RIVTOX - one dimensional model for the simulation of the transport of radionuclides in a network of river channels
Management Summary

The one-dimensional model RIVTOX, developed at IMMSP, Cybernetics Centre, Kiev, simulates the radionuclide transport in networks of river channels. The sources of radionuclide can be a direct release into a river or the runoff from a catchment. In the latter case, the output from RETRACE-2 is used as the input of RIVTOX. The stream functions, the concentrations of suspended sediment and radionuclide are averaged over a cross-section of a river. A 'diffusion wave' model, derived from the one-dimensional Saint-Venant's equation, describes the water discharge. An advection-diffusion equation simulates the transport of the suspended sediments in the river channel. Its sink/source terms describe the rate of sedimentation and resuspension as a function of the difference between the actual and equilibrium concentration of suspended matter with respect to the transport capacity of the flow. The latter is calculated on the basis of semi-empirical relations. The dynamics of the upper contaminated river bed is driven by the equation for the erosion of the bottom layer.

The radionuclide transport submodel of RIVTOX describes the dynamics of the cross-sectionally averaged concentrations of activity in solution, in suspended sediments and in bottom depositions.

The report presents the model, numerical methods and some of the validation studies results.
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1 Overview of the modelling approaches

1.1 Modelling of radionuclide transport in rivers

The one-dimensional model RIVTOX was developed at IPMMS, Cybernetics Centre, Kiev, Ukraine to solve water contamination/use problems of Ukrainian rivers after the Chernobyl accident (Zheleznyk et al., 1992, Tkalich et al. 1994). The radionuclide transport part of the model is similar to the TODAM model (Onishi, 1982), however simplifications have been done to receive practically applicable model with not too much set of the input data. On the other hand, nowadays RIVTOX includes the more detailed description of the adsorption-desorption processes (e.g. non equal rates of the desorption and adsorption, different Kd for bottom sediments and suspended sediments) that was included into the model on the basis of validation on Chernobyl data. RIVTOX was validated for the Clinch River the Tennessee river in the frame of IAEA VAMP program (Zheleznyak et al. 1995) and for the Dudvah River-the Vah River that is the Danube tributary (Slavik et al., 1997). During last study the possibility of the use in the RIVTOX two-step kinetics has been analysed.

The studies of the environmental impact of radionuclide releases demonstrate that after the initial atmospheric fallout, the large river systems are the main pathways for radionuclide transport from the point of deposition to places which are hundreds of kilometres far away.

The modelling of the radionuclide dispersion in rivers has some peculiarities compared to the modelling of lakes. The radionuclide dispersion in rivers is affected by different flow velocities, short retention times, large variability in water discharge during the year and, as a result, strong temporal variations in sedimentation-resuspension rates. There are also channel and floodplain interactions during floods, strong impacts of the hydraulic structures on flow parameters, as well as rapid water level changes due reservoir management. The simulation of these processes requires certain special approaches in radionuclide modelling. Some of these modelling methods have been reviewed in the early eighties (see e.g. IAEA Safety Series No.50-SG-S6, 1985; Codell et al., 1982; Onishi et al., 1981, Santschi and Honeyman 1989). The further development of the computer technology during the last decade and the urgent need to increase the predictability of models in order to provide adequate information for making decision concerning the remedial measures in the most contaminated water bodies after the Chernobyl accident has led to the intensive development of river modelling.

Mathemathical models describing the radionuclide transport and dispersion in rivers and reservoirs can be classified according to two different approaches - (1) spatial averaging of the variables and (2) the
individual treatment of variables describing radionuclides in different physical-chemical forms.

Variables averaged over compartments represent the highest level of averaging and, as a result, are used in models of the lowest spatial dimension. These box-type (zero dimension) models treat the entire body of water (including the sediment layer, etc.) or a part of the entire body (e.g. one box for water and one for sediments) as a homogeneous compartment.

Cross-sectionally averaged variables are often used in the channel models and in the models for narrow reservoirs. This 1-D approach is used to simulate pollutant transport from the distances larger than tenths of river width downstream the point-source term (i.e. after full mixing o contaminant over crossection) up to the hundreds of kilometres. The time scale for river 1-D models is from minutes up to tens of years (e.g. for long term sedimentation studies).

The Two dimensional (2-D) vertical models operate with width averaged variables. These models are used to describe a current, a suspended sediment and a radionuclide transport in case of a significant variability with respect to the channel depth.

Depth averaged variables are used in the lateral-longitudinal 2-D models which describe flow pattern and radionuclide dispersion in shallow reservoirs, parts of the river channels and flood plains.

The lowest level of averaging takes place in the 3-D models solving primitive or basic governing equations. The real spatial averaging scale of these models is based on the width of the computational grid but not on the a certain parameterization or averaging procedure.

The 1-D model (RIVTOX) was taken as the basic model in HDM to provide the radionuclide transport simulation in the river net in the short-term and the middle-term post accidental phase. The main processes governing the radionuclide transport in river systems are presented on the scheme of Figure 1. The pollutants in rivers are transported by the water flow (advection processes) with the simultaneous influence of the turbulent diffusion processes. The radionuclides can interact with the suspended sediments and bottom depositions. A pollutant transfer between the river water and the suspended sediment is described by the adsorption-desorption processes. The transfer between the river water and the upper layer of the bottom deposition is under the influence of adsorption-desorption and diffusion processes. The sedimentation of contaminated suspended sediments and the bottom erosion are also important pathway of the “water column-bottom” radionuclides exchange. Different types of river models describe these processes at different levels of parametrisation.
River models, independently of their spatial resolution, include two main submodels: hydraulic ones, describing water, suspended sediment and bottom dynamics and submodels concerning the fate of radionuclides in the different phases driven by these hydraulic processes.

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**Figure 1: Flow diagram of the key-processes of the radionuclide transport in rivers**

The main physical exchange mechanisms are the sedimentation of the contaminated suspended matter into the river bed and the resuspension of the sediments into water. They are controlled by hydraulic factors (e.g., river flow, sediment transport), and strongly depend on the sediment size fractionation (e.g., clay, silt, sand and gravel). The Radionuclide diffusion through interstitial water is a process which accounts for migration phenomena not related to the sediment transport. Adsorption and desorption of a radionuclide by the surface bed sediment are the main chemical exchange processes. These processes are not always completely reversible and controlled by geochemical reactions of the dissolved radionuclides with the sediment. Uptake and subsequent excretion of radionuclides by aquatic biota and, in general, perturbation of sediments due to the action of living organisms represent biological processes which are responsible for the exchange of radionuclides between water and the bed sediment.
Modelling the fate of the radionuclides in all three different phases - radionuclides in solution, in suspension and deposited on sediments is very important. Such an approach of the simulation of radionuclide dispersion has been considered by Onishi et al. (1977, 1979, 1981, 1982) and Zheleznyak et al. (1990-1999) for one-, two- and three-dimensional models and by Booth (1975), Schückler et al. (1976), Monte (1992), Benes and Černic (1990), and Hofer and Bayer (1993) for full-mixed box models.

The simplified approach of radionuclides-sediments interaction was used in models of White and Gloyna (1969), Shih and Gloyna (1970), CHNSED (Fields, 1976), HOTSED (Fields, 1977).

For the simulation of radionuclide transport in several United States rivers, the one-dimensional channel model TODAM has been used (Onishi et al., 1982). The model describes radionuclide transport attached on three typical fracture of the suspended sediments - sand, silt and clay with the specific Kd values for each of them. The Radionuclide transport module is supported by the comprehensive suspended sediment transport module, that describes the transport of cohesive and non-cohesive sediments. TODAM does not include the river hydodynamic module. It was used on the base of river hydrodynamics calculated by specific codes (DKWAV or HEC-2 or CHARIMA). TODAM was used to simulate PU-239 transport during flush-flood events in the Mortandad Canyon, New Mexico, USA (Whelan and Onishi, 1983), to reconstruct bottom contamination of the Clinch-River- Tennessee River System due to releases from the Oak Ridge National Laboratory (Onishi, private communication), to simulate Sr-90 and Cs-1237 transport in Dnieper Reservoir after the Chernobyl accident (Zheleznyak, Blaylock and al., 1995).

