d}}_h^n|^2 + \|\widetilde{\mathbf{d}}_h\|_{H^1}^2) \leq C\left(\frac{C_d}{\lambda} + K_l^2\right) \leq C$ in (21),

$$I_3 \leq C \frac{k}{h^2 \varepsilon^6} \left(k \nu |\nabla \mathbf{u}_h^{n+1}|^2 + \lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \right).$$

Using hypothesis (S1), we can select $(k_0, h_0, \varepsilon_0)$ such that for all $k \leq k_0$, $h \leq h_0$, and $\varepsilon \leq \varepsilon_0$, one has

$$C \frac{k}{h^2 \varepsilon^6} \leq 1$$

and arrives at

$$I_3 \leq k \left(\nu |\nabla \mathbf{u}_h^{n+1}|^2 + \lambda \gamma |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \right).$$

Therefore, we obtain inequality (14) using this estimate of I_3 in (18). This is finished the proof. \square

In order to get stability estimates for scheme (9)-(12), we will need the following properties of the initial approximations \mathbf{d}_h^0 , $\widehat{\mathbf{d}}_h^0$, and \mathbf{u}_h^0 :

$$\lambda|\nabla\widehat{\mathbf{d}}_h^0|^2 \leq K_1, \quad |\mathbf{u}_h^0|^2 \leq K_2, \quad 2\lambda \int_{\Omega} F_{\varepsilon}(\mathbf{d}_h^0) d\mathbf{x} \leq K_3,$$

where $K_i > 0$ ($i = 1, 2, 3$) are constants independent of h and k .

These properties can be guaranteed thanks to hypotheses (H0) and (H2), considering $\mathbf{d}_h^0 = I_h \mathbf{d}_0$ and $\mathbf{u}_h^0 = J_h \mathbf{u}_0$. Indeed, in view of the stability of the interpolation operators, $\|\mathbf{d}_h^0\|_{H^1(\Omega)} \leq C\|\mathbf{d}_0\|_{H^1(\Omega)}$ and $|\mathbf{u}_h^0| \leq C|\mathbf{u}_0|$. Therefore, there exist $K > 0$ and $K_2 > 0$ such that $\lambda\|\mathbf{d}_h^0\|_{H^1}^2 \leq K$ and $|\mathbf{u}_h^0|^2 \leq K_2$. Since $\widehat{\mathbf{d}}_h^0 = \mathbf{d}_h^0 - \widetilde{\mathbf{d}}_h$, we conclude that there exists $K_1 > 0$ so that $\lambda|\nabla\widehat{\mathbf{d}}_h^0|^2 \leq K_1$. Finally, since the initial orientation of the liquid crystal molecules verifies the constraint $|\mathbf{d}_0| = 1$, we can write

$$\begin{aligned} \int_{\Omega} F_{\varepsilon}(\mathbf{d}_h^0) &= \frac{1}{\varepsilon^2} \int_{\Omega} (|\mathbf{d}_h^0|^2 - |\mathbf{d}_0|^2)^2 \leq \frac{2}{\varepsilon^2} \int_{\Omega} |\mathbf{d}_0 - \mathbf{d}_h^0|^4 + \frac{2}{\varepsilon^2} \int_{\Omega} (\mathbf{d}_0 - \mathbf{d}_h^0, 2\mathbf{d}_0)^2 \\ &\leq \frac{1}{\varepsilon^2} \|\mathbf{d}_0 - \mathbf{d}_h^0\|_{L^4(\Omega)}^4 + \frac{4}{\varepsilon^2} |\mathbf{d}_0 - \mathbf{d}_h^0|^2 \leq \frac{C}{\varepsilon^2} \left(\|\mathbf{d}_0 - \mathbf{d}_h^0\|_{L^4(\Omega)}^4 + |\mathbf{d}_0 - \mathbf{d}_h^0|^2 \right), \end{aligned}$$

where we have used the identity $|a|^2 - |b|^2 + |b - a|^2 = (a - b, 2a)$. Now, using the approximation properties (H2) and the stability condition (S2), we find a positive constant K_3 such that

$$2\lambda \int_{\Omega} F_{\varepsilon}(\mathbf{d}_h^0) \leq C \frac{h}{\varepsilon^2} \leq K_3.$$

We now state our stability result for scheme (9)-(12):

Theorem 5 *There exist h_0 , k_0 , and ε_0 so that for any $h \leq h_0$, $k \leq k_0$, and $\varepsilon \leq \varepsilon_0$ satisfying the stability condition (S), the corresponding solution of the discrete problem (9)-(12) verifies the estimates:*

$$\begin{aligned} \text{i)} \quad \max_{0 \leq n \leq N} |\mathbf{u}_h^n| &\leq C, & \text{ii)} \quad k \sum_{n=0}^{N-1} |\nabla \mathbf{u}_h^{n+1}|^2 &\leq C, & \text{iii)} \quad \sum_{n=0}^{N-1} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 &\leq C, \\ \text{iv)} \quad \max_{0 \leq n \leq N} \|\mathbf{d}_h^n\|_{H^1(\Omega)} &\leq C, & \text{v)} \quad k \sum_{n=0}^{N-1} |P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 &\leq C & \text{vi)} \quad \sum_{n=0}^{N-1} \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{H^1(\Omega)}^2 &\leq C, \\ \text{vii)} \quad \max_{0 \leq n \leq N} \int_{\Omega} F_{\varepsilon}(\mathbf{d}_h^n) &\leq C & \text{viii)} \quad \frac{1}{\varepsilon^2} \sum_{n=0}^{N-1} \int_{\Omega} (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2)^2 &\leq C & \text{ix)} \quad \frac{1}{\varepsilon^2} \sum_{n=0}^{N-1} \int_{\Omega} |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 &\leq C, \end{aligned}$$

where $C > 0$ is independent of (h, k, ε) .

Proof: It suffices to prove (14) for all $n = 0, \dots, N - 1$. For this, we argue by induction on n . Let us define $C_d = K_1 + K_2 + K_3$ with K_i the bounds for the initial data. Then, in particular,

$(\mathbf{u}_h^0, \mathbf{d}_h^0)$ verifies the hypothesis of Lemma 4 for $n = 0$: $|\mathbf{u}_h^0|^2 + \lambda|\nabla\widehat{\mathbf{d}}_h^0|^2 \leq C_d$, then (14) holds for $n = 0$ (and, in particular, $|\mathbf{u}_h^1|^2 + \lambda|\nabla\widehat{\mathbf{d}}_h^1|^2 \leq C_d$).

Now, we assume that $(\mathbf{u}_h^s, \mathbf{d}_h^s)$ verifies (14) for $s = 1, \dots, n-1$. Adding (14) for $s = 1, \dots, n-1$, one has $|\mathbf{u}_h^n|^2 + \lambda|\nabla\widehat{\mathbf{d}}_h^n|^2 \leq |\mathbf{u}_h^0|^2 + \lambda|\nabla\widehat{\mathbf{d}}_h^0|^2 + 2\lambda \int_{\Omega} F_{\varepsilon}(\mathbf{d}_h^0) \leq K_1 + K_2 + K_3 = C_d$, which implies from Lemma 4 that (14) holds for n . \square

Definition 6 One defines $\mathbf{u}_{h,k,\varepsilon}$ ($\mathbf{u}_{h,k,\varepsilon}^0$ and $p_{h,k,\varepsilon}$, respectively) as the piecewise constant functions taking values \mathbf{u}_h^{n+1} on $(t_n, t_{n+1}]$ (\mathbf{u}_h^n and p_h^{n+1} , respectively). Analogously, we define $\mathbf{w}_{h,k,\varepsilon}$, $\mathbf{d}_{h,k,\varepsilon}$ and $\mathbf{d}_{h,k,\varepsilon}^0$. Moreover, one defines $\mathbf{u}_{h,k,\varepsilon}^l \in C^0([0, T]; \mathbf{V}_h)$ and $\mathbf{d}_{h,k,\varepsilon}^l \in C^0([0, T]; \mathbf{D}_h)$ as the piecewise linear functions such that $\mathbf{u}_{h,k,\varepsilon}^l(t_n) = \mathbf{u}_h^n$ and $\mathbf{d}_{h,k,\varepsilon}^l(t_n) = \mathbf{d}_h^n$, respectively.

With the previous notations, Theorem 5 says us:

$$\begin{aligned} \mathbf{u}_{h,k,\varepsilon}^l, \mathbf{u}_{h,k,\varepsilon}^0, \mathbf{u}_{h,k,\varepsilon} \quad \text{is bounded in} \quad & L^{\infty}(0, T; \mathbf{L}^2(\Omega)) \cap L^2(0, T, \mathbf{H}_0^1(\Omega)), \\ \mathbf{d}_{h,k,\varepsilon}^l, \mathbf{d}_{h,k,\varepsilon}^0, \mathbf{d}_{h,k,\varepsilon} \quad \text{is bounded in} \quad & L^{\infty}(0, T; \mathbf{H}^1(\Omega)), \end{aligned} \quad (25)$$

Moreover, from *iii*) and *vi*), $\mathbf{u}_{h,k,\varepsilon}^0 - \mathbf{u}_{h,k,\varepsilon} \rightarrow 0$ and $\mathbf{u}_{h,k,\varepsilon}^l - \mathbf{u}_{h,k,\varepsilon} \rightarrow 0$ in $L^2(0, T; \mathbf{L}^2(\Omega))$, with the same convergence for $\mathbf{d}_{h,k,\varepsilon}^l, \mathbf{d}_{h,k,\varepsilon}^0, \mathbf{d}_{h,k,\varepsilon}$ in $L^2(0, T; \mathbf{H}^1(\Omega))$.

Therefore, there exist subsequences of $\{\mathbf{u}_{h,k,\varepsilon}^l\}_{h,k,\varepsilon}$, $\{\mathbf{u}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, $\{\mathbf{u}_{h,k,\varepsilon}^0\}_{h,k,\varepsilon}$, $\{\mathbf{d}_{h,k,\varepsilon}^l\}_{h,k,\varepsilon}$, $\{\mathbf{d}_{h,k,\varepsilon}^0\}_{h,k,\varepsilon}$ and $\{\mathbf{d}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$ (denoted in the same way) and limit functions \mathbf{u} and \mathbf{d} verifying the following weak convergence as $(h, k, \varepsilon) \rightarrow 0$:

$$\begin{aligned} \mathbf{u}_{h,k,\varepsilon}^l \rightarrow \mathbf{u}, \quad \mathbf{u}_{h,k,\varepsilon}^0 \rightarrow \mathbf{u}, \quad \mathbf{u}_{h,k,\varepsilon} \rightarrow \mathbf{u} \quad \text{in} \quad & \begin{cases} L^2(0, T; \mathbf{H}_0^1(\Omega))\text{-weak}, \\ L^{\infty}(0, T; \mathbf{L}^2(\Omega))\text{-weak*}, \end{cases} \\ \mathbf{d}_{h,k,\varepsilon}^l \rightarrow \mathbf{d}, \quad \mathbf{d}_{h,k,\varepsilon}^0 \rightarrow \mathbf{d}, \quad \mathbf{d}_{h,k,\varepsilon} \rightarrow \mathbf{d} \quad \text{in} \quad & L^{\infty}(0, T; \mathbf{H}^1(\Omega))\text{-weak*}. \end{aligned} \quad (26)$$

3 Compactness for \mathbf{d} and \mathbf{u}

Lemma 7 Under the conditions of Theorem 5, one has

$$k \sum_{n=0}^{N-1} \left\| \frac{\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n}{k} \right\|_{L^{3/2}(\Omega)}^2 \leq C,$$

where $C > 0$ is independent of (h, k, ε) .

Note that, since $\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n = \mathbf{d}_h^{n+1} - \mathbf{d}_h^n$, one also has

$$k \sum_{n=0}^{N-1} \left\| \frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k} \right\|_{L^{3/2}(\Omega)}^2 \leq C.$$

Proof: Let $\bar{\mathbf{w}} \in \mathbf{L}^3(\Omega)$. Setting as a test function $\bar{\mathbf{w}}_h = P_h \bar{\mathbf{w}}$ into (11), P_h being the orthogonal projector from $\mathbf{L}^2(\Omega)$ onto \mathbf{W}_h , and using that $\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n \in \mathbf{W}_h$ and $(\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n \in \mathbf{W}_h$ (thanks to (H4)), this yields

$$\begin{aligned} \left(\frac{\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n}{k}, \bar{\mathbf{w}} \right) &= - \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n, \bar{\mathbf{w}} \right) - \gamma \left(\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)), \bar{\mathbf{w}} \right). \\ &\leq C \|\mathbf{u}_h^{n+1}\|_{L^6(\Omega)} \|\nabla \mathbf{d}_h^n\| \|\bar{\mathbf{w}}\|_{L^3(\Omega)} + |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))| |\bar{\mathbf{w}}| \end{aligned}$$

The result follows using the duality definition of the $L^{3/2}$ -norm and the estimates of Theorem 5.

□

From Definition 6, Lemma 7 and (25), we have $\frac{d}{dt} \mathbf{d}_{h,k,\varepsilon}^l$ is bounded in $L^2(0, T; \mathbf{L}^{3/2}(\Omega))$ and $\mathbf{d}_{h,k,\varepsilon}^l$ is bounded in $L^\infty(0, T; \mathbf{H}^1(\Omega))$. Then, a compactness result of the Aubin-Lions type implies that the sequence $\mathbf{d}_{h,k,\varepsilon}^l$ is compact in $C(0, T; \mathbf{L}^r(\Omega))$ for any $1 \leq r < 6$.

As a consequence of estimate **vi**) of Theorem 5 and (25), one obtains

$$\mathbf{d}_{h,k,\varepsilon}^0, \mathbf{d}_{h,k,\varepsilon} \rightarrow \mathbf{d} \text{ in } L^q(0, T; L^r(\Omega)) \text{ as } (h, k) \rightarrow 0,$$

with $1 \leq r < 6$ and $1 \leq q < \infty$.

The rest of this section is devoted to obtaining compactness for the discrete velocity. Let

$$\mathbf{V}_h = \{\mathbf{v}_h \in \mathbf{X}_h : (\nabla \cdot \mathbf{v}_h, q_h) = 0 \forall q_h \in Q_h\}$$

and consider $A_h^{-1} : \mathbf{V}_h \rightarrow \mathbf{V}_h$ the inverse discrete Stokes operator defined as

$$(\nabla A_h^{-1} \mathbf{u}_h, \nabla \mathbf{v}_h) = (\mathbf{u}_h, \mathbf{v}_h) \quad \forall \mathbf{v}_h \in \mathbf{V}_h. \quad (27)$$

Notice that (27) is well-defined thanks to the *Inf-Sup* condition (H3).

Observe that $|\nabla A_h^{-1} \mathbf{u}_h|$ and $\|\mathbf{u}_h\|_{\mathbf{V}'_h}$ are equivalent norms in \mathbf{V}'_h (the dual space of \mathbf{V}_h). Indeed, we take $\mathbf{v}_h = A_h^{-1} \mathbf{u}_h$ in (27), then

$$|\nabla A_h^{-1} \mathbf{u}_h|^2 = (\mathbf{u}_h, A_h^{-1} \mathbf{u}_h) \leq C \|\mathbf{u}_h\|_{\mathbf{V}'_h} |\nabla A_h^{-1} \mathbf{u}_h|,$$

whence

$$|\nabla A_h^{-1} \mathbf{u}_h| \leq C \|\mathbf{u}_h\|_{\mathbf{V}'_h}.$$

Conversely, we take any $\mathbf{v}_h \in \mathbf{V}_h$ in (27), then

$$(\mathbf{u}_h, \mathbf{v}_h) = (\nabla A_h^{-1} \mathbf{u}_h, \nabla \mathbf{v}_h) \leq |\nabla A_h^{-1} \mathbf{u}_h| |\nabla \mathbf{v}_h| \quad \forall \mathbf{v}_h \in \mathbf{V}_h.$$

A dual definition of \mathbf{V}'_h provides $\|\mathbf{u}_h\|_{\mathbf{V}'_h} \leq |\nabla A_h^{-1} \mathbf{u}_h|$.

Lemma 8 *Under the conditions of Theorem 5, one has*

$$\int_0^{T-\delta} \|\mathbf{u}_{h,k,\varepsilon}(t+\delta) - \mathbf{u}_{h,k,\varepsilon}(t)\|_{\mathbf{V}'_h}^2 dt \leq C \delta^{1/2} \quad \forall \delta : 0 < \delta < T, \quad (28)$$

where $C > 0$ is independent of (h, k, ε) .

Proof: As $\mathbf{u}_{h,k}$ is a piecewise constant function, it suffices to suppose that δ is proportional to the time step k , i.e., $\delta = r k$ for any $r = 0, \dots, N$. Then, to obtain (28) it suffices to prove

$$k \sum_{m=0}^{N-r} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{\mathbf{V}'_h}^2 \leq C (r k)^{1/2}, \quad \forall r : 0 < r < N. \quad (29)$$

Multiplying (9) by k and summing for $n = m, \dots, m-1+r$, we have

$$\begin{aligned} \left(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m, \bar{\mathbf{u}}_h \right) &= -k \sum_{n=m}^{m-1+r} c(\mathbf{u}_h^n, \mathbf{u}_h^{n+1}, \bar{\mathbf{u}}_h) - \nu k \sum_{n=m}^{m-1+r} \left(\nabla \mathbf{u}^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\ &+ \lambda k \sum_{n=m}^{m-1+r} \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) - \lambda k \sum_{n=m}^{m-1+r} \left(F_\varepsilon(\mathbf{d}_h^n) - \tilde{p}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right). \end{aligned} \quad (30)$$

Setting $\bar{\mathbf{u}}_h = A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)$ as a test function in (30), observing that

$$\left(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m, A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) = |\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2$$

(which is easily seen by taking $\mathbf{u}_h = \mathbf{u}_h^{m+r} - \mathbf{u}_h^m$ and $\bar{\mathbf{u}}_h = A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)$ in (27)), multiplying by k , and summing for $m = 0, \dots, N-r$, we get

$$\begin{aligned} k \sum_{m=0}^{N-r} |\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 &= -k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c(\mathbf{u}_h^n, \mathbf{u}_h^{n+1}, A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)) \\ &+ \nu k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\nabla \mathbf{u}^{n+1}, \nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \\ &+ \lambda k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \\ &- \lambda k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(F_\varepsilon(\mathbf{d}_h^n), \nabla \cdot A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right) \\ &:= J_1 + J_2 + J_3 + J_4. \end{aligned} \quad (31)$$

The right-hand side of (31) can be estimated as follows:

$$J_1 \leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\mathbf{u}_h^n\| \|\mathbf{u}_h^{n+1}\| \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|.$$

Applying Fubini's discrete rule, we infer

$$J_1 \leq C k^2 \sum_{n=0}^{N-1} \|\mathbf{u}_h^n\| \|\mathbf{u}_h^{n+1}\| \sum_{m=n-r+1}^{\bar{n}} \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|.$$

where

$$\bar{n} = \begin{cases} 0 & \text{if } n < 0, \\ n & \text{if } 0 \leq n \leq N - r, \\ N - r & \text{if } n > N - r. \end{cases}$$

Finally, using $\|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\| \leq |\mathbf{u}_h^{m+r} - \mathbf{u}_h^m|$, Theorem 5, Hölder's inequality and that $|\bar{n} - \overline{n - r + 1}| \leq r$, one has

$$\begin{aligned} k \sum_{m=\bar{n}-r+1}^{\bar{n}} \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\| &\leq C \left(k \sum_{m=\bar{n}-r+1}^{\bar{n}} \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|^2 \right)^{1/2} \left(k \sum_{m=\bar{n}-r+1}^{\bar{n}} 1^2 \right)^{1/2} \\ &\leq C (rk)^{1/2}; \end{aligned}$$

hence

$$J_1 \leq C (rk)^{1/2} k \sum_{n=0}^{N-1} \|\mathbf{u}_h^n\| \|\mathbf{u}_h^{n+1}\| \leq C (rk)^{1/2}.$$

Once J_1 has been bounded, there are no additional difficulties in checking that $J_2 \leq C (rk)^{1/2}$.

