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Assessment, validation and intercomparison of operational models for predicting tritium migration from routine discharges of nuclear power plants: the case of Loire River

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Abstract

During last decades, a number of projects have been launched to validate models for predicting the behaviour of radioactive substances in the environment. The project of the ''Aquatic'' working group of the project EMRAS (Environmental Modelling for Radiation Safety) organised by the International Atomic Energy Agency (IAEA) was based on the validation and assessment of models for predicting the behaviour of radionuclides in the aquatic ecosystems.

The present paper describes a blind test of models aimed at assessing the dispersion of tritium releases in the Loire River (France), on a large domain (~350 km) and on a period of six months, by comparing the results obtained by operational-to-experimental values of tritium concentration at Angers, a city along the Loire River.

The common conclusion is that the models used by the different participants namely 1D models and models based on a schematic hydraulic (box models) are reliable tools for tritium transport modelling. Nevertheless, the importance of proper and detailed hydrological data for the appropriate prediction of pollutant migration in water is demonstrated by the example provided during this study.

Keywords: Radionuclide; River propagation; Tritium; Modelling; Transport and dispersion; Loire River

1. Introduction

During last decades, a number of projects have been launched to validate models for predicting the behaviour of radioactive substances in the environment. Some of these projects were dedicated to the prediction of the behaviour of the radionuclides in the fresh-water environment (Onishy, 1994; Popov and Heling, 1996).

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Both the BIOMOVS (BIOspheric Model Validation Study; BIOMOVS, 1990) and the VAMP (VAlidation of Model Predictions; IAEA, 2000) projects stimulated intensive efforts at improving the reliability of the models aimed at predicting the migration of ^{137}Cs in lakes and of ^{137}Cs and ^{90}Sr in rivers (Smith et al., 2004).

The project EMRAS (Environmental Modelling for Radiation Safety, http://www-ns.iaea.org/projects/emras/), organised by the International Atomic Energy Agency (IAEA), continues some of the work of previous International Programmes in the field of radioecological modelling (BIOMOVS II, 1996; BIOMASS, 2003; IAEA, 1985, 1994, 2001). In particular, the working group ''Aquatic'' of the EMRAS project focused on the validation and assessment of models for predicting the behaviour of radionuclides in the aquatic ecosystem (Monte et al., 2005a,b; 2006a,b; Smith et al., 2002, 2003; Holly et al., 1990).

The activities of the ''Aquatic'' working group were based on the extensive data sets of measured radionuclide concentrations in the components of fresh-water ecosystems available following the Chernobyl and the Kysthym accidents or from routine releases of radionuclides in the aquatic environment. In particular, the present work aims at assessing the performances of operational models for predicting the migration of tritium through large rivers, an issue which was not addressed by the previous above-mentioned projects although several studies concerning the behaviour and the modelling of tritium in the environment were published in the International Literature (Amiro, 1997; Raskob and Barry, 1997; Barry et al., 1999).

As tritium does not interact with particulate matter in rivers, the results of this work can help at assessing the capabilities of the models to deal with the physical processes of convection and dispersion which drive the transport of dissolved substances in the aquatic system. The modelling exercise presented in this paper was performed for routine tritium releases of four nuclear power plants (NPPs) located along the Loire River. This exercise is part of a more complete study on the evaluation of the increase of radionuclides in the Loire River system due to routine releases of nuclear power plants (Siclet, 2001; Siclet et al., 2002).

2. Description and objectives of the Loire scenario

The present paper describes a blind test of models aimed at assessing the dispersion of tritium releases in the Loire River (France), on a large domain (~350 km) and on a period of six months, with different conditions of water flow. It compares the results obtained by operational models to experimental values of radionuclide concentration at Angers, a city along the Loire River.

Fig. 1a and b shows a general view of the Loire River system.

The following data were supplied to the modellers as follows:

- the geometry of the River Loire (~370 transversal profiles gathered by the DIREN[1] Centre, with a spacing of approx. 1 km);
- the description of the singularities (18 weirs and little dams along the river), through their crest height and the corresponding hydraulic law (law $Z = f(Q)$, where Z is the water level (m) and Q is the flow rate ($m^3\ s^{-1}$));
- the hydraulic boundary conditions for simulation and calibration (upstream flow rate condition, the flow rates of the main tributaries and the downstream hydraulic law), with a time step of 1 h, from the 1st of June to the 31st of December 1999;
- the tritium discharges for each nuclear power plant, expressed by a tritium flux in kBq/s, and the concentration of tritium coming from the Vienne River (where another NPP is located), with a time step of 1 h, from the 1st of June to the 31st of December 1999 and
- hydraulic data for calibration: water level measurements and flow rates data collected by the DIREN Centre at low, medium and high flow regimes, and data coming from field water tracings made by the CEA[2] and EDF[3], providing information about mean velocities in different parts of the Loire River.

[1] Direction Régionale de l'Environnement.
[2] Commissariat à l'Energie Atomique.
[3] Electricité de France.

