

# Software and numerical discretisation module development for radioecological dose consequence modelling

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## 1. INTRODUCTION

For supporting authority's independent modelling capacity in reviewing of safety assessment for radioactive waste disposal, a numerical software, Ecolego Toolbox, has been developed. The Toolbox is based on the commercial packages Matlab and Simulink used to solve differential equation systems, which are the cases of the assessment models. In the paper we illustrated an example of application of a newly developed module within the Toolbox, Discretisation Module. Radionuclide transport in a stream is modelled by the module with 250 compartments in main transport direction and 2 compartments in sediments corresponding to each compartment in the main direction. The solution converges when the number of compartments increases and is identical to the semi-analytical solution (Wörman et al., 2002).

## 2. DESCRIPTIONS OF THE TOOLBOX

### 2.1 Ecolego Toolbox

The Ecolego Toolbox is a set of Simulink blocks created to facilitate the creation and modelling of ordinary differential equation (compartment based) systems in the Simulink environment. Specifically the blocks have been designed to be used in the field of radionuclide transport and radioecological modelling. The name Ecolego Toolbox comes from the fact that the underlying principle for how the blocks function is the same as that of the blocks constituting a Simulink model created in the tool Ecolego (Avila et al., 2003). Thus a user of the Ecolego Toolbox will immediately recognize the structure and functionalities in an Ecolego created Simulink model, even though some layout and design differences exists between the two tools. Also, a model created with the Ecolego Toolbox can be imported to Ecolego. This allows for the use of Ecolego's data visualization capabilities and parameter handling as well as its probabilistic simulation engine, etc.

Except for those functionalities which are included in Simulink, the following five Blocks are used in the Ecolego Toolbox to facilitate model construction. The detailed description of the blocks can be found in Broed and Xu (2008).

- Compartment Block
- Function Block
- Radionuclide Block
- Transfer Function Block
- Conversion Blocks (Bq to Mole, Mole to Bq)

### 2.2 The Discretisation Module

Compartment models are traditionally used to analyse the migration of radionuclides in radioecological modelling. In application of compartment models for radionuclide transport a number of compartments can not be chosen arbitrarily but the effect of the model structure and the boundary condition on the model behaviour should be taken into account (Xu et al., 2007). Moreover, there is similarity between a finite difference approximation of an

advection-dispersion (A/D) type equation and compartmental model. Therefore, a numerical discretisation module has been newly developed within the numerical software Ecolego Toolbox, which allows us to easily set up a number of compartments in two dimensions to meet various modelling requirements.

The original version of the Discretisation Block was for 1 dimensional transport only. To be able to model systems with 2 dimensions, such as for example water transport in a rock fracture with matrix diffusion, the original block had to be extended. Due to the fact that only 2D matrix operations are allowed in Simulink, a workaround solution had to be devised. The solution was to write code that added a Compartment for each of the discretisations along the second dimension, while maintaining the original discretisation along the first dimension. Thus if the system is discretised in 10 levels along the first dimension, and 5 along the second dimension, the total number of Compartments would be 60 (10 + 5 \* 10). Were this to be constructed manually, 60 Compartments, with potentially 120 Transfer Functions linking them, would need to be set up. In such modelling it is often the case that the effect of discretisation on system behaviour is part of the study and therefore a manual method is impractical. Using the Discretisation Module the task is greatly simplified by just changing the values given for the number of required discretisation elements to get the required size of the system.

### 3. IMPLEMENTATIONS OF THE TOOLBOX

#### 3.1 The transport problem in streams

Radionuclide transport in streams can be described by processes such as advection, dispersion and exchange with hyporheic zones as well as adsorption. We use the Advective-Storage-Path (ASP) model to describe radionuclide transport in streams. The governing equations of the ASP model (Wörman et al., 2002) are written as:

$$\frac{\partial C}{\partial t} + \frac{1}{A_T} \frac{\partial(AUC)}{\partial x} - D \frac{\partial^2 C}{\partial x^2} = J_s \quad (1)$$

$$J_s = \frac{1}{2} \int_0^\infty f(T) \frac{P}{A} \xi (-V_z(\tau, T)|_{\tau=0} c_d + (V_z(\tau, T)|_{\tau=T} g_d) dT \quad (2)$$

