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User's manual for Ecolego Toolbox and the Discretization Block

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Statens strålskyddsinstitut
Swedish Radiation Protection Authority

SSI's Activity Symbols

Ultraviolet, solar and optical radiation
Ultraviolet radiation from the sun and solariums can result in both long-term and short-term effects. Other types of optical radiation, primarily from lasers, can also be hazardous. SSI provides guidance and information.

Solariums
The risk of tanning in a solarium are probably the same as tanning in natural sunlight. Therefore SSI's regulations also provide advice for people tanning in solariums.

Radon
The largest contribution to the total radiation dose to the Swedish population comes from indoor air. SSI works with risk assessments, measurement techniques and advises other authorities.

Health care
The second largest contribution to the total radiation dose to the Swedish population comes from health care. SSI is working to reduce the radiation dose to employees and patients through its regulations and its inspection activities.

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According to the Radiation Protection Act, a licence is required to conduct activities involving ionising radiation. SSI promulgates regulations and checks compliance with these regulations, conducts inspections and investigations and can stop hazardous activities.

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SSI requires that nuclear power plants should have adequate radiation protection for the generalpublic, employees and the environment. SSI also checks compliance with these requirements on a continuous basis.

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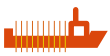
Mobile telephones and base stations emit electromagnetic fields. SSI is monitoring developments and research in mobile telephony and associated health risks.



Transport
SSI is involved in work in Sweden and abroad to ensure the safe transportation of radioactive substances used in the health care sector, industrial radiation sources and spent nuclear fuel.

Environment
"A safe radiation environment" is one of the 15 environmental quality objectives that the Swedish parliament has decided must be met in order to achieve an ecologically sustainable development in society. SSI is responsible for ensuring that this objective is reached.

Biofuel
Biofuel from trees, which contains, for example from the Chernobyl accident, is an issue where SSI is currently conducting research and formulating regulations.

Cosmic radiation
Airline flight crews can be exposed to high levels of cosmic radiation. SSI participates in joint international projects to identify the occupational exposure within this job category.

Electromagnetic fields
SSI is working on the risks associated with electromagnetic fields and adopts countermeasures when risks are identified.

Emergency preparedness
SSI maintains a round-the-clock emergency response organisation to protect people and the environment from the consequences of nuclear accidents and other radiation-related accidents.

SSI Education
is charged with providing a wide range of education in the field of radiation protection. Its courses are financed by students' fees.

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SUMMARY: The CLIMB modelling team (Catchment LInked Models of radiological effects in the Biosphere) was instituted in 2004 to provide SSI with an independent modelling capability when reviewing SKB's assessment of long-term safety for a geological repository. Modelling in CLIMB covers all aspects of performance assessment (PA) from near-field releases to radiological consequences in the surface environment. Software used to implement assessment models has been developed within the project. The software comprises a toolbox based on the commercial packages Matlab and Simulink used to solve compartment based differential equation systems, but with an added user friendly graphical interface. This report documents the new simulation toolbox and a newly developed Discretisation Block, which is a powerful tool for solving problems involving a network of compartments in two dimensions

SAMMANFATTNING: År 2004 initierade SSI modelleringsgruppen CLIMB (Catchment LInked Models of radiological effects in the Biosphere) för att bygga upp en oberoende modelleringskompetens för granskning av SKB:s säkerhetsanalyser. Modelleringen inom CLIMB täcker alla aspekter av säkerhetsanalysen från utläckage från de tekniska barriärerna till radiologiska konsekvenser i ytmiljön. En mjukvara för implementeringen av säkerhetsanalysmodeller utvecklades inom CLIMB-projektet. Mjukvaran är en Toolbox baserad på det kommersiella paketet Matlab och Simulink för att lösa differentialekvationssystem kopplade till compartment-modeller, men med mer användarvänligt användargränssnitt. Den här rapporten dokumenterar den nya Toolbox:en och ett nyligen utvecklat diskretiseringsblock som är ett kraftfullt verktyg för att lösa problem med en serie av compartments i två dimensioner.

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Contents

1. Ecolego Toolbox

1.1 Introduction

Ecolego Toolbox is a set of Simulink blocks created to facilitate the creation and modelling of compartment based systems in the Simulink environment. Specifically the blocks has been designed to be used in the field of radionuclide transport 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.