The 1-D model of SPA "TYPHOON" State Hydrometeorological Committee of USSR (Borzilov et al., 1989 ) used empirical data on the sediment transport rate and flow. The model includes more detailed descriptions of the transfer between different forms of radionuclides. Model parameters have been identified on the basis of experimental data of the Pripyat River spring floods.

The 1-D model by Smitz and Everbecq (1986) considers kinetics of radionuclide interaction with two size fractions of suspended solids. The model was verified for migration of radionuclides in the Meuse River, and subsequently was extensively applied elsewhere (Smitz, private communication).

Several 1-D numerical models have been developed to simulate non-radioactive pollutant transport in the rivers. These models do not take into consideration the specification of the radionuclide transport and radionuclide interaction with sediments, however some of them could be, in principal, modified for such purposes. One of the most well known European 1-D modelling system of the pollutant transport in the
river net is MIKE11, developed by the Danish Hydraulic Institute (Havno et al., 1995). MIKE-11 is a modelling system for the simulation of flows, sediment transport and water quality in estuaries, rivers, irrigation systems and other water bodies. MIKE11 has been designed for an integrated modular structure with basic computational modules for hydrology, hydrodynamics, advection-dispersion, water quality and cohesive and non-cohesive sediment transport. It also includes modules for the surface runoff. MIKE-11 has a well-developed graphical user interface integrated with the pre- and post-processors that support the system interaction with the GIS (Sorensen et al., 1996a).

One-dimensional model RIVTOX was developed to simulate the radionuclide transport in the solute, on the suspended sediments and in the bottom depositions. After the Chernobyl accident it has been applied for the prediction of the radionuclide transport in the river systems (Zheleznyak et al., 1992, Tkalich et al., 1993, Slavik, Zheleznyak et al. 1997). The model includes a submodel of the radionuclide transport and two submodels of the “driving forces” – a hydrodynamic (hydraulics) submodel and a sediment transport submodel.

1.2 Modelling of 1-D river hydrodynamics and sediment transport

To simulate the radionuclide transport in rivers, it is necessary to estimate beforehand the river flow and the suspended sediment transport driven by the river hydrodynamic processes. There are a lot of models to simulate river hydraulics and hydrodynamics. The Overviews of the methods are presented in M. Abott, 1979; Cunge J., Holly F. and Verwey A., 1986; Orlob, 1983 and others. The contemporary “state-of-the-art” in the field is presented by Rutherford, 1994 and demonstrated by Jobson, 1989, Zheleznyak and Marinets, 1993.

The one-dimensional models based on cross-sectionally averaged variables seem to be the most important for the determination of the river flow. Well known are computer codes such as HEC-6 and HEC-2SR (Hydrological Engineering Center, 1977, 1982), REDSED (Chen, 1988), FLUVIAL 11 (Chang, 1988), IALLUVIAL (Karim et al., 1981, 1987) and CHARIMA (Holly et al., 1990) which expands the IALLUVIAL approaches, as well as MIKE-11 (Danish Hydraulics Institute), and TELMAC (Laboratory of Hydraulics, EDF, France). The two last ones are commercially distributed modelling systems which include models of different dimensions. HEC-2SR, FLUVIAL 11, CHARIMA, MIKE-11, and TELMAC contain river hydraulic modules based on a numerical solution of the Saint-Venant equation. The possibility of an efficient estimation of river hydraulics on the base of the numerical solution of the “diffusive wave” equation and the simplified version of the Saint-Venant equation were
Suspended sediments act as a carrier of radionuclides in the river/reservoir flow. The amount of radionuclides transported by the sediments depends on the suspended sediment concentration in the river flow and the Kd value. After the Chernobyl accident, for example, up to the half of CS-137 transported by the Pripyat River from the vicinity of the Chernobyl NPP was bound on suspended sediments (Voitsekhovitch et al., 1992). The sedimentation and bottom erosion processes play a key role in the flow self-purification and in the secondary contamination.

The mathematical modelling of the sediment and the transport is a large branch of hydraulics where overviews could be found in Ackers and White (1973), Grishanin (1976), Cunge, Holly and Verwey (1986), Engelund and Fredsoe (1976), Holly et al. (1990), Karim et al. (1981,1987), Mehta et al. (1989), Onishi (1993), Raudkivi (1967), van Rijn (1984). For the steady state conditions, the sediment discharges are calculated by the empirical and semi-empirical formulae which connect the sediment discharge with the sediment parameters, the flow velocities and the river cross-section characteristics or shear stress acting on the bed. In case of the cohesive sediments (finest silt and clay) and hesive bonds between the particles it has to be taken into account (Mehta et al. 1989). The variability of the streams and sediment parameters lead to the situation that up to nowadays several different formulae are used for the practical applications. It was demonstrated within validation studies (Onishi, 1993) that the approaches of Ackers -White, Engelund-Hansen, Rijn and Toffaleti show the most acceptable results for non-cohesive sediments over a wide range of flow and sediment conditions. However, for an individual river, the best result can be also obtained by the empirical formulae especially tuned for this river.

The sediment transport models are based on the suspended sediment-mass conservation equation (advection-diffusion equation with the sink-source term describing sedimentation resuspension rate) and the equation of bottom deformation (Exner equation). The most important problem for modelling is the parametrisation of the sedimentation and resuspension rates. A physically based approach calculates these rates as a function of the difference between the actual and the equilibrium concentration of the suspended sediments. This is often titled “suspended sediment capacity” and can be derived on the base of the above mentioned formulae.

The Suspended sediments models include different formulae for calculating the equilibrium sediment concentration. The most comprehensive models (e.g. CHARIMA) contain modules of the river hydraulic computation and methods to simulate the bottom erosion dependent on the sediment grain distribution in the upper bottom layer (bottom armouring calculation) and to calculate the bottom friction dependent on the simulated dynamics of the bottom forms.
The sediment transport models are also a part of the radionuclide transport models described in Onishi et al. (TODAM, SERATRA, FETRA, FLESQOT) and RIVTOX, COASTOX and THREETOX models included into the RODOS –HDM.

The 1-D models describe the cross-sectionally averaged flow and contamination parameters in channels. This kind of models is more widely used to simulate dynamics of the radionuclide transport in the network of river channels.
2 Submodels

2.1 Submodel of river hydraulics

RIVTOX includes two submodels for simulation crosssectional averaged flow velocity and water elevation in a network of river canals. The First one is based on the full set of the Saint-Venant equations. The Second one is “diffusive wave” simplified form of the Saint-Venant equations. The latter one as it was demonstrated (e.g. Jobson, 1989; Marinets, Zheleznyak 1993) could give a good accuracy in the results for the flood routing in the river net that does not include structures (dams, gates) which could have significant upstream influence on the flow parameters. Full Saint-Venant equations should be used in the situation with significant upstream influence of the river structure, including e.g. pumping to the water intakes of the irrigation channels and so on.

The hydraulic parameters of a stream (depth, sectional area, velocity) could be calculated using the full dynamic model or the diffusive wave model. The Full dynamic model is used for rivers with dams other obstacles in the channel and for accelerated flows. The Diffusive wave approximation of full dynamic model could be used in case of the insignificant upstream influence of peculiarities in a channel.

The next assumptions should be valid to use the Saint-Venant equations for water flow modelling:

- flow is mainly one-dimensional (velocity is constant in the cross section), fluid which is incompressible and homogeneous;
- curvature of current-flow lines is small, and vertical acceleration is insignificant;
- bottom slope is small, and parameters change slightly along a stream;
- turbulence and friction influence could be taken into account in accordance with resistance laws for constant flows;

The system of Saint-Venant equations include continuity equation (mass conservation law) \(\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_i\) and momentum equation \(\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{Q^2}{A} \right) + gA \left( \frac{\partial h}{\partial x} + S_f \right) = 0\)

The glossary of terms used in the models is presented at the end of the subsection.
The components of the equation \(2\) mean: local acceleration, hydrostatic gradient, gravity, and friction.

The total water depth and bed slope are defined as follows:

\[
h = y - y_b \quad (3)
\]

\[
S_b = -\frac{\partial y_b}{\partial x} = tg \alpha \quad (4)
\]

Figure 2: River stream parameters

The momentum equation \(2\) could be rewritten on the basis of above notation as follows

\[
\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \frac{Q^2}{A} \right) + g A \left( \frac{\partial y}{\partial x} + S_f - S_a \right) = 0 \quad (5)
\]

The friction slope \(S_f\) is calculated using one of the empirical resistance laws, such as Chezy’s or Manning’s, for example:

\[
S_f = \frac{Q |Q|}{K^2} \quad (6)
\]

here \(K\) is a stream metering characteristics.