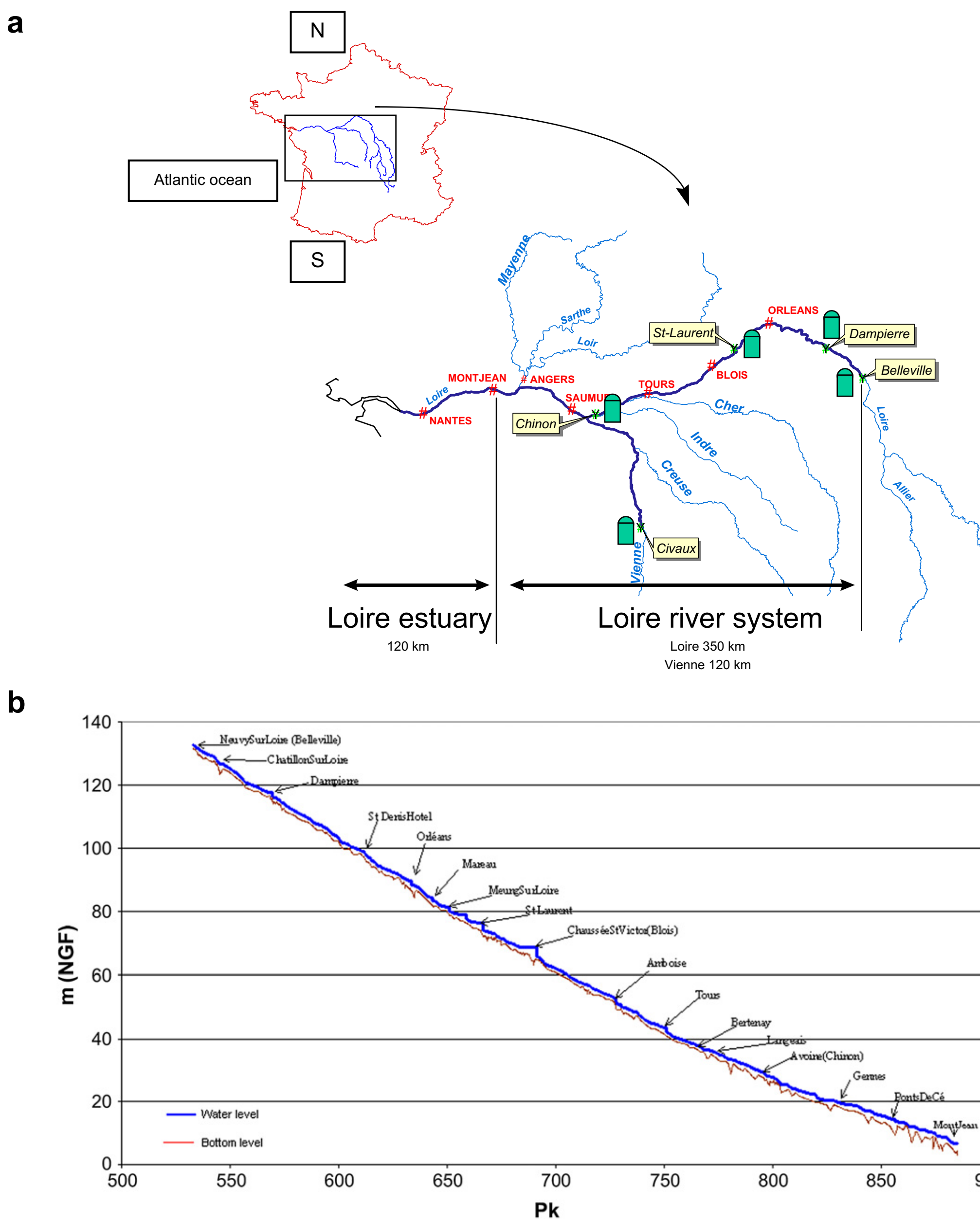

Fig. 1. (a) The Loire River system and (b) Longitudinal view of the Loire River.

The results of the modelling (temporal series of the tritium concentration with a time step of 1 h) were compared to measurements of tritium concentration made in Angers, a city along the Loire River, located downstream of all the tritium discharges (approx. 59 km downstream of the last nuclear power plant and 52 km downstream of the confluence with the River Vienne).

In order to obtain the tritium concentration in Angers, water samples were usually collected every 8 h in the downstream section of the river basin (city of Angers) from July to December 1999, and were analysed for tritium concentrations.

Fig. 2 presents the measured tritium concentrations in the water of each sample collected at Angers, with their counting uncertainties.

The mean uncertainty of the measurement is 9%, with values ranging from 0 to 19%.

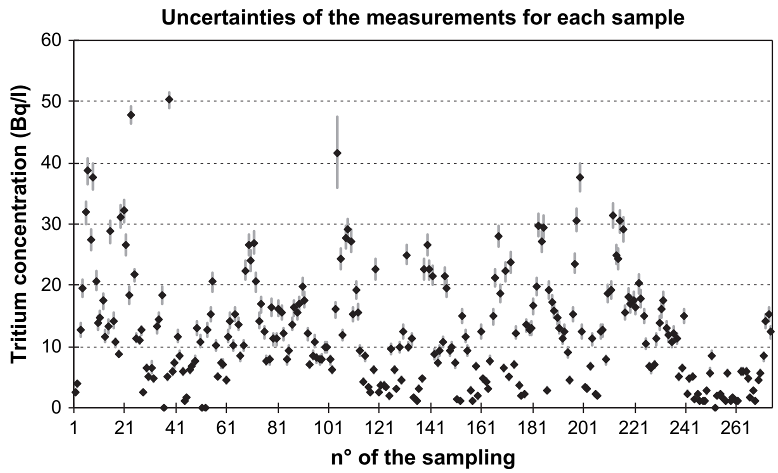

Fig. 2. Tritium concentrations and their uncertainties for each sample collected at Angers.

3. Main features of the models

3.1. Physical processes

In principle, the main processes governing radionuclides transport to be taken into account for modelling tritium propagation in rivers are as follows:

- advection of the pollutant by river flow that defines the position of the pollution peak in time and space (advection is fully defined by average river flow velocities) and
- eddy diffusion due to river turbulence and dispersion due to flow shearing that influence the magnitude of the pollution peak and its spatial spreading (Won Seo and Sung Cheong, 1998).

