Experiences from a case study of multi-model application to assess the behaviour of pollutants in the Dnieper–Bug Estuary

Luigi Monte [a,*], *Lars Håkanson* [b], *Raul Periañez* [c], *Gennady Laptev* [d], *Mark Zheleznyak* [e], *Vladimir Maderich* [f], *Giacomo Angeli* [g], *Vladimir Koshebutsky* [h]

[a] *ENEA, CR Casaccia, via P. Anguillarese, 301, 00100 Rome, Italy*
[b] *Institute of Earth Sciences, Uppsala University, Sweden*
[c] *Departamento Fisica Aplicada, University of Sevilla, Spain*
[d] *Ukrainian Institute for Hydrometeorology, Ukraine*
[e] *Institute of Mathematical Machines and System Problems, Ukraine*
[f] *Institute of Mathematical Machines and System Problems, Ukraine*
[g] *ENEA, CR Casaccia, Italy*
[h] *Institute of Mathematical Machines and System Problems, Ukraine*

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A B S T R A C T

The present paper describes the results of the application of four state-of-the-art models to predict the concentrations of pollutants in the abiotic components of the Dnieper–Bug Estuary (Ukraine). The estuary was contaminated by the radioactive substances introduced in the environment following the Chernobyl accident. The scope, the methodological approaches and the theoretical foundations underpinning the examined models are presented and compared. The model performances were assessed by comparison with available empirical data of water contamination. The main factors influencing the inherent uncertainty of the models were examined: incomplete knowledge, paucity of extensive data sets relevant to some environmental quantities, the vagueness and the ambiguity of certain information about environmental processes that can be hardly parameterised in quantitative way, etc. Model performances reflect the intrinsic uncertainty of knowledge concerning the quantitative behaviour of the involved environmental process, the ambiguity of interpretation and parameterisation of such processes, the inherent variability of environmental quantities, etc. The difficulties in selecting the “best performance” model and the benefits arising from a multi-model approach to afford complex environmental problems are presented and discussed. Multi-model approach helps to get an insight into complex problems of environmental management, to promote co-operation among modellers and to profit by the different perspectives of the models.

* *Corresponding author*. Tel.: +39 06 30484645; fax: +39 06 30486716.
E-mail address: monte@casaccia.enea.it (L. Monte).

1. Introduction

The present paper, although dealing with the behaviour of radioactive contaminants in coastal areas, affords some problems of general nature concerning the application of models to complex environmental systems. It should be recognised that the accident at the Chernobyl nuclear power plant in 1986 occurred when, owing to a great deal of previous theoretical and experimental studies, some disciplines, like radioecology, had reached mature stages of development. Therefore, the number of international projects launched for the assessment of model applications to the environmental contamination from the abovementioned accident (BIOMOVS, 1991; IAEA, 2000) offered the unique opportunity of learning more about problems of general relevance concerning the validity, the usage and the usefulness of environmental modelling for solving complex problems of environmental management. This work will try to discuss and analyse such lessons.

Due to the biological value of the coastal zone and the different demands on the utilisation of coastal waters, it is easy to understand why so much interest concerns this ecosystem and, more generally, the marine environment (Baxter et al., 1998; Aarkrog, 1998; Kryshev and Sazykina, 1995). In particular, estuaries are the object of research and environmental management in view of their high biological productivity, of their economic exploitation and of their importance for the whole biological and ecological cycles of many living species. However, in the framework of international projects on model validations in radioecology, much more efforts have been focused on lakes and rivers than on coastal areas and seas. Recently, some reviews of state-of-the-art models for the management of lakes, catchments and rivers polluted by radioactive substances have been presented (Monte et al., 2003, 2004, 2005a). These reviews were done within the thematic network EVANET-HYDRA ("Evaluation and Network of EC-Decision Support Systems in the field of Hydrological Dispersion Models and of Aquatic Radioecological Research"; http://info.casaccia.enea.it/evanet-hydra) financed by the European Commission.

In spite of the attention that coastal environment deserves, it seems that no similar studies are available for models aimed at predicting the behaviour of radionuclides in estuarine systems. One of the aims of the present work is to bridge this gap. We will outline an assessment of the methodologies used by state-of-the-art models that can be applied to the coastal environment. A particular attention will be devoted to the assessment of the results of an exercise of the application of different coastal models to a specific estuarine scenario, the Dnieper–Bug Estuary (DBE). The benefits from a multi-modelling approach will be analysed and assessed in view of the difficulties, such as the shortage of input data and information, encountered by modellers when dealing with complex environmental problems.

2. Overview of modelling approaches

2.1. General remarks

In this section, we will briefly outline the general, theoretical foundations underpinning the models for assessing the behaviour of pollutants in estuarine systems. More detailed descriptions of the models object of the present study are reported in Appendix A.

In principle, most approaches for predicting the migration of radionuclides through estuaries are similar to the ones implemented in models for lakes and rivers (Monte et al., 2003, 2005a). It is, however, necessary to account for the particular environmental conditions and processes that significantly influence the behaviour of contaminants in coastal environments.

Generally speaking, the overall structure of models for predicting the behaviour of radionuclides in estuaries comprises the following sub-models:

(a) modules for predicting the physical, hydrological, the hydraulics and the biotic processes that occur in the estuarine system (such as water temperature and salinity profiles, water fluxes and current velocities, erosion-sedimentation processes and dynamics of suspended matter in water, growth rates of organisms, tidal cycles, etc.) and are supposed to influence the contaminant migration;
(b) modules for predicting the radionuclide transfer:
   1. to the estuary from its catchment;
   2. through the abiotic components of the estuary and
   3. from the abiotic components to the biota.

As for the other water bodies, the main processes that control the migration of contaminants in estuaries are, basically, the diffusion of dissolved substances due to water turbulent motion (eddy diffusion), the transport due to the water current, the interaction of dissolved pollutant with suspended matter and bottom sediment, the mixing processes between different layers of water and, finally, the migration of pollutants from the water to the bottom sediments (sedimentation) and from the bottom sediment to the water (re-suspension). An example of sub-model for predicting hydrodynamic processes is described in Appendix A (University of Seville model). In general, several different configurations may be adopted for this kind of models. The most general equations are the full 3D hydrodynamic equations including baroclinic terms (density differences). However, "2D vertical depth-averaged" models are often used when a vertical mixing of the water column can be hypothesised (Periañez et al., 1996). These models provide predictions of the water current. Suspended sediment transport is also described by transport/diffusion equation accounting for water velocity and erosion and deposition processes (Eisma, 1993; Periañez, 2002).

It is obvious that not all the models make use of hydrological/hydraulic sub-models for assessing the quantitative behaviour of the environmental processes influencing the migration of pollutants through the components of an estuary ecosystem. Some models make use of empirical values of those parameters that relate the migration of pollutants to the environmental processes and that are averaged over finite regions of space and intervals of time (for instance, monthly averages of time-dependent quantities, average water fluxes among different sections of a water body, etc.).

The sub-models for predicting the interaction of radionuclide in the water column with suspended matter and bottom sediments show different degrees of complexity ranging from simple k_d-based assumptions (it is supposed that a reversible equilibrium between dissolved and particulate phases of radionuclide is quickly achieved) to complex multi-stage interactions (Periañez, 2004; Ciffroy et al., 2001). These sub-models assess the complicated problem of radionuclide interaction with sediment particles from various perspectives emphasising, for instance, the stochastic nature of such a process (Børretzen and Salbu, 2002), the variety of physical and chemical characteristics that influence its variability (Abril and Fraga, 1996; Matsunaga et al., 2004; Smith and Comans, 1996) or the different modelling approaches (Monte et al., 2005b). As many of the mentioned aspects were described in previous papers (Monte et al., 2003, 2005a), we do not deem necessary to repeat the results of assessments that have been discussed in the scientific literature.

Some particular environmental conditions and processes are typical of the estuarine ecosystem and significantly influence the migration of toxic substances. For instance, the different density between sea and fresh waters generates a vertical stratification that affects the diffusion of pollutants through the water column. Moreover, tidal cycle is a further factor that should be considered and modelled for assessing both the hydrodynamics of estuaries and the dispersion of contaminants through estuaries (Dyer, 1980).

The mentioned principles and approaches underpin the great deal of models developed to predict the dispersion of radionuclide through the marine and the coastal environment (Prandle, 1984; Breton and Salomon, 1995; Salomon et al., 1995; Schonfeld, 1995; Aldridge et al., 2003; Aldridge, 1998; Goshawk et al., 2003; Smith et al., 2003; Abril and Abdel-Aal, 2000; Harms, 1997; Håkanson, 1999, 2000; Cetina et al., 2000; Fisher et al., 1999).