The usual approach in river hydraulics is to use empirical Chezy’s friction coefficient \(C_{cz}\).

\[
K = C_{cz} A \sqrt{R} \quad (7)
\]

The hydraulic radius of the flow \(R\) is defined as \(A/P\), where \(P\) is “wetted perimeter” of the stream. For a wide river channel \(P\) value is close to a river width \(b\) \((P = b)\) and then \(R = h\).

On the basis of the Mannings’s empirical “friction parameter” \(n\) (average value is 0.02÷0.03 for the plain rivers) \(C_{cz}\) is determined as

\[
C_{cz} = \frac{1}{n R^\frac{3}{2}} \quad (8)
\]

In the kinematic wave approximation only two lass terms are considered in the equation \((5)\) i.e. \(S_f = S_a\), that leads to formula
\[ K = \frac{Q}{\sqrt{S_0}} \]  \hspace{1cm} (9)

In this approximation using (6)-(8), could be obtained Chezy’s formula for steady state flow

\[ Q/A = C_s\sqrt{RS_0}. \]  \hspace{1cm} (10)

The substitution of (11) into the mass balance equation (1) using the assumptions \( A = bR, R = h \) and Manning’s formula (8) will lead to kinematic wave equation

\[ \frac{\partial (bh)}{\partial t} + S_n \frac{\partial (bh^2)}{\partial x} = q_i, \]  \hspace{1cm} (12)

The diffusive wave approximation of Saint-Venant equations (1, 5) could be derived by the neglecting the first two terms in the momentum equation (5). In this case after differentiation (1) on \( x \) and (5) on \( t \) and assuming

\[ \frac{\partial K}{\partial t} = \frac{dK}{dh} \frac{\partial h}{\partial t} = \frac{dK}{dh} \left( -\frac{1}{b} \frac{\partial Q}{\partial x} - \frac{1}{b} q_i \right) \]  \hspace{1cm} (13)

we obtain:

\[ \frac{\partial Q}{\partial t} + V_v \frac{\partial Q}{\partial x} - E_{vd} \frac{\partial^2 Q}{\partial x^2} - V_v q_i = 0 \]  \hspace{1cm} (14)

here \( V_v \) is the wave propagation velocity (wave celerity), and \( E_{vd} \) is the diffusion coefficient

\[ V_v = \frac{Q}{bK} \frac{\partial K}{\partial h}, \quad E_{vd} = \frac{K^2}{2bQ} \]  \hspace{1cm} (15)

As a result it is received one parabolic equation instead of the system of two hyperbolic equations.

The formulas (15) could be simplified on the basis of assumption (9) that leads to

\[ V_v = \frac{1}{b} \frac{dQ}{dh}, \quad E_{vd} = \frac{Q}{2bS_0} \]  \hspace{1cm} (16)

On the basis of formula (10) and approximations \( A = bR, R = h \) the formula for the wave propagation velocity could be further simplified:

\[ V_v = \frac{3}{2} \frac{Q}{bh}, \quad E_{vd} = \frac{Q}{2bS_0} \]  \hspace{1cm} (17)
The functional relation between water discharge and water elevation (depth) is established on the basis of Chezy formulae.

The numerical solver for diffusive wave equation \([14] [17]\) is included into the main hydraulic module of the RIVTOX –HDM. The module of the numerical solution of the full Saint-Venant equations is included only as the option for rivers with dams and gates (without support via GUI).

**Glossary of terms used in the section 2.1**

- \(Q\) m\(^3\)/sec water discharge
- \(A\) m\(^2\) water sectional area
- \(b\) M water width
- \(h\) M water depth
- \(y\) M depth, (calculated from reference level)
- \(y_b\) M river-bed level, (calculated from reference level)
- \(q_l\) m\(^3\)/sec\(^2\) water discharge of lateral inflow, distributed along stream
- \(g\) m\(^2\)/sec gravitational acceleration
- \(S_f\) Stream friction slope
- \(S_b\) Stream bed slope
- \(K\) m\(^3\)/sec Metering characteristic
- \(V\) m\(^2\)/sec Water velocity
- \(E_{rel}\) m\(^2\)/sec Water longitudinal diffusion coefficient

### 2.2 Sediment transport submodel

The suspended sediment transport in river channels is described by the 1-D advection -diffusion equation that includes a sink-source term describing sedimentation and resuspension rates and lateral distributed inflow of sediments

\[
\frac{\partial(A S)}{\partial t} + \frac{\partial(Q S)}{\partial x} - \frac{\partial}{\partial x}\left(E_S \frac{\partial (A S)}{\partial x}\right) = \Phi_b + \Phi_f, \tag{18}
\]

where \(\Phi_b\) is a vertical sediment flux at the bottom, describing sedimentation or resuspension processes in the dependence on the flow dynamical parameters and size of bottom sediments.

\[
\Phi_b = \frac{A}{h} (q_{res} - q_{sed}). \tag{19}
\]

The fluxes are calculated as a difference between actual and equilibrium suspended sediment concentration multiplied on fall velocity of sediment grains:
where $F(x)$ is a function defined as
\[ F(x) = \frac{x + |x|}{2}, \quad x > 0 \]
\[ F(x) = 0, \quad x < 0 \] (21)

The coefficient of the erodibility $\beta$ characterizes the bottom protection from erosion due to cohesion and natural armoring of the upper layer of river bed, vegetation. This empirical coefficient as usually has values of magnitude $0.1 - 0.01$.

The equilibrium suspended sediment concentration (flow capacity) $S_{\ast}$ can be calculated by different approaches. The first empirical formula used in RIVTOX (Zheleznyak et al. 1993) was taken from Bijker’s method (Bijker, 1998).

The equilibrium discharge of the suspended sediments $p = QS_{\ast}$ is calculated as a function of the bed load $p_b$:

\[ p = 183p_b(I_1 \ln \frac{h}{z_0} + I_2) \] (22)

where $I_1$ and $I_2$ are the functions of the undimensional fall velocity $w_* = w_0 / (kU_*)$ and bottom roughness $r_* = r / h$

\[ I_1 = 0.216 - \frac{r_*}{w_*} \int_{r_*}^{0} \left[ \frac{1 - z'}{z} \right] dz' \] (23)

\[ I_2 = 0.216 - \frac{r_*}{w_*} \int_{r_*}^{0} \left[ \frac{1 - z'}{z} \right] \ln z' dz' \] (24)

where

$z' = z/h$, $r = 30 \ r_0$ - typical size of the bottom inhomogeneity, $k$ - von Karman parameter (k=0.4), $U_*$ - bottom shear stress velocity

\[ U_* = \sqrt{F_\gamma / \rho_*} = \sqrt{ghS_f} \] (25)
The bottom sediment equilibrium flow is described as follows:

\[
\tilde{p}_b = 5D \frac{T_c}{\sqrt{T_{cw}}} \left( \frac{\mu}{\rho} \right)^{0.5} \exp \left( -0.27 \frac{\rho D}{T_{cw}} \right)
\]  \hspace{1cm} (26)

where

\(T_c\) - current driven bottom shear stress,

\(\tilde{T}_c\) - bottom shear stress driven by joint action of the currents and waves,

\(D\) - averaged size of sediments,

\(\mu\) - the parameter of the bottom ripples.

The formula (26) was proposed for coastal areas and for rivers mainly used for the large reservoirs parts. In recent versions of RIVTOX van Rijn’s methods of calculation of suspended sediment transport is included into the module library.

The lateral inflow of suspended sediments to the river net \(\Phi_i\) in the equation (18) could be presented as follows

\[
\Phi_i = q_i S_i
\]  \hspace{1cm} (27)

The distributed runoff inflow to the river net \(q_i\) and the suspended sediment concentration in the runoff \(S_i\) are simulated by the HDM RETRACE model.