where  $C$  is the activity concentration in stream water [ $\text{Bq m}^{-3}$ ],  $A_T$  [ $\text{m}^2$ ] is the cross-sectional area of the main stream including side pockets,  $A$  is the cross-sectional area of the main stream excluding side pockets,  $U$  is the flow velocity in the main stream [ $\text{m s}^{-1}$ ],  $D$  is the main stream dispersion coefficient [ $\text{m}^2 \text{s}^{-1}$ ],  $g_d$  is activity concentration of the pore water in the hyporheic zone [ $\text{Bq m}^{-3}$ ],  $V_z$  is the infiltration velocity [ $\text{m s}^{-1}$ ] into the bed in the direction of the streamlines denoted by  $V_z(\tau, T)|_{\tau=0}$  and exfiltration velocity out of the bed in the direction of the streamlines by  $V_z(\tau, T)|_{\tau=T}$ ,  $f(T)$  is the probability density function (PDF) of  $T$  weighted by the velocity component normal to the bed surface,  $V_n$ ,  $T$  is the total residence time from inlet to exit of hyporheic flow path [s],  $\tau$  is the exfiltration residence time [s] ( $0 < \tau < T$ ),  $P$  is the wetted perimeter [m],  $\xi$  is an area reduction factor equal to  $V_n/V_z$  that accounts for the fact that the streamlines are not necessarily always perpendicular to the bed surface.

Similar to the APS model the mass balance for the compartments in the stream and the sediment can be written as:

$$\frac{dM_i}{dt} = -\underbrace{\frac{U}{L/n_{riv}}}_{TR_{adv}} M_i - \underbrace{\frac{D}{(L/n_{riv})^2}}_{TR_{dis}} M_i + \underbrace{\frac{D}{(L/n_{riv})^2}}_{TR_{dis}} M_{i+1} - \underbrace{\frac{\xi V_z}{2h}}_{TR_{wat\_sed}} M_i + \underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{sed\_wat}} \frac{m_j}{R_j} - \lambda M_i \quad (3)$$

$$\frac{dm_j}{dt} = -\underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{up\_down}} \frac{m_j}{R_j} + \underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{down\_up}} \frac{m_{j+1}}{R_{j+1}} - \underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{sed\_wat}} \frac{m_j}{R_j} + \underbrace{\frac{\xi V_z}{2h}}_{TR_{wat\_sed}} M_i - \lambda m_j \quad (4)$$

Where  $M_i$  is the total inventory in stream compartment  $i$  [Bq],  $m_j$  is the total inventory in sediment compartment  $j$  [Bq],  $h$  is the depth of the river [m] and equivalent to A/P in ASP model,  $\lambda$  is decay constant for radionuclide [ $s^{-1}$ ],  $L$  is the transport length in the  $x$ -direction [m],  $Z$  is the depth of the sediment [m],  $n_{riv}$  is number of compartments in the  $x$ -direction and  $n_{sed}$  is number of compartments in the  $z$ -direction,  $R_i$  is the sorption capacity of compartment  $j$  and can be expressed as  $R_j = 1 + k_{d,j}\rho/\varepsilon_j$ , where  $\varepsilon_j$  is the porosity of the sediment compartment  $j$ ,  $k_{d,j}$  is the distribution coefficient in the compartment  $j$ ,  $\rho$  is the bulk density of the sediment in compartment  $j$ .  $\varepsilon_j$  is the porosity of the sediment compartment  $j$ ,  $k_{d,j}$  is the distribution coefficient in the compartment  $j$ ,  $\rho$  is the bulk density of the sediment in compartment  $j$ .

Further, the total inventories in stream and sediment compartments are expressed as:  $M_i = C_i V_i$  and  $m_j = g_j (\varepsilon_j v_j + k_{d,j} \rho)$ , where  $C_i$  is the activity concentration same as in eq. (1),  $V_i$  is the volume of compartment  $i$  [ $m^3$ ],  $g_j$  is the activity concentration in the sediment pore water same as in eq. (2),  $v_j$  is the volume of the sediment compartment  $j$  [ $m^3$ ].