To estimate J_3 , let us define $\mathbf{d}^{n+1}(h) \in \mathbf{H}^2(\Omega)$ as the solution of the nonhomogeneous Dirichlet problem

$$\begin{cases} -\Delta \mathbf{d}^{n+1}(h) = \mathbf{w}_h^{n+1} & \text{in } \Omega, \\ \mathbf{d}^{n+1}(h) = \mathbf{l} & \text{on } \partial\Omega. \end{cases}$$

Thus, for $\bar{\mathbf{u}}_h = A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)$ we can be rewritten the term $-\lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right)$ as

$$\begin{aligned} -\lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) &= \lambda \left((\nabla \mathbf{d}_h^{n+1})^t \Delta \mathbf{d}^{n+1}(h), \bar{\mathbf{u}}_h \right) + \lambda \left((\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ &= \lambda \left((\nabla \mathbf{d}^{n+1}(h))^t \Delta \mathbf{d}^{n+1}(h), \bar{\mathbf{u}}_h \right) + \lambda \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1})^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\ &\quad + \lambda \left((\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right). \end{aligned}$$

Next, integrating by parts in the first term on the right-hand side, one gets

$$\begin{aligned} \lambda \left((\nabla \mathbf{d}^{n+1}(h))^t \Delta \mathbf{d}^{n+1}(h), \bar{\mathbf{u}}_h \right) &= -\lambda \left((\nabla \mathbf{d}^{n+1}(h))^t \nabla \mathbf{d}^{n+1}(h), \nabla \bar{\mathbf{u}}_h \right) - \frac{\lambda}{2} \left(\nabla (|\nabla \mathbf{d}^{n+1}(h)|^2), \bar{\mathbf{u}}_h \right) \\ &= -\lambda \left((\nabla \mathbf{d}^{n+1}(h))^t \nabla \mathbf{d}^{n+1}(h), \nabla \bar{\mathbf{u}}_h \right) + \frac{\lambda}{2} \left(|\nabla \mathbf{d}^{n+1}(h)|^2, \nabla \cdot \bar{\mathbf{u}}_h \right) \\ &:= L_1 + L_2. \end{aligned}$$

Playing with $\mathbf{d}^{n+1}(h)$ as before until finding the discrete terms $-\lambda \left((\nabla \mathbf{d}_h^{n+1})^t \nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right)$ and $\frac{\lambda}{2} \left(|\nabla \mathbf{d}_h^{n+1}|^2, \nabla \cdot \bar{\mathbf{u}}_h \right)$, we transform

$$\begin{aligned}
L_1 &= -\lambda \left((\nabla \mathbf{d}_h^{n+1})^t \nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}_h^{n+1})^t (\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}^{n+1}(h)), \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1})^t (\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}^{n+1}(h)), \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}^{n+1}(h))^t \nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right), \\
L_2 &= +\frac{\lambda}{2} \left(|\nabla \mathbf{d}_h^{n+1}|^2, \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}) : \nabla \mathbf{d}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}) : (\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}), \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left(\nabla \mathbf{d}_h^{n+1} : (\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}), \nabla \cdot \bar{\mathbf{u}}_h \right),
\end{aligned}$$

where $:$ denotes the inner product of two matrices, that is, let $A = (a_{ij})_{ij}$ and $B = (b_{ij})_{ij}$ be two matrices, then $A : B = \sum_{i,j} a_{ij} b_{ij}$. Finally, recompiling the previous identities, we find the discrete integration by parts

$$\begin{aligned}
-\lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) &= -\lambda \left((\nabla \mathbf{d}_h^{n+1})^t \nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}_h^{n+1})^t (\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}^{n+1}(h)), \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1})^t (\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}^{n+1}(h)), \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}^{n+1}(h))^t \nabla \mathbf{d}_h^{n+1}, \nabla \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left(|\nabla \mathbf{d}_h^{n+1}|^2, \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}) : \nabla \mathbf{d}_h^{n+1}, \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}) : (\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}), \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \frac{\lambda}{2} \left(\nabla \mathbf{d}_h^{n+1} : (\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}), \nabla \cdot \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1})^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\
&\quad + \lambda \left((\nabla \mathbf{d}_h^{n+1} - \nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \bar{\mathbf{u}}_h \right) \\
&:= I_1 + I_2 + I_3 + I_4 + I_5 + I_6 + I_7 + I_8 + I_9 + I_{10},
\end{aligned} \tag{32}$$

Comparing the problems verified by \mathbf{d}_h^{n+1} and $\mathbf{d}^{n+1}(h)$, the following property holds ([3]):

$$|\nabla \mathbf{d}^{n+1}(h) - \nabla \mathbf{d}_h^{n+1}| \leq C h |\mathbf{w}_h^{n+1}|. \tag{33}$$

Therefore, the term $-\lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m) \right)$ is estimated by taking into account the Sobolev embedding $H^1(\Omega) \hookrightarrow L^p(\Omega)$ with $p \leq 6$ and Theorem 5 as follows:

$$I_1 \leq C |\nabla \mathbf{d}_h^{n+1}|^2 \|\nabla A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \leq C \|\nabla A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)},$$

$$\begin{aligned}
I_2 &\leq C h |\nabla \mathbf{d}_h^{n+1}| |\mathbf{w}_h^{n+1}| \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \\
&\leq C \left(\frac{h}{\varepsilon^2} (\|\mathbf{d}_h^n\|_{H^1(\Omega)}^3 + \|\mathbf{d}_h^n\|_{H^1(\Omega)}) + h |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))| \right) \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \\
&\leq C \left(\frac{h}{\varepsilon^2} + h |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))| \right) \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)}, \\
I_3 &\leq C h^2 |\mathbf{w}_h^{n+1}|^2 \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \\
&\leq C \left(\frac{h^2}{\varepsilon^4} + h^2 |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 \right) \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)}.
\end{aligned}$$

The terms I_i , for $i = 4, \dots, 8$, are bounded in the same way as before. We continue with I_9 :

$$\begin{aligned}
I_9 &\leq C h |\mathbf{w}_h^{n+1}|^2 \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \\
&\leq C \left(\frac{h}{\varepsilon^4} + h |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 \right) \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)}.
\end{aligned}$$

To finish, we treat the term I_{10} :

$$\begin{aligned}
I_{10} &\leq C |\nabla(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)| |\mathbf{w}_h^{n+1}| \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \\
&\leq C \left(\frac{1}{\varepsilon^4} |\nabla(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)|^2 + |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 + 1 \right) \|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)}.
\end{aligned}$$

In view of all these bounds of I_i , the bound of term J_3 remains

$$\begin{aligned}
J_3 &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\frac{h}{\varepsilon^4} + \frac{1}{\varepsilon^4} |\nabla(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)|^2 \right) \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \\
&\quad + C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} (1 + |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2) \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)}
\end{aligned}$$

In [6] it is proven the following bound in maximum norm

$$\|A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{W^{1,\infty}(\Omega)} \leq C \|A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{W^{1,\infty}(\Omega)},$$

where A^{-1} is the continuous Stokes resolvent. Thanks to the Sobolev imbedding $W^{2,r}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$ with $r > 3$ and hypothesis (H1), one gets

$$\|\nabla A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \leq C \|A^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{W^{2,r}(\Omega)} \leq C \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^r(\Omega)}, \quad (34)$$

but r must not be bigger than 6, because we only have the estimate $k \sum_{n=0}^{N-1} \|\mathbf{u}_h^{n+1}\|_{H^1(\Omega)}^2 \leq C$ (see Theorem 5).

Therefore,

$$\begin{aligned}
J_3 &\leq C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \left(\frac{h}{\varepsilon^4} + \frac{1}{\varepsilon^4} |\nabla(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)|^2 \right) \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^r(\Omega)} \\
&\quad + C k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} (1 + |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2) \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^r(\Omega)} \\
&:= J_3^1 + J_3^2 + J_3^3 + J_3^4.
\end{aligned}$$

Due to the stability condition (S2), one has $J_3^1 \leq C(rk)^{1/2}$. In the same way, one also has $J_3^3 \leq C(rk)^{1/2}$ and $J_3^4 \leq C(rk)^{1/2}$. To estimate J_3^2 , we use the estimate $\sum_{n=0}^{N-1} |\nabla(\mathbf{d}^{n+1} - \mathbf{d}_h^n)|^2 \leq C$ (Theorem 5), Fubini's discrete rule and the stability condition (S1), obtaining

$$J_3^2 \leq C \frac{k}{\varepsilon^4} \sum_{n=0}^{N-1} |\nabla(\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)|^2 k \sum_{m=n-r+1}^{\bar{n}} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{L^r(\Omega)} \leq C \frac{k}{\varepsilon^4} (rk)^{1/2} \leq C(rk)^{1/2}.$$

Finally,

$$J_4 \leq k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|F_\varepsilon(\mathbf{d}_h^n)\|_{L^1(\Omega)} \|\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{L^\infty(\Omega)} \leq C(rk),$$

where we have used that $\|F_\varepsilon(\mathbf{d}_h^n)\|_{L^1(\Omega)} \leq C$ for all n, h .

Therefore, we can conclude

$$k \sum_{m=0}^{N-r} |\nabla A_h^{-1}(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 \leq C(rk)^{1/2}$$

which is equivalent to (29), thanks to $|\nabla A_h^{-1} \mathbf{u}_h|$ and $\|\mathbf{u}_h\|_{\mathbf{V}'_h}$ are equivalent norms. \square

The first idea to obtain compactness of the discrete velocities $\{\mathbf{u}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$ is to use the following compactness result (see *J. Simon*[18]):

“Let $X \mapsto B \hookrightarrow Y$ be three Banach spaces with continuous imbeddings, with the imbedding $X \mapsto B$ compact. Then, the following imbedding is compact

$$L^q(0, T; X) \cap \{\phi \in L^q(0, T; Y) : \|\phi(t + \delta) - \phi(t)\|_{L^q(0, T-\delta; Y)} \leq C \delta^\alpha\} \hookrightarrow L^q(0, T; B), \quad (35)$$

for $1 \leq q \leq \infty$ and $0 < \alpha < 1$.”

But one observes that the fractional time derivative estimate for the discrete velocities (28) has been done in the norm \mathbf{V}'_h which moves with respect to the space parameter h . In these conditions, the previous result does not work. The following idea is to find a fixed norm where the fractional time derivative can be bounded. For this, we consider the space

$$\mathbf{V} = \{\mathbf{v} \in \mathbf{H}_0^1(\Omega) : \nabla \cdot \mathbf{v} = 0\}$$

and the orthogonal projection $R_h : \mathbf{V}_h \rightarrow \mathbf{V}$ defined as $(\nabla(R_h \mathbf{u}_h - \mathbf{u}_h), \nabla \mathbf{v}) = 0$ for all $\mathbf{v} \in \mathbf{V}$.

We will use here the following properties of the operator R_h :

- $\|R_h \mathbf{u}_h\| \leq \|\mathbf{u}_h\|$ (H^1 -continuous dependency)
- $|R_h \mathbf{u}_h - \mathbf{u}_h| \leq C h |\nabla \cdot \mathbf{u}_h|$ (L^2 -error estimate).

Indeed, setting $\mathbf{v} = R_h \mathbf{u}_h$ as a test function, the estimate $\|R_h \mathbf{u}_h\| \leq \|\mathbf{u}_h\|$ is easily obtained. To prove the L^2 -error estimate, we consider the following Stokes problem: find $(\varphi, \chi) \in (\mathbf{V} \cap \mathbf{H}^2(\Omega)) \times (L_0^2(\Omega) \cap H^1(\Omega))$ such that

$$\begin{cases} -\Delta \varphi - \nabla \chi = R_h \mathbf{u}_h - \mathbf{u}_h & \text{in } \Omega \\ \nabla \cdot \varphi = 0 & \text{in } \Omega, \quad \varphi = 0 \quad \text{on } \partial\Omega. \end{cases} \quad (36)$$

Multiplying (36) by $R_h \mathbf{u}_h - \mathbf{u}_h$ and making use of the definition of R_h

$$|R_h \mathbf{u}_h - \mathbf{u}_h|^2 = \left(\chi, \nabla \cdot (R_h \mathbf{u}_h - \mathbf{u}_h) \right).$$

In view of $\mathbf{u}_h \in \mathbf{V}_h$ and $R_h \mathbf{u}_h \in \mathbf{V}$, the previous equality can be converted into

$$|R_h \mathbf{u}_h - \mathbf{u}_h|^2 = \left(\chi - q_h, \nabla \cdot (R_h \mathbf{u}_h - \mathbf{u}_h) \right) = - \left(\chi - K_h \chi, \nabla \cdot \mathbf{u}_h \right),$$

where $K_h \chi \in Q_h$ is the interpolation operator defined in hypothesis (H2). Thus, using the approximation property $|\chi - K_h \chi| \leq C h \|\chi\|_{H^1}$ and the continuous dependency of the Stokes problem (36), $\|\varphi\|_{H^2(\Omega)} + \|\chi\|_{H^1} \leq C |R_h \mathbf{u}_h - \mathbf{u}_h|$, one has

$$|R_h \mathbf{u}_h - \mathbf{u}_h|^2 \leq |\nabla \cdot \mathbf{u}_h| |\chi - K_h \chi| \leq C h \|\chi\|_{H^1(\Omega)} |\nabla \cdot \mathbf{u}_h| \leq C h |R_h \mathbf{u}_h - \mathbf{u}_h| |\nabla \cdot \mathbf{u}_h|;$$

hence the error estimate $|R_h \mathbf{u}_h - \mathbf{u}_h| \leq C h |\nabla \cdot \mathbf{u}_h|$ holds.

Next, we will prove that $\|R_h \mathbf{u}_h\|_{\mathbf{V}'} \leq C \left(\|\mathbf{u}_h\|_{\mathbf{V}'_h} + h |\nabla \cdot \mathbf{u}_h| \right)$. For this, we define the orthogonal projection $\tilde{P}_h : \mathbf{V} \rightarrow \mathbf{V}_h$ defined as $(\tilde{P}_h \mathbf{v} - \mathbf{v}, \mathbf{v}_h) = 0$ for all $\mathbf{v}_h \in \mathbf{V}_h$. Indeed, let $\mathbf{v} \in \mathbf{V}$ and consider the $L^2(\Omega)$ -inner product of \mathbf{v} with $R_h \mathbf{u}_h$:

$$\left(R_h \mathbf{u}_h, \mathbf{v} \right) = \left(R_h \mathbf{u}_h - \mathbf{u}_h, \mathbf{v} \right) + \left(\mathbf{u}_h, \tilde{P}_h \mathbf{v} \right) \leq C h |\nabla \cdot \mathbf{u}_h| |\mathbf{v}| + \left(\mathbf{u}_h, \tilde{P}_h \mathbf{v} \right).$$

The definition of dual norms in \mathbf{V}' and \mathbf{V}'_h , jointly with the stability property $|\tilde{P}_h \mathbf{v}| \leq |\mathbf{v}|$ gives

$$\|R_h \mathbf{u}_h\|_{\mathbf{V}'} \leq C h |\nabla \cdot \mathbf{u}_h| + \sup_{\mathbf{v} \in \mathbf{V}} \frac{\left(\mathbf{u}_h, \tilde{P}_h \mathbf{v} \right)}{\|\mathbf{v}\|} \leq C h |\nabla \cdot \mathbf{u}_h| + \sup_{\mathbf{v}_h \in \mathbf{V}_h} \frac{\left(\mathbf{u}_h, \mathbf{v}_h \right)}{|\mathbf{v}_h|};$$

hence,

$$\|R_h \mathbf{u}_h\|_{\mathbf{V}'} \leq C h |\nabla \cdot \mathbf{u}_h| + \|\mathbf{u}_h\|_{\mathbf{V}'_h}.$$

Taking $\mathbf{u}_h = \mathbf{u}_h^{m+r} - \mathbf{u}_h^m$ and using (29), one has

$$\begin{aligned} k \sum_{m=0}^{N-r} \|R_h(\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)\|_{\mathbf{V}'}^2 &\leq C k \sum_{m=0}^{N-r} \|\mathbf{u}_h^{m+r} - \mathbf{u}_h^m\|_{\mathbf{V}'_h}^2 + C h^2 k \sum_{m=0}^{N-r} |\nabla \cdot (\mathbf{u}_h^{m+r} - \mathbf{u}_h^m)|^2 \\ &\leq C (r k)^{1/2} + C h^2. \end{aligned}$$

This inequality can be written as

$$\int_0^{T-\delta} \|R_h \mathbf{u}_{h,k,\varepsilon}(t+\delta) - R_h \mathbf{u}_{h,k,\varepsilon}(t)\|_{\mathbf{V}'}^2 dt \leq C \delta^{1/2} + C h^2.$$

We again observe that the previous fractional time derivative does not verify the hypotheses of the compactness result (35), because of the additional term $C h^2$ on the right-hand side. For this reason, we use the following ‘‘compactness by perturbation’’ result due to *P. Azérad* and *F. Guillén* ([1]):

Theorem 9 *Let $X \hookrightarrow B \hookrightarrow Y$ be three Banach spaces with continuous imbeddings, with the imbedding from X to B being compact. Let $\{f_\varepsilon\}_{\varepsilon>0}$ be a family of functions of $L^p(0, T; X)$, $1 \leq p \leq \infty$, with the extra condition $\{f_\varepsilon\}_{\varepsilon>0} \subset C(0, T; Y)$ if $p = \infty$ such that*

(C1) $\{f_\varepsilon\}_{\varepsilon>0}$ is bounded in $L^p(0, T; X)$,

(C2) $\|f_\varepsilon(t+\delta) - f_\varepsilon(t)\|_{L^p(0, T; Y)} \leq \varphi(\delta) + \psi(\varepsilon)$ with

$$\lim_{\delta \rightarrow 0} \varphi(\delta) = 0, \quad \lim_{\varepsilon \rightarrow 0} \psi(\varepsilon) = 0.$$

Then, the family $\{f_\varepsilon\}_{\varepsilon>0}$ possesses a cluster point in $L^p(0, T; B)$ as $\varepsilon \rightarrow 0$.

Therefore, if we select $X = \mathbf{V}$, $B = \mathbf{H}$ and $Y = \mathbf{V}'$, then there exists $\mathbf{u} \in \mathbf{V}$ such that $R_h \mathbf{u}_{k,h,\varepsilon} \rightarrow \mathbf{u}$ in $L^2(0, T; \mathbf{L}^2(\Omega))$ -strong as $(k, h, \varepsilon) \rightarrow 0$. To conclude, we prove that

$$\mathbf{u}_{h,k,\varepsilon} \rightarrow \mathbf{u} \quad \text{in } L^2(0, T; \mathbf{L}^2(\Omega))\text{-strong as } (k, h, \varepsilon) \rightarrow 0.$$

Indeed,

$$\begin{aligned} \|\mathbf{u}_{h,k,\varepsilon} - \mathbf{u}\|_{L^2(0, T; \mathbf{L}^2(\Omega))} &\leq \|\mathbf{u}_{h,k,\varepsilon} - R_h \mathbf{u}_{h,k,\varepsilon}\|_{L^2(0, T; \mathbf{L}^2(\Omega))} + \|R_h \mathbf{u}_{h,k,\varepsilon} - \mathbf{u}\|_{L^2(0, T; \mathbf{L}^2(\Omega))} \\ &\leq C h + \|R_h \mathbf{u}_{h,k,\varepsilon} - \mathbf{u}\|_{L^2(0, T; \mathbf{L}^2(\Omega))} \rightarrow 0. \end{aligned}$$

4 Convergence for the d -system

Let us denote by the symbol \wedge the vectorial product. The convergence for (11)-(12) is based on the following result, whose proof can be found in [2] Lemma 2.2 (see also Lemma 7.1 in [15]) without the convective terms.

Lemma 10 *The next two systems are equivalent:*

$$\partial_t \mathbf{d} + \mathbf{u} \cdot \nabla \mathbf{d} - \gamma \Delta \mathbf{d} - \gamma |\nabla \mathbf{d}|^2 \mathbf{d} = \mathbf{0} \quad \text{in } Q, \tag{37}$$

and

$$|\mathbf{d}| = 1, \quad \partial_t \mathbf{d} \wedge \mathbf{d} + \mathbf{u} \cdot \nabla \mathbf{d} \wedge \mathbf{d} - \gamma \nabla \cdot (\nabla \mathbf{d} \wedge \mathbf{d}) = \mathbf{0} \quad \text{in } Q. \tag{38}$$

To check that \mathbf{d} verifies the constraint $|\mathbf{d}| = 1$, where \mathbf{d} is the limit function which we have found in (26), we only need to prove that

$$\int_{\Omega} (|\mathbf{d}_h^{n+1}|^2 - 1)^2 \rightarrow 0 \quad \text{as} \quad (h, k, \varepsilon) \rightarrow 0,$$

which can be easily deduced from the following bound (obtained in Theorem 5)

$$\int_{\Omega} F_{\varepsilon}(\mathbf{d}_h^{n+1}) = \frac{1}{4\varepsilon^2} \int_{\Omega} (|\mathbf{d}_h^{n+1}|^2 - 1)^2 \leq C.$$

Considering $\bar{\mathbf{w}}_h = P_h \bar{\mathbf{w}}$ into (11) for any $\bar{\mathbf{w}} \in \mathbf{L}^2(\Omega)$, with P_h being the orthogonal projection onto \mathbf{W}_h respect to the $\mathbf{L}^2(\Omega)$ -norm, and using that $\mathbf{d}_h^{n+1} - \mathbf{d}_h^n \in \mathbf{W}_h$ and $(\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n \in \mathbf{W}_h$ (thanks to (H4)), one has the system:

$$\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k} + (\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n + \gamma(P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}) = 0 \quad \text{in } \Omega. \quad (39)$$

Taking vectorial product of (39) by \mathbf{d}_h^n , we write

$$\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k} \wedge \mathbf{d}_h^n + (\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n \wedge \mathbf{d}_h^n + \gamma \mathbf{w}_h^{n+1} \wedge \mathbf{d}_h^n + \gamma(P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) \wedge \mathbf{d}_h^n = 0 \quad \text{in } \Omega,$$

since $\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n) \wedge \mathbf{d}_h^n = 0$. Next, multiplying by any test function $\bar{\mathbf{d}}_h \in \mathbf{D}_{0h}$, we infer the discrete weak formulation

$$\begin{aligned} & \left(\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k} \wedge \mathbf{d}_h^n, \bar{\mathbf{d}}_h \right) + \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n \wedge \mathbf{d}_h^n, \bar{\mathbf{d}}_h \right) \\ & + \gamma \left(\mathbf{w}_h^{n+1} \wedge [\mathbf{d}_h^{n+1} + (\mathbf{d}_h^n - \mathbf{d}_h^{n+1})], \bar{\mathbf{d}}_h \right) + \gamma \left((P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) \wedge \mathbf{d}_h^n, \bar{\mathbf{d}}_h \right) = 0, \end{aligned} \quad (40)$$

on which we will pass to the limit rewriting the last two terms. For this, let us define a special vectorial product, which we will denote by \odot , such that

$$\left(\mathbf{w} \wedge \mathbf{d}, \bar{\mathbf{d}} \right) := \left(\mathbf{w}, \mathbf{d} \odot \bar{\mathbf{d}} \right) \quad \forall \mathbf{w}, \mathbf{d}, \bar{\mathbf{d}} \in \mathbb{R}^3. \quad (41)$$

Thus, we write the last term of (40) as follows:

$$\begin{aligned} \left((P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) \wedge \mathbf{d}_h^n, \bar{\mathbf{d}}_h \right) &= \left((P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^n)), \mathbf{d}_h^n \odot \bar{\mathbf{d}}_h \right) \\ &= \left(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n), P_h(\mathbf{d}_h^n \odot \bar{\mathbf{d}}_h) - \mathbf{d}_h^n \odot \bar{\mathbf{d}}_h \right) := R^n. \end{aligned}$$

On the other hand, we want to obtain a discrete version of the continuous identity

$$-\Delta \mathbf{d} \wedge \mathbf{d} = -\nabla \cdot (\nabla \mathbf{d} \wedge \mathbf{d}) - \nabla \mathbf{d} \wedge \nabla \mathbf{d} = -\nabla \cdot (\nabla \mathbf{d} \wedge \mathbf{d}).$$

Taking $P_h^1[\widehat{\mathbf{d}}_h^{n+1} \odot \bar{\mathbf{d}}_h]$ as a test function in (12), with P_h^1 being the orthogonal projection onto \mathbf{D}_{0h} with respect to the \mathbf{H}_0^1 -inner product, one has

$$\left(\nabla \widehat{\mathbf{d}}_h^{n+1}, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h] \right) = \left(\mathbf{w}_h^{n+1}, P_h^1[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h] \right).$$

Therefore,

$$\left(\nabla\widehat{\mathbf{d}}_h^{n+1}, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right) = \left(\mathbf{w}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h\right) + R_1^{n+1},$$

where

$$R_1^{n+1} = \left(\mathbf{w}_h^{n+1}, P_h^1[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h] - [\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right).$$

From the definition of $\mathbf{d}_h^{n+1} = \widehat{\mathbf{d}}_h^{n+1} + \widetilde{\mathbf{d}}_h$, we get

$$\left(\nabla\mathbf{d}_h^{n+1}, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right) = \left(\mathbf{w}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h\right) + R_1^{n+1} + R_2^{n+1},$$

where

$$R_2^{n+1} = \left(\nabla\widetilde{\mathbf{d}}_h, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right).$$

Now, we will see that $\left(\nabla\mathbf{d}_h^{n+1}, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right) = \left(\nabla\mathbf{d}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \nabla\bar{\mathbf{d}}_h\right)$. Indeed,

$$\begin{aligned} \left(\nabla\mathbf{d}_h^{n+1}, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right) &= \sum_{i=1}^3 \left(\partial_i \mathbf{d}_h^{n+1}, \partial_i [\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]\right) \\ &= \sum_{i=1}^3 \left(\partial_i \mathbf{d}_h^{n+1}, \partial_i \mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h + \mathbf{d}_h^{n+1} \odot \partial_i \bar{\mathbf{d}}_h\right) \\ &= \sum_{i=1}^3 \left(\partial_i \mathbf{d}_h^{n+1} \wedge \partial_i \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h\right) + \left(\partial_i \mathbf{d}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \partial_i \bar{\mathbf{d}}_h\right) \\ &= \sum_{i=1}^3 \left(\partial_i \mathbf{d}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \partial_i \bar{\mathbf{d}}_h\right) \\ &= \left(\nabla\mathbf{d}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \nabla\bar{\mathbf{d}}_h\right). \end{aligned}$$

Therefore, we have obtained

$$\left(\nabla\mathbf{d}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \nabla\bar{\mathbf{d}}_h\right) = \left(\mathbf{w}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \bar{\mathbf{d}}_h\right) + R_1^{n+1} + R_2^{n+1}.$$

Then, from (40) one has

$$\begin{aligned} &k \sum_{n=0}^{N-1} \left\{ \left(\frac{\mathbf{d}_h^{n+1} - \mathbf{d}_h^n}{k} \wedge \mathbf{d}_h^n, \bar{\mathbf{d}}_h\right) + \left((\mathbf{u}_h^{n+1} \cdot \nabla) \mathbf{d}_h^n \wedge \mathbf{d}_h^n, \bar{\mathbf{d}}_h\right) + \gamma \left(\nabla\mathbf{d}_h^{n+1} \wedge \mathbf{d}_h^{n+1}, \nabla\bar{\mathbf{d}}_h\right) \right\} \\ &= \gamma k \sum_{n=0}^{N-1} (R^n + R_1^{n+1} + R_2^{n+1}) + k \sum_{n=0}^{N-1} \gamma \left(\mathbf{w}_h^{n+1} \wedge (\mathbf{d}_h^{n+1} - \mathbf{d}_h^n), \bar{\mathbf{d}}_h\right) \quad (42) \\ &:= \gamma k \sum_{n=0}^{N-1} (R^n + R_1^{n+1} + R_2^{n+1}) + J_1. \end{aligned}$$

As mentioned, our intention is to pass to the limit in (42) and to obtain (38). We just analyze that the residual terms in (42) go to zero as (h, k, ε) go to zero.

$$\begin{aligned}
J_1 &\leq C k \sum_{n=0}^{N-1} |\mathbf{w}_h^{n+1}| \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{H^1(\Omega)} \|\bar{\mathbf{d}}_h\|_{L^3(\Omega)} \\
&\leq C k \sum_{n=0}^{N-1} \left(|\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))| + |\mathbf{f}_\varepsilon(\mathbf{d}_h^n)| \right) \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{H^1(\Omega)} \\
&\leq C \left(k \sum_{n=0}^{N-1} \left(|\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 + |\mathbf{f}_\varepsilon(\mathbf{d}_h^n)|^2 \right) \right)^{1/2} \left(k \sum_{n=0}^{N-1} \|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n\|_{H^1(\Omega)}^2 \right)^{1/2} \\
&\leq C \frac{k^{1/2}}{\varepsilon^2} \rightarrow 0 \text{ as } (h, k, \varepsilon) \rightarrow 0
\end{aligned}$$

Using the approximation inequality $|\bar{\mathbf{d}} - P_h^1 \bar{\mathbf{d}}| \leq C h \|\bar{\mathbf{d}}\|_{H^1}$ for all $\bar{\mathbf{d}} \in \mathbf{H}_0^1(\Omega)$ (which is obtained by a duality argument jointly with the approximation inequality $\|\bar{\mathbf{d}} - P_h^1 \bar{\mathbf{d}}\|_{H^1(\Omega)} \leq C h \|\bar{\mathbf{d}}\|_{H^2(\Omega)}$, $\forall \bar{\mathbf{d}} \in \mathbf{H}^2(\Omega)$), one has

$$|\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h - P_h^1[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]| \leq C h \|\mathbf{d}_h^{n+1}\|_{H^1(\Omega)} \|\bar{\mathbf{d}}_h\|_{W^{1,\infty}(\Omega)}.$$

Then, it is easy to prove as in J_1 that the term $k \sum_{n=0}^{N-1} (R^n + R_1^{n+1}) \leq C \frac{h}{\varepsilon^2}$, whence the limit is zero thanks to (S2).