Most methodologies of radioecological modelling are similar to the ones used to predict the distribution and the effect of other kinds of toxicants, such as heavy metals, in water

Table 1 – Main features of the models that participated in the exercise

Model	Developer	Main model features	Horizon
CoastMab	Uppsala University, Sweden	Generic, process-based, dynamic, high emphasis on ecological aspects. TRP = monthly averages, SRP = the entire coastal system	Compartment model to predict monthly average values of radionuclide concentrations in water and fish accounting for prevailing ecological and environmental processes when radionuclide concentrations in sea and direct radionuclide deposition over the coastal area are available (for the specific applications also direct radionuclide flux from rivers are supplied as input data)
U. Sevilla	University of Sevilla, Spain	2D (depth-averaged) based on advection-diffusion equation, high emphasis on hydrodynamic processes TRP and SRP: in principle the model can supply very detailed information	2D model. The hydrological characteristics of the system that influence the migration of pollutant (water current velocity field) are modelled from fundamental equations accounting for meteorological conditions
ENEA	ENEA, Italy	Generic, process-based, dynamic, emphasis on radionuclide flux balance and migration to sediment TRP = monthly averages SRP = for the present application the coastal system is subdivided in three sectors	Compartment model to predict monthly average values of radionuclide concentrations in deep and surface water accounting for prevailing radionuclide fluxes when radionuclide concentrations in sea and direct radionuclide deposition over the coastal area are available. Balance of radionuclide in the system is evaluated using, as input data (a) the radionuclide fluxes from the rivers flowing into the coastal system; or (b) the deposition of radionuclide over the whole Dnieper catchment (regional model for ^{90}Sr)
THREETOX	IMMSP, Ukraine	3D model based on advection-diffusion equation, high emphasis on hydrodynamic processes TRP and SRP: in principle the model can supply very detailed information	3D model for predicting concentration in water when radionuclide input into the system is known. The hydrodynamics is simulated on the base of 3D, time-dependent, free surface, primitive equation model The hydrological characteristics of the system that influence the migration of pollutant (water current velocity field) are modelled from fundamental equations accounting for meteorological conditions. The model account for the processes governing the exchange of radionuclide between water and suspended/bottom sediment

TRP: time resolving power, SRP: spatial resolving power.

systems (Jørgensen, 1979; Ciffroy et al., 2000). On the other hand, the environmental processes, such as sedimentation, sediment re-suspension, tidal dynamics, water stratification, etc., that control the behaviour of a contaminant in water, are common to both radioactive and non-radioactive substances (Håkanson et al., 2004). Nevertheless, particular chemical processes affecting the behaviour of specific contaminants need to be considered and appropriately modelled (mercury is an obvious example; Rajar et al., 2004). The situation is even more complicated for pollutants, like organic compounds, whose fate is intimately linked to the cycling of organic matter in the aquatic ecosystem (DeBruyn and Gobas, 2004; Gobas, 1993; Jimenez-Montealegre et al., 2002) or is controlled by processes of degradation like photolysis and hydrolysis (Mossman and AlMulki, 1996) that do not affect the behaviour of radionclides or heavy metals.

Today, many user-friendly software tools are available to implement models in computer codes and many models have been developed and tested. Modellers can exchange data and information assessing and comparing their results in a very dynamic and interactive environment dominated by the information technologies. How can we take advantage of all that?

2.2. Outline of model features

The main features of the models used for the present exercise are described in Appendix A and summarised in Table 1. It can be useful to classify models according to their horizon and to their time and spatial resolving powers (TRP and SRP) in view of their scopes and aims.

Horizon, the range of information (knowledge obtained from investigation and study, instructions and requested input data) that the model is meant to process and of the outcomes that is meant to predict. The horizon defines the starting and the end points of a model. For instance, a model can use as input data the deposition of radionuclide onto the water surface and the catchment area of the estuary. The model horizon is different when the input data are the deposition onto the water surface and the empirical values of radionuclide flowing from the tributary rivers. Obviously in the first example, the model aim is more ambitious and the model is more informative as it does not require information (input of contaminant from rivers) that can be difficult or impossible to obtain for some scenarios (for instance, in case of an accident). Nevertheless, a larger horizon generally implies a higher uncertainty.

The resolving power of a model is a measure of the level of detail of its predictions. The "time resolving power" (TRP) is the ability of a model to predict differences in the system behaviour over a given interval of time. In other words, the model is supposed to describe the average behaviour of the system over a defined time interval. Example of factors affecting the TRP are the intervals of time necessary to assure the damping of some transient processes which are not intended to be modelled in a sufficient detailed time scale (for instance, the time necessary to approach a homogeneous distribution of the contaminant in the water column, a condition that, obviously, is not immediately achieved, when box models are used; the sorption and de-sorption processes of radionuclide on suspended matter when the model is based on the hypothesis of an "instantaneous" equilibrium between the dissolved and the particulate contaminant phases, etc.).

Similarly the spatial resolving power (SRP) is the ability of a model to predict differences in the system behaviour over a given spatial grid. For instance, the SRP of box models for predicting the spatial distribution of a substance in water is the size of the boxes. The horizon, the TRP and the SRP are "a priori" characteristics of a model. They are planned and set up by model developers according to their expert judgement. It is quite obvious that the aim is to properly identify such model attributes to maximise the predictive power of the model.

3. Model applications

3.1. Introductory remarks: the ideal case

The main aim of the present work is to analyse the performance of different models for application to real coastal systems, accounting for the available empirical information and input data and in view of the benefit from a multi-modelling approach. Therefore, our scope is somewhat more than a simple validation study.

It can be useful to summarise the possible options of the problem-solving process in view of environmental modelling applications.

The simplest kind of exercise that can be performed is what we can call a "school-boy problem". Candidates are requested to answer a specific question on the basis of a complete set of preliminary data and information. The answer is univocal and the exercise has only two possible outcomes: the answer can be right or wrong. A more elaborate exercise consists in formulating a problem that supplies not only the necessary input data and information but also some more data that are unnecessary to answer the problem itself. It is quite obvious that the previous examples of problems are typical of academic exercises. There are only two kinds of actors playing different roles in these exercises: an "omniscient" referee and one or more candidates. It is quite obvious that, in real circumstances, the situation is more complicated.

In relation to complex, natural systems, we can summarise a traditional perspective as follows: a theoretical "ideal model" inherent to the nature does exist: the "MODEL". The aim of science is to reveal such a "MODEL". Due to objective difficulties, only approximate realisations of such a "MODEL" are available although these can be incessantly improved. The different realisations of the "MODEL" can be temporarily accepted or definitely rejected by "verification–falsification" procedures.

If we accept the above point of view, we should conclude that, when performing blind test exercises of model validation and comparison, the modellers have to prove that the performances of the models they developed are close to the ideal one by showing that model results fit empirical data. The modeller that got the results more close to the empirical outcome wins the game. Moreover, in general, a "rule" exists to decide whether the model is "right" or "wrong". Such a rule is based on statistical tests of significance to ascertain if the model output are in agreement with the empirical data when the uncertainty of the model outcome and of the measurements are accounted for.

It is out of the scope of this paper to debate about the existence of such an "ideal" model, nevertheless it is quite obvious that the assessment of the correctness of the realisation of the "ideal" model is based on several assumptions: experiments can be performed and repeated "ad libitum" (reproducibility); uncertainties of empirical data can be reduced at will by repeated measurements (accuracy); it is possible to perform "crucial experiments" having two possible outcomes, false or true, for assessing the validity of a model (falsification). The above assumptions straightforwardly imply that ever more accurate empirical data can be compared with ever more reliable model output (it is sufficient that modellers and experimentalists are clever enough to achieve high quality results in their respective fields).

From a theoretical point of view the assessment of the uncertainty of the model output has a sound mathematical foundation. According to the most general formulation, any model can be defined as follows:

$$L(m_1, \ldots, m_n)X = Y \tag{1}$$

where L is an operator acting on vector X (the unknown quantities that should be predicted and that depends on time t and space position x), vector Y is the set of input functions and $m_1, \ldots, m_n$ are a set of parameters. Together with Eq. (1) initial/boundary conditions should be considered. Model parameter values, initial/boundary conditions and input functions are obtained from experimental evaluations corresponding, respectively, to the empirical characteristics of the examined environmental system, to the initial status of environmental system and of the contamination and to the "forcing functions" corresponding to the pollution of the system from external sources. Similarly, repeated experiments, model test, hypothesis verifications give the opportunity of deepening our knowledge of the complex set of quantitative rules and laws that underlie the many processes occurring in the environment. This corresponds to the improvement of information about the structure and the parameters of operator L. In the ideal case, initial/boundary conditions, model parameters and input functions are characterised by expected values and the relevant probability distributions. When these distributions are known, it is possible to determine the average values and the distribution of the model output by analytical mathematical techniques or by numeric procedures such as Monte Carlo routines. More optimistically, repeated experimental activities and the improvement of measurement methods can allow one to reduce the "dispersion" of the empirical values associated with the model parameter and the initial/boundary conditions.

