



The role of physical processes controlling the behaviour of radionuclide contaminants in the aquatic environment: a review of state-of-the-art modelling approaches

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ABSTRACT

This paper is aimed at presenting and discussing the methodologies implemented in state-of-the-art models for predicting the physical processes of radionuclide migration through the aquatic environment, including transport due to water currents, diffusion, settling and re-suspension. Models are briefly described, model parameter values reviewed and values recommended. The different modelling approaches are briefly classified and the advantages and disadvantages of the various model approaches and methodologies are assessed.

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1. Introduction

Physical processes in water bodies play a major role in controlling the behaviour of contaminants in the aquatic environment. These processes may directly determine the spatial distributions of pollutants through water movements (currents, waves, turbulence) and may affect the ecological conditions of the aquatic system.

In principle, modelling the behaviour of contaminants in aquatic ecosystems requires the quantitative assessment of hydraulic, geochemical, sedimentological, ecological and anthropogenic phenomena (Monte et al., 2005). The main aim of the present paper is to review and assess the methodological approaches implemented in state-of-the-art models to deal with those phenomena that are predominantly physical in nature:

- (1) Transport by the water current;
- (2) Dispersion caused by gradients of concentration and the turbulent motion of water.

Physical processes are also involved in the settling and re-suspension of contaminated sediments, although geochemical,

geological and sedimentological phenomena play more important roles in determining the radionuclide fluxes from the water column to bottom sediments and vice-versa (Monte et al., 2003).

An analysis of available experimental values of the empirical quantities that parameterise the processes is undertaken.

2. Fluid dynamics

The migration of contaminants through a water body is primarily controlled by the dynamics of water masses. State-of-the-art models are based on various approaches to solve this complex problem. However two main methodologies are generally applied.

The first approach is based on the use of the water balance equation and on the correlation of the water body morphometry (average width, depth and length) with the water fluxes. This methodology requires the knowledge of averaged values of some input quantities such as the precipitation rates, the contribution of water from the catchments, etc. to determine the water fluxes averaged over a specific time interval (for instance, one month). The balance equation can be written as follows:

$$q = RS - ES + F_{in} - \frac{dV}{dt} \quad (1)$$

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where q is the water outflow ($\text{m}^3 \text{s}^{-1}$), S and V are the surface (m^2) and the volume (m^3) of the water body, respectively, R is the rainfall rate onto the water surface (m s^{-1}), E is the evaporation rate (m s^{-1}) and F_{in} is the total contribution of water flux ($\text{m}^3 \text{s}^{-1}$) to the water body from the catchment or from any other water source. The approach is frequently used by the “box models”, aimed at assessing the contaminant concentrations averaged over defined region of the water body.

In case of rivers, the morphometric characteristics of the water body are often related to the water fluxes (IAEA, 2001; Håkanson, 2005). It is assumed that depth (h), width (W), water flux (q) and water velocity (U) in a river are related by the following empirical relationships (Leopold and Maddock, 1953):

$$h = aq^\alpha; \quad W = bq^\beta; \quad U = cq^\gamma \quad (2)$$

Since $q = hWU$ the constraints are

$$\alpha + \beta + \gamma = 1; \quad abc = 1 \quad (3)$$

From Eq. (2), it is possible to obtain the flux q as function of the volume and the water body length (L):

$$q = \left(\frac{V}{abL} \right)^{1/(\alpha+\beta)} \quad (4)$$

Substituting Eq. (4) in (1) we obtain a non-linear differential equation that yields the volume and, therefore, the flux q as function of time when F_{in} , R and E are known. If it is possible to hypothesise that the derivative of the water volume with respect to time is negligible (constant volume), (1) becomes an algebraic equation. This hypothesis is often assumed for lakes.