As tritium does not interact with suspended matter and bottom sediment, the considered scenario of tritium transport in Loire River, well supported by the detailed sets of measured data, was an excellent example to assess how efficiently the models simulate the advection and the diffusion/dispersion in river water of pollutants that are entirely in dissolved form (non-reactive pollutants).

Each model is composed of the following sub-models:

- modules for predicting the hydrological and hydraulic processes (the water fluxes, the hydraulic parameters and the current velocities) and
- modules aimed to the transport–dispersion of a pollutant in a river.

Box and 1D models were tested as they are appropriated for the modelling of pollutant migration in the Loire River when transversal non-homogeneity of pollutant is negligible.

3.2. Description of the models

The tested models are listed in Table 1.

Each of the models tested and their application to the propagation of tritium in the River Loire are described in detail in Appendices and the features of the different components are summarized in Tables 2 and 3.

3.2.1. Hydrological module

We can distinguish two kinds of hydraulic/hydrological modules:

Table 1
Participants to the exercise and models used

Model	Organization	Country
Casteaur v0.1	IRSN	France
Mascaret – module Tracer v5.0 (not in blind test)	EDF – LNHE	France
Moira – module Marte, in three cases: - with standard monthly data, - with customised monthly data, - with customised hourly data.	ENEA	Italy

- the module developed by EDF – LNHE is based on the solution of the full shallow-water equations with real geometry of the river and the possibility to deal with steady and unsteady flows and
- the modules Casteaur and Moira are based on a schematic hydraulic (see the precise description in Appendices A.1 and A.3) accounting for average empirical evaluations of water flux.

The features of the modules are summarized in Table 2.

The inputs of the hydraulic modules are the river geometry, the fluxes at the boundaries conditions and the fluxes of water from the tributaries. The outputs of the hydraulic modules are flow velocities, water levels and water fluxes.

3.2.2. Transport module

The unidimensional (1D) modelling is well appropriated for the hydraulic modelling of the Loire River. Consequently, the model of a pollutant transport in a river is based on the numerical solution of the 1D advection–diffusion equation written in a conservative form:

$$\frac{\partial AC}{\partial t}+\frac{\partial QC}{\partial x}=\frac{\partial}{\partial x}\left(AK\frac{\partial C}{\partial x}\right) \tag{1}$$

where t is the time, x is the abscissa along the river, $A(x,t)$ is the hydraulic section, $Q(x,t)$ is the discharge, $C(x,t)$ is the concentration of the pollutant and $K(x,t)$ is the dispersion coefficient.

Taking into account that advection and diffusion are driven by the hydraulic processes, success of the modelling efforts to predict tritium concentration depends mainly on model ability to simulate crucial hydraulic parameters (discharge, cross-section area and its derivatives: cross-sectional averaged velocity and bottom shear stress) or to accept such basic data from some ‘‘external’’ hydrological calculations and/or empirical hydrological data. All the models solve an advection–diffusion equation in a conservative (1) or non-conservative form (A7). The main features of the different modules are given in Table 3.

The output of the modules is the concentration of the pollutant.

Table 2
Features of the hydrological/hydraulic modules

Models features	Casteaur	Mascaret	Moira
- Full 1D St-Venant equations - Real geometry of the river - Steady and unsteady flows		X	
- Continuity equation for the discharge - Manning–Strickler equations - Steady and unsteady flows	X (with simplified geometry of the river)		
- Power relationships between the geometrical features of the river (width and depth) and the water fluxes - Continuity equation for the discharge - Steady flow			X (Moira consider also non-steady flow)

Table 3
Features of the advection–diffusion module

Models features	Casteaur	Mascaret	Moira
Form of the transport equation:			
- Non-conservative form		X (v5.0)	
- Conservative form	X		X
Physical diffusion		X (v5.0)	
Numerical resolution:			
- Finite volumes or box model	X		X
- Characteristics method		X (v5.0)	

4. Results of the blind test

4.1. Comparisons with measurements

The calculated temporal series of tritium concentrations were compared to the measured ones in Angers, a city along the Loire River, located downstream of all the tritium discharges (approx. 320 km, 290 km, 190 km and 60 km downstream of the four discharges of the Loire NPP).

We plotted these comparisons on graphs, each of them covering two successive months (graph 1: July and August 1999; graph 2: September and October 1999 and graph 3: November and December 1999) (cf. Fig. 3).

In Table 4, the correlation factor between computed results and measurements are given.

It is important to notice that in the case of propagation of peak release where the tritium concentration is quickly time-dependant, this models' performance indicator is not very relevant. For instance, a model can give good results in terms of peak magnitude but with a time shift. In this case, the factor will not reflect the ability of the model to simulate peak release propagation.

4.2. Analysis of the models' results

4.2.1. Casteaur v0.1

The comparison at Angers between the measurements and the results given by Casteaur v0.1 shows an acceptable approximation of the real situation. As Casteaur v0.1 is a dynamic box model, its calculations have to be considered as an assessment of the average conditions at the scales of the considered temporal and spatial steps: one day and the length of the reaches (some kilometers) in this case. In this configuration, it can be noted that the calculation duration on a personal computer is in the range of 1 s.

The empirical data correspond to punctual and instantaneous values locally obtained with a temporal step of 8 h. The first and simpler way to improve the precision of this model will be to reduce the temporal and spatial calculation steps (see Section 5.1).