Thus, for a given input, the "dispersion" (uncertainty) of the output values can be lowered at will. This is the most traditional and reassuring recipe for managing model uncertainty.

3.2. *The practical case: applications of state-of-the-art models*

Unfortunately, we have to cope with less optimistic circumstances:

(a) the available values of model parameters (chiefly the transfer parameters) for many environmental systems are scanty, consequently it is almost impossible to obtain their statistical distributions (it is preferable to say that, in general, only few empirical evaluations of many parameters are available and these should be considered as "reference" values);
(b) input functions can be affected by significant uncertainty that cannot be rigorously quantified chiefly in connection with the emergency phase of an accident;
(c) the structure itself of the model (the operator L) is uncertain.

Traditional approaches for assessing model validity are not applicable to environmental modelling. Most knowledge is often obtained by accidental events (like the Chernobyl incident), whereas laboratory experiments can never reproduce the complex environmental processes and situations occurring in real circumstances (Peters, 1986). It is, in general, impossible to perform ad hoc experiments to reduce uncertainties and to falsify a model. Therefore, reproducibility, accuracy and falsification principles can be difficult to apply.

Generally, different modellers make use of different experimental data and information to develop, to test and to calibrate their models. All that can make it difficult to parameterise in a quantitative and univocal way the key processes and mechanisms regulating the value of a target variable. In principle, it is, therefore, hard to select a unique, optimal model (the model closest to the "ideal" one).

Several authors have discussed these problems (Hornberger and Spear, 1981). According to the "equifinality" principle, it was claimed that, given a certain level of process-understanding, different model structures and parameter values can be equally acceptable in assessing the behaviour of complex environmental systems (Beven and Freer, 2001). In other words, we are usually dealing with many plausible models whose results are expert estimates entailing certain commitment based on scientific knowledge (Giles, 1981).

There are several other difficulties that modellers face for the application of environmental models such as vagueness, ambiguity and incompleteness of information and input data relevant to the examined environmental scenario. Input data demands from modellers rarely correspond to the input data offered by experimentalists. In spite of all that, we have the urge of getting the best from the available information for the most effective exploitation of existing knowledge in view of practical applications.

Therefore, we should consider a complex scenario that includes several actors: firstly the "customers" (those who are formulating questions to which modellers should answer); secondly, the data/information suppliers ("scenario developers"); and thirdly, the modellers. In this respect, the present exercise is not simply aimed at evaluating the assessed models in order to rank the quality of their performances. In this work, we are concerned with the evaluation of potential advantages of a multi-modelling approach for the management of a complex environmental problem when input data are insufficient and non-univocal. In such conditions, the so-called "expert judgment” is an essential factor. The main question is: can a multi-model approach contribute to achieve an expert-based consensus concerning the prediction of the evolution of the considered environmental system?

3.3. *Description of the Dnieper–Bug Estuary case study*

The Dnieper–Bug Estuary (DBE) (Fig. 1) is the largest of all the Black Sea Estuaries (surface area = $1006.3\,km^2$, volume = $4.24\,km^3$). The DBE water system consists of the Dnieper Estuary and the Bug Estuary. The length of the DBE is 63 km with a width of up to 15 km. The DBE is connected with the Black Sea through the Strait of Kirnburn. The average depth of the DBE is 4.4 m. There is a narrow, 10–12 m deep channel suitable for shipping along the estuary to the Black Sea. The bottom is covered mainly by clay (50%) and sand. The main factor affecting the regime of the system is the process of mixing fresh river waters with saline marine waters. This forms the saline wedge in the estuary, which in the summer months can reach Kherson city. Stratification in the estuary ranges from almost none in the eastern part at the Dnieper mouth to a defined two-layer system in the western marine part of the DBE. These processes are highly dependent on season. The regime of this drowned-river estuary varies from stratified to partially mixed. The average discharge of the Dnieper ranges from about 400 to about $6000\,m^3\,s^{-1}$ in spring, whereas average discharge of the Southern Bug ranges from 80 to $1000\,m^3\,s^{-1}$. The average mean water retention time in the estuary can be estimated of the order of 1 month. The Dnieper discharge, unlike the Southern Bug, is not simple seasonal because it is regulated from Kakhovka reservoir dam placed at 70 km from Dnieper mouth. Therefore, in the summer the saline wedge penetrates much further into the estuary than in the spring. Also, the salinity of the upper stratum in the summer is much higher than in the spring. In addition to the fresh water input, other key factors governing the transport of contaminants are wind and sea level variability. The estuary is ice covered in January to February and wind surges cause short-term excursions of salt wedge into the river mouths. All these factors force complicate 3D time-dependent stratified flows in DBE (Kostyanitsyn, 1964).

The following input data were available for modellers:

- Bathymetry of DBE and coastal area of the Black Sea were provided (2 km grid).
- Daily water discharges of Dnieper River and S. Bug River in 1984–1987.
- Sea level in Kinbourn Strait (Ochakiv) 1986–1987.
- Daily sea level in Kinbourn Strait (Ochakiv) 1986–1987.
- Daily temperature and salinity (ppt) at water surface.
- Three-hour values of wind, air temperature, relative humidity and cloudiness (0–10).
- Survey data in 1986 of temperature and salinity measurements.
- Survey data in 1987 of temperature, salinity and velocity.

Other parameters of DBE hydrology were not available: temperature in the Dnieper River and S. Bug River, temperature and salinity profiles in the Kinbourn Strait. Information was supplied on their seasonal changes.

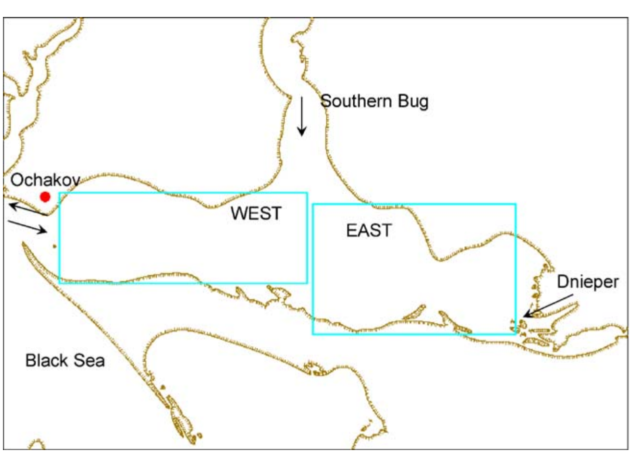

Fig. 1 – Outline of the Dnieper–Bug Estuary. The boxes correspond to the sectors for which empirical radiological data were available: data relevant to West DBE (Table 5); data relevant to Southern Bug (Table 3); data relevant of East DBE (Table 6); data relevant to Dnieper mouth (Table 2); data relevant to Black Sea (Table 4).

3.4. *Radionuclide data*

The Dnieper–Bug Estuary was contaminated by radionuclides introduced in the environment following the accident occurred at the Chernobyl nuclear power plant. The contamination was caused by direct deposition onto the estuary and by the radioactive substances transported by River Dnieper and, to a lesser extent, by River Bug.

Whereas very much data relevant to the morphometry, the hydrology and the meteorological conditions of DBE were available, radiological input data were more difficult to find. Existing data were gathered by two different Ukrainian Institutes (Institute of Mathematical Machines and System Problems and Ukrainian Institute for Hydrometeorology) on the basis of experimental campaigns carried out by several laboratories (Kanivets et al., 1997; Katrich et al., 1993). It should be noticed that a significant effort of selection and evaluation of the empirical data were performed to assure the quality of these data sets.

The input data were the time dependent radionuclide concentrations in Black Sea, in River Dnieper and in southern Bug outlet. Table 2 shows radionuclide concentrations in River Dnieper, the main tributary to the coastal area. Tables 3 and 4 show the concentrations of radionuclides in Southern Bug outlet and North west Black Sea (input data). Tables 5 and 6 show data of measured radionuclide concentrations in water of the West and East part of DBE (data for the assessment of the model performances). Abbreviations in the tables indicate the Institutes that collected samples and performed the radiological measurements:

- IBSS, Institute for Biology of the Southern Seas, Sevastopol.
- IEM, Institute of Experimental Meteorology (Typhoon), Obninsk.
- MHI, Marine Hydrophysical Institute, Sevastopol.