IAEA (2001) recommends the following values: $a = 0.163$, $\alpha = 0.447$, $b = 10$, $\beta = 0.460$ (provided that lengths are in m and time in s). EPA (1997) suggests that α ranges from 0.3 to 0.5 and β from 0 to 0.2. Seasonal estimates of R , E and F_{in} are available for specific geographic regions and aquatic systems in most cases. Nevertheless, methods have been developed to evaluate these quantities from information that can be easily achieved. For instance, when empirical evaluations are not available, the mean annual value of F_{in} can be approximated by the following semi-empirical formula (Håkanson, 2005):

$$F_{\text{in}} = \frac{10^{-8}RS_c}{650} \quad (5)$$

where S_c is the catchment area measured in m^2 , R is measured in mm y^{-1} and F_{in} is in $\text{m}^3 \text{s}^{-1}$. Moreover, Håkanson (2005) suggests that the river length can be estimated from the catchment area as follows:

$$L = 10^{-5}S_c \left(L \text{ is in m and } S_c \text{ in } \text{m}^2 \right) \quad (6)$$

The above formulae were obtained by assessing morphometric data of European rivers and are recommended for watercourses characterised by an average water discharge ranging from 1 to $500 \text{ m}^3 \text{ s}^{-1}$.

It should be noted that, in case of rivers, the evaporation in Eq. (1) can be, generally, neglected whereas evaporation is an important term in the water balance of lakes. Models for predicting evaporation from lake surfaces are based on complex thermodynamic processes occurring at the lake surface (Jørgensen et al., 1983).

The second approach to predict the dynamics of water makes use of fundamental laws of physics implemented in the so-called Navier–Stokes and continuity partial-derivative equations to determine the velocity field of water (water current as function of time and of spatial co-ordinates) and the water elevation. Any

attempt to treat this complex subject in the present paper is pretentious. Consequently, we will try to outline some of the main methodological principles underpinning it. The Navier–Stokes equation is basically derived from the Newton’s second law. Therefore, the application of such an equation requires the evaluation of the forces acting on the water mass. Among these, the Coriolis’ force due to the earth rotation can be significant in large water bodies like seas. Other forces are the wind stress and the bed friction. Their assessment can be done by semi-empirical formulae (Periáñez, 2005a). The motivations of the Navier–Stokes and continuity equations can be found in specialised textbooks (Daily and Harleman, 1973), while an application of the methods to practical cases of radionuclide migration through rivers can be found in Zheleznyak et al. (1992).

The solution of Navier–Stokes equation requires the application of suitable numerical methods (finite differences or finite elements). As the descriptions of the principles of these methods are beyond the scope of the present paper, interested readers are referred to the literature (Vreugdenhil, 1998; Kowalick and Murty, 1993).

3. Diffusion and dispersion

Diffusion is the process that implies a movement of molecules from regions of space of high concentration to regions of low concentration. The radionuclide flux, \mathbf{F} ($\text{Bq m}^{-2} \text{ s}^{-1}$), due to diffusion is related to the concentration gradient (Fick’s first law):

$$\mathbf{F} = -\mathbf{K}^* \mathbf{C} \quad (7)$$

where \mathbf{grad} is the gradient of C ($C = \mathbf{i}(\partial/\partial x)C + \mathbf{j}(\partial/\partial y)C + \mathbf{k}(\partial/\partial z)C$), C is the radionuclide concentration in water, and \mathbf{i} , \mathbf{j} and \mathbf{k} are the unit vectors along the coordinate axes x , y and z . \mathbf{K} is a 3×3 component symmetric tensor (the diffusion tensor).

The diffusion process is due to the thermal motion of molecules (molecular dispersion) and depends on the mass of the particles. Nevertheless, the dispersion of pollutant due to disordered, turbulent motion of water is usually modelled by Eq. (7) by analogy with Fick’s first law (eddy diffusion).

The turbulent motion of water is the major component of the overall diffusion process (molecular and eddy). Consequently, the dispersion of a pollutant, being mainly due to turbulence, is independent of the characteristics of the pollutant itself.

The tensorial form of Eq. (7) highlights that, in principle, dispersion is a non-hisotropic processes occurring in the three dimensions. When the dispersion tensor is reduced to the principal axes, the radionuclide flux due to the dispersion processes occurring in longitudinal (x), transversal (y) and vertical directions (z) is as follows:

$$\mathbf{F}(x, y, z, t) = -\mathbf{K}_x \cdot \frac{\partial C(x, y, z, t)}{\partial x} \mathbf{i} - \mathbf{K}_y \cdot \frac{\partial C(x, y, z, t)}{\partial y} \mathbf{j} - \mathbf{K}_z \cdot \frac{\partial C(x, y, z, t)}{\partial z} \mathbf{k} \quad (8)$$

We assess the three terms in Eq. (8) separately.