4.2.2. Mascaret – module Tracer

LNHE who was the provider of empirical data for model testing did not participate in the blind test.

The calculated tritium concentrations resulting from the application of Mascaret to the River Loire are in good agreement with the measured concentrations at Angers.

The module Tracer represents quite well the high tritium discharges of short duration, with a low numerical dispersion. It seems particularly suitable for high flow rates (for example in November and December 1999), when physical dispersion is less important than advection (which is the main process).

Nevertheless, for low flow rates, when physical dispersion becomes important compared to advection, even if the mean levels of tritium concentration are reproduced, the peaks of tritium concentrations are not enough smoothed and the module overpredicts the tritium concentrations (as seen from the results of July and August 1999).

4.2.3. Moira – module Marte

Three applications of model Marte to River Loire were undertaken. The performed exercise aims at showing the functioning of the model when information at different levels of detail are used (see Appendix A.3).

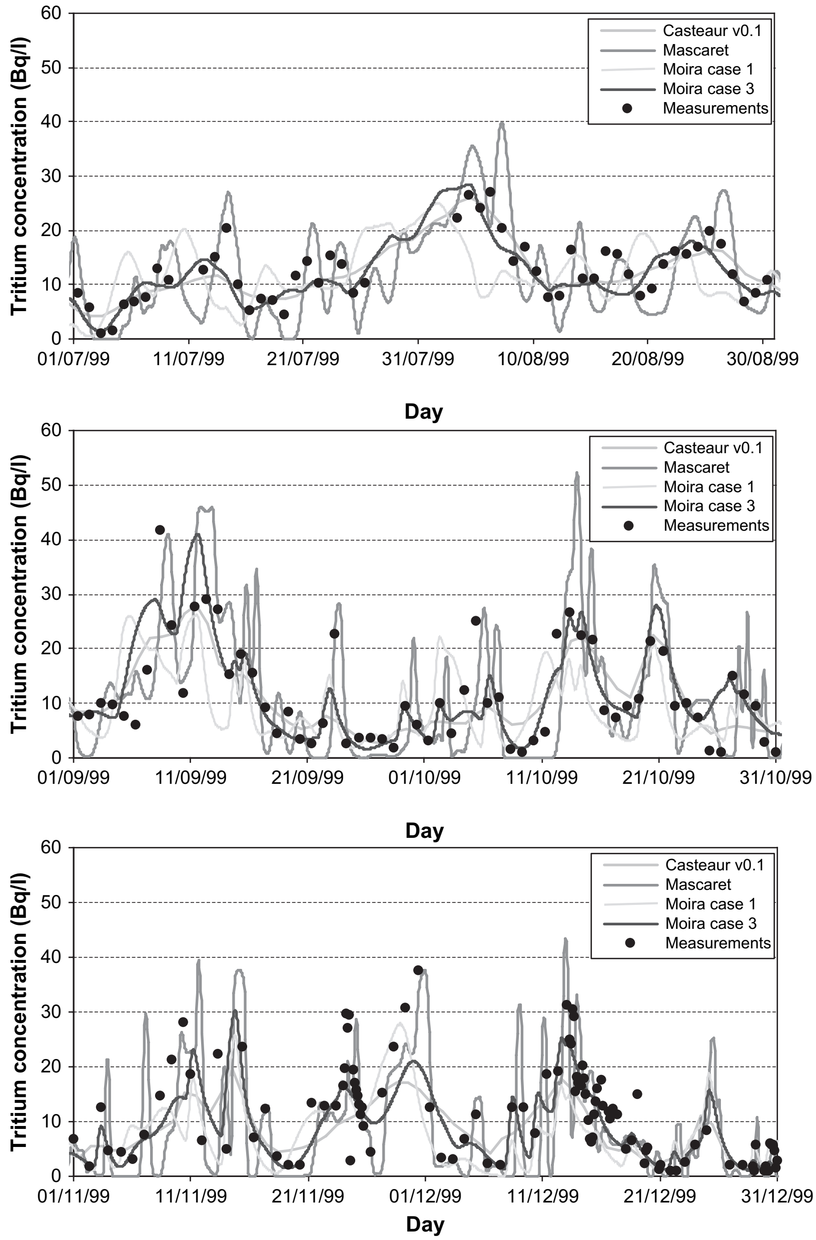

Fig. 3. Comparison between calculated and measured tritium concentration at Angers.

As seen from Fig. 3, in general, the results of the model applications are apparently in reasonable agreement with the measured data. It is obvious that the performances of the model improve when more site-specific information relevant to the hydrologic regime of the river are used.

Water velocity and water fluxes are the most important factors to be accounted for a reliable prediction of the migration of tritium through the river. Therefore, the performances of the model are essentially controlled by appropriate estimates of those time-dependant quantities.

5. Models' improvements

In a second step of the study, after presentation of the results of the blind test, some participants made new tests, with improvements of their models or with new models.

Table 4
Correlation factors between simulation and measurements

Model	Correlation coefficient
Mascaret	0.68
Moira 1	0.49
Moira 3	0.78
Casteaur	0.73

The participants who have presented new computations on the scenario and the models they tested are listed in Table 5.

Each of the models tested and its application to the River Loire are described hereafter. Results of the comparisons with measurements are plotted in Fig. 4.

5.1. Casteaur

In view to improve the simulations and on the basis of the results of the blind test, some improvements have been implemented in Casteaur v0.1. These evolutions concern two levels: the numerical method and the spatial discretisation.