Let us consider the non-homogeneous Dirichlet problem

$$-\Delta \tilde{\mathbf{d}} = 0 \quad \text{in } \Omega, \quad \tilde{\mathbf{d}} = \mathbf{l} \quad \text{on } \partial\Omega.$$

Thus, one observes that each term of $k \sum_{n=0}^{N-1} R_2^{n+1}$ can be rewrite as

$$\begin{aligned}
(\nabla \tilde{\mathbf{d}}_h, \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]) &= ((\nabla(\tilde{\mathbf{d}}_h - \tilde{\mathbf{d}}), \nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]) \\
&\leq |\nabla(\tilde{\mathbf{d}}_h - \tilde{\mathbf{d}})| |\nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]| \rightarrow 0
\end{aligned}$$

using the fact that $\nabla \tilde{\mathbf{d}}_h \rightarrow \nabla \tilde{\mathbf{d}}$ in $\mathbf{L}^2(\Omega)$ -strong and $|\nabla[\mathbf{d}_h^{n+1} \odot \bar{\mathbf{d}}_h]|$ is bounded. Thus, we obtain that $k \sum_{n=0}^{N-1} R_2^{n+1} \rightarrow 0$ as $(h, k, \varepsilon) \rightarrow 0$.

In conclusion, we get that the limit function \mathbf{d} verifies (38). Therefore, the limit \mathbf{d} -system (37) holds at least in a weak sense.

5 Compactness for the gradient of \mathbf{d}

Let us define $\mathbf{z}_{h,k,\varepsilon}(t) = \mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^{n+1}))$ and $\mathbf{d}_{h,k,\varepsilon}(t) = \mathbf{d}_h^{n+1}$ if $t \in (t_n, t_{n+1}]$. Then, $\mathbf{d}_{h,k,\varepsilon}(t)$ is a minimum of the following optimization problem:

$$J_{h,k,\varepsilon}(\mathbf{d}_{h,k,\varepsilon}(t)) = \min_{\mathbf{d}_h \in \mathbf{D}_{t_h}} J_{h,k,\varepsilon}(\mathbf{d}_h) \quad (43)$$

where $J_{h,k,\varepsilon} : \mathbf{D}_{\mathbf{l}_h} \rightarrow \mathbb{R}$ is defined as

$$J_{h,k,\varepsilon}(\mathbf{d}_h) = \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{d}_h|^2 + F_{\varepsilon}(\mathbf{d}_h) - \mathbf{z}_{h,k,\varepsilon}(t) \cdot \mathbf{d}_h \right)$$

and

$$\mathbf{D}_{\mathbf{l}_h} = \{\mathbf{d}_h \in \mathbf{D}_h : \mathbf{d}_h = \mathbf{l}_h \text{ on } \partial\Omega\}.$$

Indeed, the *Euler-Langrange* equation associated to this problem at the time $t \in (t_n, t_{n+1}]$ is

$$\mathbf{d}_h \in \mathbf{D}_{\mathbf{l}_h} \text{ such that } (\nabla \mathbf{d}_h, \nabla \bar{\mathbf{d}}_h) + (\mathbf{f}_{\varepsilon}(\mathbf{d}_h), \bar{\mathbf{d}}_h) = (\mathbf{z}_{h,k,\varepsilon}(t), \bar{\mathbf{d}}_h) \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_{0h}. \quad (44)$$

Next, taking into account the definitions of $\mathbf{z}_{h,k,\varepsilon}$ and P_h , we find that $\mathbf{d}_{h,k,\varepsilon}(t)$ verifies the previous problem for all $t \in (t_n, t_{n+1}]$. Then, $\mathbf{d}_{h,k,\varepsilon}(t)$ is a minimum of (43).

On the other hand, we define $\mathbf{d}^* : [0, T] \rightarrow \mathbf{H}_{\mathbf{l}}^1(\Omega)$ as a solution of the (constrained) optimization problem

$$J(\mathbf{d}^*(t)) = \min_{\{\mathbf{d} \in \mathbf{H}_{\mathbf{l}}, |\mathbf{d}|=1\}} J(\mathbf{d}) \quad (45)$$

where

$$J(\mathbf{d}) = \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{d}|^2 - \mathbf{z}(t) \cdot \mathbf{d} \right), \quad (46)$$

$$\mathbf{H}_{\mathbf{l}}^1 = \{\mathbf{d}_h \in \mathbf{H}^1(\Omega) : \mathbf{d} = \mathbf{l} \text{ on } \partial\Omega\}.$$

and the function $\mathbf{z} \in \mathbf{L}^2(Q)$ is defined as a limit of $\mathbf{z}_{h,k,\varepsilon}$. Indeed, we shall see that \mathbf{z} exists. For this, it suffices to prove that $(\mathbf{z}_{h,k,\varepsilon})$ is bounded in $\mathbf{L}^2(Q)$ independently of (h, k, ε) . For any $t \in (t_n, t_{n+1}]$:

$$|\mathbf{z}_{h,k,\varepsilon}(t)|^2 = |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^{n+1}))|^2 \leq C|\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n))|^2 + C|\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^{n+1})|^2.$$

Now, decomposing the last term as follows:

$$\begin{aligned} |\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^{n+1})|^2 &\leq \frac{C}{\varepsilon^2} (|\mathbf{d}_h^{n+1}|^2 - 1) (\mathbf{d}_h^{n+1} - \mathbf{d}_h^n)^2 + \frac{C}{\varepsilon^2} (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2) |\mathbf{d}_h^n|^2 \\ &\leq \frac{C}{\varepsilon^2} (\|\mathbf{d}_h^{n+1}\|_{L^\infty(\Omega)}^2 + 1) |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 + \frac{C}{\varepsilon^2} \|\mathbf{d}_h^n\|_{L^\infty(\Omega)} \left(|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2 \right)^2. \end{aligned}$$

Using the inverse inequality $\|\bar{\mathbf{d}}_h\|_{L^\infty(\Omega)} \leq C h^{-1/2} \|\bar{\mathbf{d}}_h\|_{H^1(\Omega)}$ for all $\bar{\mathbf{d}}_h \in \mathbf{D}_h$ and the estimate $\|\mathbf{d}_h^n\|_{H^1(\Omega)} \leq C$ for all n , we get

$$|\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n) - \mathbf{f}_{\varepsilon}(\mathbf{d}_h^{n+1})|^2 \leq \frac{C}{h^2 \varepsilon^2} \left(|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 + \left| |\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2 \right|^2 \right).$$

Therefore, we have obtained the bound

$$|\mathbf{z}_{h,k,\varepsilon}(t)|^2 \leq C|\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_{\varepsilon}(\mathbf{d}_h^n))|^2 + \frac{C}{h^2 \varepsilon^2} \left(|\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 + \left| |\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2 \right|^2 \right).$$

Finally, multiplying by k , summing over n , taking into account the bounds of Theorem 5, and the stability condition (S1), we find that $(z_{h,k,\varepsilon})$ is bounded in $\mathbf{L}^2(Q)$.

Next, using the interpolator operator $I_h : \mathbf{H}^1 \rightarrow \mathbf{D}_h$, which verifies $I_h(\mathbf{H}_l^1) \subset \mathbf{D}_{l_h}$, we deduce

$$J_{h,k,\varepsilon}(\mathbf{d}_{h,k,\varepsilon}(t)) \leq J_{h,k,\varepsilon}(I_h \mathbf{d}^*(t)).$$

Taking into account that $F_\varepsilon(\mathbf{d}_{h,k,\varepsilon}(t)) \geq 0$, we have

$$\int_\Omega \left(\frac{1}{2} |\nabla \mathbf{d}_{h,k,\varepsilon}(t)|^2 - z_{h,k,\varepsilon}(t) \cdot \mathbf{d}_{h,k,\varepsilon}(t) \right) \leq J_{h,k,\varepsilon}(I_h \mathbf{d}^*(t)). \quad (47)$$

Next, let us see that

$$\lim_{(h,k,\varepsilon) \rightarrow 0} \int_0^T J_{h,k,\varepsilon}(I_h \mathbf{d}^*(t)) = \int_0^T J(\mathbf{d}^*(t)).$$

To start with, we prove that

$$\int_0^T \int_\Omega \frac{1}{2} |\nabla I_h \mathbf{d}^*(t)|^2 \rightarrow \int_0^T \int_\Omega \frac{1}{2} |\nabla \mathbf{d}^*(t)|^2,$$

which can be easily deduced from dominated convergence theorem, since $\int_\Omega |\nabla I_h \mathbf{d}^*(t)|^2 \leq C \|\mathbf{d}^*(t)\|_{H^1(\Omega)}$ and $\int_\Omega \frac{1}{2} |\nabla I_h \mathbf{d}^*(t)|^2 \rightarrow \int_\Omega \frac{1}{2} |\nabla \mathbf{d}^*(t)|^2$ as $h \rightarrow 0$ for almost everywhere $t \in [0, T]$.

Using the following approximation properties of I_h (imposed in (H2)):

$$|I_h \mathbf{d}^*(t) - \mathbf{d}^*(t)| \leq C h \|\mathbf{d}^*(t)\|_{H^1(\Omega)},$$

$$\|I_h \mathbf{d}^*(t) - \mathbf{d}^*(t)\|_{L^4(\Omega)} \leq C h^{1/4} \|\mathbf{d}^*(t)\|_{H^1(\Omega)},$$

we are going to prove that $\int_0^T \int_\Omega F_\varepsilon(I_h \mathbf{d}^*(t)) \rightarrow 0$ as $(h, \varepsilon) \rightarrow 0$. Indeed, since $|\mathbf{d}^*(t, \mathbf{x})| = 1$ and using $|a|^2 - |b|^2 + |a - b|^2 = (a - b, 2a)$, we observe that

$$\begin{aligned} \int_0^T \int_\Omega F_\varepsilon(I_h \mathbf{d}^*(t, \mathbf{x})) &= \frac{1}{\varepsilon^2} \int_0^T \int_\Omega (|I_h \mathbf{d}^*(t, \mathbf{x})|^2 - |\mathbf{d}^*(t, \mathbf{x})|^2)^2 \\ &\leq \frac{C}{\varepsilon^2} \int_0^T \int_\Omega (|\mathbf{d}^*(t, \mathbf{x}) - I_h \mathbf{d}^*(t, \mathbf{x})|^4 + \frac{C}{\varepsilon^2} \int_0^T \int_\Omega |(\mathbf{d}^*(t, \mathbf{x}) - I_h \mathbf{d}^*(t, \mathbf{x})) \cdot \mathbf{d}^*(t, \mathbf{x})|^2 \\ &\leq C \frac{h}{\varepsilon^2} \int_0^T \|\mathbf{d}^*(t)\|_{H^1(\Omega)}^4 + C \frac{h^2}{\varepsilon^2} \int_0^T \|\mathbf{d}^*(t)\|_{H^1(\Omega)}^2. \end{aligned}$$

Therefore, thanks to (S) we will obtain convergence to zero if we prove that $\int_0^T \|\mathbf{d}^*(t)\|_{H^1(\Omega)}^4 < \infty$, which is deduced from $\mathbf{z} \in L^2(0, T; \mathbf{L}^2(\Omega))$ and from the definition of \mathbf{d}^* . Indeed, from (45) and (46) and using that $|\mathbf{d}^*| = 1$, we have $\|\mathbf{d}^*(t)\|_{H^1(\Omega)}^2 \leq C(|\mathbf{z}(t)| + 1)$; hence

$$\int_0^T \|\mathbf{d}^*(t)\|_{H^1}^4 \leq C \left(\int_0^T |\mathbf{z}(t)|^2 + 1 \right) < \infty.$$

The convergence $\int_0^T \left(\mathbf{z}_{h,k,\varepsilon}(t), I_h \mathbf{d}^*(t) \right) \rightarrow \int_0^T \left(\mathbf{z}(t), \mathbf{d}^*(t) \right)$ is deduced by using that $\mathbf{z}_{h,k,\varepsilon} \rightarrow \mathbf{z}$ in $L^2(0, T; \mathbf{L}^2(\Omega))$ -weakly and $I_h \mathbf{d}^* \rightarrow \mathbf{d}^*$ in $L^2(0, T; \mathbf{L}^2(\Omega))$ -strongly.

From (46), the previous convergences and the lower continuity of the $L^2(\Omega)$ -norm, we get

$$\begin{aligned} \int_0^T J(\mathbf{d}(t)) &\leq \liminf_{(h,k,\varepsilon) \rightarrow 0} \int_0^T \int_{\Omega} \frac{1}{2} |\nabla \mathbf{d}_{h,k,\varepsilon}(t)|^2 - \mathbf{z}_{h,k,\varepsilon}(t) \cdot \mathbf{d}_{h,k,\varepsilon}(t) \\ &\leq \liminf_{(h,k,\varepsilon) \rightarrow 0} \int_0^T J_{h,k,\varepsilon}(I_h \mathbf{d}^*(t)) = \int_0^T J(\mathbf{d}^*(t)). \end{aligned}$$

The opposite inequality is easily shown since $|\mathbf{d}(t, \mathbf{x})| = 1$ and \mathbf{d}^* is the solution of (45). Then,

$$\int_0^T J(\mathbf{d}(t)) = \int_0^T J(\mathbf{d}^*(t)),$$

whence

$$\lim_{(h,k,\varepsilon) \rightarrow 0} \int_0^T \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{d}_{h,k,\varepsilon}(t)|^2 - \mathbf{z}_{h,k,\varepsilon}(t) \cdot \mathbf{d}_{h,k,\varepsilon}(t) \right) = \int_0^T \int_{\Omega} \left(\frac{1}{2} |\nabla \mathbf{d}(t)| - \mathbf{z}(t) \cdot \mathbf{d}(t) \right).$$

In particular,

$$\lim_{(h,k,\varepsilon) \rightarrow 0} \int_0^T \int_{\Omega} |\nabla \mathbf{d}_{h,k,\varepsilon}(t)|^2 = \int_0^T \int_{\Omega} |\nabla \mathbf{d}(t)|^2,$$

arriving at

$$\mathbf{d}_{k,h,\varepsilon} \rightarrow \mathbf{d} \quad \text{in } L^2(0, T; \mathbf{H}^1(\Omega)) \text{ - strong.}$$

6 Convergence for the discrete momentum system

Since we do not have any estimate for the discrete pressure p_h^{n+1} , we must choose a discrete test function which eliminates the the discrete pressure term.

Lemma 11 *Let $\mathbf{v} \in \mathbf{C}_c^\infty(\Omega)$. Then there exists $\bar{\mathbf{u}}_h \in \mathbf{X}_h$ such that:*

$$\mathbf{v}_h \rightarrow \mathbf{v} \quad \text{in } \mathbf{W}_0^{1,\infty}(\Omega) \quad \text{and} \quad \left(\nabla \cdot \mathbf{v}_h, q_h \right) = \left(\nabla \cdot \bar{\mathbf{u}}, q_h \right), \quad \forall q_h \in Q_h.$$

A proof of this lemma can be seen in [8], but for a convergence in the $\mathbf{H}^1(\Omega)$ -norm. Some minor changes can be introduced in order to get the convergence in the $\mathbf{W}^{1,\infty}(\Omega)$ -norm, using inverse inequality $\|\nabla \bar{\mathbf{u}}_h\|_{L^\infty(\Omega)} \leq C h^{-3/2} |\nabla \bar{\mathbf{u}}_h| \quad \forall \bar{\mathbf{u}}_h \in \mathbf{X}_h$, and the approximation properties $\|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{\mathbf{W}^{1,\infty}(\Omega)} \leq C h^{1/2} \|\bar{\mathbf{u}}\|_{\mathbf{H}^3(\Omega)}$ and $\|\bar{\mathbf{u}} - J_h \bar{\mathbf{u}}\|_{\mathbf{H}^1(\Omega)} \leq C h^2 \|\bar{\mathbf{u}}\|_{\mathbf{H}^3(\Omega)} \quad \forall \bar{\mathbf{u}} \in \mathbf{H}^3(\Omega)$.

We consider $\mathbf{v} \in C^1([0, T]; \mathbf{C}_c^\infty(\Omega))$ with $\nabla \cdot \mathbf{v} = 0$ and $\mathbf{v}(T) = 0$. Let \mathbf{v}_h^n be the projection of $\mathbf{v}(t^n)$ furnished by Lemma 11. We define $\mathbf{v}_{h,k} \in L^\infty(0, T; \mathbf{V}_h)$ as the piecewise constant functions taking values \mathbf{v}_h^{n+1} on $(t_n, t_{n+1}]$ and $\tilde{\mathbf{v}}_{h,k} \in C^0([0, T]; \mathbf{V}_h)$ as the piecewise linear, globally continuous functions such that $\tilde{\mathbf{v}}_{h,k}(t_n) = \mathbf{v}_h^n$. It is known that as $(h, k) \rightarrow 0$,

$$\mathbf{v}_{h,k} \rightarrow \mathbf{v} \quad \text{in } L^\infty(0, T; \mathbf{W}_0^{1,\infty}(\Omega)),$$

$$\tilde{\mathbf{v}}_{h,k} \rightarrow \mathbf{v} \quad \text{in } W^{1,\infty}(0, T; W_0^{1,\infty}(\Omega)),$$

Taking $\bar{\mathbf{u}}_h = \mathbf{v}_h^{n+1}$ as a test function in (9), multiplying by k , summing over n , and using the expression (discrete integration by parts in time)

$$\sum_{n=0}^{N-1} \left(\mathbf{u}_h^{n+1} - \mathbf{u}_h^n, \mathbf{v}_h^{n+1} \right) = \left(\mathbf{u}_h^N, \mathbf{v}_h^N \right) - \sum_{n=0}^{N-1} \left(\mathbf{u}_h^n, \mathbf{v}_h^{n+1} - \mathbf{v}_h^n \right) - \left(\mathbf{u}_h^0, \mathbf{v}_h^0 \right)$$

and the fact that $\mathbf{v}_h^N = 0$ (since $\mathbf{v}(T) = 0$), the following formulation holds:

$$\left\{ \begin{array}{l} -k \sum_{n=0}^{N-1} \left(\mathbf{u}_h^n, \frac{\mathbf{v}_h^{n+1} - \mathbf{v}_h^n}{k} \right) - \left(\mathbf{u}_h^0, \mathbf{v}_h^0 \right) + \nu k \sum_{n=0}^{N-1} \left(\nabla \mathbf{u}_h^{n+1}, \nabla \mathbf{v}_h^{n+1} \right) \\ +k \sum_{n=0}^{N-1} \left\{ c \left(\mathbf{u}_h^n, \mathbf{u}_h^{n+1}, \mathbf{v}_h^{n+1} \right) - \lambda \left((\nabla \mathbf{d}_h^n)^t \mathbf{w}_h^{n+1}, \mathbf{v}_h^{n+1} \right) + \lambda \left(\nabla \cdot \mathbf{v}_h^{n+1}, F_\varepsilon(\mathbf{d}_h^n) \right) \right\} \end{array} \right\} = 0.$$

Next, taking into account Definition 6, the previous equality reads

$$\left\{ \begin{array}{l} -\int_0^T \left(\mathbf{u}_{h,k,\varepsilon}^0, \frac{\partial}{\partial t} \tilde{\mathbf{v}}_{h,k} \right) - \left(\mathbf{u}_h^0, \mathbf{v}_h^0 \right) + \nu \int_0^T \left(\nabla \mathbf{u}_{h,k,\varepsilon}^0, \nabla \mathbf{v}_{h,k} \right) \\ + \int_0^T \left\{ c \left(\mathbf{u}_{h,k,\varepsilon}^0, \mathbf{u}_{h,k,\varepsilon}, \mathbf{v}_{h,k} \right) - \lambda \left((\nabla \mathbf{d}_{h,k,\varepsilon})^t \mathbf{w}_{h,k,\varepsilon}, \mathbf{v}_{h,k} \right) + \lambda \left(\nabla \cdot \mathbf{v}_{h,k}, F_\varepsilon(\mathbf{d}_{h,k,\varepsilon}) \right) \right\} \end{array} \right\} = 0.$$

At this point, we will only pass to the limit in the last two terms (denoted by Q_1 and Q_2 , respectively) because the rest of the terms are quite standard in the framework of the Navier-Stokes equations.