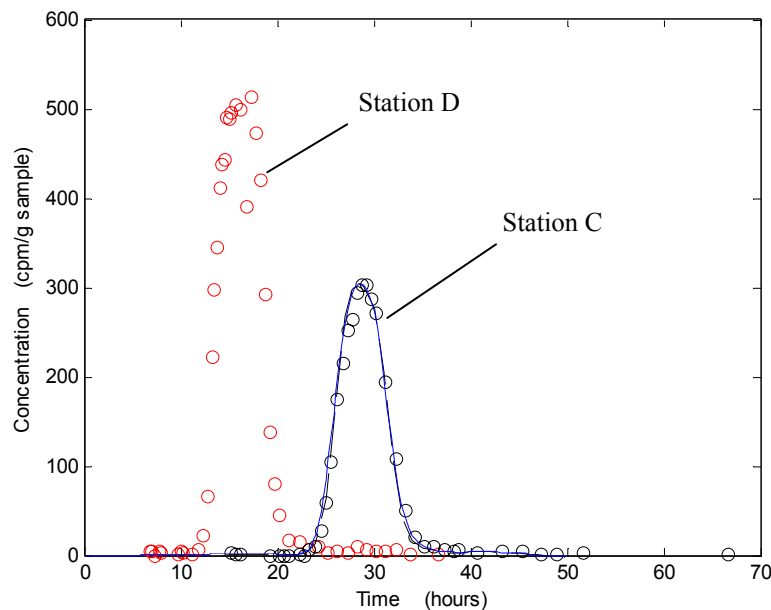
### 3.2 Model implementation and results

Data obtained from a tracer experiment performed in Säva Brook in Uppland County (Wörman et al., 2002) was used to verify the compartment model of the stream. In the experiment, moderately sorbing  $^{51}\text{Cr}$ , was used as the tracer. The concentration-time-distributions were obtained at eight stations along a distance of 30 km.

The input data used in this application are based on the distance between station C and D. The model, eq. (3) and (4), was implemented in the Discretisation Module. First, we tuned the number of compartments in the  $x$ -direction. The breakthrough curve converges when the number of compartments is large than 200. Then, we tuned the number of compartments in sediments ( $z$ -direction). The number of compartments in  $z$ -direction is not sensitive either the depth of the sediment on the model predictions in this case. The reason for this might be the residence time of radionuclide in the studied domain is much shorter than the residence time of radionuclide in the sediment, therefore, the discretisation of sediment has no effect on the model response.

Finally, the lumped parameter  $TR_{wat\_sed}$  was obtained by fitting the simulated breakthrough curve with experimental data when 250 compartments are used (Fig. 1). The calibrated lumped parameter value of  $TR_{wat\_sed}$  is 0.033 [ $\text{hour}^{-1}$ ] which is a factor of 0.55 of the value used for ASP model (Wörman, et. al., 2002). The reason for this is that in ASP model mass flux from water into sediment is integrated over the distribution of transport pathways while in the compartmental model no such a distribution function is employed. All the parameters used in the compartment model are exact the same as the one used in ASP model except the

$TR_{\text{wat\_sed}}$ . The simulated breakthrough curve of the compartmental model is closely aligned with the one of the ASP model obtained by a semi-analytical solution (Wörman et al., 2002).



**Figure 1.** Measured concentration-time distribution for  $^{51}\text{Cr}$  at station D (marked with 'o') in Säva Brook experiment (Wörman, et. al., 2002) and predicted curve (solid line) at station D using compartmental river model with 250 compartments and  $TR_{\text{wat\_sed}}$  as  $0.033 [\text{hour}^{-1}]$  and dashed line (hidden by the solid curve) by ASP model.

#### 4. CONCLUSIONS

Simulink is very powerful and flexible but also rather complicated and obscure. Ecolego and Ecolego Toolbox offer a set of tools and functionalities to facilitate environmental fate modelling of radionuclides and other contaminants. Specifically the Ecolego Toolbox contains code blocks to facilitate handling decay chains, unit conversion (Bq to Mole or Mole to Bq), and the discretisation module which could be a powerful tool in radioecological modelling.

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