Substitution of the (19) and (27) into (18) leads to the following equation:

\[
\frac{\partial (AS)}{\partial t} + \frac{\partial (QS)}{\partial x} - \frac{\partial \left( E_s \frac{\partial (AS)}{\partial x} \right)}{\partial x} = \frac{A}{h} (q_{res} - q_{sed}) + q_i S_i
\]  \hspace{1cm} (28)

which could be taken into account the water balance equation (1) presented in such a form

\[
\frac{\partial S}{\partial t} + U \frac{\partial S}{\partial x} - \frac{1}{A} \frac{\partial}{\partial x} \left( AE_s \frac{\partial S}{\partial x} \right) = \frac{1}{h} (q_{res} - q_{sed}) + \frac{q_i}{A} (S_i - S)
\]  \hspace{1cm} (29)

where \(U = Q/A\) -crossectionally averaged flow velocity, \(E_s\) - dispersion coefficient for suspended sediments. It is assumed, that for suspended sediments could be used the same dispersion coefficient as for a soluble tracer in water flow. The overview of the methods of the calculation of the dispersion coefficient for 1-D channel flow has been presented by F.Holly (1985) and recently by Won Seo (1998).
The widely used formulas are as follows:

Elder (1958):

\[ E_x = \alpha_E U_e h \]  

(30)

The calibration constant \( \alpha_E \) has a constant value of 5.9.

Fischer (1973) (in presentation of van Majzik, 1992):

\[ E_x = \alpha_F b^2 U^2 \frac{U}{U_*} \]  

(31)

The calibration constant \( \alpha_F \), e.g. for the Rhine River has a value of 0.011.

Won Seo (1998):

\[ E_x = \alpha_W \left( \frac{b}{h} \right)^{1.23} \left( \frac{U}{U_*} \right)^{1.25} \]  

(32)

The calibration constant \( \alpha_W \) is given in the literature having a value of 0.64.

The simplest approach based on the Elder formula (30), shear stress velocity definition (25) and Chezy’s and Manning’s formula (3)-(6), is used in RIVTOX

\[ E_x = E_s = \alpha_E U_e h = \alpha_E \sqrt{g n U} \ h^{\frac{1}{2}} \]  

(33)

The values of the parameter \( \alpha_E \) should be calibrated if trace experiment data are available for the river of the model implementation.

The Other longitudinal dispersion formulas could be used optionally.

The fluxes of the sedimentation and the resuspension (20) control the dynamics of the upper most contaminated layer of the bottom sediments. The thickness of this layer \( Z^* \) could be calculated from the mass balance equation

\[ \rho_s (1 - \epsilon) \frac{dZ'}{dt} = q_{sed} - q_{er} \]  

(34)

After the simulation of stream hydrodynamics, the numerical solution of the equations (21), (24) is used with the appropriate empirical formulas for the modelling of the suspended sediment transport in the river flow.
Glossary of terms used in section 2.2

\begin{itemize}
  \item \textit{s} \quad \text{kg/m}^3 \quad \text{Suspended sediment concentration}
  \item \textit{s}_* \quad \text{kg/m}^3 \quad \text{Suspended sediment equilibrium concentration}
  \item \textit{\Phi}_b \quad \text{kg/m} \cdot \text{sec} \quad \text{total vertical flux of sediments at water-river bed interface per unit of river branch length}
  \item \textit{q}_{res} \quad \text{kg/m}^2 \cdot \text{sec} \quad \text{Resuspension (erosion) rate per unit area of the bottom (upward directed flux)}
  \item \textit{q}_{sed} \quad \text{kg/m}^2 \cdot \text{sec} \quad \text{Sedimentation rate per unit area of the bottom (dawnward directed flux)}
  \item \textit{\beta} \quad \text{Erodibility empirical coefficient}
  \item \textit{w}_0 \quad \text{m}^2/\text{sec} \quad \text{Sediment fall velocity}
  \item \textit{\Phi}_l \quad \text{kg/m} \cdot \text{sec} \quad \text{Suspended sediment flux from lateral inflow per unit of river branch length}
  \item \textit{s}_l \quad \text{kg/m}^3 \quad \text{suspended sediment concentration in the lateral water inflow}
  \item \textit{E}_s \quad \text{m}^2/\text{sec} \quad \text{longitudinal dispersion coefficient for sediments}
  \item \textit{E}_x \quad \text{m}^2/\text{sec} \quad \text{longitudinal dispersion coefficient for soluble tracer}
  \item \alpha_E \quad \text{parameter of the longitudinal dispersion for Elder’s formula}
  \item \textit{u} \quad \text{m/sec} \quad \text{crosssectionally averaged flow velocity}
  \item \textit{U}_* \quad \text{m/sec} \quad \text{bottom shear stress velocity}
  \item K \quad \text{von Karman parameter}
  \item \textit{T}_c \quad \text{kg/} \text{(m sec}^2) \quad \text{current driven bottom shear stress}
  \item D \quad \text{M} \quad \text{averaged size of sediments,}
  \item \textit{Z}_* \quad \text{M} \quad \text{thickness of the bottom sediment upper layer}
  \item \textit{\rho}_s \quad \text{Kg/m}^3 \quad \text{density of the suspended sediments ( default value 2600 )}
  \item \textit{\rho}_w \quad \text{Kg/m}^3 \quad \text{water density ( default value 1000 )}
  \item \epsilon \quad \text{porosity of the bottom sediments}
\end{itemize}
2.3 Submodel of radionuclide transport

This submodel of RIVTOX describes the advection diffusion transport of the cross-sectionally averaged concentrations of radionuclides in the solution $C$, the concentration of radionuclides on the suspended sediments $C^s$ and the concentration $C^b$ in the top layer of the bottom depositions. The adsorption/desorption and the diffusive contamination transport in the systems "solution - suspended sediments" and "solution - bottom deposition" is treated via the Kd approach for the equilibrium state, additionally taking into account the exchange rates $a_{ij}$ between solution and particles for the more realistic simulation of the kinetic processes.

The present version of RIVTOX uses different values of the sorption and desorption rates $a_{1,2}$ and $a_{2,1}$ for the system "water-suspended sediment" and $a_{1,3}$ and $a_{3,1}$ for the system "water-bottom deposits" because this fits better with the real physical-chemical behaviour of radionuclides in the water systems. Furthermore, the use of the different exchange rates gives a better fit in the simulations

\[
\frac{\partial C}{\partial t} + Q \frac{\partial C}{\partial x} - \frac{1}{A} \frac{\partial}{\partial x} \left( AE_c \frac{\partial C}{\partial x} \right) = f^C \left( S, C, C^s, C^b, Z', \bar{p}^c \right) + f^{C_i} \left( C, C_i \right)
\]

\[
\frac{\partial C^s}{\partial t} + Q \frac{\partial C^s}{\partial x} - \frac{1}{A} \frac{\partial}{\partial x} \left( AE_c \frac{\partial C^s}{\partial x} \right) = f^C \left( S, C, C^s, C^b, Z', \bar{p}^c' \right) + f^{C_i} \left( C, C^s, C_i, C_i^c \right)
\]

\[
\frac{\partial C^b}{\partial t} = f^C \left( S, C, C^s, C^b, Z', \bar{p}^c' \right)
\]

\[
\frac{\partial Z'}{\partial t} = f^C \left( S, \bar{p}^c' \right)
\]

where

\[
f^C = -\lambda C - a_{1,2} \left( K_{as} SC - C^s \right) - a_{1,3} \left( K_{as} C - C^b \right) \frac{\rho_s (1-\varepsilon) Z'}{h}
\]

\[
f^{C_i} = \frac{Q}{A} \left( C_i - C \right)
\]

\[
f^{C^s} = -\lambda C^s + a_{1,2} \left( K_{as} C - C^s \right) + \frac{\rho_{\text{inj}} \left( C^b - C^s \right)}{hS}
\]

\[
f^{C^b} = \frac{Q S_i \left( C^s - C^b \right)}{AS}
\]

\[
f^{C_i} = a_{1,3} \left( K_{as} C - C^b \right) - \frac{\rho_{\text{inj}} \left( C^b - C^s \right)}{\rho_s (1-\varepsilon) Z'} - \lambda C^b
\]

The numerical solver for the system of the equations \ref{36} is included into the RIVTOX code.
### Glossary of terms used in section 2.3