Using the discrete integration by parts (32) and replacing $\bar{\mathbf{u}}_h$ by \mathbf{v}_h^{n+1} , the term Q_1 is rewritten as

$$Q_1 = -\lambda \int_0^T \left(\nabla \mathbf{d}_{h,k,\varepsilon} \odot \nabla \mathbf{d}_{h,k,\varepsilon}, \nabla \mathbf{v}_{h,k} \right) + k \sum_{n=0}^{N-1} \sum_{i=2}^{10} I_i^{n+1} := Q_1^a + Q_1^b.$$

Clearly, we have the convergence

$$Q_1^a = -\lambda \int_0^T \left(\nabla \mathbf{d}_{h,k,\varepsilon} \odot \nabla \mathbf{d}_{h,k,\varepsilon}, \nabla \mathbf{v}_{h,k} \right) \rightarrow -\int_0^T \left(\nabla \mathbf{d} \odot \nabla \mathbf{d}, \nabla \mathbf{v} \right), \quad \text{as } (h, k, \varepsilon) \rightarrow 0,$$

due to the fact that $\nabla \mathbf{d}_{h,k,\varepsilon} \rightarrow \nabla \mathbf{d}$ in $L^2(0, T; \mathbf{L}^2(\Omega))$ and $\nabla \mathbf{v}_{h,k} \rightarrow \nabla \mathbf{v}$ in $L^\infty(0, T; W_0^{1,\infty}(\Omega))$ strongly as $(h, k, \varepsilon) \rightarrow 0$.

In view of the proof of Lemma 8, the term Q_1^b is bounded as $Q_1^b \leq C \left(\frac{h}{\varepsilon^4} + \frac{k^{1/2}}{\varepsilon^2} \right)$ which goes to zero thanks to hypothesis (S).

Finally, we have that $Q_2 = \int_0^T \lambda \left(\nabla \cdot \mathbf{v}_{h,k}, F_\varepsilon(\mathbf{d}_{h,k,\varepsilon}) \right) \rightarrow 0$ as $(h, k, \varepsilon) \rightarrow 0$, thanks to the fact that $F_\varepsilon(\mathbf{d}_{h,k,\varepsilon})$ is bounded in $L^\infty(0, T; \mathbf{L}^1(\Omega))$ and $\|\nabla \cdot \mathbf{v}_{h,k}\|_{L^\infty(\Omega)} \rightarrow 0$ as $(h, k) \rightarrow 0$ (since $\nabla \cdot \mathbf{v} = 0$ and $\mathbf{v}_{h,k} \rightarrow \mathbf{v}$ in $L^\infty(0, T; W_0^{1,\infty}(\Omega))$ strongly as $(h, k) \rightarrow 0$).

7 The 2D case

To approximate 2D liquid crystal flows we may avoid to impose $(\mathbf{X}_h \cdot \nabla)\mathbf{D}_h \subset \mathbf{W}_h$ in hypothesis (H4). In fact, it will be seen that we may choose C^0 finite elements for the discrete Laplacian of the orientation vector. Moreover, we will specify some new hypotheses (S1') and (H2') to be used instead of (S1) and (H2). In particular, hypothesis (S1') will be better in the sense it will require a weaker relation between the parameters h , k , and ε .

Next, we will describe the new hypotheses (S1') and (H2') which will be completed with the original hypotheses (S2), (H1), and (H3), and from (H4) only $\mathbf{D}_h \subset \mathbf{W}_h$ is imposed.

(S1') Stability conditions:

$$\lim_{(h,k,\varepsilon)=0} \frac{k}{h^{2/3+2\alpha\varepsilon^6}} = 0,$$

for a fixed $\alpha > 0$ defined below.

(H2') The triangulation of Ω and the discrete spaces verify:

- the inverse inequalities:

$$\begin{aligned} \|\nabla \bar{\mathbf{u}}_h\|_{L^\infty(\Omega)} &\leq C h^{-1} |\nabla \bar{\mathbf{u}}_h| \quad \forall \bar{\mathbf{u}}_h \in \mathbf{X}_h, \\ \|\bar{\mathbf{d}}_h\|_{W^{1,3}(\Omega)} &\leq C h^{-1/3} \|\bar{\mathbf{d}}_h\|_{H^1(\Omega)} \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_h, \\ \|\bar{\mathbf{d}}_h\|_{L^\infty(\Omega)} &\leq C h^{-\alpha} \|\bar{\mathbf{d}}_h\|_{H^1(\Omega)} \quad \forall \bar{\mathbf{d}}_h \in \mathbf{D}_h, \end{aligned}$$

with $\alpha > 0$.

- the approximation properties:

$$\|\mathbf{u} - J_h \mathbf{u}\| + h \|\mathbf{u} - J_h \mathbf{u}\|_{H^1(\Omega)} \leq C h^3 \|\mathbf{u}\|_{H^3(\Omega)} \quad \forall \mathbf{u} \in \mathbf{H}^3(\Omega) \cap \mathbf{H}_0^1(\Omega),$$

$$\|\mathbf{u} - J_h \mathbf{u}\|_{W^{1,\infty}(\Omega)} \leq C h \|\mathbf{u}\|_{H^3(\Omega)} \quad \forall \mathbf{u} \in \mathbf{H}^3(\Omega),$$

$$|p - K_h p| \leq C h \|p\|_{H^1(\Omega)} \quad \forall p \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\|\mathbf{d} - I_h \mathbf{d}\| + h \|\mathbf{d} - I_h \mathbf{d}\|_{H^1(\Omega)} \leq C h^2 \|\mathbf{d}\|_{H^2(\Omega)} \quad \forall \mathbf{d} \in \mathbf{H}^2(\Omega),$$

$$\|I_h \mathbf{d} - \mathbf{d}\|_{L^4(\Omega)} \leq C h^{1/2} \|\mathbf{d}\|_{H^1(\Omega)} \quad \forall \mathbf{d} \in \mathbf{H}^1(\Omega),$$

$$|P_h \mathbf{w} - \mathbf{w}| \leq C h^\beta \|\mathbf{w}\|_{W^{1,p}(\Omega)} \quad \forall \mathbf{w} \in \mathbf{H}^1(\Omega),$$

for $p < 2$ and $1/3 < \beta < 1$, where J_h , K_h and I_h are interpolation operators in \mathbf{X}_h , Q_h , and \mathbf{D}_h , respectively, and P_h is the $L^2(\Omega)$ -projection onto \mathbf{W}_h .

- the stability property

$$\|P_h \mathbf{w}\|_{L^q(\Omega)} \leq C \|\mathbf{w}\|_{L^q(\Omega)} \quad \forall \mathbf{w} \in \mathbf{L}^q(\Omega),$$

for some $q > 2$ where P_h is the $L^2(\Omega)$ -projection onto \mathbf{W}_h .

(H4') Compatibility condition between $(\mathbf{W}_h, \mathbf{D}_h)$:

$$\mathbf{D}_h \subset \mathbf{W}_h.$$

Remark 12 Hypothesis (H4') is valid for \mathbf{W}_h defined by finite elements of degree 1 in each triangle of \mathcal{T}_h . Moreover, in the 2D domains we have better inverse inequalities than for 3D domains. This is the reason why we can modified hypothesis (S1) by (S1').

Throughout this section we only focus on those steps to be worthy of remark with respect to the previous analysis for three-dimensional domains. First, we note the appearance of the extra term $C \frac{h^{2(\beta-1/3)}}{\varepsilon^4} k$ on the right hand side of inequality (14) in Lemma 4 which converges to zero under condition (S1').

Lemma 13 Suppose that, there exists a constant $C_d > 0$ independent of h , k and ε such that

$$|\mathbf{u}_h^n|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 \leq C_d.$$

Then, there exist $h_0 > 0$, $k_0 > 0$ and $\varepsilon_0 > 0$ such that for all $h \leq h_0$, $k \leq k_0$ and $\varepsilon \leq \varepsilon_0$ satisfying hypothesis (S1'), the corresponding solution $(\mathbf{u}_h^{n+1}, \mathbf{d}_h^{n+1}, \mathbf{w}_h^{n+1})$ of the discrete problem (9)-(12) verifies the following inequality:

$$\left\{ \begin{array}{l} \left(|\mathbf{u}_h^{n+1}|^2 - |\mathbf{u}_h^n|^2 + |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 \right) + \nu k |\nabla \mathbf{u}_h^{n+1}|^2 \\ + \lambda \left(|\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 - |\nabla \widehat{\mathbf{d}}_h^n|^2 + |\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 \right) + \lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \\ + 2\lambda \int_{\Omega} (F_\varepsilon(\mathbf{d}_h^{n+1}) - F_\varepsilon(\mathbf{d}_h^n)) + \frac{\lambda}{\varepsilon^2} \int_{\Omega} \left(\frac{1}{4} (|\mathbf{d}_h^{n+1}|^2 - |\mathbf{d}_h^n|^2)^2 + |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n|^2 \right) \end{array} \right\} \leq C \frac{h^{2(\beta-1/3)}}{\varepsilon^4} k, \quad (48)$$

where P_h is the $L^2(\Omega)$ -projection onto \mathbf{W}_h .

Proof: Let us only indicate how the proof of Lemma 4 changes. There are two bounds which have an important modification. To begin with, identity (16) takes the form

$$\begin{aligned} & \lambda \left(|\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 - |\nabla \widehat{\mathbf{d}}_h^n|^2 + |\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 \right) + 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) \\ & + 2\lambda k \left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{w}_h^{n+1} + \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) + 2\lambda \gamma k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \\ & = 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) \right) + 2\lambda k \left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) \right), \end{aligned}$$

owing to the fact that the convective term $(\mathbf{u}^{n+1} \cdot \nabla) \mathbf{d}_h^n$ and $\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n$ do not belong to \mathbf{W}_h , in general, because now we do not consider hypothesis (H4). Bounding the right-hand side using the new hypothesis (H2')

$$\begin{aligned}
2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) \right) &\leq |\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n| |\mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))| \\
&\leq C |\mathbf{d}_h^{n+1} - \mathbf{d}_h^n| \frac{h^\beta}{\varepsilon^2} \|(|\mathbf{d}_h^n|^2 - 1) \mathbf{d}_h^n\|_{W^{1,p}(\Omega)} \\
&\leq C |\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n| \frac{h^\beta}{\varepsilon^2} \left(\|\mathbf{d}_h^n\|_{H^1(\Omega)}^3 + \|\mathbf{d}_h^n\|_{H^1(\Omega)} \right) \\
&\leq \frac{\nu}{3} k \|\mathbf{u}_h^{n+1}\|^2 + \frac{\gamma \lambda}{2} k |P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) + \mathbf{w}_h^{n+1}|^2 \\
&\quad + C \frac{h^{2(\beta-1/3)}}{\varepsilon^4} k,
\end{aligned}$$

where $p < 2$ and we have carried out the last bound using estimate (19) and the hypothesis $\|\mathbf{d}_h^n\|_{H^1(\Omega)} \leq C$. Analogously, we bound the next term as follows

$$\begin{aligned}
2\lambda k \left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) \right) &\leq k \|\mathbf{u}_h^{n+1}\|_{L^6(\Omega)} \|\nabla \mathbf{d}_h^n\|_{L^3(\Omega)} |\mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))| \\
&\leq C k \|\mathbf{u}_h^{n+1}\| h^{-1/3} |\nabla \mathbf{d}_h^n| \frac{h^\beta}{\varepsilon^2} \|(|\mathbf{d}_h^n|^2 - 1) \mathbf{d}_h^n\|_{W^{1,p}(\Omega)} \\
&\leq C k \frac{h^{\beta-1/3}}{\varepsilon^2} \|\mathbf{u}_h^{n+1}\| |\nabla \mathbf{d}_h^n| \left(\|\mathbf{d}_h^n\|_{H^1(\Omega)}^3 + \|\mathbf{d}_h^n\|_{H^1(\Omega)} \right) \\
&\leq \frac{\nu}{2} k \|\mathbf{u}_h^{n+1}\|^2 + C \frac{h^{2(\beta-1/3)}}{\varepsilon^4} k.
\end{aligned}$$

Next, identity (22) is replaced by

$$\begin{aligned}
&\left(|\mathbf{u}_h^{n+1}|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 \right) + \left(|\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + \lambda |\nabla (\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n)|^2 \right) \\
&+ 2k \left(\nu |\nabla \mathbf{u}_h^{n+1}|^2 + \gamma \lambda |\mathbf{w}_h^{n+1} + P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n))|^2 \right) \\
&\leq \left(|\mathbf{u}_h^n|^2 + \lambda |\nabla \widehat{\mathbf{d}}_h^n|^2 \right) - 2\lambda \left(\widehat{\mathbf{d}}_h^{n+1} - \widehat{\mathbf{d}}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) \right) \\
&+ 2\lambda k \left(\mathbf{u}_h^{n+1} \cdot \nabla \mathbf{d}_h^n, \mathbf{f}_\varepsilon(\mathbf{d}_h^n) - P_h(\mathbf{f}_\varepsilon(\mathbf{d}_h^n)) \right),
\end{aligned}$$

from which we extract by using the foregoing bound for the last term on the right hand side and (23) that

$$|\nabla \widehat{\mathbf{d}}_h^{n+1}|^2 \leq C \left(|\nabla \widehat{\mathbf{d}}_h^n|^2 + |\mathbf{u}_h^n|^2 + \frac{1}{\varepsilon^4} \left(\|\mathbf{d}_h^n\|_{H^1(\Omega)}^6 + \|\mathbf{d}_h^n\|_{H^1(\Omega)}^2 \right) + C \frac{h^{2(\beta-1/3)}}{\varepsilon^4} k \right).$$

Consequently, again (24) holds.

The rest of analysis does not change. \square

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Capítulo 6

Unconditional stability and convergence for non-isothermal phase-field model

Unconditional stability and convergence for non-isothermal phase field model

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Abstract

We propose and analyze two C^0 finite element schemes with \mathbb{P}_1 -approximation for solving a phase field model of a binary alloy with thermal properties. The first scheme is nonlinear, unconditionally stable and convergent. The other scheme is linear but conditionally stable and convergent. A maximum principle for the discrete concentration is avoided using a truncation operator in both schemes.

1 Introduction

1.1 Model

The phase field method provides a mathematical description for free-boundary problems associated to physical processes with phase transitions. It postulates the existence of a function, called the phase field, whose value identifies the phase at a particular point in space and time. The method is particularly suitable for cases with complex growth structures occurring during phase transitions. The mathematical model studied in this work describes the solidification process occurring in a binary alloy with temperature-dependent properties. It is based on a highly nonlinear parabolic system of partial differential equations with three dependent variables: phase-field, solute concentration and temperature. Moreover, the temperature equation has nonlinear degenerate diffusion.

Let $\Omega \subseteq \mathbb{R}^d$ ($d = 2$ or 3) be a bounded domain with boundary Γ . Denote by $[0, T]$ the time interval ($T > 0$). We use the notation $Q = \Omega \times (0, T)$, $\Sigma = \Gamma \times (0, T)$ and $\mathbf{n}(\mathbf{x})$ is the outwards unit normal vector to Ω at the point $\mathbf{x} \in \Gamma$. We consider the following differential problem,

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related to a phase field model of a binary alloy with thermal properties ([1]):

$$\begin{cases} \alpha\varepsilon^2\phi_t - \varepsilon^2\Delta\phi = \frac{1}{2}(\phi - \phi^3) + \beta(\theta - \theta_Ac - \theta_B(1 - c)) & \text{in } Q, \\ C_V\theta_t + \frac{l}{2}\phi_t = \nabla \cdot [K_1(\phi)\nabla\theta] & \text{in } Q, \\ c_t = K_2(\Delta c + M\nabla \cdot [c(1 - c)\nabla\phi]) & \text{in } Q, \end{cases} \quad (1)$$

This model is completed with the Neumann boundary conditions

$$\frac{\partial\phi}{\partial\mathbf{n}}\Big|_{\Sigma} = 0, \quad (K_1(\phi)\nabla\theta) \cdot \mathbf{n}\Big|_{\Sigma} = 0, \quad \frac{\partial c}{\partial\mathbf{n}}\Big|_{\Sigma} = 0 \quad (2)$$

and the initial conditions

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \quad \theta(\mathbf{x}, 0) = \theta_0(\mathbf{x}), \quad c(\mathbf{x}, 0) = c_0(\mathbf{x}) \quad \mathbf{x} \in \Omega. \quad (3)$$

The unknowns for this problem are: $\phi : Q \rightarrow \mathbb{R}$ (phase-field) is the state variable characterizing the different phases so that $\phi = 1$ represents the liquid phase and $\phi = -1$ represents the solid phase, $\theta : Q \rightarrow \mathbb{R}$ is the temperature of the material, $c : Q \rightarrow [0, 1]$ (concentration) represents the fraction of one of the two materials in the mixture. The parameter $\alpha > 0$ is the relaxation scaling; the parameter β is given by $\beta = \varepsilon[s]/3\sigma$, where $\varepsilon > 0$ is the measure of the interface thickness, σ the surface tension and $[s]$ the entropy density difference between phases; θ_A, θ_B are the melting temperatures of each of the two materials in the alloy; $C_V > 0$ is the specific heat; $l > 0$ the latent heat; $K_1 \geq 0$ the thermal conductivity; $K_2 > 0$ is the solute diffusivity; $M \in \mathbb{R}$ is a constant related to the slopes of solid and liquid lines.

We will assume $K_1 = K_1(\phi)$ to be a globally Lipschitz continuous function satisfying that $0 \leq K_1(r) \leq b$ for all $r \in \mathbb{R}$, with $b > 0$. In this sense, the problem is singular with respect to the temperature when $K_1(\phi) = 0$.

The phase field model for solidification (1) is used to treat phenomena such as crystal growth and the fusion of materials.

Definition 1 A triplet (ϕ, θ, c) is called a weak solution of (1), (2)-(3) in $(0, T)$ if:

1. $\phi \in L^2(0, T; H^2(\Omega)) \cap L^\infty(0, T, H^1(\Omega))$, $\phi_t \in L^2(Q)$, $\phi(0) = \phi_0$, $\frac{\partial\phi}{\partial\mathbf{n}} = 0$ a.e. on Σ ,
2. $\theta \in L^\infty(0, T; L^2(\Omega))$, $\theta_t \in L^2(0, T, H^1(\Omega)')$, $\theta(0) = \theta_0$,
3. $c \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$, $c_t \in L^2(0, T; H^1(\Omega)')$, $c(0) = c_0$, $0 \leq c \leq 1$ a.e. in Q ,
4. $J := \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi) \in L^2(Q)$,

and verifying

$$\alpha\varepsilon^2\phi_t - \varepsilon^2\Delta\phi = \frac{1}{2}(\phi - \phi^3) + \beta(\theta - \theta_Ac - \theta_B(1 - c)) \quad \text{a.e. in } Q,$$

$$C_V \int_0^T \langle \theta_t, \eta \rangle dt + \frac{l}{2} \int_0^T (\phi_t, \eta) dt + \int_0^T (J, \nabla \eta) = 0,$$

$$\int_0^T \langle c_t, \eta \rangle dt + K_2 \int_0^T (\nabla c, \nabla \eta) dt + K_2 M \int_0^T (c(1-c) \nabla \phi, \nabla \eta) = 0,$$

for each $\eta \in L^2(0, T; H^1(\Omega))$. If, in addition, $K_1 \geq b_0 > 0$, then $\theta \in L^2(0, T; H^1(\Omega))$ and $J = K_1(\phi) \nabla \theta$.

Here and in the sequel, $\langle \cdot, \cdot \rangle$ denotes the duality $H^1(\Omega)', H^1(\Omega)$ and (\cdot, \cdot) the inner product in $L^2(\Omega)$.

1.2 Known results

In [1], existence of weak solutions for problem (1), (2)-(3) is obtained via the introduction of a regularized problem approximating the thermal conductivity K_1 by a strictly positive, regular function followed by the derivation of suitable a priori estimates and the application of compactness arguments. More concretely, the following existence result was established in [1].

Theorem 2 *Let Ω be an open bounded domain of \mathbb{R}^d , $d = 2$ or 3 , with smooth boundary Γ . Assume $\phi_0 \in H^{1+\gamma}(\Omega)$ with $1/2 < \gamma \leq 1$ such that $\frac{\partial \phi_0}{\partial \mathbf{n}} = 0$ on Γ , $\theta_0 \in L^2(\Omega)$ and $c_0 \in H^1(\Omega)$ such that $0 \leq c_0 \leq 1$ a.e. in $\bar{\Omega}$. Then, there exists (ϕ, θ, c) a weak solution of (1)-(3) (with $K_1 > 0$ a constant) in $(0, T)$.*

In [7], optimal order error estimates are given for a fully discrete numerical scheme of a more simplified phase field model than (1) without the concentration, paying special attention on the dependency of the parameter ε . In particular, it is shown that all error bounds depend only on a lower polynomial order for $\frac{1}{\varepsilon}$ as ε is small. Moreover, error estimates are used to establish convergence of the fully discrete scheme to solutions of the sharp interface limits under different scaling in its coefficients.

In [2] a semi-discretization in time scheme is proposed considering a problem with only the temperature and the phase field variables and replacing in the equation for the temperature the term $\frac{l}{2} \phi_t$ by a more general term $\frac{l}{2} f(\theta, \phi)_t$, where f is a generic function satisfying some adequate properties. Convergence of the semi-discrete in time solutions is proved, obtaining existence and regularity results of the limit problem.

1.3 Main results of the paper

In this work we consider two numerical schemes in order to approximate problem (1) using continuous \mathbb{P}_1 -finite elements. Since a maximum principle cannot be satisfied by the discrete concentration, we introduce a discrete truncation operator ([4]) in order to guarantee a L^∞ bound for some terms in the discrete concentration equation.

First of all, we will present in Section 2 the nonlinear numerical scheme (4)-(6) which will be unconditionally stable and convergent

Theorem 3 (Unconditionally stable, convergent nonlinear scheme) *Assume $\phi_0 \in H^1(\Omega)$, $\theta_0 \in L^2(\Omega)$ and $c_0 \in H^1(\Omega)$ such that $0 \leq c_0 \leq 1$ a.e. in $\bar{\Omega}$. Let \mathcal{T}_h , $0 < h < 1$, be a regular, quasi-uniform family of triangulations of a polyhedral domain Ω . Then, there exists a convergent subsequence of functions $\phi_{h,k}, \hat{\phi}_{h,k}, \tilde{\phi}_{h,k}, \theta_{h,k}, \hat{\theta}_{h,k}, \tilde{\theta}_{h,k}, c_{h,k}, \hat{c}_{h,k}$ and $\tilde{c}_{h,k}$ associated to scheme (4)-(6) (see Definition 7) towards a weak solution (ϕ, θ, c) of problem (1), (2)-(3) in $(0, T)$, as $(h, k) \rightarrow 0$ in the following sense:*

$$\begin{aligned} \theta_{h,k} &\rightarrow \theta, \quad \hat{\theta}_{h,k} \rightarrow \theta, \quad \tilde{\theta}_{h,k} \rightarrow \theta \quad \text{in } L^\infty(0, T; L^2(\Omega))\text{-weak*}, \\ c_{h,k} &\rightarrow c, \quad \hat{c}_{h,k} \rightarrow c, \quad \tilde{c}_{h,k} \rightarrow c \quad \text{in } \begin{cases} L^2(0, T; H^1(\Omega))\text{-weak}, \\ L^\infty(0, T; L^2(\Omega))\text{-weak*}, \end{cases} \\ \phi_{h,k} &\rightarrow \phi, \quad \hat{\phi}_{h,k} \rightarrow \phi, \quad \tilde{\phi}_{h,k} \rightarrow \phi \quad \text{in } L^\infty(0, T; H^1(\Omega))\text{-weak*}, \\ \frac{d}{dt} \tilde{\phi}_{h,k} &\rightarrow \frac{d}{dt} \phi \quad \text{in } L^2(0, T; L^2(\Omega))\text{-weak}, \\ \frac{d}{dt} \tilde{\theta}_{h,k} &\rightarrow \frac{d}{dt} \theta, \quad \frac{d}{dt} \tilde{c}_{h,k} \rightarrow \frac{d}{dt} c \quad \text{in } L^2(0, T; H^1(\Omega)')\text{-weak}. \end{aligned}$$

Second, we construct the linear numerical scheme (23)-(25) which will be conditionally stable, using the original ideas in [5].