1.2 Blocks in the Ecolego Toolbox

Except for those functionalities which are included in Simulink, the following Blocks shown in Fig. 1-1 are used in the Ecolego Toolbox to facilitate model construction:

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

Below follows a description of each block in the Ecolego Toolbox library.

1.2.1 Compartment Block

The Compartment block represents a section of the system in which the concentration of the radionuclides are homogenously distributed, i.e. a single Compartment has exactly one value of the concentration for any given radionuclide. Each Compartment has an unlimited number of inputs and outputs, as selected by the user. The inputs represent the time-dependent flux of radionuclides into the Compartment, and the outputs the time-dependent outflux of radionuclides over time. Mathematically the Compartment integrates the difference between the total influx and total outflux over time. In addition to this, the radioactive decay, including ingrowth of possible daughter nuclides, is calculated inside the Compartment.

The compartment has an Initial Condition setting, that by default is zero. If the user wishes to have an initial condition other than this, it is possible to select “Display Initial Condition Port” on “Compartment” window (see Fig. 1-2). The “Compartment” window will be displayed by double-clicking on the Compartment symbol. This adds an additional input port to the Compartment block and whatever value(s) are input here becomes the new initial conditions for the Compartment.

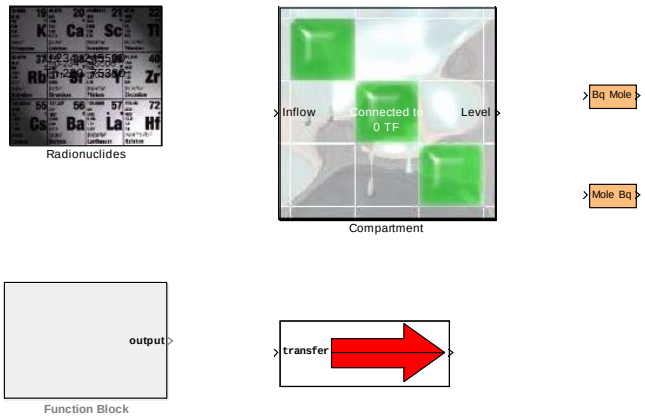


Fig. 1-1 Symbols of various Blocks in Ecolego Toolbox library.

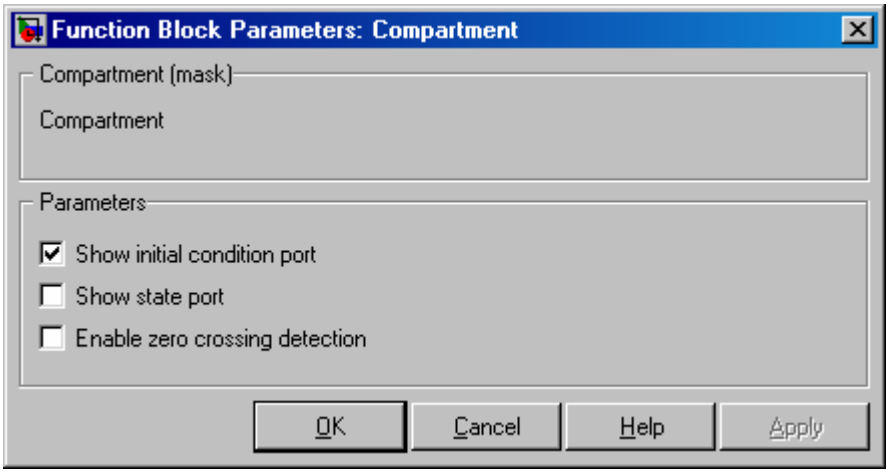


Fig. 1-2 Example of “Compartment” block dialog window.

1.2.2 Function Block

The Function Block is a higher level maths expression block, compared to the built-in maths blocks in Simulink. It allows complex mathematical expressions to be entered (in ordinary Matlab syntax) on the Function Block dialog window (shown in Fig. 1-3), which is displayed when double-clicking the Function Block. The expressions then are parsed and built as a set of Simulink low-level math operations blocks, representing the mathematical expression. Each variable and/or parameter used in the expression is added as an input to the Function Block. Each such input can be time-varying, thus allowing for fully time-dependent functions.