Table 2 – Fluxes of ^{137}Cs and ^{90}Sr from River Dnieper to the estuary

Date	Data gathered by institute of mathematical machines and system problems			Data gathered by ukrainian institute for hydrometeorology	
	^{137}Cs (dissolved) (Bq m^{-3})	^{137}Cs (suspended) (Bq m^{-3})	^{90}Sr (Bq m^{-3})	^{137}Cs (total) (Bq m^{-3})	^{90}Sr (Bq m^{-3})
Pre-accident				3.0	23–33
May 1986	27.8	20.4	18.5	76.0	
June 1986	12.2–14.1	14.8	37	4–11/16/7	26–92
July 1986	7.8	12.2	100	7.0	58–61
August 1986	7.4	12.2	78		
September 1986	6.7	4.4	56		
October 1986	7.0	4.1	63–89		
November 1986	7.4	3.7	59–104	10.0	37–55
December 1986	7.8	3.7	89		
January 1987					
February 1987	14.1		48.		
March 1987					
April 1987				3–11/5.2	660–470
May 1987					
June 1987	5.6–19.2	3.7–6.7	40–278		
July 1987					
August 1987					
September 1987	8.1–14.8	5.2			
October 1987					
November 1987					
December 1987					300–330

Table 3 – Concentration of radionuclides in the Southern Bug outlet (data gathered by Ukrainian Institute for Hydrometeorology)

Date	^{137}Cs (Bq m^{-3})	^{90}Sr (Bq m^{-3})
Pre-accident	3.5–7 (NOSS)	7–10.5 (NOSS)
June 1986	16 (UCME)	
October 1986	10 (UCME)	
December 1987	3.5 (UCME)	

In parentheses the acronyms of the Institutes that carried out sampling and measurements.

- UCME, Ukrainian Centre for Marine Ecology, Odessa.
- NOSS, Nikolaevskaya Oblast Sanitary Station, Nikolaev.
- CGO, Central Geophysical Observatory, Kiev.

3.5. *The exercise*

The main goal of the exercise is to simulate the response of a multi-actor system comprised of modellers and data suppliers in the occasion of an environmental emergency. Therefore, the actors are urged to carry out a cooperative effort rather than hampered by a conflicting competition.

Modellers were asked to supply predictions of both ^{137}Cs and ^{90}Sr in water on the basis of the supplied data and/or using further information from other sources they deemed useful and trustworthy. Among the input data not supplied by the "scenario developers", modellers deemed important the depositions of radionuclides over the estuary. These data were obtained from the literature (De Cort et al., 1998) for ^{137}Cs. Data of deposition of ^{90}Sr of Chernobyl origin were estimated on the basis of the relative low mobility in atmosphere of this radionuclide compared with ^{137}Cs (a negligible or very low ^{90}Sr deposition was the common hypothesis of the modellers).

4. Discussion

As previously stated many models for predicting the migration of radionuclides through large estuaries require the preliminary assessment of hydrological characteristics such as the water current field, the water temperature and salinity profiles, etc. Examples of results of such kind of models are reported in Figs. 2 and 3. Comparisons of model output

Table 4 – Concentration of radionuclide in the North-west Black Sea (data gathered by Ukrainian Institute for Hydrometeorology)

Date	^{137}Cs (Bq m^{-3})	^{90}Sr (Bq m^{-3})
Pre-accident	18 (IEM), 15 (IBSS)	22 (IEM), 18-20 (MHI)
June 1986	55–80 (IEM), 125–185 (IBSS)	26–33 (IEM), 30–130 (IBSS)
October 1986	110 (UCME)	
April 1987	33–140 (IBSS)	19–63 (IBSS)
June 1987	52 (UCME)	

In parentheses the acronyms of the Institutes that carried out sampling and measurements.

Table 5 – Concentration of radionuclides in West DBE (validation data; data gathered by Ukrainian Institute for Hydrometeorology)

Date	^{137}Cs ($Bq\,m^{-3}$)	^{90}Sr ($Bq\,m^{-3}$)
Pre-accident	3.5–7 (NOSS)	7–10.5 (NOSS), 28 ± 5 (MHI)
June 1986	12–34 (UCME)	26–41 (IBSS)
October 1986	14–18 (UCME)	
April 1987	14–30 (UCME)	220 (IBSS)
December 1987		220 (IBSS)

In parentheses the acronyms of the Institutes that carried out sampling and measurements.

Table 6 – Concentration of radionuclides in the East DBE (validation data; the data were gathered by Ukrainian Institute for Hydrometeorology)

Date	^{137}Cs ($Bq\,m^{-3}$)	^{90}Sr ($Bq\,m^{-3}$)
Pre-accident	3.5–7 (NOSS)	7–10.5 (NOSS), 28 ± 5 (MHI)
June 1986	12–19 (UCME)	26–41 (IBSS)
October 1986	14–18 (UCME)	
April 1987	3–10 (UCME)	400 (IBSS)
December 1987		260 (IBSS)

In parentheses the acronyms of the Institutes that carried out sampling and measurements.

and empirical data of radionuclide concentration in water are reported in Figs. 4 and 5.

From the assessment of many models (Monte et al., 2005a) it seems quite obvious that a main factor of uncertainty is represented by the difficulties for predicting quantitatively the complex interaction with bottom sediment of the pollutant in water (contaminant diffusion from the water column to sediment, sedimentation and re-mobilisation). Nevertheless in the present exercise, due to the fast dynamic of the water within the estuary and the relatively low interaction of considered radionuclide with sediment in sea water, this difficulty did not significantly affect the model performances. Indeed, in spite of the different approaches, parameter values and algorithms used by the models (one of these has quite neglected the interaction of radionuclides with sediments), there are no significant differences in model performances that can be attributed to the methodologies employed for predicting the contaminant removal from the water column due to the mentioned processes.

The modellers made use of different values of radionuclide deposition onto the estuary. An estimated value of 2000–5000 $Bq\,m^{-2}$ of ^{137}Cs initial deposition onto the DBE was obtained from graphical data reported by De Cort et al. (1998). The differences among the output of the models at initial time reflect the uncertainty of the assumed ^{137}Cs initial deposition. Unfortunately, empirical evaluations of ^{90}Sr deposition are not available. Although several evidences indicate negligible contamination levels of the environment due to the initial fall-out of ^{90}Sr in areas far from the Chernobyl power plant, one of the modellers used a cautionary, conservative value of 1000 $Bq\,m^{-2}$. This gives reason of the predicted initial peak of ^{90}Sr contamination in water (Fig. 5).

Fig. 5 shows the results from an application of the ENEA model at a regional scale. The input data of this ”regional model” was the deposition of ^{90}Sr onto the catchment of the Dnieper system around the Chernobyl power plant. The contribution of contaminant to the estuary from River Dnieper was evaluated by an application of model MARTE (see the ENEA model description in Appendix A) to the whole basin of the river. In spite of the larger horizon of this particular model application, the predictions of the time behaviour of radionuclide concentration in the estuary were within the range of the results obtained by the other models. This is a further evidence that the transport of pollutants characterised by weak adsorption on bottom sediment can be predicted with a sufficient accuracy although migration occurs over large distances.

An important question is whether or not all the approaches used can be integrated in a single model. Although this is considered categorical in many traditional fields, in principle, it is not so obvious in case of environmental models. The perspectives, the horizons, the features, the structures of the models are often not fully consistent. The integration of these

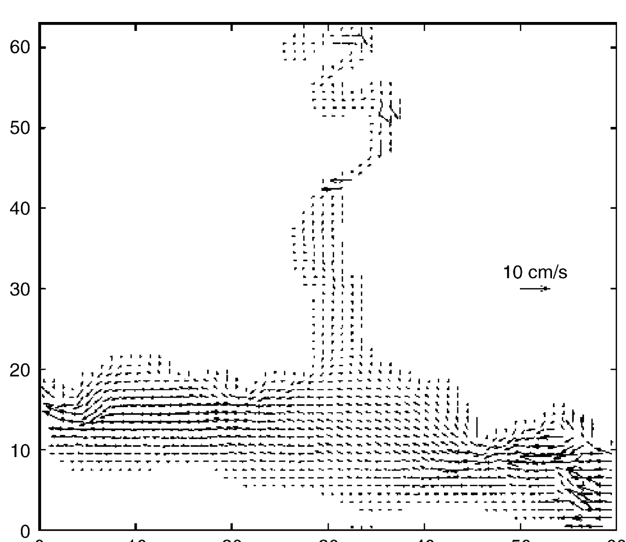

Fig. 2 – A graphical output showing the results of the hydrological model developed by the University of Sevilla.