For the blind test, the hydraulic module was solved with an explicit semi-unsteady method and the radioecological model by a pure implicit mode. Now, all the models are solved with this last method. This allows to obtain a more realistic propagation of the water masses (and so of the pollutants) and to improve the numerical stability of the system.

From this first evolution, the next improvement is the integration of methods to refine the spatial discretisation. For the user, it is now possible to define a spatial resolution allowing to refine the discretisation of the spatial grid to a scale lower than the one of the river reaches. Particularly, this last point allows to apply and to test different associations between spatial and temporal steps.

From these evolutions and with exactly the same input parameters than the ones used for the blind test, a new computation has been realized with a spatial step $dx = 0.5$ km and a temporal step $dt = 0.5$ h.

Comparatively to the results previously presented for the blind test (Fig. 3), this new simulation highlights significant improvements of the predicted concentrations at Angers (Fig. 4). This result illustrates well how the box models could be improved simply by refining the space grid and the time resolution. Considering that the targets are the instantaneous values punctually measured at Angers, this result has to be associated to the theoretical bases of the box approaches. In these approaches, the objectives are not to compute punctual values in space and time but to compute integrated values on a spatio-temporal domain.

So, the more the spatio-temporal scales are near those of the measured conditions, the best the results are. Nevertheless, considering that the diffusion process is not implicitly considered in Casteaur v0.1, it could be surprising to obtain a precision equivalent to this of more advanced numerical tools as Mascaret, where this process is taken into account. It can be deduced that for the temporal and spatial scales associated to this scenario, the dominant transfer's processes are the dilution and the advection.

In comparison to complex models, it can be noted that the simplified parameterization, the calculation duration (*one to some seconds on a personal computer*) and the precision of the results justify using this type of box model for equivalent scenario.

5.2. Elementary Algebraic Model for Dilution/Transport

5.2.1. Description of the new calculation

The application of an Elementary Algebraic Model for Dilution/Transport (EAMDT) was made by ENEA to predict the migration of tritium through River Loire.

Table 5
Participants who improved their modelling or tested new models

Models used for the exercise	Organization	Country
Casteaur v0.1, with improvement of the numerical method and the spatial discretisation, and for different couple (time step and space step)	IRSN	France
EAMDT, without/with smoothing	ENEA	Italy

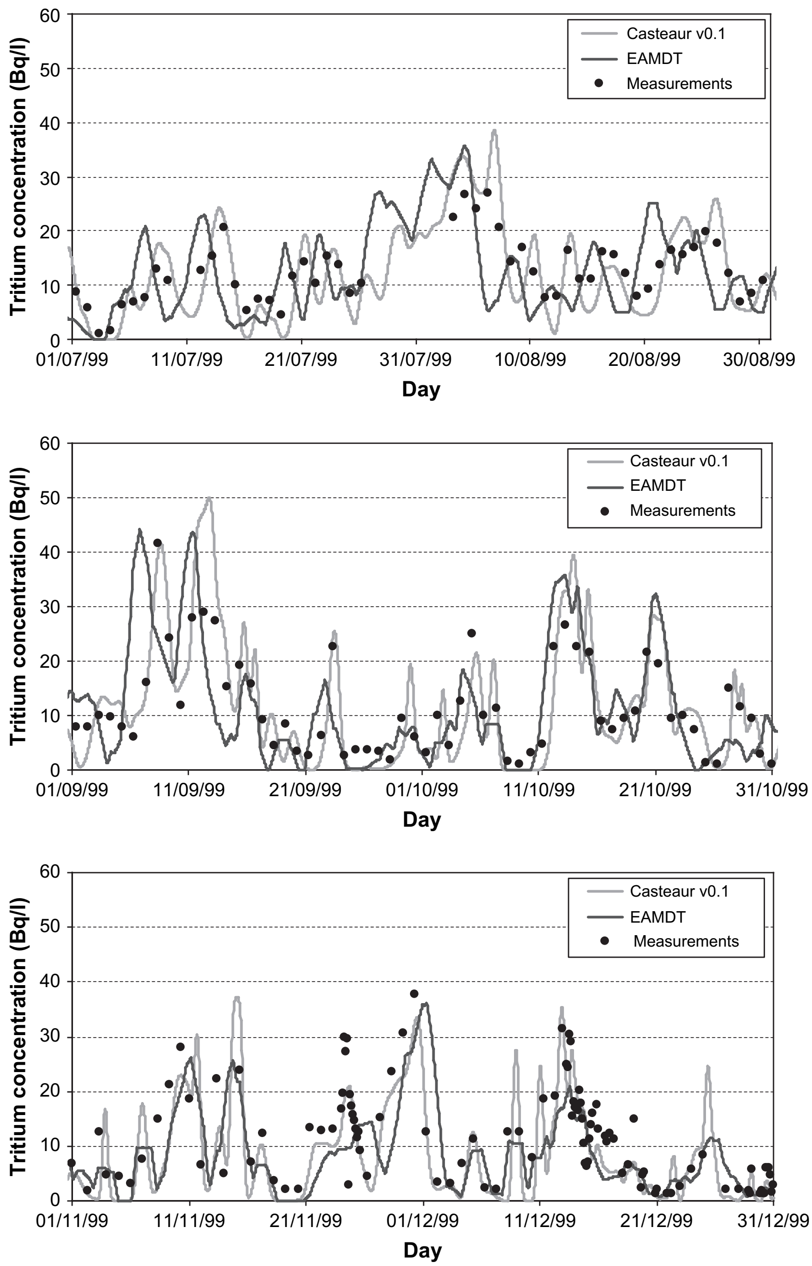

Fig. 4. Comparison between improved calculated and measured tritium concentration at Angers for Casteaur and EAMDT.