3.1. Vertical dispersion

In shallow or well-mixed water bodies vertical dispersion is a rapid process. Consequently, it is commonly assumed that the concentration of a radionuclide in the water column quickly reaches a homogeneous vertical profile.

The vertical dispersion coefficient in a river can be assessed by the following approximate equation (Fisher et al., 1979):

$$K_z = 6.7 \times 10^{-2} \cdot h \cdot u^* \quad (9)$$

where u^* is the friction velocity (m s^{-1}). The geometric mean of the ratio u^*/U , calculated from the analysis of data reported by IAEA (2001) and EPA (1997) concerning more than 30 rivers in North America, is 0.12 with a standard deviation of the natural logarithm of 0.78. For instance, a current velocity of the order of 1 m s^{-1} and a depth of few meters, would give a vertical dispersion coefficient of the order of $10^{-2} \text{ m}^2 \text{ s}^{-1}$.

In deep water bodies, different densities of water layers may induce stratification that will give low values of the vertical dispersion coefficient K_z . A typical example is the thermal stratification of water characterised by the formation of a thermocline, a sharp vertical gradient in temperature, in an intermediate layer of the water column. Different salinity levels in coastal areas can also give rise to stratification (halocline). Similarly, a chemocline is defined as the water layer showing a significant gradient of a dissolved chemical substance and a lutocline is a gradient in suspended matter concentrations. Stratification can be responsible for the inhomogeneous distribution of pollutants, dissolved substances and planktonic biota in the water column.

Several empirical estimates of the vertical eddy dispersion coefficient are available from the literature (Table 1). These were generally obtained by calibration of the dispersion equation for predicting the distribution of dissolved substances in the water column. Furthermore, K_z may be evaluated from the water thermal conductivity. From thermodynamic and hydrodynamic considerations (Daily and Harleman, 1973) it follows:

$$\rho c_p K_z = k \quad (10)$$

where ρ is the water density (kg m^{-3}), c_p is the specific heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$) of water (constant pressure) and k is the thermal conductivity ($\text{J s}^{-1} \text{m}^{-1} \text{K}^{-1}$).

A selection of values of vertical eddy diffusion coefficient was reported by Jørgensen (1979) from an analysis of literature data on parameters used in ecological models. The values for the epilimnion (the upper well-mixed water layer in stratified lakes) were of the order of 10^{-2} – $10^{-4} \text{ m}^2 \text{ s}^{-1}$. Such high values are induced by mechanical processes of water turbulence, such as the wind action, and by the diurnal cycles of warming and cooling.

The vertical diffusion coefficient through the thermocline (or chemocline/halocline), during stratification is orders of magnitude lower (6×10^{-9} – $10^{-6} \text{ m}^2 \text{ s}^{-1}$). The lowest values of K_z in Quay et al. (1979) were measured at specific hours of the day. In general, the daily maximum values were at least one order of magnitude higher.

Deep lakes show higher values of the vertical diffusion coefficient in the epilimnion than shallow lakes. Consequently, from the values reported here, it is possible to conclude that the contaminant is homogeneously distributed in the epilimnion of a lake after a few days. Intermediate values of K_z were obtained for the hypolimnion. A selection of recommended values of vertical diffusion coefficient for practical applications is reported in Table 2.

Stratification in rivers is less frequent than in lakes and coastal waters due to turbulence. Nevertheless, deep, gently meandering rivers may stratify.

The vertical diffusion coefficient in the sea depends on depth and stability of the water column. Typical values of the vertical diffusion coefficient representative of coastal waters, used in several models, are of the order of $10^{-3} \text{ m}^2 \text{ s}^{-1}$ (Parker, 1991; Perriáñez, 2004; Schonfeld, 1995). These values are similar to those for lake epilimnion (Table 1).