Theorem 4 (Conditionally stable, convergent linear scheme) *Assume the constraint*

$$(S) \quad \lim_{(h,k) \rightarrow 0} \frac{k}{h} = 0.$$

Under the assumptions of Theorem 3. Then, there exists a convergent subsequence of functions $\phi_{h,k}, \hat{\phi}_{h,k}, \tilde{\phi}_{h,k}, \theta_{h,k}, \hat{\theta}_{h,k}, \tilde{\theta}_{h,k}, c_{h,k}, \hat{c}_{h,k}$ and $\tilde{c}_{h,k}$ associated to scheme (23)-(25) (see Definition 7) towards a weak solution (ϕ, θ, c) of problem (1), (2)-(3) in $(0, T)$, as $(h, k) \rightarrow 0$ in the same sense of Theorem 3.

The rest of the paper is described as follows. In Section 2 a nonlinear scheme is presented, obtaining its unconditional stability in Section 3. In Section 4 some necessary compactness results are proved, passing to the limit in Section 5 and concluding the proof of Theorem 3. Finally, a conditional stable and convergent linear scheme is studied in Section 6 given an outline of the proof of Theorem 4.

2 A nonlinear Scheme

In what follows, let us consider a uniform partition $t_n = nk$ of the time interval $[0, T]$ with $k = T/N$ the time step and let $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) be a domain with polyhedral boundary such that there is a family of triangulations \mathcal{T}_h with $\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K$. Here $h := \max_{K \in \mathcal{T}_h} h_K$ with h_K the diameter of K . Let X_h be the finite element subspace of $H^1(\Omega)$ furnished by globally continuous, piecewise linear functions, that is,

$$X_h = \{x_h \in C^0(\bar{\Omega}) : x_h|_K \in \mathbb{P}_1(K), \forall K \in \mathcal{T}_h, \}.$$

To approximate numerically problem (1), (2)-(3), we propose the following scheme:

Initialization: Let $(\phi_h^0, \theta_h^0, c_h^0) \in X_h \times X_h \times X_h$ be suitable approximations of (ϕ_0, θ_0, c_0) as $h \rightarrow 0$.

Step $n + 1$: Given $(\phi_h^n, \theta_h^n, c_h^n) \in X_h \times X_h \times X_h$.

Find $\phi_h^{n+1} \in X_h$ as solution of the problem:

$$\begin{cases} \alpha \varepsilon^2 \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) + \varepsilon^2 (\nabla \phi_h^{n+1}, \nabla x_h) + \frac{1}{2} ((\phi_h^{n+1})^3, x_h) \\ = \frac{1}{2} (\phi_h^n, x_h) + \beta (\theta_h^n - \theta_A c_h^n - \theta_B (1 - c_h^n), x_h), \quad \forall x_h \in X_h. \end{cases} \quad (4)$$

Find $\theta_h^{n+1} \in X_h$ and $c_h^{n+1} \in X_h$ as solution of the decoupled variational problems:

$$C_V \left(\frac{\theta_h^{n+1} - \theta_h^n}{k}, x_h \right) + (K_1^k (\phi_h^{n+1}) \nabla \theta_h^{n+1}, \nabla x_h) = -\frac{l}{2} \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right), \quad \forall x_h \in X_h, \quad (5)$$

$$\left(\frac{c_h^{n+1} - c_h^n}{k}, x_h \right) + K_2 (\nabla c_h^{n+1}, \nabla x_h) = -K_2 M \left([c_h^n]_T (1 - [c_h^n]_T) \nabla \phi_h^n, \nabla x_h \right), \quad \forall x_h \in X_h. \quad (6)$$

Here, $K_1^k = K_1 + k$ and $[\cdot]_T$ is a truncation operator defined as follows: given $x_h \in X_h$, then $[x_h]_T \in X_h$ such that:

$$[x_h]_T(\mathbf{x}_i) = \begin{cases} x_h(\mathbf{x}_i) & \text{if } x_h(\mathbf{x}_i) \in [0, 1], \\ 0 & \text{if } x_h(\mathbf{x}_i) < 0, \\ 1 & \text{if } x_h(\mathbf{x}_i) > 1, \end{cases}$$

where \mathbf{x}_i are the nodes of the mesh \mathcal{T}_h . Notice that, since X_h is defined by \mathbb{P}_1 finite elements, one has that $0 \leq [x_h]_T(\mathbf{x}) \leq 1$ for each $\mathbf{x} \in \bar{\Omega}$.

Since (5) and (6) are quadratic linear systems, it is easy to check the existence and uniqueness of solutions. On the other hand (4) is a discrete nonlinear variational problem and its existence and uniqueness can be proved as follows: we define

$$J(\phi_h) = \frac{\alpha \varepsilon^2}{2k} \int_{\Omega} |\phi_h|^2 + \frac{\varepsilon^2}{2} \int_{\Omega} |\nabla \phi_h|^2 + \frac{1}{8} \int_{\Omega} |\phi_h|^4 - \int_{\Omega} g \phi_h,$$

where $g = \frac{\alpha\varepsilon^2}{k}\phi_h^n + \frac{1}{2}\phi_h^n + \beta\left(\theta_h^n - \theta_A c_h^n - \theta_B(1 - c_h^n)\right)$. Clearly, J is a strictly convex functional on X_h , then the minimum problem $\min_{\phi_h \in X_h} J(\phi_h)$ has a unique solution characterized by its *Euler* equation (4).

We will denote by C generic positive constants always independent of the discretization parameters h and k .

3 A priori estimates and weak convergences

Let us denote by $|\cdot|$ the $L^2(\Omega)$ -norm and by $\|\cdot\|_{H^1(\Omega)}$ the $H^1(\Omega)$ -norm. With such a notation we establish the following

Lemma 5 *Under the hypotheses of Theorem 2, the discrete solution of scheme (4)-(6) verifies the following estimates:*

$$\begin{aligned}
\text{i)} \max_{0 \leq n \leq N} \|\phi_h^n\|_{H^1(\Omega)} &\leq C, & \text{ii)} \sum_{n=0}^{N-1} \|\phi_h^{n+1} - \phi_h^n\|_{H^1(\Omega)}^2 &\leq C, & \text{iii)} k \sum_{n=0}^{N-1} \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 &\leq C, \\
\text{iv)} \max_{0 \leq n \leq N} |\theta_h^n| &\leq C, & \text{v)} \sum_{n=0}^{N-1} |\theta_h^{n+1} - \theta_h^n|^2 &\leq C, & \text{vi)} k \sum_{n=0}^{N-1} |\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}|^2 &\leq C, \\
\text{vii)} \max_{0 \leq n \leq N} |c_h^n| &\leq C, & \text{viii)} \sum_{n=0}^{N-1} |c_h^{n+1} - c_h^n|^2 &\leq C, & \text{ix)} k \sum_{n=0}^{N-1} |\nabla c_h^{n+1}|^2 &\leq C,
\end{aligned}$$

where $C > 0$ depends only on the data (ϕ_0, θ_0, c_0) but is independent of (h, k) .

Proof: We take $x_h = 2k\phi_h^{n+1}/\alpha\varepsilon^2$, $x_h = 2k\theta_h^{n+1}/C_V$ and $x_h = 2kc_h^n$ as test functions in (4), (5) and (6) respectively, use the identity $(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2$ and bound adequately the right hand-side, resulting

$$\begin{aligned}
&|\phi_h^{n+1}|^2 - |\phi_h^n|^2 + |\phi_h^{n+1} - \phi_h^n|^2 + \frac{2k}{\alpha} |\nabla \phi_h^{n+1}|^2 + \frac{k}{2\alpha\varepsilon^2} \|\phi_h^{n+1}\|_{L^4(\Omega)}^4 \\
&\leq Ck|\phi_h^n|^2 + Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck,
\end{aligned} \tag{7}$$

$$\begin{aligned}
&|\theta_h^{n+1}|^2 - |\theta_h^n|^2 + |\theta_h^{n+1} - \theta_h^n|^2 + \frac{2k}{C_V} |\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}|^2 = -\frac{l}{C_V} k \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, \theta_h^{n+1} \right) \\
&\leq \frac{k}{2} |\theta_h^{n+1} - \theta_h^n|^2 + \frac{k}{2} |\theta_h^n|^2 + \frac{2l^2}{C_V^2} k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2,
\end{aligned} \tag{8}$$

$$|c_h^{n+1}|^2 - |c_h^n|^2 + |c_h^{n+1} - c_h^n|^2 + kK_2 |\nabla c_h^{n+1}|^2 \leq Ck |\nabla \phi_h^n|^2, \tag{9}$$

In order to control the terms $k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2$ and $k |\nabla \phi_h^n|^2$ on the right hand-side of (8) and (9) respectively, we consider $x_h = k \frac{4l^2}{\alpha C_V^2 \varepsilon^2} \frac{\phi_h^{n+1} - \phi_h^n}{k}$ as a test function in (4) getting

$$\begin{aligned} & \frac{2l^2}{\alpha C_V^2} \left(|\nabla \phi_h^{n+1}|^2 - |\nabla \phi_h^n|^2 + |\nabla (\phi_h^{n+1} - \phi_h^n)|^2 \right) + \frac{4l^2}{2\alpha C_V^2 \varepsilon^2} \left((\phi_h^{n+1})^3, \phi_h^{n+1} - \phi_h^n \right) \\ & + \frac{4l^2}{C_V^2} k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 \leq C k |\phi_h^n|^2 + C k |\theta_h^n|^2 + C k. \end{aligned} \quad (10)$$

Now, using again the identity $(a - b, a) = \frac{1}{2} (|a|^2 - |b|^2 + |a - b|^2)$, we can rewrite

$$\begin{aligned} \left((\phi_h^{n+1})^3, \phi_h^{n+1} - \phi_h^n \right) &= \frac{1}{2} \int_{\Omega} (\phi_h^{n+1})^2 \left((\phi_h^{n+1})^2 - (\phi_h^n)^2 + (\phi_h^{n+1} - \phi_h^n)^2 \right) \\ &= \frac{1}{4} \left(\int_{\Omega} (\phi_h^{n+1})^4 - \int_{\Omega} (\phi_h^n)^4 + \int_{\Omega} ((\phi_h^{n+1})^2 - (\phi_h^n)^2)^2 \right) \\ &+ \frac{1}{2} \int_{\Omega} (\phi_h^{n+1})^2 (\phi_h^{n+1} - \phi_h^n)^2. \end{aligned}$$

Next, adding (7), (8), (9) and (10), summing over n and applying the discrete Gronwall lemma, we get the desired estimates and this completes the proof. \square

Consider the linear operator $\Delta_h : X_h \rightarrow X_h$ defined as:

$$-(\Delta_h \phi_h, x_h) = (\nabla \phi_h, \nabla x_h) \quad \forall x_h \in X_h. \quad (11)$$

Then, the discrete phase-field equation (4) can be rewritten as:

$$\begin{aligned} & \alpha \varepsilon^2 \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) - \varepsilon^2 (\Delta_h \phi_h^{n+1}, x_h) + \frac{1}{2} \left((\phi_h^{n+1})^3, x_h \right) \\ & = \frac{1}{2} (\phi_h^n, x_h) + \beta (\theta_h^n - \theta_A c_h^n - \theta_B (1 - c_h^n), x_h). \end{aligned} \quad (12)$$

Taking $x_h = -\Delta_h \phi_h^{n+1}$ as test function in (12) and using the estimates of Lemma 5 we establish the following result.

Corollary 6 *It holds*

$$k \sum_{n=0}^{N-1} |\Delta_h \phi_h^{n+1}|^2 \leq C.$$

Definition 7 *One defines $\phi_{h,k}$ (respectively $\widehat{\phi}_{h,k}$) as the piecewise constant functions in time taking values ϕ_h^{n+1} on $(t_n, t_{n+1}]$ (respectively ϕ_h^n). Analogously, we define $\theta_{h,k}$, $\widehat{\theta}_{h,k}$, and $c_{h,k}$, $\widehat{c}_{h,k}$. Moreover, one defines $\widetilde{\phi}_{h,k}, \widetilde{\theta}_{h,k}, \widetilde{c}_{h,k} \in C^0([0, T]; X_h)$ as the piecewise linear functions in time such that $\widetilde{\phi}_{h,k}(t_n) = \phi_h^n$, $\widetilde{\theta}_{h,k}(t_n) = \theta_h^n$, $\widetilde{c}_{h,k}(t_n) = c_h^n$, respectively.*

An easy consequence of the previous definition and Lemma 5 and Corollary 6 is the following result.

Lemma 8 *The following estimates (independent of h and k) hold:*

$$\begin{aligned}
\{\theta_{h,k}\}_{h,k}, \{\widehat{\theta}_{h,k}\}_{h,k}, \{\widetilde{\theta}_{h,k}\}_{h,k} & \text{ in } L^\infty(0, T; L^2(\Omega)), \\
\{c_{h,k}\}_{h,k}, \{\widehat{c}_{h,k}\}_{h,k}, \{\widetilde{c}_{h,k}\}_{h,k} & \text{ in } L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)), \\
\{\phi_{h,k}\}_{h,k}, \{\widehat{\phi}_{h,k}\}_{h,k}, \{\widetilde{\phi}_{h,k}\}_{h,k} & \text{ in } L^\infty(0, T; H^1(\Omega)), \\
\left\{ \frac{d}{dt} \widetilde{\phi}_{h,k} \right\}_{h,k} & \text{ in } L^2(0, T; L^2(\Omega)). \\
\{-\Delta_h \phi_{h,k}\}_{h,k} & \text{ in } L^2(0, T; L^2(\Omega)) \\
\{K_1^k(\phi_{h,k}) \nabla \theta_{h,k}\}_{h,k} & \text{ in } L^2(0, T; L^2(\Omega))
\end{aligned}$$

In addition, there exist a subsequence of (h, k) (denoted in the same way) and limit functions ϕ , θ , c , w and J verifying the following weak convergences as $(h, k) \rightarrow 0$:

$$\begin{aligned}
\theta_{h,k} \rightarrow \theta, \quad \widehat{\theta}_{h,k} \rightarrow \theta, \quad \widetilde{\theta}_{h,k} \rightarrow \theta & \text{ in } L^\infty(0, T; L^2(\Omega))\text{-weak*}, \\
c_{h,k} \rightarrow c, \quad \widehat{c}_{h,k} \rightarrow c, \quad \widetilde{c}_{h,k} \rightarrow c & \text{ in } \begin{cases} L^2(0, T; H^1(\Omega))\text{-weak}, \\ L^\infty(0, T; L^2(\Omega))\text{-weak*}, \end{cases} \\
\phi_{h,k} \rightarrow \phi, \quad \widehat{\phi}_{h,k} \rightarrow \phi, \quad \widetilde{\phi}_{h,k} \rightarrow \phi & \text{ in } L^\infty(0, T; H^1(\Omega))\text{-weak*}, \\
\frac{d}{dt} \widetilde{\phi}_{h,k} \rightarrow \frac{d}{dt} \phi & \text{ in } L^2(0, T; L^2(\Omega))\text{-weak}, \\
-\Delta_h \phi_{h,k} \rightarrow w & \text{ in } L^2(0, T; L^2(\Omega))\text{-weak}, \\
K_1^k(\phi_{h,k}) \nabla \theta_{h,k} \rightarrow J & \text{ in } L^2(0, T; L^2(\Omega))\text{-weak}.
\end{aligned}$$

4 Strong convergences

Next, let us show some compactness results in order to identify firstly $w = -\Delta\phi$ and $J = \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi)$ and then pass to the limit as $(h, k) \rightarrow 0$.

First of all, since $\{\widetilde{\phi}_{h,k}\}_{h,k}$ is bounded in $L^\infty(0, T, H^1(\Omega))$ and $\{\partial_t \widetilde{\phi}_{h,k}\}_{h,k}$ is bounded in $L^2(0, T; L^2(\Omega))$, applying a compactness theorem of Aubin-Lions type ([8]), one has that

$$\widetilde{\phi}_{h,k} \rightarrow \phi \text{ in } C(0, T; L^p(\Omega)) \text{ strongly as } (h, k) \rightarrow 0,$$

with $p < 6$. Moreover, due to Lemma 5

$$\|\widetilde{\phi}_{h,k} - \phi_{k,h}\|_{L^2(0, T; L^2(\Omega))}^2 \leq \|\widehat{\phi}_{h,k} - \phi_{k,h}\|_{L^2(0, T; L^2(\Omega))}^2 = k \sum_{n=0}^{N-1} |\phi_h^{n+1} - \phi_h^n|^2 \leq Ck.$$

Therefore, $\phi_{h,k} \rightarrow \phi$, $\widehat{\phi}_{h,k} \rightarrow \phi$ in $L^2(0, T; L^2(\Omega))$ strongly as $(h, k) \rightarrow 0$. As $\{\phi\}_{h,k}$ and $\{\widehat{\phi}\}_{h,k}$ are bounded in $L^\infty(0, T; H^1(\Omega))$, Sobolev's imbedding gives us the strong convergences

$$\phi_{h,k}, \widehat{\phi}_{h,k} \rightarrow \phi \quad \text{in } L^q(0, T; L^p(\Omega)) \text{ strongly as } (h, k) \rightarrow 0,$$

with $q < \infty$ and $p < 6$.

Lemma 9 *The following estimates hold*

$$\int_0^T \|\partial_t \widetilde{\theta}_{h,k}(t)\|_{H^1(\Omega)'}^2 dt \leq C, \quad (13)$$

$$\int_0^T \|\partial_t \widetilde{c}_{h,k}(t)\|_{H^1(\Omega)'}^2 dt \leq C, \quad (14)$$

where $C > 0$ is independent of (h, k) .

Proof: Consider P_h the orthogonal projection operator from $L^2(\Omega)$ onto X_h . Let $x \in H^1(\Omega)$. Then, by taking $x_h = P_h x$ as test function in (5) and (6) respectively, we obtain

$$C_V \left\langle \frac{\theta_h^{n+1} - \theta_h^n}{k}, x \right\rangle \leq C |K_1^k(\phi_h^{n+1}) \nabla \theta_h^{n+1}| \|x\|_{H^1(\Omega)} + \frac{l}{2} \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right| |x|,$$

$$\left\langle \frac{c_h^{n+1} - c_h^n}{k}, x \right\rangle \leq C |\nabla c_h^{n+1}| \|x\|_{H^1(\Omega)} + C |\nabla \phi_h^n| \|x\|_{H^1(\Omega)},$$

where we have used the stability properties of the L^2 -projection $|P_h x| \leq |x|$ and $\|P_h x\|_{H^1} \leq C \|x\|_{H^1}$ (the stability in the H^1 -norm can be obtained by means of a duality argument and comparing with the H^1 -projector). Finally, multiplying by k , summing over n , using Definition 7 and the dual definition of the $H^1(\Omega)'$ -norm, the proof is finished. \square

As a consequence of Lemmas 8 and 9, one can use a compactness result ([8]) obtaining the following strong convergences as $(h, k) \rightarrow 0$:

$$\widetilde{\theta}_{h,k} \rightarrow \theta \quad \text{strongly in } L^2(0, T; H^1(\Omega)'),$$

$$\widetilde{c}_{h,k} \rightarrow c \quad \text{strongly in } L^2(0, T; L^p(\Omega)),$$

with $p < 6$. In fact, we also have that $\widehat{\theta}_{h,k}, \theta_{h,k} \rightarrow \theta$ strongly in $L^2(0, T; H^1(\Omega)'),$ $\widehat{c}_{h,k}, c_{h,k} \rightarrow c$ strongly in $L^2(0, T; L^2(\Omega))$ as $(h, k) \rightarrow 0$, since

$$\begin{aligned} \|\widetilde{\theta}_{h,k} - \theta_{h,k}\|_{L^2(0, T; H^1(\Omega)')}^2 &\leq \|\theta_{h,k} - \widehat{\theta}_{h,k}\|_{L^2(0, T; H^1(\Omega)')}^2 \\ &\leq C \|\widehat{\theta}_{h,k} - \theta_{h,k}\|_{L^2(0, T; L^2(\Omega))}^2 = C k \sum_{n=0}^{N-1} |\theta_h^{n+1} - \theta_h^n|^2 \leq C k \end{aligned}$$

and $\|\widetilde{c}_{h,k} - c_{h,k}\|_{L^2(0, T; L^2(\Omega))}^2 \leq \|c_{h,k} - \widehat{c}_{h,k}\|_{L^2(0, T; L^2(\Omega))}^2 = k \sum_{n=0}^{N-1} |c_h^{n+1} - c_h^n|^2 \leq C k$ (due to Lemma 5).

Remark 10 We can change the hypothesis $c_0 \in H^1(\Omega)$ by $c_0 \in L^2(\Omega)$ by imposing the constraint $k/h^2 \leq C$. Indeed, since $k\|c_h^0\|_{H^1(\Omega)}^2 \leq C \frac{k}{h^2} |c_h^0|^2 \leq C \frac{k}{h^2} |c_0|^2$, assuming $k/h^2 \leq C$ one has that $\{\tilde{c}_{h,k}\}_{h,k}$ is still bounded in $L^2(0, T; H^1(\Omega))$ and $\tilde{c}_{h,k} \rightarrow c$ strongly in $L^2(0, T; L^2(\Omega))$.

To prove the compactness of $\{\phi_{h,k}\}_{h,k}$ in $L^2(0, T; H^1(\Omega))$ we firstly must identify $w = -\Delta\phi$. Indeed, we consider $\eta \in C_c^\infty(Q)$ and choose $\eta_h^n \in X_h$ a suitable approximation of $\eta(t_n)$ such that $\eta_{h,k} \rightarrow \eta$ in $L^2(0, T; H^1(\Omega))$ strongly as $(h, k) \rightarrow 0$ (here, $\eta_{h,k}$ is defined by η_h^n as in Definition 7). Then, setting $\phi_h = \phi_h^{n+1}$ and $x_h = \eta_h^{n+1}$ in the discrete laplacian definition (11), multiplying by k and summing over n and tending $(h, k) \rightarrow 0$,

$$\int_Q (\nabla\phi, \nabla\eta) \leftarrow \int_Q (\nabla\phi_{h,k}, \nabla\eta_{h,k}) = \int_Q (-\Delta_h\phi_{h,k}, \eta_{h,k}) \rightarrow \int_Q (w, \eta).$$

Therefore, it is clear that $w = -\Delta\phi$ in $L^2(\Omega)$. Next, taking $\eta \in C^\infty(Q)$ and proceeding in the same manner, we recover the boundary condition $\frac{\partial\phi}{\partial\mathbf{n}} = 0$ on Σ .