This model is based on transport and dilution processes. Tritium concentration at Angers is simply calculated by the following equation:

$$C(t) = \frac{\sum_i F_i(t - \tau_i)}{\Phi(t)} \tag{2}$$

where $C(t)$ (Bq m^{-3}) and $\Phi(t)$ (m^3 s^{-1}) are, respectively, the concentration of tritium and the water flux at Angers at instant t, and $F_i(t)$ (Bq s^{-1}) is the input flux of tritium into River Loire at source point i and at time t. The argument $(t - \tau_i)$ of function F_i accounts for the delay due to the transport of the contaminant from the release point to Angers.

The delay time is

$$\tau_i = \frac{x_i}{v}$$

v (m/s) is the average water velocity and x_i (m) is the distance of Angers from the ith source point.

5.2.2. Application to the scenario

We used $v = 0.67$ m/s for the present application.

The dispersion of radionuclide due to turbulent diffusion was simulated by a time-moving average to smooth the output.

The software realisation of the model is a simple Excel file.

The model was applied by using different time intervals for averaging the concentrations of radionuclide in water at Angers (smoothing procedure):

- order of smoothing = 0 h;
- order of smoothing = 11 h;
- order of smoothing = 41 h;
- order of smoothing = 121 h and
- order of smoothing = 201 h.

5.2.3. Conclusions of this application to the scenario

The present applications of EAMDT clearly demonstrate that the water transport and the dilution due to the river water fluxes are the most important processes controlling, from a quantitative point of view, the behaviour of dissolved contaminants in water when the interaction with sediments is negligible. The comparison of the results of EAMDT with other more advanced models suggests that the appropriate quantitative evaluations of these processes are necessary to assure acceptable performances of a model.

It seems, therefore, that the predictive power of a migration model for assessing the transport of (non-reactive) dissolved substances in a water body is mainly related to the accuracy that characterises the simulation of the above processes.

EAMDT is, in principle, the most simple model that can be applied for predicting the migration of dissolved radionuclides through rivers. The present application shows that such models supply reasonable estimates of the radionuclide concentration in water when approximate and quick evaluations are required.

6. Conclusions

The common conclusion of the study is that the models used by the participating institutes, namely 1D model (Mascaret) and models based on a schematic hydraulic (Casteaur and Moira), are reliable tools for tritium transport modelling and, consequently, for the simulation of advection and diffusion of non-reactive pollutants in rivers. In the blind test, all the models give results in good agreement with the measurements in Angers.

The refinement of the discretisation allows a better accuracy for sharp release of pollutants and a better adaptation to the hydraulic variability. The box models Moira and Casteaur v0.1 are indeed more diffusive and consequently the peaks are smoothed.

The importance of proper and detailed hydrological data for the appropriate prediction of pollutant migration in water is demonstrated by the examples provided during this study:

- Moira "case 3" run, based on the site-specific hourly averaged data on water discharges, provides results closer to the experimental data than the Moira "case 1" and "case 2" runs that are based on generic monthly averaged data and site-specific monthly averaged data, respectively (Fig. 3).
- The comparison of the results of Moira with 20 boxes against the other results with more refined spatial discretisation emphasizes the different mathematical features of the model solutions.

- Implementation of box models with small temporal and spatial discretisations is, in principle, equivalent to finite-difference approximation of 1D partial differential advection equation. Therefore, the results of both kinds of models can be comparable. The main differences are due to numerical diffusion of the various finite-difference schemes and to the presence of a physical dispersion term in 1D models (Casteaur results for different size of boxes).

Therefore, 1D models or box models with small spatial resolution (scale of hundred of meters) have *ad hoc* advance for the process simulation, compared to the models that used ‘‘rough’’ spatial resolution.

Hydrological model is a common tool for hydrological forecasting. The hydrological input data necessary for the radionuclide transport model (results of simulations or empirical time series) could be obtained in each country by contacts between radiological and hydrological experts/institutions.

The steadily increasing performance of conventional computers (PC) provides new possibilities to use pre-customised 1D numerical models for simulation of emergency releases of radionuclide into rivers that was not possible earlier. Nevertheless, box models continue to be main tools for quick analysis of radionuclide transport in rivers on the basis of generic or limited sets of input data by the expert community.

When the conditions of pollutant releases approach the steady state on a river with a quite regular geometry, very simple models based on the evaluations of radionuclide dilution (contaminant input rate in water divided by the water flow) and peak transport due to the water velocity (transport time = distance from the contaminant source divided by the water average velocity) can supply results that are in reasonable agreement with the other models as demonstrated by the applications of ‘‘Elementary Algebraic Model for Dilution/Transport’’ (Fig. 4).

Acknowledgements

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Appendix A. Description of the models

A.1. Model Casteaur (IRSN)

A.1.1. General considerations

The code Casteaur v0.1 (Boyer et al., 2005; Boyer and Beaugelin-Seiller, 2002; Beaugelin-Seiller et al., 2002; Duchesne et al., 2003) is dedicated to operational assessments of the radionuclides transfers in rivers. It is based on five modelling layers: a hydrographical model, a hydraulic model, a sedimentary model, a trophic chain model and a radioecological model. As the Loire scenario aimed to assess the tritium concentration along the river, only the hydrographical model, the hydraulic model and the dissolved part of the radioecological model are involved and described hereafter.