K_z may also be calculated by turbulence models (Perriáñez, 2005b), but this is a complex and time consuming approach.

3.2. Transversal and longitudinal dispersion

Horizontal transport in lake surface water is caused by currents and is induced by the effect of wind. Changes in wind intensity and direction can induce disorganised water movements. The horizontal diffusion coefficient in lakes can be several orders of magnitude higher than K_z through the thermocline. Values ranging from 10^{-3} to $10^{-2} \text{ m}^2 \text{ s}^{-1}$ were measured by Quay et al. (1979).

Evaluations of longitudinal and transversal dispersion coefficients in rivers are available from the literature. IAEA (2001) suggests values ranging from 7.6×10^{-1} to $1.5 \times 10^3 \text{ m}^2 \text{ s}^{-1}$ and from 4.8×10^{-3} to $1.1 \text{ m}^2 \text{ s}^{-1}$ for, respectively, the longitudinal (K_x) and the transversal (K_y) dispersion coefficients in several North America rivers. It is generally recognised that values of these parameters are higher in large rivers. Moreover, the values of the dispersion coefficients in a river are strongly influenced by the water velocity. Turbulence effects imply that, in a given river, the dispersion coefficient increases with the water flux. For example, evaluations derived from dye tracer experiments in the River Thames (Smith et al., 2006) suggested the quadratic relationship $K_x = 0.0148Q^2 + 0.33Q$ between the longitudinal dispersion coefficient ($\text{m}^2 \text{ s}^{-1}$) and the water flux Q ($\text{m}^3 \text{ s}^{-1}$). The range of the corresponding empirical values of K_x was from 0.09 (low flows) to $49 \text{ m}^2 \text{ s}^{-1}$.

Table 1
Selected values of the vertical dispersion coefficient.

Values ($\text{m}^2 \text{ s}^{-1}$)	Environment	Methodology	Reference
10^{-9} – 10^{-8}	Lakes, thermocline	Injection of tritiated water in two small temperate dimictic lakes	Quay et al. (1979)
1.5×10^{-7}	Dispersion across chemocline in stagnant lake	Calibration of a model	Landing (1991)
1×10^{-6}	Dispersion across thermocline. Lakes in central Italy	Calibration of a model to predict the dispersion of dissolved ^{134}Cs of Chernobyl origin in water	Monte et al. (1991)
10^{-2}	Lakes, epilimnion	Collection of literature data	Jørgensen (1979)
3.5×10^{-4}	Irish Sea (above thermocline)	Calibration of a model to predict chlorophyll and nitrate concentrations	Parker (1991)
6×10^{-5} – 1×10^{-2}	Epilimnion, Lakes Erie and Ontario (Canada)	H_2O_2 used as a natural, photochemically produced tracer. Values were measured at specific hours of the day (minimum value at 15 h, maximum at 12 h)	Scully et al. (1998)
5×10^{-6} – 5×10^{-4}	Epilimnion, Jacks Lake (Canada)	H_2O_2 used as a natural, photochemically produced tracer. Values were measured at specific hours of the day (minimum value at 17 h, maximum at 14 h)	Scully et al. (1998)
6×10^{-4}	Lakes in central Italy. From epilimnion to deep water during mixing	Calibration of a model to predict the dispersion of dissolved ^{134}Cs of Chernobyl origin in water	Monte et al. (1991)
10^{-7} – 10^{-5}	Dispersion in deep water layer. Lake Baikal	Calibration of a model to predict dispersion of substances	Kipfer et al. (2000)
10^{-7} – 10^{-6}	Lakes, hypolimnion	Injection of tritiated water in two small temperate dimictic lakes	Quay et al. (1979)
1×10^{-4}	Dispersion in deep layers below thermocline	Literature data	Jørgensen (1979)
7×10^{-7} – 5.6×10^{-6}	Dispersion across thermocline of Lake Lugano	From an analysis of water temperature profile during water stratification (assessed data in graphical form)	Rossi et al. (1983)

Table 2
Recommended ranges and values of vertical dispersion coefficient in lakes.