Now, we continue to get the compactness of $\{\phi_{h,k}\}_{h,k}$ in $L^2(0, T; H^1(\Omega))$. Considering $\phi_h = \phi_h^{n+1}$ and $x_h = \phi_h^{n+1}$ in (11), multiplying by k and summing over n , this results

$$\int_0^T |\nabla\phi_{h,k}|^2 = - \int_0^T (\Delta_h\phi_{h,k}, \phi_{h,k}) \longrightarrow - \int_0^T (\Delta\phi, \phi) = \int_0^T |\nabla\phi|^2 \quad \text{as } (h, k) \rightarrow 0,$$

because of $\phi_{h,k} \rightarrow \phi$ strongly in $L^2(0, T; L^2(\Omega))$ and $\{-\Delta_h\phi_{h,k}\}_{h,k} \rightarrow -\Delta\phi$ weakly in $L^2(0, T; L^2(\Omega))$.

Therefore, one can obtain the convergence $\|\nabla\phi_{h,k}\|_{L^2(0, T; L^2(\Omega))} \rightarrow \|\nabla\phi\|_{L^2(0, T; L^2(\Omega))}$ as $(h, k) \rightarrow 0$. Consequently, one has

$$\|\phi_{h,k} - \phi\|_{L^2(0, T; H^1(\Omega))} \rightarrow 0 \quad \text{as } (h, k) \rightarrow 0,$$

thanks to $\phi_{h,k} \rightarrow \phi$ strongly in $L^2(Q)$ and weakly \star in $L^2(0, T; H^1(\Omega))$.

Finally, the following compactness result is established using that $\{c_{h,k}\}_{h,k}$ is compact in $L^2(0, T; L^2(\Omega))$ and bounded in $L^2(0, T; H^1(\Omega))$ (see [4] for the details).

Proposition 11 *The following convergences hold:*

$$[c_{h,k}]_T, [\tilde{c}_{h,k}]_T \rightarrow T_0^1 c \quad \text{in } L^2(0, T; L^2(\Omega))\text{-strong, as } (h, k) \rightarrow 0. \quad (15)$$

where T_0^1 is the truncation operator defined as:

$$T_0^1 c(\mathbf{x}, t) = \begin{cases} c(\mathbf{x}, t) & \text{if } c(\mathbf{x}, t) \in [0, 1], \\ 0 & \text{if } c(\mathbf{x}, t) < 0, \\ 1 & \text{if } c(\mathbf{x}, t) > 1. \end{cases}$$

Now we want to identify $J = \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi)$. Indeed, since K_1 is a globally Lipschitz continuous function on \mathbb{R} and $\phi_{h,k}$ converges to ϕ in $L^2(0, T; H^1(\Omega))$, then (see [6], Theorem 16.7)

$$K_1(\phi_{h,k}) \rightarrow K_1(\phi) \quad \text{strongly in } L^2(0, T; H^1(\Omega)). \quad (16)$$

On the other hand, using that $\theta_{h,k} \rightarrow \theta$ weakly \star in $L^\infty(0, T; L^2(\Omega))$ and (16), the following weak convergences hold:

$$\theta_{h,k} \nabla K_1(\phi_{h,k}) \rightarrow \theta \nabla K_1(\phi) \quad \text{weakly in } L^2(0; T; L^1(\Omega)), \quad (17)$$

$$\theta_{h,k} K_1(\phi_{h,k}) \rightarrow \theta K_1(\phi) \quad \text{weakly in } L^2(0; T; L^{3/2}(\Omega)). \quad (18)$$

Now, using the regularity $K_1(\phi_{h,k}) \in L^\infty(0, T; H^1(\Omega))$ and $\theta_{h,k} \in L^2(0, T; H^1(\Omega))$ (because of $0 < k \leq K_1^k$) and the Sobolev product $\|\varphi\psi\|_{W^{1,3/2}(\Omega)} \leq C\|\varphi\|_{H^1(\Omega)}\|\psi\|_{H^1(\Omega)}$ for all $\varphi, \psi \in H^1(\Omega)$, we get

$$K_1(\phi_{h,k})\theta_{h,k} \in L^2(0, T; W^{1,3/2}(\Omega))$$

and, in particular,

$$\nabla(K_1(\phi_{h,k})\theta_{h,k}) = K_1(\phi_{h,k})\nabla\theta_{h,k} + \theta_{h,k}\nabla K_1(\phi_{h,k}). \quad (19)$$

Therefore, in view of the convergences (17), (18) and the identity (19), one arrives at

$$K_1(\phi_{h,k})\nabla\theta_{h,k} \rightarrow \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi) \quad \text{in } L^2(0, T; W^{-1,1/2-\varepsilon}(\Omega)). \quad (20)$$

with $1/2 > \varepsilon > 0$.

Next, remembering the definition of $K_1^k = k + K_1$ we write

$$K_1^k(\phi_{h,k})\nabla\theta_{h,k} = k\nabla\theta_{h,k} + K_1(\phi_{h,k})\nabla\theta_{h,k}. \quad (21)$$

Now, taking into account that $\|k^{1/2}\nabla\theta_{h,k}\|_{L^2(Q)} \leq \|\sqrt{K_1^k(\phi_{h,k})}\nabla\theta_{h,k}\|_{L^2(Q)} \leq C$ with $C > 0$ independent of (k, h) , one obtains

$$k\nabla\theta_{h,k} \rightarrow 0 \quad \text{in } L^2(Q)$$

that jointly with (20) and (21), this gives us

$$K_1^k(\phi_{h,k})\nabla\theta_{h,k} \rightarrow \nabla(K_1(\phi)\theta) - \theta\nabla K_1(\phi) \quad \text{in } L^2(0, T; W^{-1,3/2-\varepsilon}(\Omega)).$$

5 Passing to the limit

In order to pass to the limit in the c -equation, we will use the following result, which is easy to prove because the first equation (22) satisfies the maximum principle:

Lemma 12 *The following two systems are equivalent:*

$$c_t = K_2(\Delta c + M\nabla \cdot [T_0^1 c(1 - T_0^1 c)\nabla\phi]) \quad \text{in } Q, \quad (22)$$

and

$$0 \leq c \leq 1, \quad c_t = K_2(\Delta c + M\nabla \cdot [c(1 - c)\nabla\phi]) \quad \text{in } Q,$$

To pass to the limit in scheme (4)-(6), we rewrite the scheme as follows: taking $x_h = \eta_h^{n+1} \in X_h$ a suitable approximation at time t_{n+1} of a test function $\eta \in C^0([0, T]; C_c^\infty(\Omega))$ such that $\eta(T) = 0$ (clearly $\eta_h^N = 0$) as a test function in (4), (5) and (6), multiplying by k , summing over n and denoting $\eta_{h,k}$, similarly to Definition 7, one arrives at

$$\begin{cases} \alpha \varepsilon^2 \int_0^T \left(\frac{d}{dt} \tilde{\phi}_{h,k}, \eta_{h,k} \right) + \varepsilon^2 \int_0^T \left(\nabla \phi_{h,k}, \nabla \eta_{h,k} \right) + \int_0^T \frac{1}{2} \left((\phi_{h,k})^3, \eta_{h,k} \right) \\ - \frac{1}{2} \int_0^t \left(\hat{\phi}_{h,k}, \eta_{h,k} \right) - \beta \int_0^t \left(\hat{\theta}_{h,k} - \theta_A [\hat{c}_{h,k}]_T - \theta_B (1 - [\hat{c}_{h,k}]_T), \eta_{h,k} \right) = 0, \\ C_V \int_0^T \left\langle \frac{d}{dt} \tilde{\theta}_{h,k}, \eta_{h,k} \right\rangle + \frac{l}{2} \int_0^T \left(\tilde{\phi}_{h,k}, \eta_{h,k} \right) - \int_0^T \left(K_1^k(\phi_{h,k}) \nabla \theta_{h,k}, \nabla \eta_{h,k} \right) = 0, \\ \int_0^T \left\langle \frac{d}{dt} \tilde{c}_{h,k}, \eta_{h,k} \right\rangle + K_2 \int_0^T \left(\nabla c_{h,k}, \nabla \eta_{h,k} \right) + K_2 M \int_0^T \left([\hat{c}_{h,k}]_T (1 - [\hat{c}_{h,k}]_T) \nabla \hat{\phi}_{h,k}, \nabla \eta_{h,k} \right) = 0. \end{cases}$$

There are no additional difficulties in passing to the limit to obtain that (ϕ, θ, c) is a solution of (1). In particular, taking $(h, k) \rightarrow 0$ in the discrete equation for the concentration c and using (15), we arrive at the limit equation (22), hence $0 \leq c \leq 1$ and $T_0^1 c = c$. Finally, the ϕ -equation is verified pointwise in Q thanks to the strong regularity of ϕ . The proof of Theorem 3 is finished.

6 A conditionally stable, convergent linear scheme

In this section we replace the nonlinear discrete approximation (4) of $(1)_1$ by a linear discretization. Accordingly, to obtain stability we have to impose a constraint on the discrete parameters.

Let us define $f(\phi) = \frac{1}{2\varepsilon^2}(\phi^2 - 1)\phi$ associated to the potential function $F(\phi) = \frac{1}{8\varepsilon^2}(\phi^2 - 1)^2$. We proposed the following linear scheme:

Initialization: Let $(\phi_h^0, \theta_h^0, c_h^0) \in X_h \times X_h \times X_h$ be suitable approximations of (ϕ_0, θ_0, c_0) as $h \rightarrow 0$.

Step $n + 1$: Given $(\phi_h^n, \theta_h^n, c_h^n) \in X_h \times X_h \times X_h$.

Find $\phi_h^{n+1} \in X_h$ as solution of the problem:

$$\begin{aligned} & \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right) + \frac{1}{\alpha} \left(\nabla \phi_h^{n+1}, \nabla x_h \right) \\ & = -\frac{1}{\alpha} \left(f(\phi_h^n), x_h \right) + \frac{\beta}{\varepsilon^2 \alpha} \left(\theta_h^n - \theta_A c_h^n - \theta_B (1 - c_h^n), x_h \right), \quad \forall x_h \in X_h. \end{aligned} \quad (23)$$

Find $\theta_h^{n+1} \in X_h$ and $c_h^{n+1} \in X_h$ as solution of the decoupled variational problems:

$$C_V \left(\frac{\theta_h^{n+1} - \theta_h^n}{k}, x_h \right) + \left(K_1^k(\phi_h^{n+1}) \nabla \theta_h^{n+1}, \nabla x_h \right) = -\frac{l}{2} \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, x_h \right), \quad \forall x_h \in X_h, \quad (24)$$

$$\left(\frac{c_h^{n+1} - c_h^n}{k}, x_h \right) + K_2 \left(\nabla c_h^{n+1}, \nabla x_h \right) = -K_2 M \left([c_h^n]_T (1 - [c_h^n]_T) \nabla \phi_h^n, \nabla x_h \right), \quad \forall x_h \in X_h. \quad (25)$$

The stability of scheme (23)-(25) will be obtained by induction on the time step n in two steps. In the first step, we establish the following result which provides a basic recursive inequality.

Lemma 13 *Assume the constraint:*

$$(S) \quad \lim_{(h,k) \rightarrow 0} k/h = 0.$$

If there exists a constants $C_d > 0$ (independent of h and k) such that

$$\|\phi_h^n\|_{H^1(\Omega)}^2 + \frac{\alpha C_V^2}{8l^2} |\theta_h^n|^2 + |c_h^n|^2 \leq C_d, \quad (26)$$

then, there exist $k_0, h_0 > 0$ sufficiently small but independent of n such that for any $k \leq k_0$ and $h \leq h_0$, the following inequalities hold

$$\left\{ \begin{array}{l} \|\phi_h^{n+1}\|_{H^1(\Omega)}^2 - \|\phi_h^n\|_{H^1(\Omega)}^2 + \frac{1}{2} \|\phi_h^{n+1} - \phi_h^n\|_{H^1(\Omega)}^2 \\ + \frac{\alpha C_V^2}{8l^2} (|\theta_h^{n+1}|^2 - |\theta_h^n|^2 + |\theta_h^{n+1} - \theta_h^n|^2) \\ + \frac{1}{4\varepsilon^2} \int_{\Omega} \left((|\phi_h^{n+1}|^2 - 1)^2 - (|\phi_h^n|^2 - 1)^2 + \frac{1}{2} (|\phi_h^{n+1}|^2 - |\phi_h^n|^2)^2 \right) \\ + \frac{\alpha}{16} k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 + \frac{k}{2\alpha} |P_h(f(\phi_h^n)) - \Delta_h \phi_h^{n+1}|^2 + \frac{\alpha C_V k}{4l^2} |\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}|^2 \\ \leq C k |\theta_h^n|^2 + C k |\phi_h^n|^2 + C k |c_h^n|^2 + C k, \end{array} \right. \quad (27)$$

$$|c_h^{n+1}|^2 - |c_h^n|^2 + |c_h^{n+1} - c_h^n|^2 + k K_2 |\nabla c_h^{n+1}|^2 \leq C k |\nabla \phi_h^n|^2. \quad (28)$$

Proof: Let $P_h : H^1(\Omega) \rightarrow X_h$ be the L^2 -projection. Firstly, we consider $x_h = P_h(f(\phi_h^n)) - \Delta_h \phi_h^{n+1} \in X_h$ in (23), rewritten (23) using the discrete laplacian operator (similarly as in (12)), and bounding the right-hand side, one arrives at:

$$\left(\phi_h^{n+1} - \phi_h^n, f(\phi_h^n) - \Delta_h \phi_h^{n+1} \right) + \frac{k}{2\alpha} |P_h(f(\phi_h^n)) - \Delta_h \phi_h^{n+1}|^2 \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k. \quad (29)$$

Now, we handle the first term on the left hand side of (29) as follows

$$\begin{aligned} \left(\phi_h^{n+1} - \phi_h^n, -\Delta_h \phi_h^{n+1} \right) &= \frac{1}{2} \left(|\nabla \phi_h^{n+1}|^2 - |\nabla \phi_h^n|^2 + |\nabla(\phi_h^{n+1} - \phi_h^n)|^2 \right), \\ \left(\phi_h^{n+1} - \phi_h^n, f(\phi_h^n) \right) &= \frac{1}{2\varepsilon^2} \left(\phi_h^{n+1} - \phi_h^n, ((\phi_h^{n+1})^2 - 1)\phi_h^n \right) \\ &\quad + \frac{k}{2\varepsilon^2} \left(\frac{\phi_h^{n+1} - \phi_h^n}{k}, ((\phi_h^n)^2 - (\phi_h^{n+1})^2)\phi_h^n \right) := I_1 - I_2. \end{aligned}$$

Next, we continue rewriting I_1 , by using first the identity $|a|^2 - |b|^2 - |a - b|^2 = 2(a - b, b)$ and afterwards $|a|^2 - |b|^2 + |a - b|^2 = 2(a - b, a)$, as follows

$$\begin{aligned} I_1 &= \frac{1}{4\varepsilon^2} \int_{\Omega} \left((\phi_h^{n+1})^2 - 1 \right) \left((\phi_h^{n+1})^2 - (\phi_h^n)^2 - (\phi_h^{n+1} - \phi_h^n)^2 \right) \\ &= \frac{1}{8\varepsilon^2} \int_{\Omega} \left(((\phi_h^{n+1})^2 - 1)^2 - ((\phi_h^n)^2 - 1)^2 + ((\phi_h^{n+1})^2 - (\phi_h^n)^2)^2 \right) \\ &\quad + \frac{k^2}{4\varepsilon^2} \int_{\Omega} \left(1 - (\phi_h^{n+1})^2 \right) \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 \end{aligned}$$

and bounding I_2 as

$$I_2 \leq C k^2 \|\phi_h^n\|_{L^\infty(\Omega)}^2 \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 + \frac{1}{16\varepsilon^2} \int_{\Omega} ((\phi_h^{n+1})^2 - (\phi_h^n)^2)^2.$$

Finally, we get from (29)

$$\begin{aligned} & |\nabla \phi_h^{n+1}|^2 - |\nabla \phi_h^n|^2 + |\nabla(\phi_h^{n+1} - \phi_h^n)|^2 + \frac{k}{\alpha} |P_h(f(\phi_h^n)) - \Delta_h \phi_h^{n+1}|^2 \\ & + \frac{1}{4\varepsilon^2} \int_{\Omega} \left((|\phi_h^{n+1}|^2 - 1)^2 - (|\phi_h^n|^2 - 1)^2 + \frac{1}{2} (|\phi_h^{n+1}|^2 - |\phi_h^n|^2)^2 \right) \\ & \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k + C k \|\phi_h^n\|_{L^\infty(\Omega)}^2 k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 + \frac{k^2}{2\varepsilon^2} \int_{\Omega} (\phi_h^{n+1})^2 \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 \\ & \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k + C k \left(\|\phi_h^n\|_{L^\infty(\Omega)}^2 + \|\phi_h^{n+1}\|_{L^\infty(\Omega)}^2 \right) k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 \\ & \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k + C \frac{k}{h} \left(\|\phi_h^n\|_{H^1(\Omega)}^2 + \|\phi_h^{n+1}\|_{H^1(\Omega)}^2 \right) k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2, \end{aligned} \tag{30}$$

where in the last line the inverse estimate $\|x_h\|_{L^\infty(\Omega)} \leq C h^{-1/2} \|x_h\|_{H^1(\Omega)}$ has been used.

Now we are looking for the bound $\|\phi_h^{n+1}\|_{H^1(\Omega)} \leq C_1$ where $C_1 > 0$ depends on the constant C_d of hypothesis (26) but it will be independent of n . It will be carried out by bounding $\|\phi_h^{n+1}\|_{H^1(\Omega)}$ in terms of $\|\phi_h^n\|_{H^1(\Omega)}$, $|\theta_h^n|$ and $|c_h^n|$ and using hypothesis (26). Indeed, taking $x_h = \frac{\phi_h^{n+1} - \phi_h^n}{k}$ as a test function in (23) yields

$$\begin{aligned} & \alpha k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 + \left(|\nabla \phi_h^{n+1}|^2 - |\nabla \phi_h^n|^2 + |\nabla(\phi_h^{n+1} - \phi_h^n)|^2 \right) \\ & \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k + C k |f(\phi_h^n)|^2 \\ & \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k + C k \|\phi_h^n\|_{H^1(\Omega)}^6 + C k \|\phi_h^n\|_{H^1(\Omega)}^2. \end{aligned} \tag{31}$$

In particular, the previous inequality says us, by using hypothesis (26), that

$$|\nabla \phi_h^{n+1}|^2 \leq C.$$

In order to get that $\|\phi_h^{n+1}\|_{H^1(\Omega)}^2 \leq C_1$ we have to estimate $|\phi_h^{n+1}|^2 \leq C$. To this end, we take $x_h = \phi_h^{n+1}$ in (23)

$$\begin{aligned} & \frac{1}{2} \left(|\phi_h^{n+1}|^2 - |\phi_h^n|^2 + |\phi_h^{n+1} - \phi_h^n|^2 \right) + \frac{2}{\alpha} k |\nabla \phi_h^{n+1}|^2 \\ & \leq C k |\theta_h^n|^2 + C k |c_h^n|^2 + C k + C k \|\phi_h^n\|_{H^1(\Omega)}^6 + C k \|\phi_h^n\|_{H^1(\Omega)}^2. \end{aligned}$$

Therefore, it follows that there exists $C_1 > 0$ depending on C_d such that $\|\phi_h^{n+1}\|_{H^1(\Omega)}^2 \leq C_1$.

Thus, using that $\|\phi_h^{n+1}\|_{H^1}^2 \leq C_1$ in (30) and again hypothesis (26), we get

$$\begin{aligned} & |\nabla\phi_h^{n+1}|^2 - |\nabla\phi_h^n|^2 + |\nabla(\phi_h^{n+1} - \phi_h^n)|^2 + \frac{k}{\alpha}|P_h(f(\phi_h^n)) - \Delta_h\phi_h^{n+1}|^2 \\ & + \frac{1}{4\varepsilon^2} \int_{\Omega} \left((|\phi_h^{n+1}|^2 - 1)^2 - (|\phi_h^n|^2 - 1)^2 + \frac{1}{2}(|\phi_h^{n+1}|^2 - |\phi_h^n|^2)^2 \right) \\ & \leq Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck + C\frac{k}{h}k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2. \end{aligned} \quad (32)$$

In order to control the term $C\frac{k}{h}k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2$ on the right hand-side of (32), we choose

$x_h = \frac{\phi_h^{n+1} - \phi_h^n}{k}$ in (23) and arrive at

$$\frac{k}{2} \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 \leq Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck + \frac{k}{\alpha^2}|P_h(f(\phi_h^n)) - \Delta_h\phi_h^{n+1}|^2. \quad (33)$$

Balancing equations (32) and (33) and taking into account the constraint $\lim_{(h,k) \rightarrow 0} \frac{k}{h} = 0$, we have for any $k \leq k_0$ and $h \leq h_0$ (with k_0 and h_0 independent of n)

$$\begin{aligned} & |\nabla\phi_h^{n+1}|^2 - |\nabla\phi_h^n|^2 + |\nabla(\phi_h^{n+1} - \phi_h^n)|^2 + \frac{\alpha}{8}k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 \\ & + \frac{1}{4\varepsilon^2} \int_{\Omega} \left((|\phi_h^{n+1}|^2 - 1)^2 - (|\phi_h^n|^2 - 1)^2 + \frac{1}{2}(|\phi_h^{n+1}|^2 - |\phi_h^n|^2)^2 \right) \\ & + \frac{k}{2\alpha}|P_h(f(\phi_h^n)) - \Delta_h\phi_h^{n+1}|^2 \leq Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck. \end{aligned} \quad (34)$$

On the other hand, taking $x_h = \theta_h^{n+1}$ in (24), one arrives at inequality (8). Now, balancing (8) and (34), one gets

$$\begin{aligned} & |\nabla\phi_h^{n+1}|^2 - |\nabla\phi_h^n|^2 + |\nabla(\phi_h^{n+1} - \phi_h^n)|^2 + \frac{\alpha C_V^2}{8l^2} \left(|\theta_h^{n+1}|^2 - |\theta_h^n|^2 + |\theta_h^{n+1} - \theta_h^n|^2 \right) \\ & + \frac{1}{4\varepsilon^2} \int_{\Omega} \left((|\phi_h^{n+1}|^2 - 1)^2 - (|\phi_h^n|^2 - 1)^2 + \frac{1}{2}(|\phi_h^{n+1}|^2 - |\phi_h^n|^2)^2 \right) \\ & + \frac{\alpha}{16}k \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 + \frac{k}{2\alpha}|P_h(f(\phi_h^n)) - \Delta_h\phi_h^{n+1}|^2 + \frac{\alpha C_V k}{4l^2} |\sqrt{K_1^k(\phi_h^{n+1})} \nabla\theta_h^{n+1}|^2 \\ & \leq Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck. \end{aligned} \quad (35)$$

Taking now $x_h = \phi_h^{n+1}$ in (23), we obtain

$$\begin{aligned} & |\phi_h^{n+1}|^2 - |\phi_h^n|^2 + |\phi_h^{n+1} - \phi_h^n|^2 + \frac{2}{\alpha}k|\nabla\phi_h^{n+1}|^2 + \frac{k}{2\alpha\varepsilon^2} \|\phi_h^n\|_{L^4(\Omega)}^4 \\ & \leq -\frac{k}{2\alpha\varepsilon^2} \left((\phi_h^n)^3 - \phi_h^n, \phi_h^{n+1} - \phi_h^n \right) + \frac{k}{2\alpha}|\phi_h^n|^2 + Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck \\ & \leq \frac{1}{2}|\phi_h^{n+1} - \phi_h^n|^2 + Ck^2\|\phi_h^n\|_{L^6(\Omega)}^6 + Ck|\phi_h^n|^2 + Ck|\theta_h^n|^2 + Ck|c_h^n|^2 + Ck. \end{aligned}$$

Using the Sobolev imbedding $\|x_h\|_{L^6(\Omega)} \leq C\|x_h\|_{H^1(\Omega)}$ and the inverse inequality $\|x_h\|_{L^6(\Omega)} \leq h^{-1/4}\|x_h\|_{L^4(\Omega)}$, we find

$$\begin{aligned}
& |\phi_h^{n+1}|^2 - |\phi_h^n|^2 + \frac{1}{2}|\phi_h^{n+1} - \phi_h^n|^2 + \frac{2}{\alpha}k|\nabla\phi_h^{n+1}|^2 + \frac{k}{2\alpha\varepsilon^2}\|\phi_h^n\|_{L^4(\Omega)}^4 \\
& \leq Ck|\theta_h^n|^2 + Ck|\phi_h^n|^2 + Ck|c_h^n|^2 + Ck + C\frac{k}{h}\|\phi_h^n\|_{H^1(\Omega)}^2 k\|\phi_h^n\|_{L^4(\Omega)}^4 \\
& \leq Ck|\theta_h^n|^2 + Ck|\phi_h^n|^2 + Ck|c_h^n|^2 + Ck + C\frac{k}{h}k\|\phi_h^n\|_{L^4(\Omega)}^4,
\end{aligned}$$

where in the last line we have used hypothesis (26).