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$</td>
<td>Bq/m$^3$</td>
<td>radionuclide concentration in solution</td>
</tr>
<tr>
<td>$C^s$</td>
<td>Bq/kg</td>
<td>radionuclide concentration on suspended sediments</td>
</tr>
<tr>
<td>$C^b$</td>
<td>Bq/kg</td>
<td>radionuclide concentration in bottom depositions</td>
</tr>
<tr>
<td>$C_l$</td>
<td>Bq/m$^3$</td>
<td>radionuclide concentration in solution of lateral inflow</td>
</tr>
<tr>
<td>$C_{ls}$</td>
<td>Bq/kg</td>
<td>radionuclide concentration on suspended sediments in lateral inflow</td>
</tr>
<tr>
<td>$E_c$</td>
<td>m$^2$/sec</td>
<td>radionuclide longitudinal dispersion coefficient</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>sec$^{-1}$</td>
<td>decay coefficient</td>
</tr>
<tr>
<td>$a_{ls}$</td>
<td>sec$^{-1}$</td>
<td>sorption rate in “water-suspended sediments” system</td>
</tr>
<tr>
<td>$a_{ls}$</td>
<td>sec$^{-1}$</td>
<td>sorption rate in “water-bottom deposition” system</td>
</tr>
<tr>
<td>$a_{ls}$</td>
<td>sec$^{-1}$</td>
<td>desorption rate in “water-bottom deposition” system</td>
</tr>
<tr>
<td>$a_{ls}$</td>
<td>sec$^{-1}$</td>
<td>desorption rate in “water-bottom deposition” system</td>
</tr>
<tr>
<td>$K_{ds}$</td>
<td>m$^3$/kg</td>
<td>distribution coefficient in “water-suspended sediments” system</td>
</tr>
<tr>
<td>$K_{db}$</td>
<td>m$^3$/kg</td>
<td>distribution coefficient in “water-bottom deposition” system</td>
</tr>
</tbody>
</table>
3 Boundary and initial conditions in river network

3.1 River network

For a complex river net the above models are applied to the river network graph. Each equation is solved for the respective "simple channel" (branch) with the relevant initial conditions on a branch and the appropriate boundary condition in a junction of the river net. Each branch is considered as a river channel name "simple channel" means that inside this branch there are no junctions with 2 or more inflows or outflows, sharp changes in depth or width of the stream or water discharge. These points are named "special" points and define a scheme of the river net for the simulation purposes.

![River stream scheme](image)

**Figure 3: River stream scheme**

For the numerical solution of the model equations each branch is covered by the set of the grid nodes (computational mesh) as presented on Figure 3. The configuration of the graph and the size of the branches could be taken from the GIS (e.g. MapInfo map). The information about the river hydrographical characteristics (e.g. mean depth and width, typical discharge, the crossection data - A=A (h) or b=b(h) tables) is prepared for some river crossections to be interpolated into the computational nodes in the modelling system.

3.2 Boundary condition and initial conditions

a) In all models, for all influx points of the river net, the source term conditions should be set:
\[ Q(t) \big|_{t=0} = \tilde{Q}(t) \]
\[ S(t) \big|_{t=0} = \tilde{S}(t) \]
\[ C(t) \big|_{t=0} = \tilde{C}(t) \]
\[ C^s(t) \big|_{t=0} = \tilde{C}^s(t) \]

(37)

where \( \tilde{Q}(t) \), \( \tilde{S}(t) \), \( \tilde{C}(t) \), \( \tilde{C}^s(t) \) are the source functions

b) At the outflow nodes the condition of the free propagation:

\[ \left( \frac{\partial Q}{\partial t} + \frac{Q}{A} \frac{\partial Q}{\partial x} \right) \big|_{x=l} = f^Q_{\text{out}} \]
\[ \left( \frac{\partial S}{\partial t} + \frac{Q}{A} \frac{\partial S}{\partial x} \right) \big|_{x=l} = f^S_{\text{out}} \]
\[ \left( \frac{\partial C}{\partial t} + \frac{Q}{A} \frac{\partial C}{\partial x} \right) \big|_{x=l} = f^C_{\text{out}} \]
\[ \left( \frac{\partial C^s}{\partial t} + \frac{Q}{A} \frac{\partial C^s}{\partial x} \right) \big|_{x=l} = f^{C^s}_{\text{out}} \]

(38)

where \( l \) - a branch length.

c) The Conjunction node (inflow from more than one branch and outflow through one branch) conditions of the free propagation are imposed at the inflow branch.

The mass balance conditions:

\[ (Q)_{\text{in}} \big|_{t=0} = \sum_{i} (Q)_{i \rightarrow l} \]
\[ (QC)_{\text{in}} \big|_{t=0} = \sum_{i} (QC)_{i \rightarrow l} \]
\[ (QS)_{\text{in}} \big|_{t=0} = \sum_{i} (QS)_{i \rightarrow l} \]
\[ (QSC)_{\text{in}} \big|_{t=0} = \sum_{i} (QSC)_{i \rightarrow l} \]

(39)

d) The fork nodes (inflow from one branch and outflow through two or mode branches).

At the inflow branch the free propagation conditions (38) are imposed. At the outflow branches source term conditions (37) are imposed, where the source functions are equal to the output from the inflow branch.

The initial conditions should be also set for all parameters in all points of the numerical mesh at the start time.
4 Numerical solution

Choosing a numerical solver for RIVTOX system of equations several principles were followed:

1. Numerical scheme should be fast and robust, to be able to deal with high time steps;

2. Numerical solver should contain blocks, each solving a known standard problem. Reaction part in Radionuclide transport submodel should be separated, to increase additional ability of software customization to different types of chemical/nuclide pollutant.

It has been decided to use fully implicit version of any numerical schemes, for they are unconditionally stable (robust) and don’t suffer from oscillations.

Following the idea of separation of reaction part in Radionuclide transport submodel the numerical solver is constructed based on the operator splitting technique.

It has to be noted that PDEs in both cases of Sediment and Radionuclide transport submodels are of advection-dispersion-reaction with lateral inflow type. Splitting is made as follows:

1) Advection: \( \frac{\partial \Phi}{\partial t} + U \frac{\partial \Phi}{\partial x} = 0 \), \( \Phi \) is either \( S \), \( C \) or \( C_s \),

2) Dispersion: \( \frac{\partial \Phi}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} \left( AE \frac{\partial \Phi}{\partial x} \right) = 0 \), \( \Phi \) is either \( S \), \( C \) or \( C_s \),

3) Reaction with lateral inflow: \( \frac{\partial \Phi}{\partial t} = RP(\Phi) \), where \( RP \) indicates processes, involved in reaction and lateral inflow, \( \Phi \) contains several variables (depends on submodule).

It is clear that for Advection and Dispersion steps different substances – \( S \), \( C \) and \( C_s \) – are separated, so equations can be solved independently.

Reaction system of equation includes variables:

- \( S \) in case of Sediment transport submodel;
- \( C, C_s \) and \( C_b \) in case of Radiouclide transport submodel.
4.1 Advection PDE

Advection equation is solved with newly derived fully implicit version MPDATA scheme, originally appeared in an explicit form (see Smolarkiewicz, 1998). The scheme inherits unconditional stability of the first order implicit scheme with upwind differencing advection representation, and tends to a second order scheme which is the main property of MPDATA iterations. The scheme doesn’t suffer from any oscillations, so no correction of fluxes is needed (compare to different Flux Correction Transport – FCT – limiters, applied to explicit MPDATA to prevent oscillations near the wave front).

One major drawback of implicit MPDATA is high numerical dispersion, which comes from implicit first order upwind differencing scheme. From the other hand, for modelling of advection-dispersion processes of real substances the numerical dispersion is highly suppressed by physical dispersion, so application of implicit MPDATA in this case is valid.