Range ($\text{m}^2 \text{s}^{-1}$)	Value ($\text{m}^2 \text{s}^{-1}$)	Water layer
$<10^{-6}$	10^{-7}	Through thermocline
$>10^{-4}$	10^{-3}	Epilimnion
10^{-7} – 10^{-4}	10^{-4} (accounting for the different stratification conditions during the year)	Hypolimnion

EPA (1997) suggests:

$$K_x = k \frac{U^2 W^2}{hu^*} \quad (11)$$

where k is a dimensionless constant. Typical values of k range from 0.011 (EPA, 1997) to 0.033 (IAEA, 2001). The range of the empirical evaluation of K_x reported by IAEA (2001) was from <1 to $>1000 \text{ m}^2 \text{ s}^{-1}$, depending on the river's hydrological characteristics.

For rivers with little meandering, Sayre (1973) suggested that K_y can be approximated by a semi-empirical formula such as

$$K_y = 0.6 \cdot h \cdot u^* \quad (12)$$

giving ordinary values of 10^{-2} – $10^{-1} \text{ m}^2 \text{ s}^{-1}$. IAEA (2001) suggests ranges from approximately 10^{-2} to $1.1 \text{ m}^2 \text{ s}^{-1}$. Extensive descriptions of sub-models for predicting the longitudinal and transverse dispersions are available in literature (Won Seo et al., 1998; Jobson, 1997; Gharbi and Verrette, 1998).

Averaged over time, the dispersion coefficient in coastal waters can be higher (order of magnitude $10^2 \text{ m}^2 \text{ s}^{-1}$) than the values measured in rivers in view of the mixing effects produced by tides.

4. Transport by the current

Whereas diffusion is due to the turbulent components of the water flow, transport is related to the average, ordered water movement.

The radionuclide flux due to water transport is related to the concentration C of radionuclide (Bq m^{-3}) and to the water velocity U (m s^{-1}) by the following equation:

$$F = UC \quad (14)$$

Eq. (14) was obtained by dividing the total amount of substance flowing, per unit time, over the surface S , by the surface area.

It is quite obvious that parameter U in the pollutant transport equation is of hydrological nature and is independent of the pollutant. Ordinarily, U in rivers ranges from few decimetres per second to $>1 \text{ m s}^{-1}$, depending on the river characteristics and on the hydraulic regime. Water current is also a significant transport mechanism of radionuclides in coastal waters as result of the tides. Tidal currents can reach 1 m s^{-1} in dynamic environments (e.g., the Straits of Gibraltar or the English Channel).

Transport and diffusion processes are implemented in the so-called advection–diffusion equation for predicting the dispersion of contaminant in water (Onishi, 1994).

5. Migration to and from sediments

The migration of radionuclide from the water column to bottom sediments and vice-versa is a complex process involving the interaction between dissolved and solids phases of the contaminant and the sedimentation and re-suspension of particulate matter. The treatment of this subject pertains more properly to geochemistry and sedimentology rather than to physics. Nevertheless, for the sake of completeness, we give a brief review of the

methodologies used for modelling this important process of radionuclide migration.

The process of interaction of dissolved radionuclides with solids particles in suspension or deposited, is usually modelled according to the “ k_d concept” (k_d = partition coefficient “particulate form/dissolved form”) based on the notion of a reversible and rapid equilibrium between the dissolved and the adsorbed phases of the radionuclide. Recommended screening values of k_d for several radionuclides and for both marine and fresh waters are reported by IAEA (1982, 2001). However, this rapid equilibrium is not true for all contaminants. The equilibrium between the concentrations of the dissolved and the attached phases may be not instantaneously achieved and the adsorption–desorption processes are not always rapidly reversible (Ciffroy et al., 1996; Comans and Hockley, 1992; Smith and Comans, 1996; Smith et al., 2000) and can occur in several stages (Børretzen and Salbu, 2002). Moreover, the processes may depend on the different kinds of suspended matter in the water column and on the chemical characteristics of the water. Madruga (1993) reported an extensive study of the sorption–desorption process for Cs and Sr in sediments.