Finally, taking $Ck/h \leq \frac{1}{4\alpha\varepsilon^2}$ yields

$$\begin{aligned}
& |\phi_h^{n+1}|^2 - |\phi_h^n|^2 + \frac{1}{2}|\phi_h^{n+1} - \phi_h^n|^2 + \frac{2}{\alpha}k|\nabla\phi_h^{n+1}|^2 + \frac{k}{4\alpha\varepsilon^2}\|\phi_h^n\|_{L^4(\Omega)}^4 \\
& \leq Ck|\theta_h^n|^2 + Ck|\phi_h^n|^2 + Ck|c_h^n|^2 + Ck.
\end{aligned} \tag{36}$$

Adding (35) to (36) it gives (27).

Inequality (28) is easily obtained by testing (25) by c_h^{n+1} and bounding adequately as in the proof of Lemma 5. \square

Now we turn our attention to the initial approximations which must satisfy hypothesis (26) imposed in Lemma 13 in order to guarantee a correct induction argument. It is easy to check that if we select $\phi_h^0 = I_h\phi_0$, $\theta_h^0 = I_h\theta_0$, and $c_h^0 = I_hc_0$ as initial approximations, where I_h is the interpolation operator into X_h , it follows that there exists a constant $C_2 > 0$ such that

$$\frac{\alpha C_V^2}{8l^2}|\theta_h^0|^2 + |c_h^0|^2 + \|\phi_h^0\|_{H^1(\Omega)}^2 + \frac{1}{4\varepsilon^2} \int_{\Omega} (|\phi_h^0|^2 - 1)^2 \leq C_2, \tag{37}$$

thanks to the stability properties of I_h in the L^2 and H^1 norms.

Now, we are in position to give the stability result.

Lemma 14 *Under the hypotheses of Theorem 2, the discrete solution of scheme (23)-(25) satisfies the following estimates:*

$$\begin{aligned}
\mathbf{i)} \max_{0 \leq n \leq N} \|\phi_h^n\|_{H^1(\Omega)} &\leq C, & \mathbf{ii)} \sum_{n=0}^{N-1} \|\phi_h^{n+1} - \phi_h^n\|_{H^1(\Omega)}^2 &\leq C, & \mathbf{iii)} k \sum_{n=0}^{N-1} \left| \frac{\phi_h^{n+1} - \phi_h^n}{k} \right|^2 &\leq C, \\
\mathbf{iv)} \max_{0 \leq n \leq N} |\theta_h^n| &\leq C, & \mathbf{v)} \sum_{n=0}^{N-1} |\theta_h^{n+1} - \theta_h^n|^2 &\leq C, & \mathbf{vi)} k \sum_{n=0}^{N-1} |\sqrt{K_1^k(\phi_h^{n+1})} \nabla \theta_h^{n+1}|^2 &\leq C, \\
\mathbf{vii)} \max_{0 \leq n \leq N} |c_h^n| &\leq C, & \mathbf{viii)} \sum_{n=0}^{N-1} |c_h^{n+1} - c_h^n|^2 &\leq C, & \mathbf{ix)} k \sum_{n=0}^{N-1} |\nabla c_h^{n+1}|^2 &\leq C,
\end{aligned}$$

where $C > 0$ depends only on data (ϕ_0, θ_0, c_0) .

Proof: Obviously, if we let (27) and (28) hold for $n = 0, \dots, N-1$, we get all the statements of the theorem by adding (27) and (28) and applying the discrete Gronwall lemma. Therefore, it suffices to prove that (27) and (28) hold for $n = 0, \dots, N-1$.

Let us consider $C_d = e^{CT} (C_2 + CT)$ for some constant $C > 0$ independent of (h, k) with $C_2 > 0$ from (37). As the initial approximations verify hypothesis (26) for $n = 0$, inequalities (27) and (28) are satisfied for $n = 0$.

The final induction step can be easily seen assuming that inequalities (27) and (28) hold for $l = 0, \dots, n - 1$ and using again the discrete Gronwall lemma

$$\begin{aligned} & \frac{\alpha C_V^2}{8l^2} |\theta_h^n|^2 + |c_h^n|^2 + \|\phi_h^n\|_{H^1(\Omega)}^2 + \frac{1}{4\varepsilon^2} \int_{\Omega} (|\phi_h^n|^2 - 1)^2 \\ & \leq e^{C(n-1)k} \left(\frac{\alpha C_V^2}{8l^2} |\theta_h^0|^2 + |c_h^0|^2 + \|\phi_h^0\|_{H^1(\Omega)}^2 + \frac{1}{4\varepsilon^2} \int_{\Omega} (|\phi_h^0|^2 - 1)^2 + C(n-1)k \right) \\ & \leq e^{CT} (C_2 + CT) := C_d. \end{aligned}$$

Then, we find that hypothesis (26) is satisfied. Therefore, in view of Lemma 13, inequalities (27) and (28) hold. \square

To finish the proof of Theorem 4 it is necessary to prove the convergence of the linear scheme (23)-(25). But, as the argument for this is similar to that developed for the nonlinear scheme (4)-(6), it is left to the reader.

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Capítulo 7

Experiencias numéricas de cristales líquidos nemáticos

Experiencias numéricas de cristales líquidos nemáticos

F. Guillén-González*, J.V. Gutiérrez-Santacreu*

En este capítulo, presentamos algunas simulaciones numéricas de un modelo simplificado de cristales líquidos nemáticos, usando el esquema numérico desarrollado en [2].

La literatura sobre simulaciones numéricas de cristales líquidos no es muy amplia. Los tests numéricos que realizamos en la Sección 1 son extraídos del trabajo [3] de *Liu y Walkington*, con los que comparamos los resultados. Estos tests exhiben el curioso comportamiento de los flujos de cristales líquidos en presencia de singularidades. En la Sección 2, mostramos otros tests numéricos inspirados en los realizados en [1], aunque con distintas condiciones de contorno.

Todos los ejemplos numéricos que se exhiben son computados en un dominio bidimensional $\Omega = (-1, 1) \times (-1, 1)$. El par velocidad y presión (\mathbf{u}, p) es aproximado usando el par de elementos finitos estable conocido como mini-elemento $(\mathbb{P}_1 + \text{burbuja}, \mathbb{P}_1)$. El par vector de orientación y su laplaciano $(\mathbf{d}, -\Delta \mathbf{d})$ es aproximado usando el par de elementos finitos $(\mathbb{P}_1, \mathbb{P}_0)$. Estos ejemplos son calculados sobre una malla uniforme de 32×32 y 160 pasos por unidad de tiempo (i.e. $h = 1/16$ y $k = 1/160$). Como en [3], seleccionamos los parámetros λ , ν y γ iguales a uno. Respecto al parámetro de penalización ε asociado a la función \mathbf{f}_ε haremos varias elecciones que se especificará más tarde. La resolución numérica se lleva a cabo con la ayuda del software de *Freefem++* usando una formulación penalizada en norma L^2 de la presión en la ecuación de la divergencia discreta nula siendo el parámetro de penalización del orden de 10^{-6} . El sistema lineal que queda en cada etapa de tiempo es resuelto usando el método directo de sistemas lineales LU.

Los cálculos han sido ejecutados con un procesador Intel(R) Core(TM)2 CPU 4300 @ 1.80 GHz 1.80 GHz.

1. Aniquilación de singularidades de *Liu-Walkington*

1.1. Aniquilación de dos singularidades de distinto signo

Para mostrar la aniquilación de singularidades que presentan los flujos de cristales líquidos consideramos el ejemplo dado en [3]. La velocidad inicial cero y el vector de orientación $\mathbf{d}_0 = \widehat{\mathbf{d}} / \sqrt{|\widehat{\mathbf{d}}|^2 + 0,05^2}$, donde

$$\widehat{\mathbf{d}} = (x^2 + y^2 - 0,25, y).$$

Este vector de orientación tiene dos singularidades en $(\pm 1/2, 0)$ (puntos en los que $\widehat{\mathbf{d}} = (0, 0)$) como muestra la Figura 1. Como condición de contorno para el vector de orientación tomamos el valor de \mathbf{d}_0 sobre la frontera del dominio Ω en todos los ejemplos.

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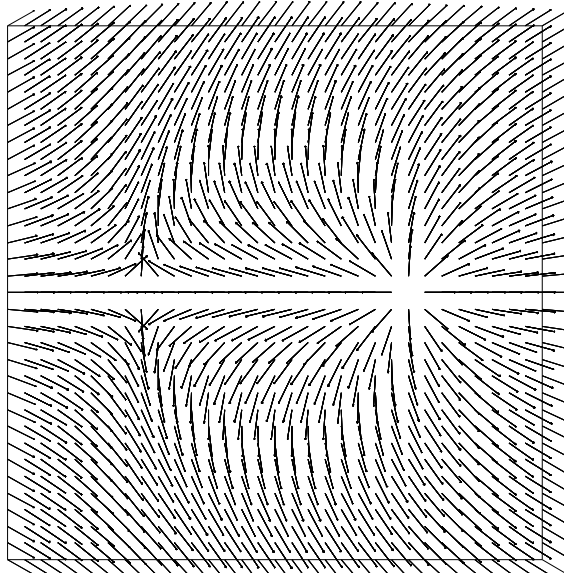


Figura 1: Vector director inicial

A continuación, mostramos en las Figuras 2, 3, 4 y 5 la evolución de estos datos iniciales tomando primero el valor para el parámetro de penalización $\varepsilon = 0,06$.

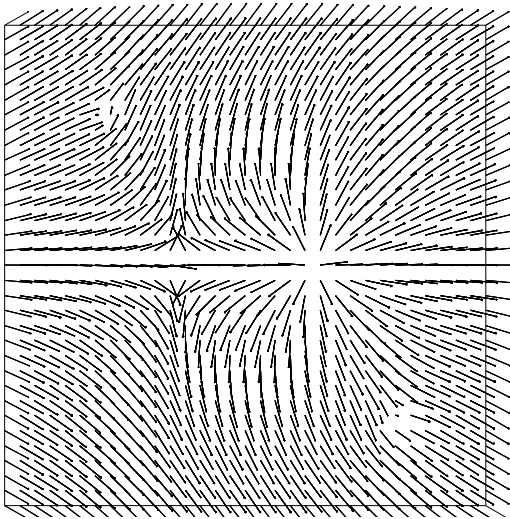


Figura 2: Vector director $t=0.25$

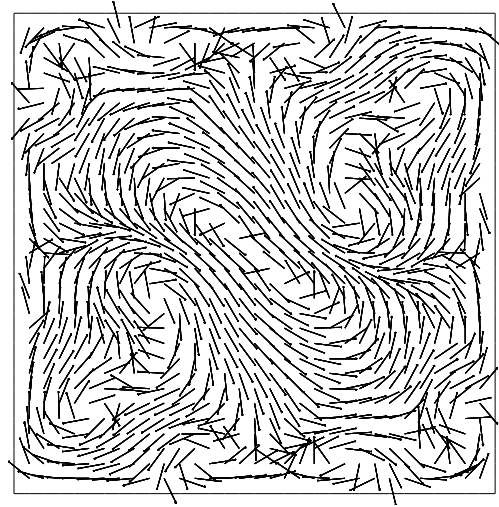


Figura 3: Velocidad $t=0.25$

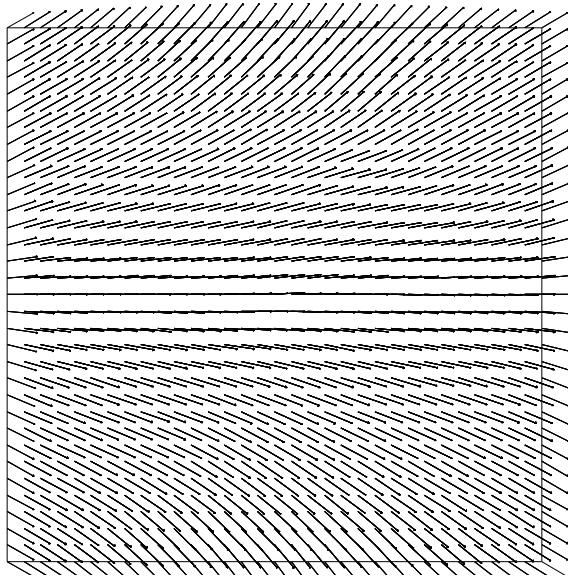


Figura 4: Vector director $t=0.75$

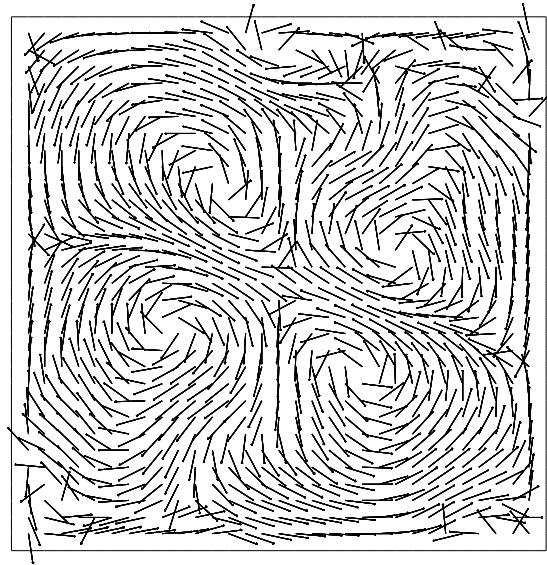


Figura 5: Vector director $t=0.75$

La evolución de los datos iniciales para $\varepsilon = 0,07$ se muestra en las Figuras 6, 7, 8 y 9. En ambos casos, se observa la aniquilación de las dos singularidades que se atraen.

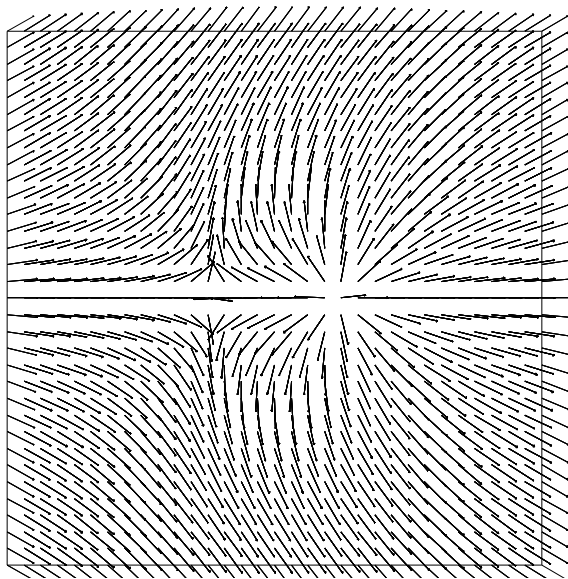


Figura 6: Vector director $t=0.25$

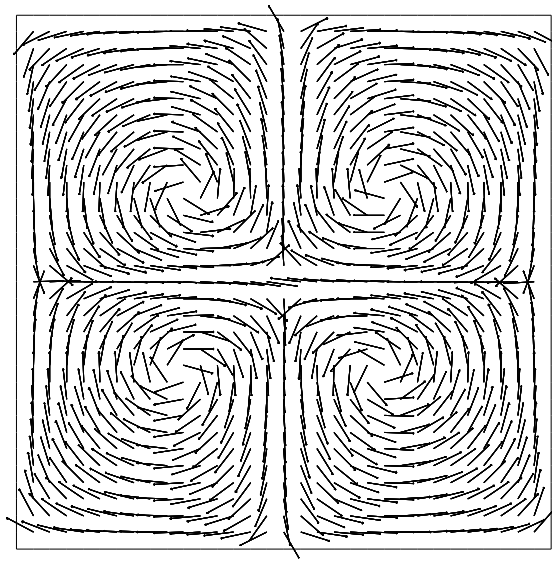


Figura 7: Velocidad $t=0.25$

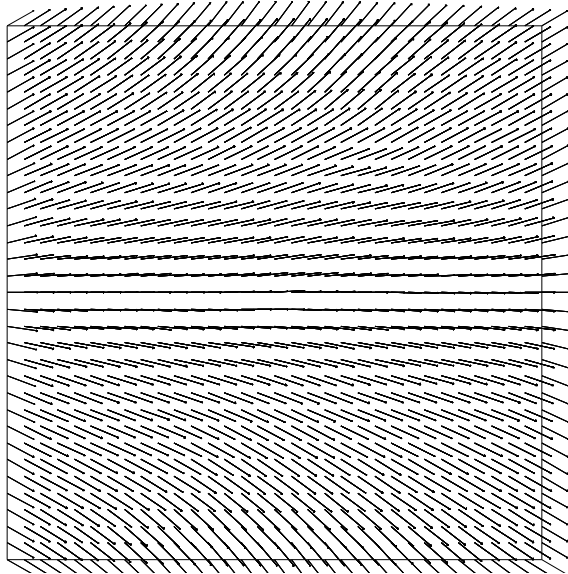


Figura 8: Vector director $t=0.75$

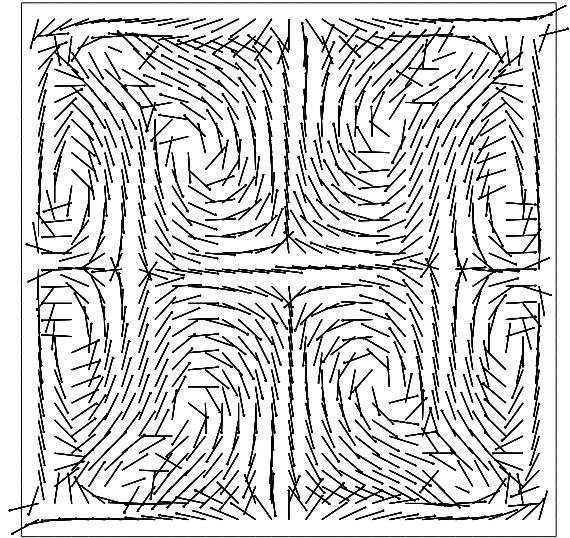


Figura 9: Velocidad $t=0.75$

Es curioso observar la sensibilidad de los resultados del campo de velocidades respecto al parámetro de penalización ε .

En los resultados obtenidos en el artículo [3] se toma $\varepsilon = 0,05$ siendo el tiempo de aniquilación de las singularidades $t = 0,25s$. Para este valor del parámetro de penalización nuestro esquema numérico no converge, lo que nos indica que nuestro sistema lineal no muestra tanta robustez con respecto al parámetro de penalización como el esquema no lineal de [3]. Para $\varepsilon = 0,06$ se recupera la dinámica de las singularidades (siendo el tiempo de aniquilación $t = 0,41875s$, casi el doble que en [3]) observando oscilaciones del vector de orientación como muestra la Figura 2 y un campo de velocidades diferente del obtenido en [3], que es el que se muestra en las Figuras 3 y 4. Todo lo contrario sucede si elegimos $\varepsilon = 0,07$; que muestra un comportamiento cualitativo análogo al de [3], siendo el tiempo de aniquilación $t = 0,30625s$. Los beneficios de nuestro esquema con respecto al esquema citado [3] son obvios. En [3] se construye un esquema no lineal y se considera una aproximación de elementos finitos globalmente C^1 para el vector de orientación. Luego, nuestro esquema reduce enormemente el número de grados de libertad y la complejidad en la resolución numérica, lo que se reflejan en los tiempos de ejecución; en nuestros cálculos para $\varepsilon = 0,06$ se tardó 1234.6s y para $\varepsilon = 0,07$ se consumió 1221.31s para hacer las 160 iteraciones de tiempo. Por el contrario, el esquema de [3] precisó de tres a cuatro iteraciones del método de Newton para cada paso de tiempo lo que supuso un gasto de 6 horas en un ordenador Sun Ultra Sparc por unidad de tiempo.

1.2. Aniquilación de singularidades con flujo rotativo

Este ejemplo parte del mismo vector inicial de orientación del caso anterior (ver Figura 10). Ahora, el vector de velocidad inicial será considerado rotativo. Más concretamente, $\mathbf{u}_0(x, y) = (-20y, 20x)$. Las Figuras 11, 12 y 13 muestran el comportamiento en cuatro tiempos diferentes del campo de vectores directores para el valor $\varepsilon = 0,07$. El campo de velocidades se mantiene rotativo.