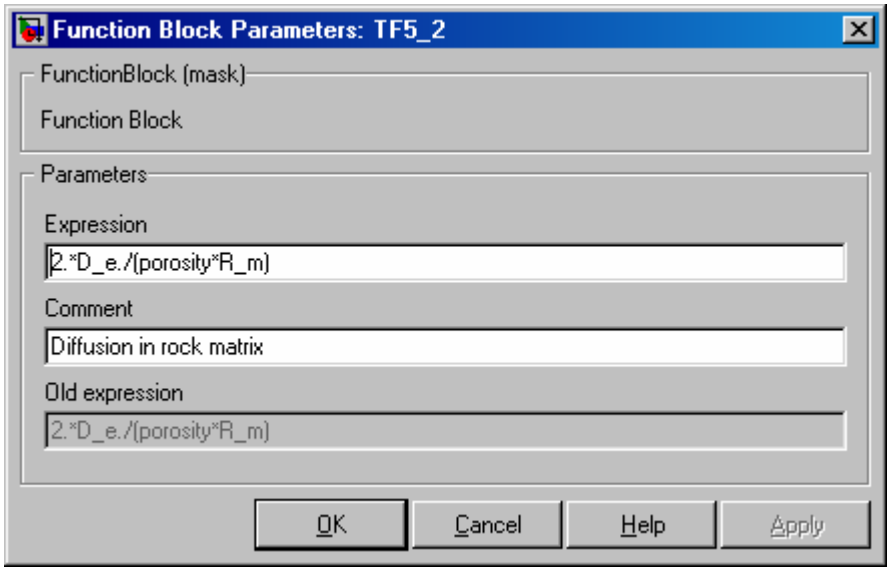


Fig. 1-3 Example of "Function" block dialog window (mathematical expressions can be typed in the Expression field).

1.2.3 Radionuclide Manager Block

The Radionuclide Block contains information about the radionuclides selected in the model. It also contains information about their respective halflives and about any eventual decay-chains. The Radionuclide Block is required in all models making use of the Compartment or Conversion blocks in a model. All information can be accessed and edited directly in the block itself (Fig. 1-4), but a special GUI (Graphical User Interface) has been written that allows for simplified graphical editing of the relevant data.

The Radionuclide Block creates an object known as the "Decaymatrix", which is a matrix containing all decay-associated data for all selected radionuclides in the model. This matrix is used within each Compartment to calculate decay and ingrowth for each radionuclide. It is also possible to select the fundamental unit for the quantity of radionuclide, whether Bq or Mole in the Radionuclide Block.

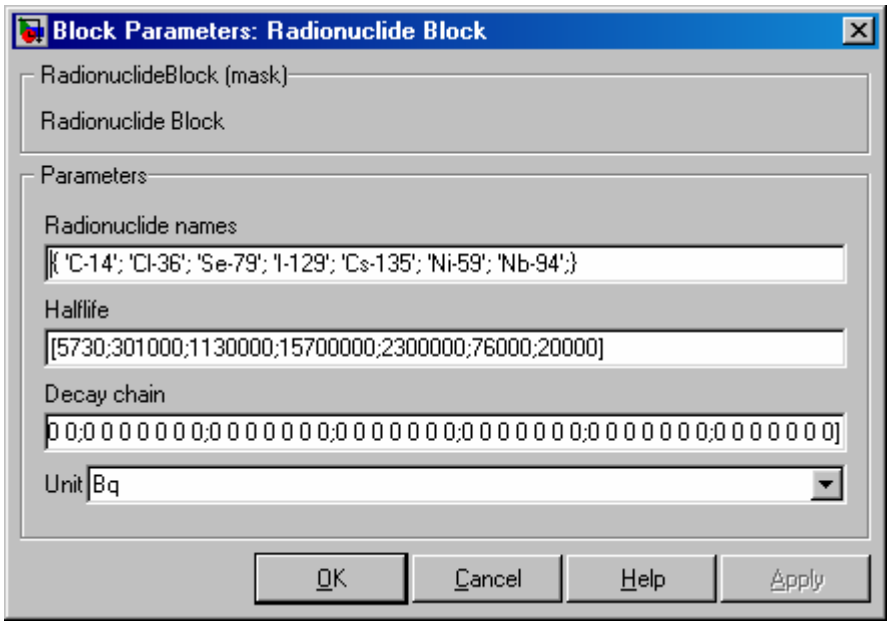


Fig. 1-4 Example of "Radionuclide" block dialog window.