The main physical process involved in the migration of radionuclide to and from bottom sediments is the settling of contaminated suspended particles and the re-suspension of contaminated sediment particles. To model these processes two main approaches are available: (a) application of fundamental equations derived from physics, such as the Stokes' theorem to calculate the settling velocity, in order to determine the particulate matter; or (b) assessment of contaminant macro-fluxes using process aggregation.

It is very difficult to apply approach (a) and very often semi-empirical formulae are used to evaluate sedimentation and re-suspension rates of particulate matter. For instance, such an approach was used to predict the behaviour of contaminants from Chernobyl in the Dnieper River (Zheleznyak et al., 1992).

The most simple and direct application of process aggregation methodology account for three main radionuclide fluxes:

- Flux of contaminant from water to bottom sediment: $F_{ws} = v_{ws} C_w$;
- Flux of contaminant from bottom sediment to water: $F_{sw} = K_{sw} D_s$;
- Flux of contaminant from “active” bottom sediment to “passive” sediment: $F_{ds} = K_{ds} D_s$.

where v_{ws} (m s^{-1}) is the radionuclide migration velocity from water to bottom sediment and K_{sw} (s^{-1}) and K_{ds} (s^{-1}) are, respectively, the rate of radionuclide migration from sediment to water and of radionuclide migration to passive sediment, C_w is the radionuclide concentration in water and D_s is the radionuclide deposition (Bq m^{-2}) in sediment. Following the analysis of data from severe accidents in recent decades, evaluations of aggregated parameters v , K_{sw} and K_{ds} are available for ^{90}Sr and ^{137}Cs . Table 3 shows indicative ranges of values for ^{90}Sr and ^{137}Cs from a literature assessment (Smith et al., 2002, 2005; Monte, 2001; Monte et al., 2002, 2003; IAEA, 2000). Data on deposition velocity of plutonium are available for the Great Lakes in North America and the relevant range is from 1×10^{-6} to $3.5 \times 10^{-6} \text{ m s}^{-1}$ (Shukla, 1993).

Table 3
Examples of model parameter values for ^{137}Cs and ^{90}Sr in freshwater environment.

Parameter	^{137}Cs	^{90}Sr
v (m s^{-1})	3×10^{-7} – 3×10^{-6}	1×10^{-8} – 1×10^{-7}
k_s (s^{-1})	6×10^{-9} – 2×10^{-8}	$<10^{-10}$ – 1×10^{-9}
k_{sw} (s^{-1})	1×10^{-8} – 3×10^{-8}	6×10^{-10} – 6×10^{-9}

6. Discussion and conclusions

Fluid dynamics processes and sedimentation–re-suspension of radionuclides in water are modelled according to two main methodological approaches. The first one makes use of equations derived from fundamental laws of physics such as the Newton's second law implemented in the Navier–Stokes equation or the Stoke's theorem to calculate particle-settling velocities. This approach is usually called “reductionist” as it is based on the principle that the functioning of complex systems can be understood and, therefore, simulated by some fundamental laws of general nature. The solution of the transport (advection–diffusion) equation in reductionistic models may be treated in an Eulerian or a Lagrangian framework. The last is very useful for models developed to support the decision-making process after an accident since the method is well suited for problems when large concentration gradients are involved (numerical dispersion is not introduced) and very fast answers may be obtained (Periáñez, 2005c, 2006).

In contrast, the second approach is based on the use of semi-empirical formulae aimed at evaluating the most important quantities necessary to model the migration processes from a low number of easily achievable data and makes an extensive usage of the principle of “process aggregation”. Section 2 shows how, when site-specific data are not available, appropriate sub-models allow one to obtain estimates of the main morphometric and hydrological parameters necessary for assessing the migration of contaminants in rivers. It is quite obvious that, at least in principle, the time and spatial resolution of the results of such a kind of models cannot achieve the detail of the “reductionist” models that are aimed at assessing values of water velocity, water elevation, water fluxes, etc. as function of time and space at any level of resolution (at least in principle).