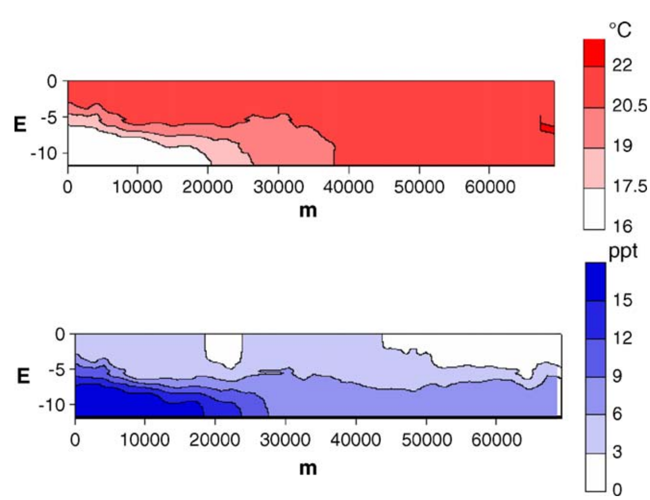

Fig. 3 – Temperature and salinity along DBE sections in summer simulated by model THREETOX.

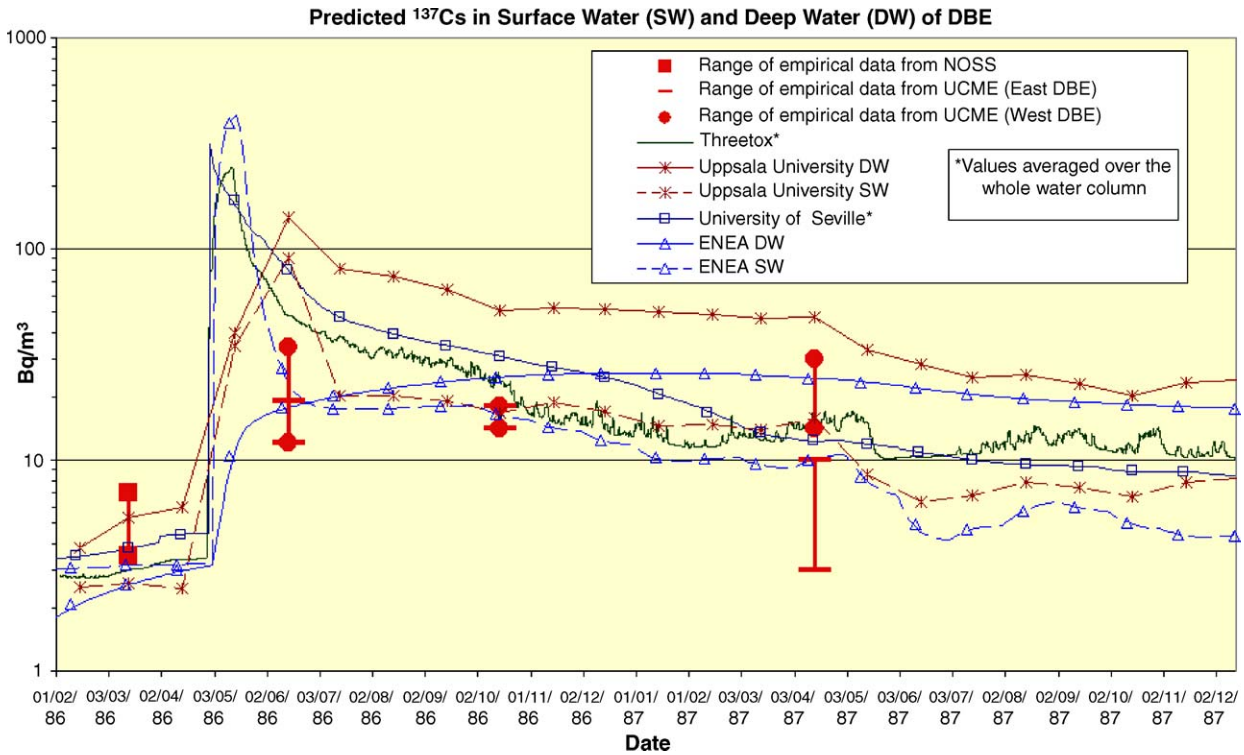

Fig. 4 – Comparison of the results of the model output with empirical data of ^{137}Cs concentration in water.

different models in a comprehensive "super-model" can be, therefore, hard to achieve.

The examined models make use of significantly different values of similar parameters (Table 7). As sufficient information on the statistical distributions of the empirical values of these parameters are not available, the results of the models cannot be framed in a probabilistic perspective for instance in terms of mean values and confidence levels. As a matter of fact, it seems more proper to state that the output of each model is one of the possible outcomes that the community of experts deems worthy of commitment.

Nothing is more instructive than a comparative graph, like Figs. 4 and 5, to show the information available for the "*customers*".

From the figures it is quite clear that, despite the above-mentioned difficulties, there is an apparent consensus among modellers concerning the time behaviour of the radionuclide in water. Figures make intuitive what information obtained from the models can be perceived worthy of consensus and in which measure model output should be considered illustrative of the empirical outcomes. For instance, a delay of radionuclide concentration peak in water is predicted for ^{90}Sr, whereas for ^{137}Cs the concentration in water shows a clear decline on time.

The range of variability of model output is comparable with the range of variability of the empirical concentrations. This clearly confirm that model performances reflect the intrinsic uncertainty of knowledge concerning the quantitative behaviour of the involved environmental process, the ambiguity of interpretation and parameterisation of such processes, the inherent variability of environmental quantities, etc.

When the exercise was carried out, data of radionuclide concentration in the estuary compartments were available from the scientific literature. This occurrence made impossible a blind validation of the assessed models. Consequently, modellers were asked to run their models avoiding preliminary calibration. It is very difficult to appreciate how much the availability of contamination data influenced the model appli-

Table 7 – Selection of parameter values used by the models

Parameter	Model	Value ($m^2\ s^{-1}$)
Vertical mixing coefficient (surface-deep waters)	CoastMab	10^{-6} (order of magnitude)
	ENEA	1.9×10^{-7}–1.9×10^{-6} (depending on the distance from the tributary river)
Horizontal diffusion coefficient	U. Sevilla	0.58
Mixing coefficient sea water-coastal waters	CoastMab	23
	ENEA	116

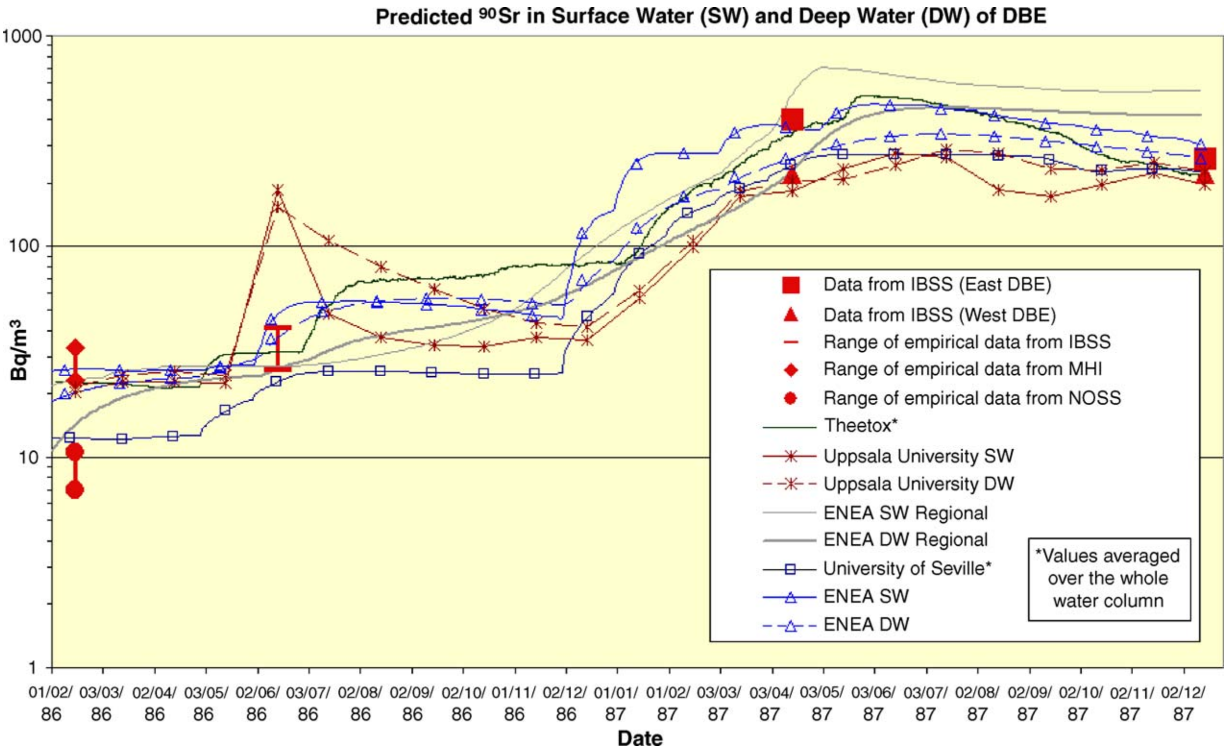

Fig. 5 – Comparison of the results of the models with empirical data of ^{90}Sr concentration in water. The initial peak predicted by the CoastMab Model (University of Uppsala) is due to the hypothesis that a direct deposition of approximately 1000 Bq m^{-2} occurred onto the estuary. Other modellers hypothesised a negligible ^{90}Sr direct deposition. It is important to notice that no empirical data of initial ^{90}Sr direct deposition were available. The model "ENEA regional" predicted the concentration of radionuclide in the estuary from the experimental deposition of ^{90}Sr onto the heavily contaminated area around the Chernobyl nuclear power plant. The contribution of contamination to the estuary from River Dnieper was evaluated by an application of model MARTE (see the ENEA model description in Appendix A) to the whole basin of the river (the main tributary of the estuary).