Radionuclide transport models often have to consider multiple nuclides, most often when the ingrowth of daughter nuclides is of interest, but also when two or more nuclides might have some relationship other than belonging to the same decay chain, for instance when there are similarities in the physico-chemical properties which might lead them to compete in adsorption processes or root-uptake processes. To handle this effectively, it was decided to look at the models implemented as being vectorised. Since a signal in Simulink can either be a scalar or a vector, this raises no big problems. Instead of multiplying the signal corresponding to one nuclide, a matrix multiplication is performed with the vector-signal. The matrix contains all information about the decay-times and also about decay chains. The goal is to calculate the change in each nuclide per time unit, either in units of nuclei or activity.

If N_1, N_2 and N_3 are the number of nuclei [Mole] in a decay chain where N_1 is the parent nuclide, and λ_1, λ_2 and λ_3 are the decay-constants, we have:

$$\begin{cases} \dfrac{dN_1}{dt} = -\lambda_1 N_1 \\ \dfrac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2 \\ \dfrac{dN_3}{dt} = \lambda_2 N_2 - \lambda_3 N_3 \end{cases} \tag{1-1}$$

Which, in matrix form, can be written as:

$$\frac{d\mathbf{N}}{dt} = \begin{bmatrix} -\lambda_1 & 0 & 0 \\ \lambda_1 & -\lambda_2 & 0 \\ 0 & \lambda_2 & -\lambda_3 \end{bmatrix} \times \begin{bmatrix} N_1 \\ N_2 \\ N_3 \end{bmatrix} = \begin{bmatrix} -\lambda_1 \cdot N_1 \\ \lambda_1 \cdot N_1 - \lambda_2 \cdot N_2 \\ \lambda_2 \cdot N_2 - \lambda_3 \cdot N_3 \end{bmatrix} \quad (1\text{-}2)$$

If the unit used in the model is activity, $A_i = \lambda_i N_i$ [Bq], we can multiply both sides of equation (1-1) with decay-constants to obtain:

$$\begin{cases} \lambda_1 \dfrac{dN_1}{dt} = \lambda_1(-\lambda_1 N_1) & \dfrac{dA_1}{dt} = -\lambda_1 A_1 \\ \lambda_2 \dfrac{dN_2}{dt} = \lambda_2(\lambda_1 N_1 - \lambda_2 N_2) \Leftrightarrow & \dfrac{dA_2}{dt} = \lambda_2 A_1 - \lambda_2 A_2 \\ \lambda_3 \dfrac{dN_3}{dt} = \lambda_3(\lambda_2 N_2 - \lambda_3 N_3) & \dfrac{dA_3}{dt} = \lambda_3 A_2 - \lambda_3 A_3 \end{cases} \quad (1\text{-}3)$$

Which now is equivalent to:

$$\frac{d\mathbf{A}}{dt} = \begin{bmatrix} -\lambda_1 & 0 & 0 \\ \lambda_2 & -\lambda_2 & 0 \\ 0 & \lambda_3 & -\lambda_3 \end{bmatrix} \times \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} = \begin{bmatrix} -\lambda_1 \cdot A_1 \\ \lambda_2 \cdot A_1 - \lambda_2 \cdot A_2 \\ \lambda_3 \cdot A_2 - \lambda_3 \cdot A_3 \end{bmatrix} \quad (1\text{-}4)$$

In the equations above, the vectors **N** and **A** are the state-vectors of any individual compartment, i.e. compartment inventories. In the example a decay-chain consisting of three nuclides is used, but the same principle holds for any number and mix of nuclides and decay chains used in a model.

1.2.4 Transfer Function Block

The Transfer Function block is what is used to make a connection (representing transfer of radionuclides) between any two Compartments, or to be used as a sink accounting for losses from the system. The Transfer Function block is basically a Function Block but with added functionality in that it automatically identifies what block is the so called donor Compartment, i.e., the Compartment from which the radionuclides are to be removed by the rate governed by the Transfer Function Block. This is accomplished via the use of a pair of matching Goto and From blocks, and a callback function that is executed whenever the connection is changed on the Transfer Function Block.