Although, it has been argued that “reductionistic” models often require huge amounts of data and information, such as the (time-dependent) boundary conditions for the Navier–Stokes partial differential equations, that are never easy to obtain or to account for (the effects of obstacles, of aquatic vegetation, etc.) or are often very uncertain and influenced by many variable environmental factors, it should be recognised that these kind of models are a powerful and essential tool for a better understanding of the processes dynamics of complex aquatic systems. The advantages from the use of different kind of models for solving similar environmental problems were presented and discussed following an exercise of model application (Monte et al., 2006) (<http://www-ns.iaea.org/projects/emras/>).

It should be noted that “aggregated” models can supply, for practical applications, more reliable results when site-specific, rather than generic values, of their parameters are used. This is possible in several cases for the hydrological sub-model if series of empirical data of precipitation rates, water fluxes and related morphometric data are available.

Generally, diffusion is a very complicated process. In rivers, the water current is not uniform across the water column, having a maximum value at the surface and decreasing with depth due to friction against the bottom. This velocity profile is the cause of the shear dispersion. If a radionuclide is released at the surface, it is partially transported downwards in the water column due to dispersion. However, radionuclides at the surface are advected faster than radionuclides at deeper locations since velocity at the surface is greater. Thus, the volume of contamination suffers a deformation along the direction of the current in the upper part of the water column. The overall result is an enhanced dispersion in the current direction. Shear dispersion is included in 3-dimensional dispersion models, since they solve the vertical current profile, but not in 2-dimensional, depth averaged models. Horizontal shear

stress also produces shear dispersion. In a river, currents are stronger at the centre than along shores due to friction. The shear effect will enhance mixing along the channel. In 2-dimensional dispersion models this is included since the hydrodynamic model automatically produces the current distribution outlined above. However, if a 1-dimensional model is applied, the effective dispersion coefficient must be increased to account for this horizontal shear.

The effective dispersion coefficient depends on the spatial grid size used in the numerical solution of the diffusion equation: coarse grids require larger dispersion coefficients because larger eddies cannot be solved and their effects have to be described as turbulent mixing. The following empirical parameterization has been proposed for the horizontal diffusion coefficient (Dick and Schonfeld, 1996) and used in several models:

$$K = 0.2055 \times 10^{-3} \Delta x^{1.15} \quad (15)$$

where Δx is the grid cell size. The values of the diffusion coefficient should be selected not only on the basis of the physical characteristics of the studied area (for instance current magnitude), but also accounting for the model structure (1-D, 2-D or 3-D) and resolution. Moreover, it should be noted that, in watercourses, the effects of dispersion of radionuclide are complicated by the presence of obstacles such as islands and aquatic vegetation. Consequently, although dispersion is an important process controlling the distribution of radionuclide in water, it is difficult to make predictions of contaminant distribution in water with a spatial resolution that requires accurate evaluations of the diffusion coefficients as function of the position.

To obtain an idea of the uncertainty associated with the diffusion coefficient in water it is sufficient to compare the results of formula (12) with empirical evaluation of the coefficient reported by IAEA (2001). The ratio “calculated/observed” values range from 0.083 to 2.68 with a geometric mean of 0.91 and a standard deviation of the natural logarithm of 0.98 (68% of values within almost one order of magnitude).

It should be noted that, on the basis of the values of diffusion coefficients, in the order of a few days or weeks are required for achieving relatively complete transversal mixing. In case of steady state (the contaminant input rate is a constant independent of time) point-source conditions, a complete transversal mixing in a river is achieved when $(x/L) \gg (K_x/K_y)$, where x is the distance from the contaminant source and L is the width of the river. Therefore, for medium and long-term predictions and for quasi-stationary contamination conditions, both transversal and longitudinal dispersion in rivers do not significantly influence the model results in view of the predominant effect of the contaminant transport by the current.

Vertical stratification of water can have a significant influence on the distribution of radionuclides in aquatic systems. When the vertical stratification shows an almost stable seasonal behaviour (as typically occurs in deep lakes) and if a fine time resolution of the model results is not necessarily required (for instance, time resolution ≥ 1 month), the distribution of contaminants in the water column can be predicted with reasonable accuracy by using the estimates of K_z reported in Table 1, as demonstrated by Monte et al. (1991).

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