Advection PDE for river network is solved in several steps:

1) for each branch for its inner points form three-diagonal matrix according to fully implicit first order upwind differencing scheme:

\[
-nn(v^n)\Phi^{n+1}_{i-1} + [1 + nn(v^n) - np(v^n)]\Phi^{n+1}_i + np(v^n)\Phi^{n+1}_{i+1} = \Phi^n_i,
\]

where

\[
v^n_i = \frac{\delta t}{\delta x} u^n_i, \quad nn(z) = \frac{z + |z|}{2}, \quad np(z) = \frac{z - |z|}{2}.
\]

This equality can be rewritten in the matrix form:

\[
A e = f,
\]

where

\[
A = \begin{bmatrix}
* & * & * & \ldots & * \\
A_{21} & A_{22} & A_{23} & \ldots & \* \\
& & & & \ddots \\
& & & & \* & A_{M-1,M-2} & A_{M-1,M-1} & A_{M-1,M} \\
& & & & \* & * & \ldots & *
\end{bmatrix},
\]

\[
f = \begin{bmatrix}
\Phi^n_{i-1} \\
\Phi^n_i \\
\Phi^n_{i+1} \\
\ldots \\
\Phi^n_{M-1} \\
\Phi^n_M
\end{bmatrix},
\]

\[
e = \begin{bmatrix}
\Phi^{n+1}_{i-1} \\
\Phi^{n+1}_i \\
\Phi^{n+1}_{i+1} \\
\ldots \\
\Phi^{n+1}_{M-1} \\
\Phi^{n+1}_M
\end{bmatrix}.
\]

2) Assume \(\Phi^{n+1}_k = e_k \Phi^n_{i+1} + f_k \Phi^M_{M} + g_k\), \(1 \leq k \leq M\). Substitute each inner point equation with this assumption and get the three-diagonal matrix system of equations:

\[
A e = e^i
\]

\[
A f = e^M
\]

\[
A g = P^n,
\]

where
\[ A = \begin{bmatrix}
1 & 0 & 0 & \ldots & 0 \\
A_{21} & A_{22} & A_{23} & \ldots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & 1
\end{bmatrix} \]

3) Find \( e, f, g \) coefficients with fast double sweep procedure (or sparse iterative solver).

4) Form the node matrix equation with rules, described in the Section “Boundary and Initial conditions in river network”. In matrix formation use coefficients \( (e,f,g) \) calculated on the previous step. Note, that node equation is always solved for implicit time level \((n+1)\), disregarding the numerical scheme for inner points.

5) Solve node matrix equation with either matrix solver (sparse iterative solver in our case).

6) Find values for inner points according to the formula

\[ \Phi_k^n = e_k \Phi_{k-1}^{n+1} + f_k \Phi_{k+1}^{n+1} + g_k. \]

7) Calculate correction velocity \( U \) according to implicit MPDATA scheme.

8) Repeat 1)-7) with the number of iteration, defined by user.

### 4.2 Dispersion PDE

Dispersion PDE is solved with the first order implicit scheme, which is unconditionally stable for dispersion parabolic equation. Numerical dispersion in most cases is much less than physical one, so the first order approximation here is quite applicable.

Numerical solver follows the same steps 1)-6) of Advection numerical solver with several changes. Step 1) uses rules of constructing first order scheme for dispersion equation.

Steps 4)-5) (node matrix subsolver) use the following trick with two substeps:
a] form a new substance

\[
G = \left| \frac{\partial \Phi}{\partial x} \right|, \quad Q_G = -AE \cdot \text{sign}\left( \frac{\partial \Phi}{\partial x} \right).
\]

In new terms dispersion equation can be written in the form of pseudo-advection one:

\[
A \frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x} (Q_G G) = 0.
\]

\(G\) is set to be non-negative for usage of stable upwind differencing operator.

Free propagation condition has a simple form \(G = 0\).

Balance equation has the form

\[
G_{\text{out}} = \frac{\sum G Q_G}{\sum Q_G}.
\]

No source term information is used, so this step can be treated as a relaxation.

b] Solve node matrix equation, find \(G_1, G_M\) for all branches.

c] Find \(\Phi_1, \Phi_M\) by solving system of equations:

\[
\begin{align*}
\Phi_2^{n+1} - \Phi_1^{n+1} &= dx \cdot G_1 \cdot \text{sign}(\Phi_2^n - \Phi_1^n), \\
\Phi_M^{n+1} - \Phi_{M-1}^{n+1} &= dx \cdot G_M \cdot \text{sign}(\Phi_M^n - \Phi_{M-1}^n),
\end{align*}
\]

\[
\begin{align*}
(e_2 - 1)\Phi_1^{n+1} + f_2 \Phi_M^{n+1} + g_2 &= dx \cdot G_1 \cdot \text{sign}(\Phi_2^n - \Phi_1^n), \\
-e_{M-1} \Phi_1^{n+1} + (1 - f_{M-1}) \Phi_M^{n+1} - g_{M-1} &= dx \cdot G_M \cdot \text{sign}(\Phi_M^n - \Phi_{M-1}^n).
\end{align*}
\]

It can be seen, that the sign of \(\frac{\partial \Phi}{\partial x}\) is preserved, with possible switching when \(\frac{\partial \Phi}{\partial x}\) is close to zero.

### 4.3 Reaction PDE

Reaction ordinary differential equation is solved in different methods for Sediment transport submodel and Radionuclide transport submodel.

In case of sediments it is possible to write an analytical solution, assumed all variables \((h, S^*)\) to be constant through the interval of integration. Indeed, reaction part for sediment transport equation can be written in the form
\[
\frac{dS}{dt} = \bar{\beta} \frac{w_0}{h} (S - S_*) ,
\]

where

\[
\bar{\beta} = \begin{cases} 
1, & S > S_* \\
\beta, & S \leq S_* 
\end{cases}
\]

Note, that in any case solution is exponent multiplied by initial \( \Delta = S - S_* \). So solution is sign preserving, and there is no “switching” in parameter \( \bar{\beta} \) once we know initial sign of \( \Delta \). Summarizing, the solution of reaction ODE in case of sediment transport model is

\[
S^{n+1} = S^n + \exp \left( -\bar{\beta} w_0 \frac{1}{h} \cdot \delta t \right) (S^n - S^n) .
\]

Lateral inflow is added then as constant rate inflow:

\[
S^{n+1} = S^{n+1} + \delta t * q_i S_i / A .
\]

For Radionuclide transport submodel PDE is solved with implicit Euler integration:

\[
\begin{bmatrix}
C_s^{n+1} \\
C_s^{n+1} \\
C_b^{n+1}
\end{bmatrix} =
\begin{bmatrix}
C_s^n \\
C_s^n \\
C_b^n
\end{bmatrix} + \Delta t
\begin{bmatrix}
M_{11} & M_{12} & M_{13} \\
M_{21} & M_{22} & M_{23} \\
M_{31} & M_{32} & M_{33}
\end{bmatrix}
\begin{bmatrix}
C_s^{n+1} \\
C_s^{n+1} \\
C_b^{n+1}
\end{bmatrix} + \Delta t
\begin{bmatrix}
q_s C_s'/A \\
q_s C_s'/AS \\
0
\end{bmatrix},
\]

where matrix \( \begin{bmatrix}
M_{11} & M_{12} & M_{13} \\
M_{21} & M_{22} & M_{23} \\
M_{31} & M_{32} & M_{33}
\end{bmatrix} \) is formed according to corresponding reaction rules. The solution for the next integration time step can be found easily:

\[
\begin{bmatrix}
C_s^{n+1} \\
C_s^{n+1} \\
C_b^{n+1}
\end{bmatrix} =
\begin{bmatrix}
M_{11} & M_{12} & M_{13} \\
M_{21} & M_{22} & M_{23} \\
M_{31} & M_{32} & M_{33}
\end{bmatrix}^{-1}
\begin{bmatrix}
C_s^n \\
C_s^n \\
C_b^n
\end{bmatrix} + \Delta t
\begin{bmatrix}
q_s C_s'/A \\
q_s C_s'/AS \\
0
\end{bmatrix} .
\]
5 RIVTOX Input and Output Data

The input data of the model are as follows:

- The Parameters of the river channel network such as the length of the branches and the positions of the junctions, the dependence of the area of crosssection of the channel from the water surface elevation, the bottom roughness, typical scenarios of the river floods for the simulation of direct releases of radionuclides into the water.

- The Typical distribution of the grain size of the suspended sediments and grain sizes of the bottom deposits.

- Time dependent information about the point sources for the simulation of the direct release and the output from RETRACE as the lateral inflow of the contamination for the modelling of the fate of pollutants which were washed out from the watershed.

The radionuclide transport parameters are defined in RIVTOX –HDM 4.0 for 7 radionuclides. The presented values in table 3.3. could be considered as the default values, that could be supplementary calibrated on the basis of processing of measured data during the direct implementation of the model.