Several Transfer Function Blocks can be connected to the same donor Compartment. Further, the block allows for direct input of mathematical expressions, describing the transfer rate in either Bq/Yr or Mole/Yr depending on the selected unit in the Radionuclide Block. However, these functions all assume that any parameter in the expression is a constant. To use time-varying parameters the user has to select the “Show External Rate Port” checkbox in the blocks dialog window (Fig. 1-5). When this is

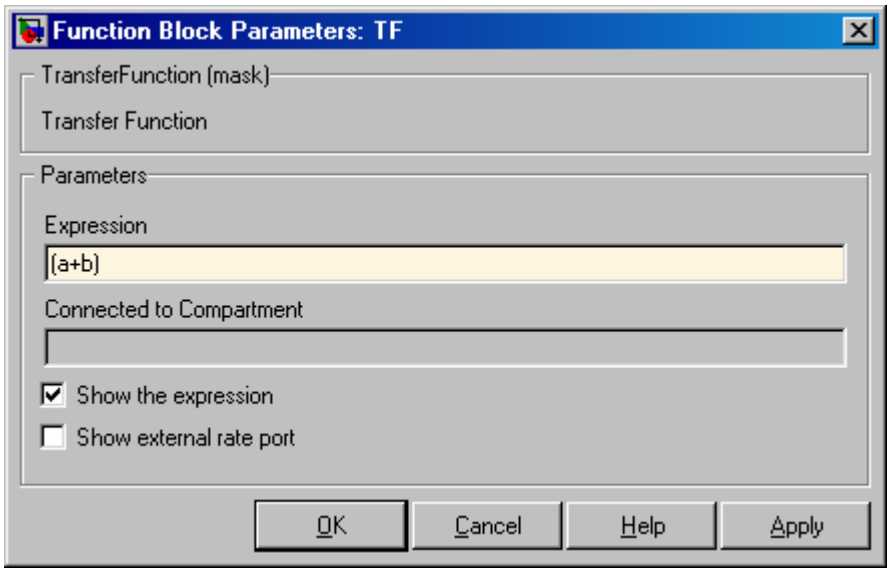


Fig. 1-5 Example of "Transfer Function" block dialog window.

selected, a new port is made available on the block where the user can input the output of a Function Block or any other required signal representing the transfer rate. Note that the expressions are not automatically assumed to be proportional to the donor Compartments value, so the donor Compartments value has to be used in the expression if this is the goal.

Example:

The expression "(a+b)" entered in the Transfer Function block (or fed as an input as described above) would mean that the amount of "(a+b)" will be removed from the donor Compartment each time-step. Thus the value of the Transfer Function Block is not proportional to the value of the donor Compartment.

*On the other hand, if the expression was instead "(a+b) * INVENTORY", where INVENTORY is the value of the donor Compartment, then the value of the Transfer Function Block will be directly proportional to the value of the donor Compartment.*

Note: the variable INVENTORY can be used to automatically access the donor Compartments value IF the expression is written directly in the Transfer Function Block, and not using the external rate port option. If the external rate port is used, this value has to be connected manually like any parameter to the inputs of the Function Block.

1.2.5 Conversion Blocks

The Conversion Blocks, when being connected with an output from another block, automatically converts the value between either Mole to Bq or Bq to Mole. These blocks also uses the information stored in the Radionuclide Block.

1.2.6 Parameter Input

Although a parameter in Simulink can be defined in several different ways, to simplify the use of Ecolego Toolbox, model parameters are by convention defined in so called subsystem masks. By following this convention, it is possible to import and export model parameters to and from Ecolego Toolbox (for example to/from MS Excel). The user still has the option of suing any valid Simulink method to define parameters, however, parameters defined in this way cannot then be included when interfacing Ecolego Toolbox with MS Excel.

A subsystem mask basically represents a workspace for a given Simulink subsystem (note: a mask also has other functionalities, that are not presented here), in which the user can define the parameters. This is similar to the ordinary Matlab workspace, the only difference being the manner in which the user defines the parameters, and how these are available in the model. In contrast to the Matlab workspace, parameters defined in a masked subsystem are only available to blocks contained within such a subsystem. In this way it is possible to construct hierarchical structures when building a model, and even use parameters with the same names but different values depending on their location in the model.