cations. It is reasonable to suppose that variability of model output around empirical data should have been higher in case of a blind test. Nevertheless, this occurrence does not influence our conclusions as these are, indeed, supported by the awareness of significant uncertainty levels of the output of the models.

It is worthwhile to notice that approximate evaluations of contaminant concentrations in water can be obtained as weighted average of pollutant concentrations in the Black Sea and in river water. The weights can be suitably chosen to account for the different proportions of sea and river waters in the estuary. Appropriate weights can be: (a) the ratio R = salinity in the estuary/salinity in the sea; and (b) $(1-R)$. By using a sea salinity of 16 ppt (value measured at Ochakov strait) and an average salinity of surface water in the estuary of, approximately, 2.5 ppt, from the data in Tables 2 and 4 (neglecting the contribution from River Bug) we can easily obtain values that are almost in the range of the results of the models here assessed. This shows that, for this specific scenario, the main processes controlling the behaviour of radionuclides in the estuary are the pollutant transport from the sea and the river. It is quite obvious that the results of this simple model can be accepted as an approximate estimate of the estuary contamination solely for this particular case. The simple model cannot supply reliable results when applied to different situations. For instance, a direct introduction of contaminant in the estuary from an external source cannot be properly modelled by the above weighted average, as radionuclide concentrations in sea and river are equal to zero in such a circumstance. In other words, the model is not sufficiently developed for application to the innumerable possible contamination scenarios, coastal systems and environmental circumstances that the other more complex and general models are meant to simulate. This is an important conclusion that should be accounted for in order to prevent the perusal of the practical principle stating that a simple model is ever better than a complex one if they supply similar results for some particular applications.

5. Conclusions

The conclusions of the present work are not derived from a deductive theory of models; they rather pertain to the assessment of model performances and of the potential exploitation of the model outcomes given the current level of process understanding. We have not argued in which measure existing models achieved the optimal, "ideal" level of knowledge of the system functioning. This paper considers model outcomes as a manifestation of the expert judgements of modellers given a state-of-the-art knowledge level.

First of all, we have to notice that, according to a traditional approach, as models should correspond to an external reality that appears as univocal, it is straightforwardly derived that the "ideal" model is unique. Therefore, a multi-model approach can be accepted if and only if different models are aimed at solving problems of different kinds for which different realisations of the "ideal" model can be appropriate (it is often claimed that different models are different realisations of the "ideal" model in view of the specific applications for which the models were designed). Moreover, in principles, a detailed analysis of users' needs and of model structures, mainly in relation to the output/input data organisation, can lead to the development of a general model encompassing almost the totality of the possible problems that should be addressed.

The above assumptions can be hardly supported in view of the discussions in the previous sections of this work. As the present exercise shows, the examined models were structurally different, make use of different set of parameters and of parameter values and were based on several different hypotheses. Nevertheless, they were applied for solving the same problem and no realistic criteria were found to ascertain what was the most appropriate for the solution. It is quite obvious that these models cannot be "unified" in a comprehensive "super-model". "Pluralism" in environmental modelling is, therefore, not an oddity but a necessity.

It is recognised that models are tools for organising available knowledge in a rational frame as reported by several authors (Gertsev and Gertseva, 2004). Still, models have a further important function that is often neglected. As demonstrated by the many exercises carried out in the framework of several international projects, multi-model approach facilitates the "mutual learning" for modellers and for the other actors involved in environmental assessment problems (Fisher et al., 2002). Models should therefore be considered as powerful tools for "communication".

This exercise clearly shows that a multi-model approach can be useful for the management of a complex problem of environmental assessment. The approach make clear what are the conclusions that obtain the largest consensus from modellers and what are the ones that should be carefully handled.

Multi-model approach is a powerful tool for strengthening co-operation, improving model credibility and consensus and exploiting available knowledge as noticed by several authors (Fisher et al., 2002).

It should be also emphasised that modern information technologies make very useful and effective an active, mutual cooperative effort among different actors that are involved in model applications for the management of environmental emergencies.

Acknowledgements

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Appendix A. Model descriptions

A.1. *The CoastMab-model (Uppsala University, Sweden)*

This is a box model based on ordinary differential equations (see Table 1A). For this model, one needs to define the borderlines, which limit the given coastal areas and its boundaries towards the sea and/or adjacent coastal areas. Such techniques and the model itself are described in details in the scientific literature (Håkanson, 2005).

The calculation time (dt) of the model is 1 month to reflect seasonal variations. An important demand, related to the practical utility of the model, is that it should be driven by variables readily accessed from standard monitoring programs or maps. The obligatory driving variables include four morphometric parameters (coastal area, section area, mean and maximum depth), latitude (to predict surface water and deep

Table 1A – Compilation of equations for the coastal model (for further information, see Håkanson, 2005)

Compartment surface water

$dM_{SW}(t)/dt = F_{sea\,SW} + F_{DW\,SWx} + F_{ET\,SW} + F_{trib} + F_{atm} - F_{SW\,sea} - F_{SW\,DW} - F_{SW\,ET} - F_{SW\,DWx} - F_{SW\,de}$

$F_{sea\,SW}$ = flow from sea to SW
$F_{DW\,SWx}$ = mixing from DW to SW
$F_{ET\,SW}$ = resuspension from ET to SW
F_{trib} = River inflow
F_{atm} = Fallout
$F_{SW\,sea}$ = flow from SW to sea
$F_{SW\,DW}$ = flow from SW to DW
$F_{SW\,ET}$ = flow from SW to ET
$F_{SW\,DWx}$ = mixing from SW to DW
$F_{SW\,de}$ = physical decay

Compartment deep water

$dM_{DW}(t)/dt = F_{SW\,DW} + F_{ET\,DW} + F_{SW\,DWx} + F_{sea\,DW} + F_{A\,DW} - F_{DW\,SWx} - F_{DW\,A} - F_{DW\,sea} - F_{DW\,de}$

$F_{ET\,DW}$ = resuspension from ET to DW
$F_{SW\,DWx}$ = mixing from SW to DW
$F_{sea\,DW}$ = flow from sea to SW
$F_{A\,DW}$ = resuspension from A-area to DW
$F_{DW\,A}$ = flow from DW to A-area
$F_{DW\,sea}$ = flow from DW to sea
$F_{DW\,de}$ = physical decay

Compartment ET-sediments

$dM_{ET}(t)/dt = F_{SW\,ET} - F_{ET\,DW} - F_{ET\,SW} - F_{de\,ET}$

$F_{ET\,de}$ = physical decay

Compartment A-sediments

$dM_{A}(t)/dt = F_{DW\,A} - F_{bur} - F_{A\,DW} = F_{de\,A}$

F_{bur} = flow from A-sediment to passive sediment
$F_{de\,A}$ = physical decay

M: mass (Bq); F: flux (Bq/month); de: decay; bur: burial; SW: surface water; DW: deep water; ET: ET-areas; A: A-areas; flux from SW to DW: $F_{SW\,DW}$, etc.

water temperatures, stratification and mixing) and the concentration of the given radionuclide in the sea outside the given coastal area, which is estimated in this paper using a simple approach based on the ecological halflife.

The model has four compartments. Two water compartments, surface water and deep water. The model also has two sediment compartments, the ET-areas, i.e., the erosion and transportation areas where fine sediments are discontinuously being deposited, and the A-areas, i.e., the accumulation areas where fine sediments are continuously being deposited. The processes accounted for are inflow and outflow via surface and deep water, direct fallout onto the water surface of the coastal area, sedimentation, burial (the transport from surficial A-sediments to underlying sediments), resuspension, diffusion and mixing between surface and deep water.