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>$K_{db}$ (m3/kg)</th>
<th>$K_{ds}$ (m3/kg)</th>
<th>$a_{12}$ (1/day)</th>
<th>$a_{21}$ (1/day)</th>
<th>$a_{13}$ (1/day)</th>
<th>$a_{31}$ (1/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cs-137</td>
<td>3</td>
<td>15</td>
<td>1</td>
<td>0.02</td>
<td>0.01</td>
<td>0.002778</td>
</tr>
<tr>
<td>Sr-90</td>
<td>0.25</td>
<td>0.8</td>
<td>1</td>
<td>0.02</td>
<td>0.04</td>
<td>0.002778</td>
</tr>
<tr>
<td>H-3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Co-60</td>
<td>5</td>
<td>20</td>
<td>1</td>
<td>0.02</td>
<td>0.01</td>
<td>0.002778</td>
</tr>
<tr>
<td>I-131</td>
<td>0.01</td>
<td>0.01</td>
<td>1</td>
<td>0.02</td>
<td>0.04</td>
<td>0.002778</td>
</tr>
<tr>
<td>Pu-239</td>
<td>200</td>
<td>800</td>
<td>1</td>
<td>0.02</td>
<td>0.01</td>
<td>0.002778</td>
</tr>
<tr>
<td>Ru-106</td>
<td>4</td>
<td>15</td>
<td>1</td>
<td>0.02</td>
<td>0.01</td>
<td>0.002778</td>
</tr>
</tbody>
</table>

The output data are as follows arrays that presents the value of variables in the nodes of the grid, constructed on river branches:

- time variable crosssectionally averaged concentration of radonuclides in the solute;
- time variable crosssectionally averaged concentration of radonuclides on the suspended sediments;
- time variable crosssectionally averaged concentration of radonuclides in the upper layer of the bottom sediments.
The output data of the RIVTOX module is used by the special module “PREPARATION” to be transferred into the RODOS dose calculation module FDMA.
6 Model testing and validation studies

6.1 Numerical methods testing on the basis of the analytical solutions

The analytical solutions of the advection-diffusion equation could be obtained for the simplified cases. The diffusive wave equation could be presented as:

\[ \frac{\partial Q}{\partial t} + V \frac{\partial Q}{\partial x} = E \frac{\partial^2 Q}{\partial x^2}, \]  

(40)

\[ \frac{\partial Q}{\partial t} + V \frac{\partial Q}{\partial x} = E \frac{\partial^2 Q}{\partial x^2} \]  

(41)

Assuming the constant values of the wave propagation velocity and the diffusion coefficient the following analytical solution of the above equation could be obtained

\[ Q(x,t) = \frac{M}{2B\sqrt{\pi Et}} \exp \left( \frac{(x-Vt)^2}{4Et} \right) \]  

(42)

The simulated results (Figure 4) are in good correspondence with the analytical solution.
6.2 Validation studies for the Rhine River watershed

6.2.1 High flood at Christmas 1993

RIVTOX was tested coupled with RETRACE to simulate the extremely high flood event took place in the Rhine River for a period of December 1993 - January 1994.

The main objective of the validation study was to compare the model chain results with the daily averaged measured discharges in four outlets of the Rhine river. It should be mentioned that elevation data for the Rhine watershed channel net (orographical) data used in validation have been obtained from the maps with the different spatial resolution. This discrepancy in data resolution resulted in problems with the definition of runoff directions based on relief. Therefore, due to input data resolution discrepancy of some misplacements of the lateral inflow has been inserted into the simulation. Unfortunately, it is impossible now to estimate the magnitude of the errors dealt with input data problem.

Another problem concerned the input meteorological data. Precipitation data were provided by the German Meteorological Service for about 70 meteorological stations but the air moisture data was not available for this validation. To correct this absence of data it was supposed that for the whole period of the validation when the
intensive rains took place, the air temperature was 5°C and the relative air humidity was 90% which gives the air moisture deficit 0.873 hPa. (Popov, 1997).

Figure 5: Simulation results of the combined RIVTOX and RETRACE model for the flood event of the River Rhine in 1993. Comparison of predicted and measured discharge data for Andernach and Maxau.

Figure 6: Comparison of the simulated by RIVTOX and measured discharges for 4 sites at the River Rhine for December 1993 flood.

In Figure 5 and Figure 6 the simulation results are compared with the measurements for four crossections of the River Rhine. For two of
them – upper site the Andemach and the lower one the Maxau. On figure 7 here are presented the input precipitation data and the result of the runoff simulation by RETRACE. The model agreement with the measured data for this extreme flood situation was reasonable. The Reasons for the disagreement are associated with the more diffusive character of the discharge hydrograph simulated by RIVTOX. More precisely, RIVTOX’s hydrographs demonstrate less steepness of the fronts, and less magnitudes than measured. This behaviour might be a result of the not enough detailed data about the river crossections, used during the simulations.

6.2.2 Chernobyl radionuclides in the Rhine tributaries

Testing and tuning exercises RIVTOX was performed for two watersheds of the Mosel and the Neckar. In the first case the most complete set of data was available for water contamination which included monthly average values of $^{137}$Cs concentrations in the dissolved form and on the suspended particles [Mundschenk]. As the most contaminated region of the Mosel, catchment was situated upstream from the upper measured cross section and it was assumed, that the concentration of $^{137}$Cs in the lateral inflow was negligibly small compared to the one in the main stream. The upper cross-section was located about 222 km upstream from the junction of the Mosel with the Rhine river. The comparison with field data was performed for a cross-section located about 2 km from Koblenz. The results of the simulation for the years 1986-1988 are presented in Figure 7 and cover the Cernobyl ve fallout and runoff from the Mosel watershed.

**Figure 7: Simulation of Cs-137 concentration in the Mosel River**

The sub-module for modelling of the transport of the suspended matter was tested in the frame of the Neckar River study. Experimental data contained the daily suspended matter concentrations for two crossections at km 160 and 60.7 of the Neckar [RODOS data]. The simulation was done for the 30-day period and includes a period of 10...
days with heavy rain events (Figure 8). The inflows of the lateral water and the suspended matter were estimated from available meteorological data and from runoff coefficients.

![Neckar river, 60.7km](image1)

![Neckar river](image2)

**Figure 8: Simulation of $^{137}$Cs concentration in the Neckar River.**

### 6.3 VAMP validation study (Clinch-Tennessee and Dnieper).

The RODOS RIVTOX model was validated in the frame of the IAEA VAMP project. Two scenarios were prepared in the River and Reservoir sub-group.

The first scenario described the long term release of, $^{137}$Cs, $^{90}$Sr, $^{106}$Ru and $^{60}$Co to the Clinch-Tennessee river system from Oak Ridge National Laboratory (ORNL). Experimental data include monthly averaged water concentration values near ORNL and the water discharge rates. The simulated period was expanded from 1964 to 1983. The result of the validation is shown in Figure 9.

![Total concentration of Cs 137 in water, Centers Ferry](image3)

![Total concentration of Cs 137 in water, Watts Bar Dam](image4)

**Figure 9: Simulation for the Clinch river**
The second scenario covered the long term contamination of water and sediment by Cs$^{137}$ and Sr$^{90}$ for the set of the Dnieper reservoir cascade. The simulations were performed in two steps. In the first stage, model results were compared with unknown experimental data. The best estimate and confidence interval were obtained with the help of the uncertain analysis. In the second stage, the model parameters were tuned to reach a good agreement with the experimental data and the most sensitive parameters were defined which were the most important for the migration of radionuclides in the river systems. During the validation exercise, on the basis of the Dnieper river data the second version of RIVTOX model has been developed. Figure 10 - Figure 15 show the results of the second version of RIVTOX in comparison with the first version (curve CC) and measured data. This version differs from the previous first one by using different values for the sorption and the desorption rates $a_{1,2}$ and $a_{2,1}$ for the system "water-suspended sediment" and $a_{1,3}$ and $a_{3,1}$ for the system "water-bottom deposits". One can see that RIVTOX with those different exchange rates provides a better agreement with the measured data.