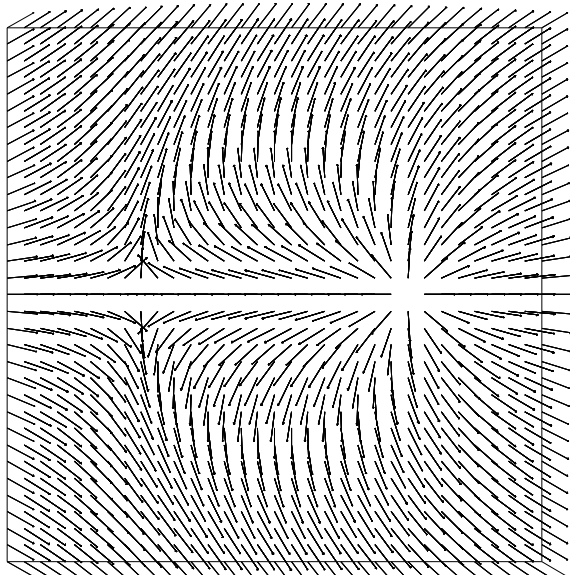


Figura 10: Vector director $t=0$

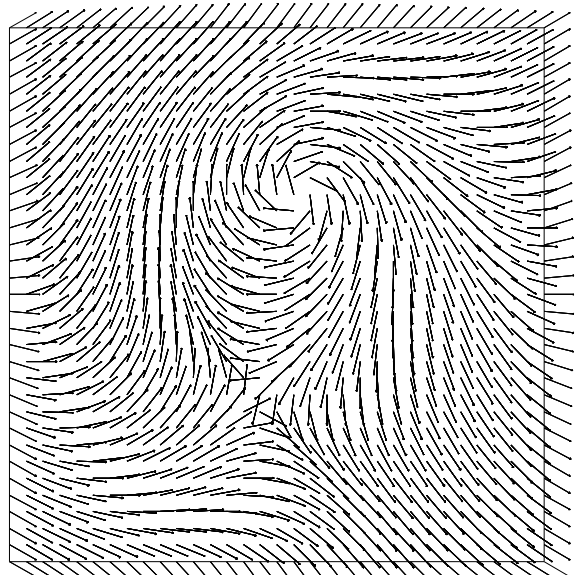


Figura 11: Vector director $t=0.1$

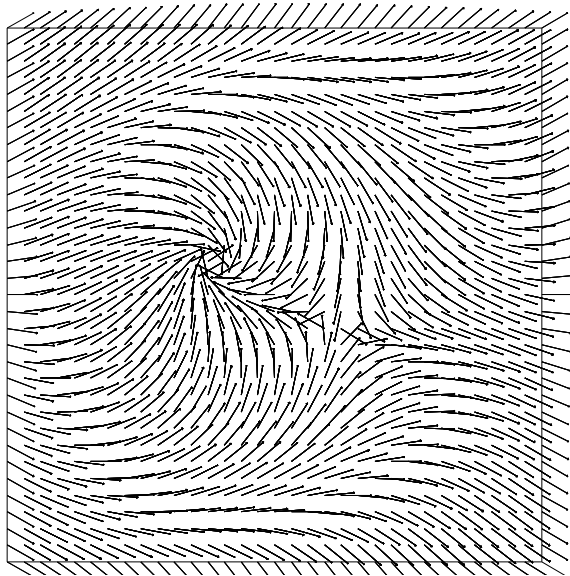


Figura 12: Vector director $t=0.2$

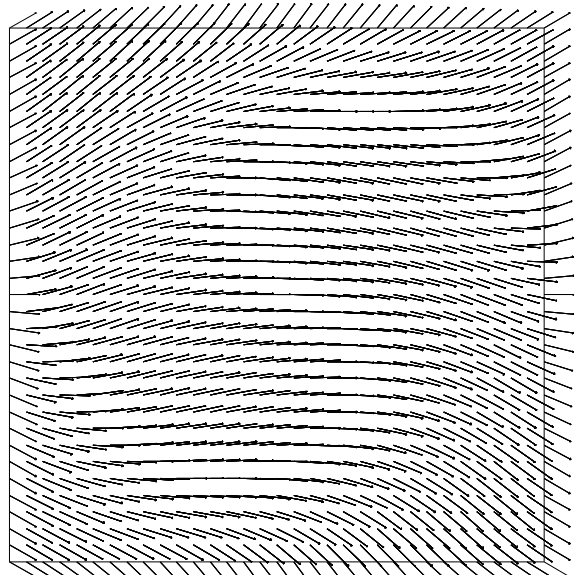


Figura 13: Vector director $t=0.5$

Cuando $\varepsilon = 0,06$ y el mismo vector director inicial (ver Figura 14) las singularidades se mueven como en $\varepsilon = 0,07$. Las gráficas en los tiempos $t = 0,1$, $t = 0,2$ y $t = 0,5$ son análogas. En las Figuras 15, 16 y 17 vemos la aparición de oscilaciones en la solución numérica del vector director, lo que puede ser debido a que el condicionamiento del sistema lineal del esquema empeora cuando ε va a cero.

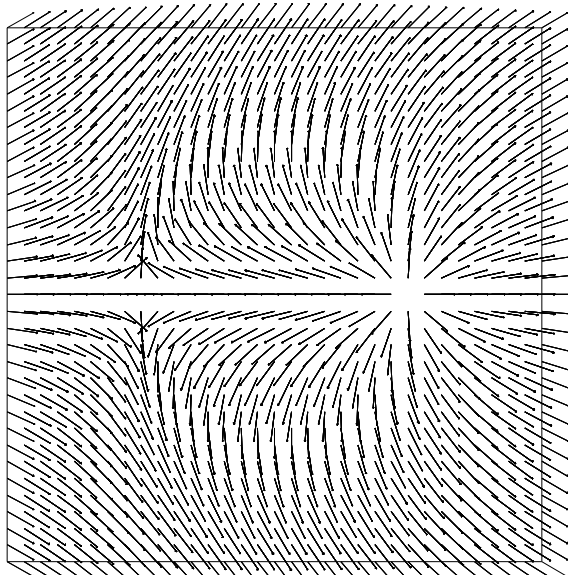


Figura 14: Vector director $t=0$

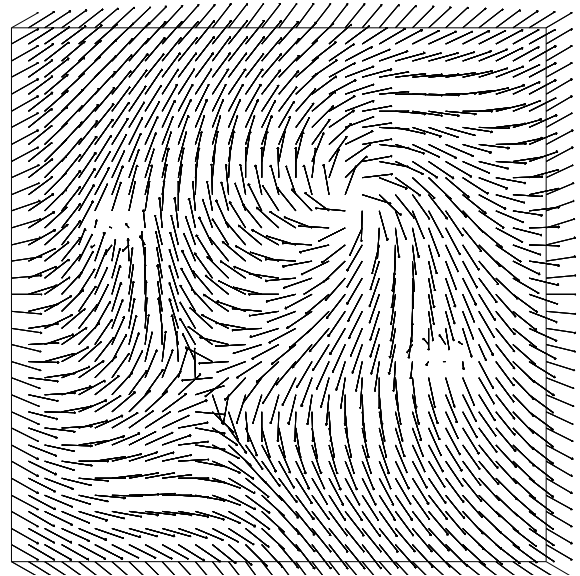


Figura 15: Vector director $t=0.06875$

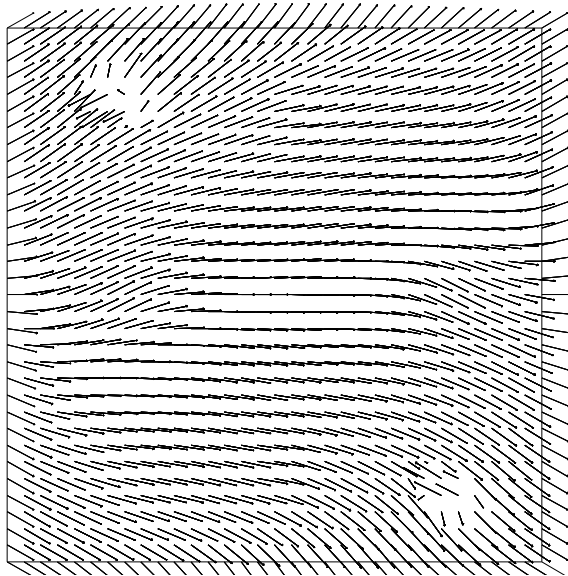


Figura 16: Vector director $t=0.3812$

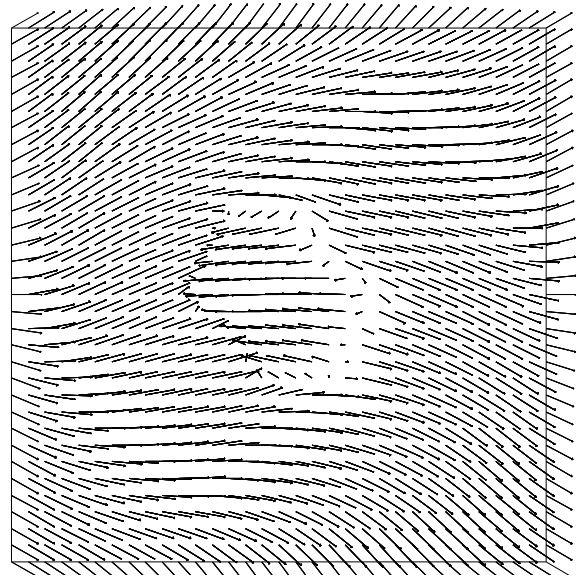


Figura 17: Vector director $t=0.5$

Esta dinámica de las singularidades para $\varepsilon = 0,06$ y $0,07$ es la misma que la obtenida en [3] para $\varepsilon = 0,05$. En nuestro esquema los tiempos de aniquilación son $t = 0,25s$ y $t = 0,28125s$ para $\varepsilon = 0,06$ y $0,07$ respectivamente frente a $t = 0,20s$ del esquema de [3].

Los tiempos de ejecución son $981.968s$ para $\varepsilon = 0,06$ y $965.409s$ para $\varepsilon = 0,07$ por unidad de tiempo.

2. Nuevas experiencias numéricas

2.1. Dos singularidades con distinto signo

Ahora estudiamos el ejemplo de dos singularidades situadas en $(\pm 1/2, 0)$ que se repelen a largo del eje x hasta una posición de equilibrio determinada por la influencia de las condiciones frontera. Tomamos ahora el vector director inicial:

$$\mathbf{d}_0 = \hat{\mathbf{d}} / \sqrt{|\hat{\mathbf{d}}|^2 + 0,025},$$

donde $\hat{\mathbf{d}}(x, y) = (x^2 - y^2 - 0,25, 4xy)$. La velocidad inicial es cero. Para esta experiencia numérica elegimos $\varepsilon = 0,06$. La evolución del vector director y velocidad es como sigue en las Figuras 18, 19, 20 y 21:

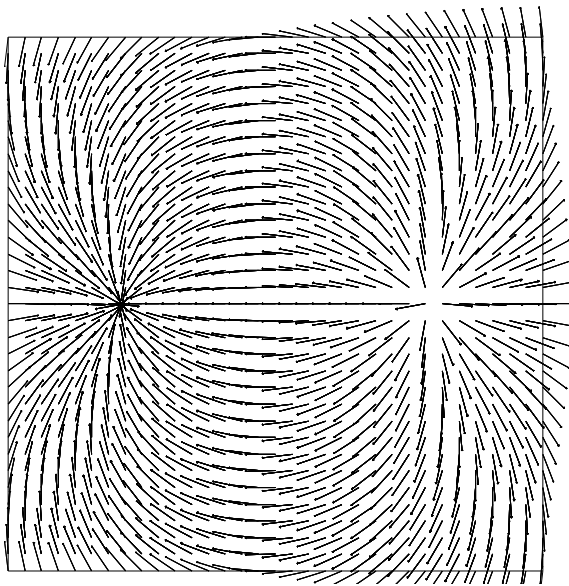


Figura 18: Vector director $t=0.0625$

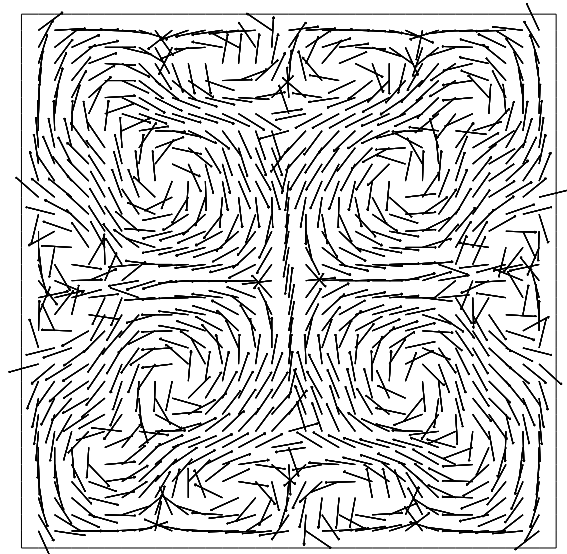


Figura 19: Velocidad $t=0.0625$

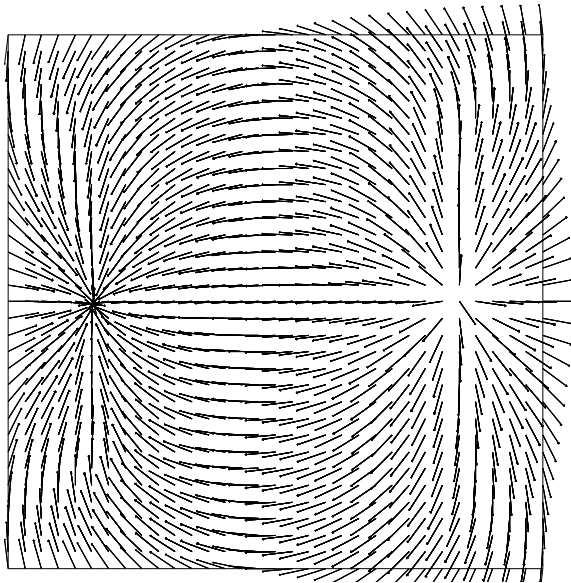


Figura 20: Vector director $t=0.5$

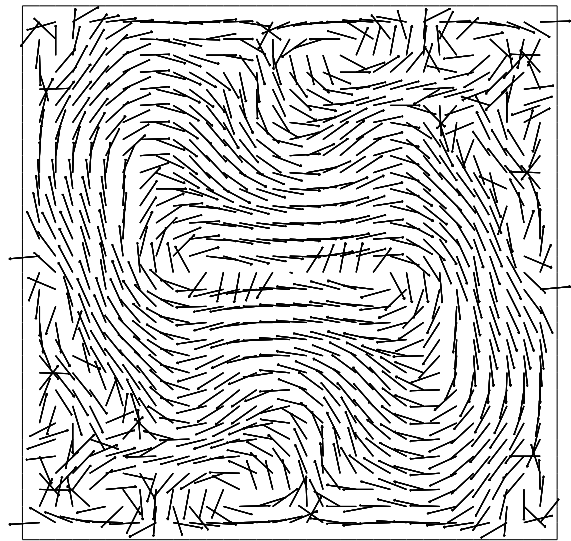


Figura 21: Velocidad $t=0.5$

Un comportamiento algo diferente en lo que se refiere a la velocidad se consigue si elegimos $\varepsilon = 0,08$ como se puede ver las Figuras 22, 23 24 y 25. De nuevo se observa la gran sensibilidad del campo de velocidades respecto al parámetro de penalización ε :

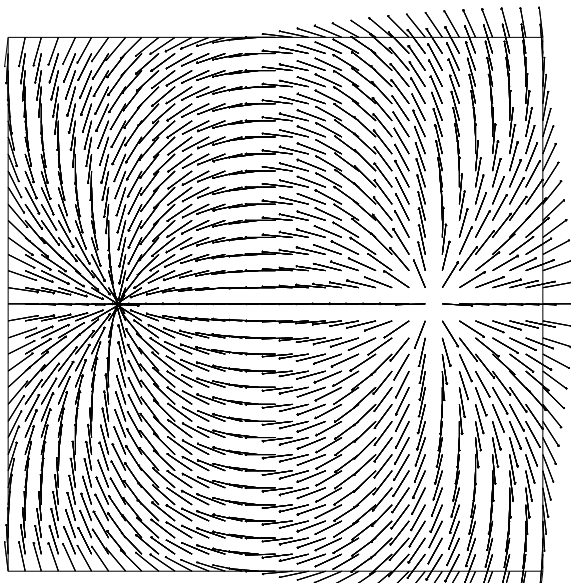


Figura 22: Vector director $t=0.0625$

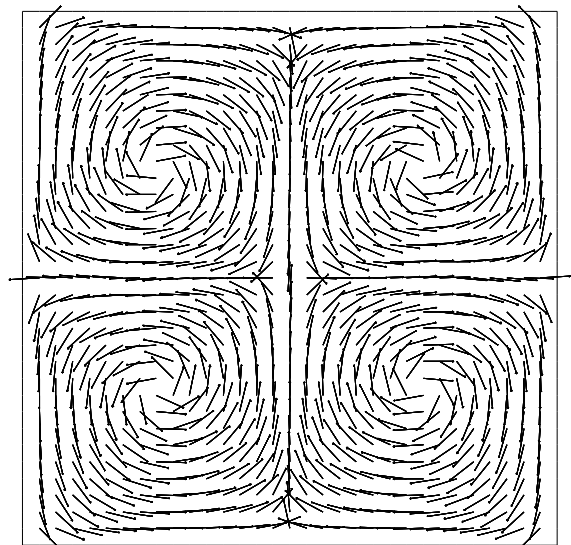


Figura 23: Vector director $t=0.0625$

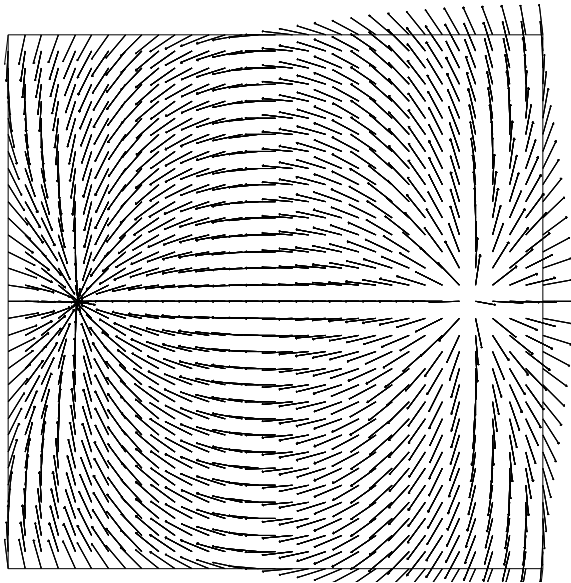


Figura 24: Vector director $t=0.5$

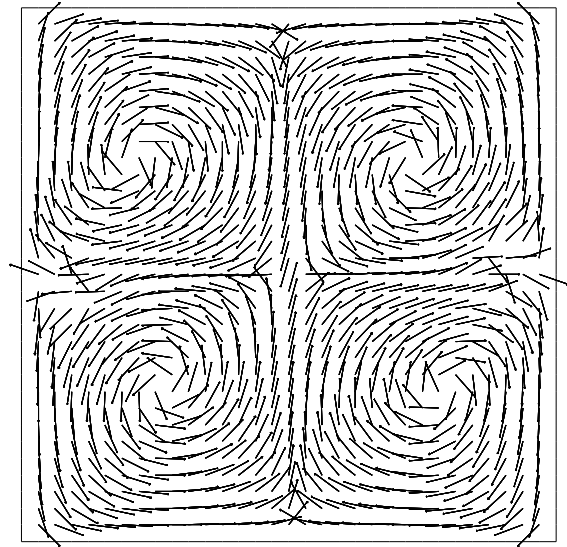


Figura 25: Vector director $t=0.5$

2.2. Una singularidad de orden cuatro

Como último ejemplo consideramos de nuevo una velocidad inicial cero y elegimos un vector de orientación que tiene una singularidad en el origen de coordenadas de orden cuatro que conseguimos eligiendo $\hat{\mathbf{d}}(x, y) = (x^4 - 6x^2y^2 + y^4, 4xy(x^2 - y^2))$ y componiendo \mathbf{d}_0 como en los casos anteriores. El parámetro de penalización es seleccionado igual a $\varepsilon = 0,06$.

La singularidad de orden 4 en el origen evoluciona descomponiéndose en cuatro singularidades que se dirigen hacia las esquinas del dominio empujadas por el campo de velocidades generado, donde se mantienen por la influencia de las condiciones de contorno. Esto se muestra en las Figuras 26, 27, 28 y 29:

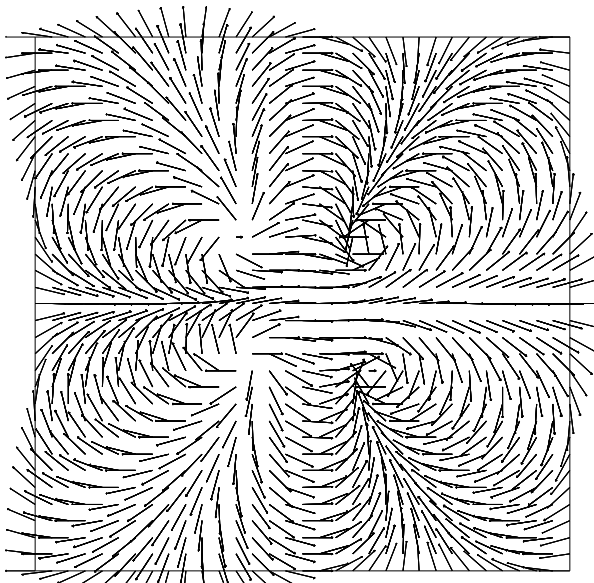


Figura 26: Vector director $t=0.0625$

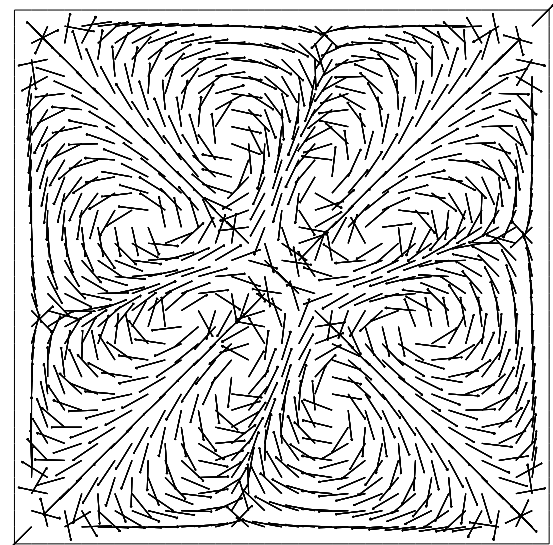


Figura 27: Vector director $t=0.0625$

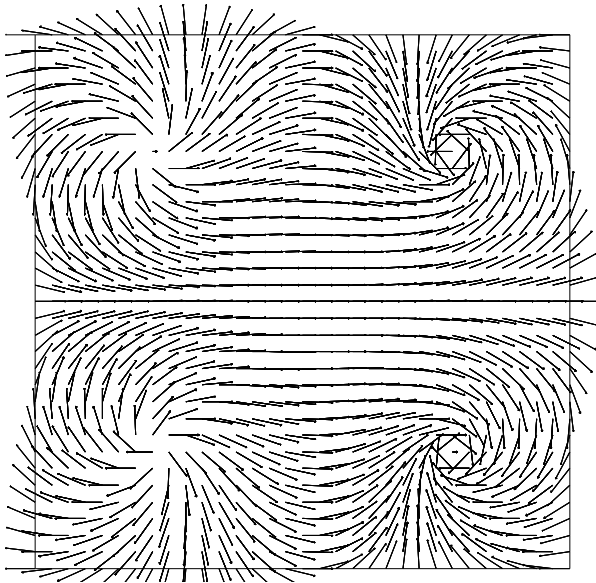


Figura 28: Vector director $t=0.2$

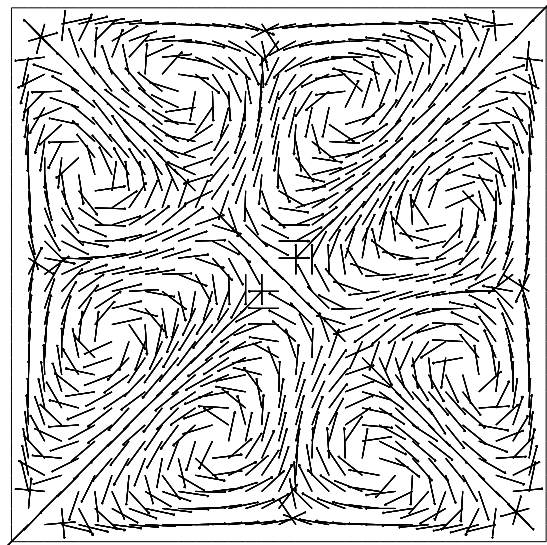


Figura 29: Vector director $t=0.2$

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