The sub-model to predict radionuclide concentrations in fish has been described by Håkanson (2005). The relevant motivations and tests will not be repeated here. Basically, the fish model relates radionuclide concentrations in water, on suspended particles and in sediments to concentrations in fish. The bioconcentration factor (BCF) is modified by factors known to influence biouptake and retention of radionuclides in biota:

- The amount in dissolved and particulate phases of the radionucide.
- The feeding habits of the fish.
- The weight of the fish.
- The trophic characteristics of the coastal system.
- Water temperature.
- Salinity.
- Chemical dilution (e.g., the K-concentration in lake water influences the biouptake of ^{137}Cs and the Ca-concentration the biouptake of ^{90}Sr).

A.2. *The ENEA model (ENEA, Italy)*

The ENEA model is based on quantitative evaluations and balance of radionuclide contents in the water system components (surface water, deep water, bottom sediment) accounting for the fluxes among these (Fig. 1A). The model structure is conceptually similar to the one adopted for the sub-model MARTE (model for assessing radionuclide transport and countermeasure effects in complex catchment) (Monte, 2001) implemented in the computerised decision support systems MOIRA (Appelgreen et al., 1996). The water body is divided in three sectors from the river mouth to the sea. Each sector is sub-divided in three compartments: surface water, deep water and bottom sediment. A fourth compartment representing the sediment interface between bottom sediment and water is considered for ^{137}Cs to simulate the quick interaction processes of such a radionuclide with particulate matter. The first order differential equations of the model were obtained by calculating radionuclide budget in the system compartments from the balance between input and output radionuclide fluxes. These are supposed proportional to the amount of radionuclide in the respective "source" compartment. Eddy diffusion (horizontal between sectors, and vertical between surface and deep waters) is simulated by two-way fluxes that are calculated as the difference between radionuclide concentrations in two contiguous sectors (or water compartments) divided by the distance of the sectors (or compartments) and multiplied by the horizontal (vertical) eddy diffusion coefficient (Monte et al., 1995). We outline briefly the principles and the equations of the model.

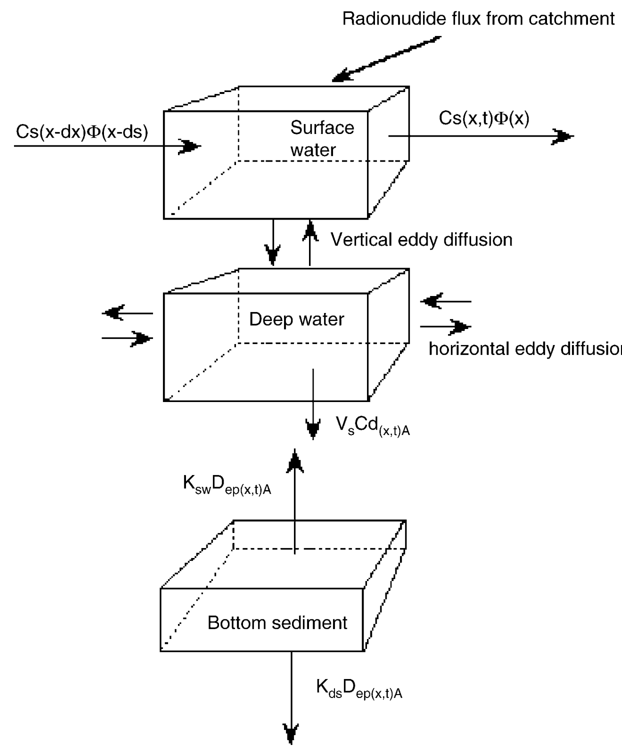

Fig. 1A – Compartments and radionuclide fluxes in the ENEA model. Cs(*x*,*t*) and Cd(*x*,*t*) are the concentrations of radionuclide in surface and deep water (sector *x*), at time *t*. *A* is the area of the interface "water/bottom sediment". v_s is the migration velocity of radionuclide from water to sediment. K_{sw} is the radionuclide resuspension rate from sediment (D_{ep} = radionuclide deposit in Bq m^{-2}) and K_{ds} is the radionuclide migration rate from bottom to deep (passive) sediments. This structure is common to many models for predicting the migration of contaminants in water systems, although a further "water-sediment" interface compartment is often considered to simulate the fast interaction processes of pollutants with sediment.

The radionuclide absorption by suspended matter and by the sediment interface layer is modelled according to the well-known "k_d concept" (k_d = partition coefficient "particulate form/dissolved form") based on the hypothesis of a reversible quick equilibrium between the dissolved (C) and the adsorbed phases (C_{ad}) of radionuclide

$$\frac{C_{ad}}{C} = k_d$$

The total amount, T_i (Bq), of radionuclide in deep water (dissolved + particulate form) and in sediment interface layer is

$$T_i = C_i L_i h_i \Delta_i + C_i k_d w_{sm} L_i h_i \Delta_i + C_i k_d D_l \delta L_i \Delta_i$$

where L_i, h_i and Δ_i are, respectively, the width, the thickness and the length of sector i, w_{sm} is the suspended matter ($kg\,m^{-3}$) and D_l and δ are the thickness and the density of the sediment interface layer.

The previous equation can be written as follows:

$$T_i = C_i\left[1 + k_d w_{sm} + \frac{k_d D_l \delta}{h_i}\right] h_i L_i \Delta_i$$

If we put

$$h_{eff\,i} = h_i + h_\Delta$$

where

$$h_\Delta = k_d w_{sm} h_i + k_d D_l \delta$$

we get

$$T_i = C_i h_{eff\,i} L_i \Delta_i$$

Similar equations govern the behaviour of radionuclide concentration C^s in surface water provided that

$$h_\Delta = k_d w_{sm} h_i$$

The time variation of radionuclide concentration obeys the following equations:

(a) deep water

$$\frac{\partial C_i}{\partial t} = -\frac{E_o}{\text{Dist}}\frac{h_i}{\Delta_i h_{eff\,i}}[-Ct_{i-1} + 2Ct_i - Ct_{i+1}] + \frac{E_v}{h/2}\frac{1}{h_{eff\,i}}[Ct_i^s - Ct_i] - \frac{v_s C_i}{h_{eff\,i}} + \frac{K_{sw}\text{Dep}_i}{h_{eff\,i}} - \lambda C_i$$

where C_i and Ct_i are, respectively, the dissolved and the total radionuclide concentrations in sector i of deep water, E_o and E_v are the horizontal and the vertical eddy diffusion coefficients, Dist is the distance between the barycentre of two contiguous sectors, h is the depth of the water column, Ct_i^s is the total radionuclide concentration in sector i of surface water, v_s is the radionuclide sedimentation velocity, K_{sw} is the rate of resuspension of radionuclide from sediment and λ is the radioactive decay constant;

(b) surface water

$$\frac{\partial C_i^s}{\partial t} = -\frac{1}{\Delta_i L h_s}[\Phi_i Ct_i^s - \Phi_{i-1} Ct_{i-1}^s] + \frac{E_v}{h/2}\frac{1}{h_s}[Ct_i - Ct_i^s] - \lambda C_i^s$$

where C_i^s is the dissolved radionuclide in sector i of surface water, h_s is the thickness of surface water, Φ_i is the surface water flux from sector i to the contiguous sector (it is supposed that the prevailing horizontal component of water movement is due to the fresh water flux from the river).

The following equation governs the deposit Dep ($Bq\,m^{-2}$) of radionuclide in sediment:

$$\frac{\partial \text{Dep}_i}{\partial t} = v_s C_i - K_{sw}\text{Dep}_i(x,t) - K_{ds}\text{Dep}_i(x,t) - \lambda \text{Dep}_i(x,t)$$

where K_{ds} is the rate of migration of radionuclide to passive sediments.

A.3. *University of seville model (Spain)*

A 2D depth-averaged model has been adopted at the University of Seville to simulate the flux of radionuclides in the Dnieper–Bug Estuarine system.

The model solves the 2D depth averaged hydrodynamic equations off-line using monthly averaged wind conditions and water discharge from the rivers. Thus 24 water current fields are obtained, corresponding to the period 1986–1987. These current fields are used to solve the advection/diffusion dispersion equation for radionuclides.