Figure 10: Concentration of Cs-137 in Kiev reservoir
Figure 11: Concentration of Sr-90 in Kiev reservoir

Figure 12: Concentration of Cs-137 in Kremenchug reservoir
Figure 13: Concentration of Sr-90 in Kremenchug reservoir

Figure 14: Concentration of Cs-137 in Dnieper reservoir
Figure 15: Concentration of Sr-90 in Dnieper reservoir
6.4 RETRACE - RIVTOX chain validation on the base of Ilya River case study

The Ilya river watershed is the first object for a validation of the whole chain of the hydrological modelling starting from the precipitation – the infiltration – the surface runoff – the sub-surface runoff – and finally the channel flow. This exercise will also include the toxicological part with the surface runoff and wash-off and the migration in the river net. The catchment of the Ilya River, which is the tributary to the Uzh River (flowing into the Kiev Reservoir), is situated mainly in the 30-km Chernobyl zone (Figure 16) and has a sizes of about 20 km in longitudinal direction and of about 15 km in the lateral direction. The data measured in 1988 by the SPA Typhoon (Obninsk, Russia) and the Ukrainian Hydrometeorological Institute (Kiev, Ukraine) were used in this validation study (Figure 17). The following set of the data is taken into account:

- the map of soil contamination;
- the meteorological scenario (daily precipitation);
- the water discharge at the outlet;
- the concentration of soluble and sorbed forms of $^{90}\text{Sr}$ and $^{137}\text{Cs}$ at the outlet;
- the contamination of bottom sediments.

Figure 16: Ilya river basin
Figure 17: Meteorological and hydrological data for the Ilya river basin

The lateral inflow into the river net is simulated by the RETRACE (Figure 18) and was then used by RIVTOX to simulate the transport in the river channels taking into account the interaction between radionuclides in the solution and on the suspended sediments (Figure 19). The limited measured data are not coincident with the exact moments of the short rainstorm floods at the river. Therefore, the comparison of the measured and calculated radionuclide concentrations should be done for averaged rather than for peak values. The uncertainties of the RIVTOX modelling were evaluated using the Monte-Carlo techniques for water-sediment exchange parameter variations. The measured data are within 90% confidence intervals of simulated $^{137}$Cs concentration on the sediments (Figure 20).
Figure 18: Measured (2) and simulated (1) hydrograph in outlet of Ilya river.

Figure 19: Cs-137 in surface runoff; daily averaged concentration in runoff from the Ilya River catchment (simulation by RETRACE)
6.5 RIVTOX implementation for the simulation of consequences of an accidental release from the Kharkov sewage system (summer 1995)

The RIVTOX was used in Ukraine in summer 1995 to evaluate the consequences of the extended accidental release of the Kharkov municipal waste water to the rivers. Within several days, the model as the part of the RODOS hydrological chain was customized and adopted by IMMSP to simulate the chemical and bacteriological contamination of the Udy River the Siversky Donets River aquatic system. Based on the request from the State Emergency Commission, several calculations have been provided to evaluate the amount of water that should be pumped to the Siversky Donets trough the channel from the Dnieper River to improve the water quality to permissible levels. This countermeasure on the basis of the RODOS’ hydromodule calculations was successfully implemented by the Ukrainian State Committee on the Water Resources (Figure 21).
6.6 Accidental releases from Bohunice NPP to Dudvah River-Vakh River

RIVTOX was implemented in collaboration with VUJE, Trnava, Slovakia to simulate the radionuclide transport in the river system of the Dudvah River-the Vakh River and the Bohunice NPP.

The waste water from the NPP “Bohunice” at Jaskovske Bohunice, Slovakia is released through the technological 15 km long pipeline into the Vah River. Another pathway for radionuclides released from the NPPs during the accident (or regularly during switch off the technological pipeline) is the 5.2 km long Manivier canal with the concrete paved bed that transports water from the NPP units cooling towers to the Dudvah River, that is right tributary of the Vah River. The last accidental release of $^{137}$Cs from the Unit A-1 occurred by this way in January 1989 that highly contaminated the bottom sediments of the canal and of the Dudvah River.

The data collected in VUJE for this accident provides a unique possibility to test the model of the direct release of radionuclide into the river system and its propagation in the river net from first hours after the accident. The implementation of the RIVTOX for this situation (Slavik et al., 1997) has demonstrated the needs to use two-step radionuclide exchange kinetic
submodels to simulate radionuclide dynamics in the first post-accidental hours.

The detailed description of these results are presented in the publication of Slavík et al., 1997.
Conclusion

The report presents the modules, the numerical algorithms and the results of the case validation studies of the one-dimensional model RIVTOX, developed at IMMSP, Cybernetics Centre, Kiev, to simulate the radionuclide transport in the networks of the river channels. The Sources can be a direct release into a river or a runoff from the catchment.

The model is implemented into the Hydrological Dispersion Module (HDM) of the RODOS coupled with the watershed radionuclide runoff model RETRACE-2.

As the part of the RODOS HDM the RIVTOX code was implemented and tested for the case studies of the River Rhine, the Dudvakh River-the Vakh River (Slovakia), the Iljya River (the Pripyat River Basin, Ukraine).

The model was tested and verified in different case studies (the Dniper River, the Clinch River-the Tennesee River and others). Some of these results are also presented in the Report.

The graphical user interface of the RIVTOX and User Manual are presented in the separate reports.
REFERENCES


ANONYMOUS, Methodology for evaluating the radiological consequences of radioactive effluents released in normal operations, National Radiological Protection Board, Chilton, United Kingdom (1994).


Benes P., Cernik M., Slavik, O., Modelling of Migration of $^{137}$Cs Accidentally Released into a Small River. J. Environ. Radioactivity 22, 279-293 (1994).

Benes P., Cernik, M., Model Calculations and Experimental Analysis of Transport of Radiocesium in the System Wastewater Channel - Dudvah (in Czech Republic). Report of the Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague 1990.


Coppe, P., Estimated models of impact used by Electricité de France within the framework of the french and European regulations, Radioprotection, Special issue, Proc. of the joint seminar from September 15th to 18th 1992, Fribourg, Switzerland, 185-189 (1993).


Ehrhardt, J. The RODOS system: decision support for off-site emergency management in Europe. -Radiation Protection Dosimetry, 1997, v.73, No.1-4, pp.35-40

Elder J.W, 1958, The dispersion of marked fluid in turbulent shear flow, Cavendish laboratory, University of Cambridge, Fluid mechanics 5


Fischer H.B, 1973, Longitudinal dispersion and turbulent mixing in open-channel flow, annual review fluid mechanics, University of California


modelling of hydrological pathways in RODOS. - Radiation Protection Dosimetry, 1997, v.73, No.1-4, pp.67-70


Hubel K., Erstellung eines dynamischen Modells zur Berechnung der Strahlenexposition über den Wasserpfad bei stehenden und fließenden Gewässern. Jahresbericht Bayerische Landesanstalt für Wasserforcsung (St.Sch.1071), Munchen 1989


IAEA, Safety Series N 100, Evaluation the Reliability of Predictions Made Using Environmental Transfer Models, IAEA, Vienna, 1989;


Mazijk van A. One dimensional approach of transport phenomena of dissolved matter in rivers. – Communication on Hydraulic and Geotechnical Engineering. – Delft University of Technology, Faculty of Civil Engineering, Report No. 96-3, September 1996, -310 p.


Modelling and study of the mechanisms of the transfer of radioactive material from terrestrial ecosystems to water bodies, (1996) Final report ECP-3 Project, CEC-Belarus, Russia, Ukraine Programme on the radiological consequences of the Chernobyl accident.

Morozov A., Zheleznyak M., Aliev K., Bilotkach U., Votsekhovitch O. Prediction of radionuclide migration in the Pripyat River and Dnieper Reservoirs and decision support of water protection measures on the basis of mathematical modelling.- Book of Extended Synopses. International Conference “One Decade after Chernobyl: Summing up the Radiological Consequences of the Accident”, Vienna, Austria 8-12 April 1996


Onishi Y. Sediment transport models and their testing. - In NATO Advanced Studies Institute Lecture Series, Pullman, WA, 1993


Raudkivi A. Loose boundary hydraulics, Pergamon Press, N.Y., (1967)


Won Seo I, Sung Cheong T, 1998, Predicting longitudinal dispersion coefficient in natural streams, J.Hydraulic Eng., Proc.ASCE. g


Zheleznyak M., Tkalich P.V., Lyashenko G.B., Marinets A.V. Radionuclide aquatic dispersion model-first approach to integration into the ÅN decision support
system on a basis of Post-Chernobyl experience. - Radiation Protection Dosimetry, N6, 1993, pp.37-43.

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