A.1.2. Hydrographical model

The river geometry is described by a succession of reaches constituting a linear hydrographic network where the reaches are limited by an important variation among one of their characteristic hydrographical parameters: length $L(b)$ (m), average slope $I(b)$ (m m^{-1}), trapezium bathymetric section defined by the width $l(b)$ (m) and the angle of the bank $\varphi(b)$ (rad). For the Loire scenario, 33 reaches have been defined.

A.1.3. Hydraulic model

The hydraulic model is a box dynamic model. It assess the temporal evolutions of the water flow $Q(b,t)$ (m^3 s^{-1}), the flow mean speed $U(b,t)$ (m/s) and the water column volume $wc(b,t)$ (m^3) from the Eqs. (A1), (A2) (continuity) and (A3) (Strickler relation):

$$\mathrm{wc}(b,t) = L(b)A(b,t) \tag{A1}$$

$$\frac{\mathrm{dwc}(b,t)}{\mathrm{d}t} = Q(b-1,t) + q(b,t) - Q(b,t) \tag{A2}$$

$$Q(b,t) = U(b,t)A(b,t) = \mathrm{Str}(b)R(b,t)^{2/3}\sqrt{I(b)} \tag{A3}$$

where $q(b,t)$ ($\mathrm{m}^3\,\mathrm{s}^{-1}$) is the specific water inflow in the reach b at the time t, $A(b,t)$ (m^2) is the wet section area, $R(b,t)$ (m) is the hydraulic radius and $\mathrm{Str}(b)$ ($\mathrm{m}^{1/3}\,\mathrm{s}^{-1}$) is the Strickler coefficient. $A(b,t)$ and $R(b,t)$ are given by the following relations:

$$A(b,t) = h(b,t)\frac{l(b)\sin(\varphi(b)) + h(b,t)\cos(\varphi(b))}{\sin(\varphi(b))} \tag{A4}$$

$$R(b,t) = h(b,t)\frac{l(b)\sin(\varphi(b)) + h(b,t)\cos(\varphi(b))}{2h(b,t) + l(b)\sin(\varphi(b))} \tag{A5}$$

A.1.4. Dissolved part of the radioecological model

The dissolved part of the radioecological model proposes also a box dynamic approach. The temporal evolutions of the total activities (Bq) in the different reaches are calculated using the following equation:

$$\frac{\mathrm{d}r(b,t)}{\mathrm{d}t} = Q(b-1,t)C(b-1,t) + S(b,t) - Q(b,t)C(b,t) - \lambda r(b,t) \tag{A6}$$

where $r(b,t)$ (Bq) is the total activity, $S(b,t)$ ($\mathrm{Bq\,s}^{-1}$) is an input data specifying the radionuclide release in the reach b at the time t and $C(b,t) = r(b,t)/\mathrm{wc}(b,t)$ is the volumes activity ($\mathrm{Bq\,m}^{-3}$).

A.2. Mascaret – module Tracer (EDF R&D – LNHE)

A.2.1. General description of Mascaret

Mascaret (Luck, 2003) is a 1D hydrodynamic system for simulating hydrodynamic flows, water quality and sediment transport. So, there are the following including modules:

- The hydrodynamic module solves the 1D shallow-water equations on a looped and branched network. According to the flow characteristics, three hydraulic components are available: steady subcritical regime, unsteady subcritical regime and unsteady mixed flow regime. In case of unsteady subcritical flow, the hydrodynamic module uses an implicit finite-difference computation method (Preissman scheme).
- The module 'Casier' simulates the flow in the floodplain by domain decomposition in basins where only the continuity equation is taken into account.
- The module 'Courlis' simulates the transport of cohesive sediments.

The module 'Tracer' simulates the dispersion of pollutants; this module can be coupled with water quality modules (in the case of interacting pollutants). The Tracer module is only coupled with the hydrodynamic module for subcritical flow regimes (steady and unsteady).

The module Tracer solves the 1D advection–diffusion equation, in its non-conservative form:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(AK\frac{\partial C}{\partial x}\right) + S \tag{A7}$$

where $C(x,t)$ is the tracer concentration ($\mathrm{kg/m}^3$), $u(x,t)$ is the flow velocity (m/s), $A(x,t)$ is the river section (m^2), $S(x,t)$ is the sources of tracer ($\mathrm{kg/m}^3$ s) and $K(x,t)$ is the dispersion coefficient (m^2/s).

In a computation involving different tracers of concentration C_i, the source terms S_i for a tracer i can depend on the concentration of other tracers C_j. As a result, the module Tracer can be applied to water quality modelling, by computing the source terms S_i, representing the interactions between the different tracers.

The resolution is made by a method with fractional steps: a convection step (using the method of characteristics in weak convection) and a diffusion step (implicit scheme).

A.2.2. Application to the River Loire

In the application on the River Loire, the hydrodynamic module of Mascaret was used in subcritical unsteady mode, with a complete description of the river geometry (all the 368 profiles were taken into account to describe the river geometry) and a fine representation of the weirs.

The step for the discretisation in space is approximatively 200 m, so that the River Loire is described by 2656 points.

The time step for the computation is 300 s. We used a constant Strickler coefficient (Str $= 30$ m$^{1/3}$ s^{-1}) and a constant dispersion coefficient in the module Tracer ($K = 100$ m^2/s).