Horizontal density gradients are included in the equations since will also affect currents in the estuary. The hydrodynamic equations also include the standard non-linear, Coriolis, gravity and horizontal friction terms. The density of water is obtained from its salinity through a standard equation of state. The hydrodynamic equations are

$$\frac{\partial z}{\partial t} + \frac{\partial}{\partial x}(Hu) + \frac{\partial}{\partial y}(Hv) = 0,$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial z}{\partial x} + \frac{Hg}{2\rho_0}\frac{\partial \rho}{\partial x} - \Omega v + k\frac{u\sqrt{u^2+v^2}}{H} - \frac{\tau_x}{\rho_0 H} = A\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right),$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial z}{\partial y} + \frac{Hg}{2\rho_0}\frac{\partial \rho}{\partial x} + \Omega u + k\frac{v\sqrt{u^2+v^2}}{H} - \frac{\tau_x}{\rho_0 H} = A\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

where u and v are the components of the water current along the x and y axis, z is the surface elevation over the mean water level, H is total water depth, k is the bed friction coefficient, A is horizontal viscosity, ρ is density of water and the wind stress components are

$$\tau_x = C_D \rho_a |W| W_x, \qquad \tau_y = C_D \rho_a |W| W_y$$

where C_D is a drag coefficient, ρ_a is air density and W is wind speed. The water density is obtained from the following standard equation of state:

$$\rho = \rho_0(1 + \alpha S)$$

where ρ_0 is a reference density taken as $998.9\,kg\,m^{-3}$ and S is water salinity. Coefficient α is 7.45×10^{-4}. Water salinity is obtained from an advection/diffusion dispersion equation with appropriate boundary conditions at the river mouths and Kinbourn Strait.

The hydrodynamic equations are forced by the monthly averaged winds, river discharges and salinity at the Kinbourn Strait (salinity at the river mouths is fixed to zero). The bed friction coefficient has been fixed as $k = 0.025$. However, the estuary is covered by ice during the winter months. In this case the friction coefficient is increased to 0.050 to account for the reduction in water velocity because of friction with the ice cover. It has been checked that a realistic order of magnitude for currents is obtained (in comparison with measurements provided with the scenario description) and that continuity is satisfied. Thus, currents into the estuary are of the order of $5\,cm\,s^{-1}$.

The hydrodynamic model is run separately for each month in the period 1986–1987. Each model run is carried out until a steady situation is achieved, starting from rest conditions. A steady situation is reached in less than 100 h of simulation.

The corresponding steady current and water surface elevation fields are stored in files that will be read by the dispersion code. Twenty-four model runs are carried out and 24 files are generated. Horizontal resolution of the model is 1000 m (the same computational grid provided with the scenario is used) and time step in the hydrodynamic calculation is 20 s due to the CFL stability condition (a explicit finite difference scheme is used to solve the equations).

A.3.1. Dispersion

The dispersion model consists of an advection/diffusion equation with appropriate boundary conditions. Files containing current fields are read to compute the advection terms. Linear interpolation between these currents fields is used to have a smooth transition from 1 month to the following. The dispersion equation is

$$\frac{\partial C_d}{\partial t} + \frac{1}{H}\left(\frac{\partial (C_d H)}{\partial x} + \frac{\partial (C_d H)}{\partial y}\right) = \frac{1}{H}\left(\frac{\partial}{\partial x}\left(HK\frac{\partial C_d}{\partial x}\right) + \frac{\partial}{\partial y}\left(HK\frac{\partial C_d}{\partial y}\right)\right)$$

where C_d is the concentration of dissolved radionuclides and K is the diffusion coefficient.

The same computational grid as in the hydrodynamic calculations is used. However, stability conditions are not so restrictive and time step could be increased to 720 s. Explicit second order accuracy finite difference schemes are used to solve the advection and diffusion terms in the dispersion equation. In particular, the MSOU (monotonic second order upstream) scheme is used for advection and a centered scheme is used for diffusion.

Radionuclide concentrations at the three open boundaries (Dnieper and Bug mouths and Kinbourn Strait) are fixed for each month from provided data. The dataset is not complete. Thus, linear interpolation is used when data is lacking for a time period. Also, the average concentration is used if a range of concentrations is provided or if there are results from different institutes. In the case of Cs, there are no data for Kinbourn Strait. Thus data corresponding to the Black Sea are used. Initial conditions must also be specified for radionuclide concentrations. These conditions consists of considering an uniform background concentration over all the estuary. It has been taken as 3 and 9 Bq/m^3 for Cs and Sr, respectively, which are the minimum measured concentrations according to the provided dataset.

The diffusion coefficient has been selected according to the model grid size, following the classical Okubo's relation. It leads to a value equal to 0.58 $m^2 s^{-1}$.

A.4. THREETOX model (IMMSP, Ukraine)

The THREETOX code is an advanced 3D surface water modelling system for hydrodynamics, sediment and radionuclide transport in lakes, reservoirs, estuaries and coastal ocean (Margvelashvili et al., 1997; Koziy et al., 1998; Margvelashvili et al., 2002; Koshebutsky et al., 2004). It is most appropriate for short-term and local prediction radionuclide transport after release. The modelling system was applied to the water bodies of different scales: cooling pond of Chernobyl NPP (Margvelashvili et al., 2002), Dnipro-Boog, Ob' and Yenisey estuaries (Margvelashvili et al., 1999; Koziy et al., 1998, 2000) and the Kara Sea (Koziy et al., 2000). THREETOX includes hydrodynamics, ice, sediment and radionuclide transport sub-models.

Hydrodynamics sub-model. The hydrodynamics is simulated on the base of 3D, time-dependent, free surface, primitive equation model. The model equations are written in Cartesian coordinates. The prognostic variables of the hydrodynamics code are the three components of the velocity fields, temperature, salinity and surface elevation. The water body is assumed to be hydrostatic and incompressible. The concept of eddy viscosity/diffusivity and $k-\varepsilon$ model of turbulence are used to define the turbulent stresses and scalar fluxes. Heat fluxes at the sea surface are derived from parameterisations that employ observed atmospheric temperatures, humidity, cloudiness and wind.

Suspended sediment transport submodel. The particulate matter is represented by three different grain size fractions. Suspended sediment transport is described by the advection-diffusion equation, taking into account the settling velocity of the sediment. For cohesive sediment the erosion and deposition rates are modelled by using the formulae of Partheniades (1965) and Krone (1962). For non-cohesive sediments the bottom boundary condition describes the resuspension or settling of sediments, which depends on the ratio between the actual and the near-bed equilibrium concentration of the sediments (Van Rijn, 1984). The effective bottom shear stresses induced by currents and wind waves are summed. The mass conservation equations for the bottom deposits describe evolution of bed level.

Radionuclides transport submodel. The sub-model of radionuclide transport describes the specific water-sediment sorption processes. It includes the advection–diffusion equations for dissolved and adsorbed by suspended sediment radioactivity in the water column, and the equations for concentration of the dissolved and adsorbed radioactivity in the bottom deposits. The exchanges between the different phases are described by diffusion, sorption, and sedimentation–resuspension processes. Adsorption and desorption of radionuclides between liquid and solid phases are described by the radionuclide exchange rates and by the distribution coefficients for suspended sediments and bottom, respectively.

Numerical method. Sigma co-ordinates are used to avoid difficulties in numerical solution of problem for realistic bottom topography. Splitting of the barotropic and baroclinic modes imposed in the code (Blumberg and Mellor, 1983). The governing equations together with the boundary conditions are solved by finite difference techniques. A horizontally and vertically staggered mesh is used for the computations.

A.4.1. Model forcing

THEETOX was customised in the Dnieper–Bug Estuary using bathymetry from navigational maps. The horizontal grid size is 1 km, whereas model has 20 sigma-layers in vertical direction. The initial thickness of the upper bottom sediment layer was taken to be 2 cm. The monthly averaged concentrations of the suspended sediment in the Dnieper and Southern Bug mouth were specified according to the State Water Cadastre. The daily discharges and temperature of Dnieper and Southern Bug were prescribed. The observed in Ochakiv atmospheric temperature, humidity, cloudiness and wind with 3 h interval were used. At the estuary mouth in the Kinbourn strait the measured daily level variations and temperature and salinity profiles were used as boundary conditions when flows were directed into the estuary. For outflow the radiation conditions were used for velocity and scalars. Scenario of ^{137}Cs and ^{90}Sr dispersion.

The following coefficients of radionuclides' equilibrium distribution in the "solute-suspended sediments" (K_{ds}) and "solute-bottom sediments" (K_{db}) systems were used: $K_{ds} = 15\,m^3\,kg^{-1}$, $K_{db} = 3\,m^3\,kg^{-1}$ for ^{137}Cs and $K_{ds} = K_{db} = 0.3\,m^3\,kg^{-1}$, in the case of ^{90}Sr. The monthly averaged concentrations of the radionuclides in the solute and attached to sediment in the Dnieper and Southern Bug mouth were prescribed using the data of Polikarpov et al. (1988, 1992) and Katrich et al. (1993). The concentrations of the radionuclides in the Kinbourn strait was prescribed from UHMI data and Katrich et al. (1993) data. The fallout of ^{137}Cs that took place 30 April 1986 was 5000 Bq m^{-2}.

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