A.3. Moira – model Marte (ENEA)

A.3.1. Model description

MARTE (Models for Assessing Radionuclide Transport and countermeasure Effects in complex catchments) is a structured set of codes implemented in MOIRA (MOdel-based computerised system for management support to Identify optimal Remedial strategies for restoring radionuclide contaminated Aquatic ecosystem and drainage areas; Monte et al., 2000) Decision Support System for applications to complex water river basins (Monte, 2001):

- HydroAV (hydrological module): MARTE sub-code simulating the temporal behaviour of the hydrological and morphologic parameters of a complex water body.
- Cat (catchment module): MARTE sub-code simulating the migration of the pollutant from the catchment to the aquatic system.
- Migra (simulation of contaminant migration through abiotic components of aquatic systems): MARTE sub-code simulating the migration of a pollutant through the abiotic components of an aquatic system.
- Biot (simulation of contaminant migration from the abiotic to the biotic components of an aquatic system): MARTE sub-code simulating the migration of a pollutant from the abiotic components of an aquatic system to the fishes' species.

For the present application modules HydroAV and Migra were used.

The river is assumed to be composed of a chain of interconnected ‘‘Elementary Boxes’’ (Ess). Therefore, the model supplies predictions averaged over a spatially defined part of the water system (the EB).

The water balance is calculated by the following simple equation:

$$Q_i = Q_0 + \sum_1^i \Delta Q_j \tag{A8}$$

where Q_i is the water flux from box ith, Q_0 is the water flux from the river source and ΔQ_i is the increment of water flux in box jth calculated as follows:

$$\Delta Q_i = \mathrm{ROFF}_i - E_i + R_i - W_{di} \tag{A9}$$

where ROFF_i is the total runoff from the sub-catchment ith, E_i and R_i are, respectively, the evaporation and the precipitation rates and W_{di} is the water withdrawal rate.

The average width (B) and depth (h) of each box are calculated as non-linear functions of the water fluxes:

$$B = aQ_i^b$$

$$h = cQ_i^d \tag{A 10}$$

where a, b, c and d are parameters.

Each ES is composed of

- the water column;
- an upper sediment layer strongly interacting with water (‘‘interface layer’’);
- an intermediate sediment layer below the ‘‘interface layer’’ (‘‘bottom sediment’’);
- a sink sediment layer below the ‘‘bottom sediment’’ and
- the right and left sub-catchments of the ES.

The model accounts for the fluxes of radionuclide due to the following processes: sedimentation, radionuclide removal due to water withdrawal, radionuclide migration from water to sediment (diffusion component), radionuclide migration from sediment to water (resuspension), radionuclide migration from catchment, radionuclide transport through the ES chain. The parameters in the equation controlling the radionuclide exchange from water and sediment were set equal to 0 for the present applications to ^3H.

In view of the present application, River Loire was subdivided in 20 segments. Each segment corresponds to an EB in the MARTE code.

A.3.2. Model applications

Case 1. Generic standard version (monthly averages of water fluxes). The hydrological module HydroAV makes use of monthly averages of runoff data.

For this application, the model makes use of generic functions (IAEA, 2001) to estimate the morphological characteristics of River Loire. Generic functions were used to determine average values of depth and width (of each river segment) as power functions of the water fluxes.

The present results were obtained by running a ‘‘stand-alone’’ version of the model.

Data input:

- monthly averages of upstream water fluxes at Belleville and of the four main tributaries (hydraulic boundary conditions) and
- $h = 0.163Q^{0.447}$ and $B = 10Q^{0.460}$, where h is the average depth (m), B is the average width (m) and Q is the monthly average water outflow ($m^3\ s^{-1}$) of each river segment.

Model outputs are monthly averaged fluxes and hourly averaged concentrations.

Case 2. Site-specific standard version (monthly averages of water fluxes). HydroAV works with monthly average data.

It makes use of site-specific functions to evaluate morphologic parameters of River Loire. Available experimental data were not sufficient to fit average depths and widths to power functions of water fluxes. Therefore, the used power functions were selected to assure that water velocity, depths and widths were reasonably close to available empirical estimates.

Data input:

- monthly averages of upstream water fluxes at Belleville and of the water fluxes from four main tributaries (hydraulic boundary conditions) and
- $h = 0.163Q^{0.384}$ and $B = 29.4Q^{0.398}$.

Functions for evaluating h and B in model MARTE ‘‘site-specific standard version’’ were obtained by fitting the experimental water velocity to power functions of the water flux ($v = aQ^b$). These functions assure that the predicted values of h and B are comparable with experimental data. The functions in MARTE ‘‘site-specific standard version’’ are more realistic for the specific conditions of River Loire in comparison with the default functions used by MARTE ‘‘generic standard version’’.

Model outputs are monthly averaged fluxes and hourly averaged concentrations.

Case 3. Site-specific customised version (hourly averages of water fluxes). Customised HydroAV works with hourly data.

Table A1
Main features of the performed exercises

Model applications	Morphometry	Water fluxes
Case 1. Generic standard	$h = 0.163Q^{0.447}$ and $B = 10Q^{0.460}$ generic default functions	Monthly averages
Case 2. Site-specific standard	$h = 0.163Q^{0.384}$ and $B = 29.4Q^{0.398}$ site-specific functions obtained by a calibration of water velocity	Monthly averages
Case 3. Site-specific customised	$h = 0.163Q^{0.384}$ and $B = 29.4Q^{0.398}$ site-specific functions obtained by a calibration of water velocity	Hourly averages

As for the above site-specific standard version application, HydroAV makes use of site-specific functions to determine morphologic parameters of River Loire.

Data input:

- hourly values of water fluxes and
- $h = 0.163Q^{0.384}$ and $B = 29.4Q^{0.398}$.

Model outputs are hourly averaged fluxes and hourly averaged concentrations.

The description of the main characteristics of the exercises of model application is summarized in Table A1.

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