To define a parameter, the user must right-click a masked subsystem in the model, and then select “edit mask”. This opens a dialog window, where the user should select the “Parameters” tab. In this view, the user can add, remove and edit the order of the list of defined parameters. Each parameter has a “prompt” and a “variable” which needs to be defined. The “prompt” is the text that will appear when the user left double-clicks on the masked subsystem after the parameter has been defined. The “variable” contains a variable name that is used by the model. For instance, if a parameter has assigned the variable “kd”, the value for kd is available anywhere within the masked subsystem in question by simply writing “kd” in the appropriate location (this could be in the “value” field of a constant block, in any dialog parameter for any Simulink block, or in an expression of a transfer function block).

Once the parameters are defined in a masked subsystem, and the user has pressed “apply” or “ok”, the mask dialog will open the next time the user left double-clicks the subsystem. For an example of this see Fig. 1-6a and 1-6b. In the opened mask dialog, the user can specify any values to the listed parameters.

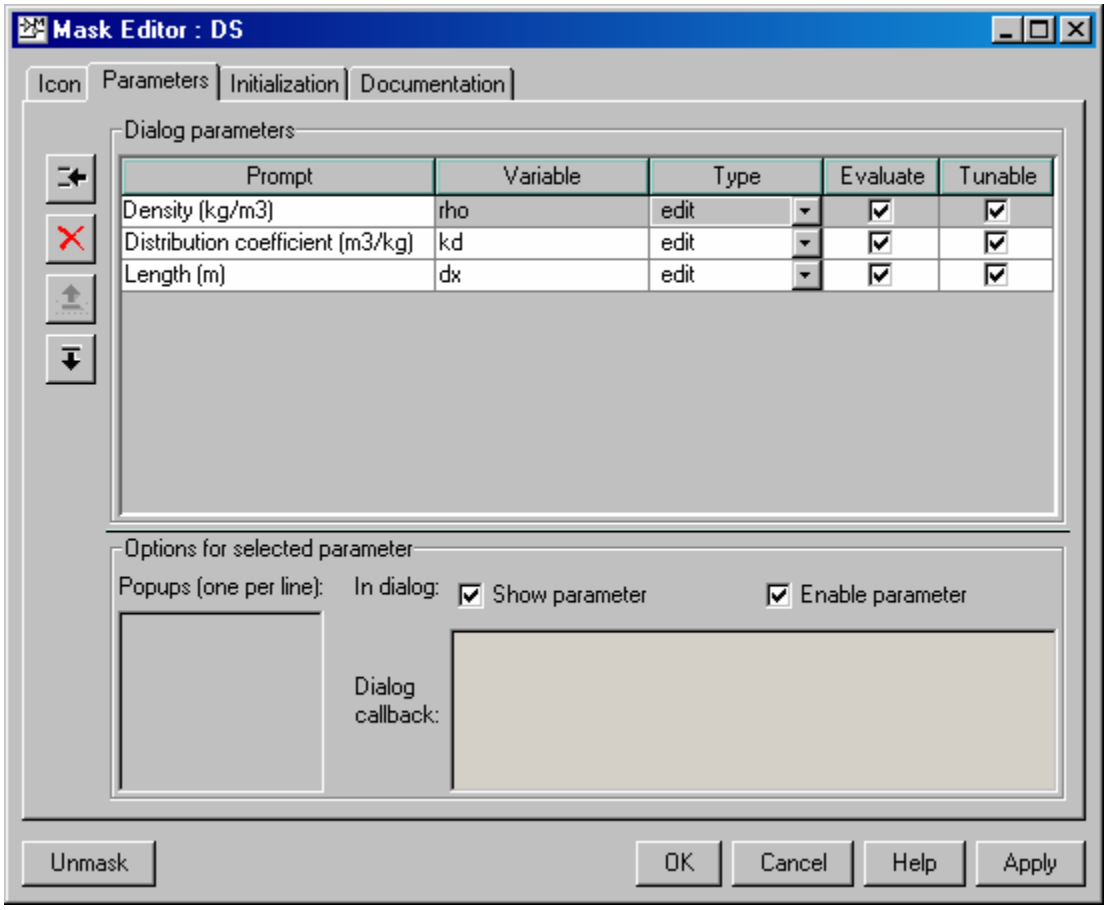


Fig. 1-6a Example of the editing of a masked subsystems parameters.

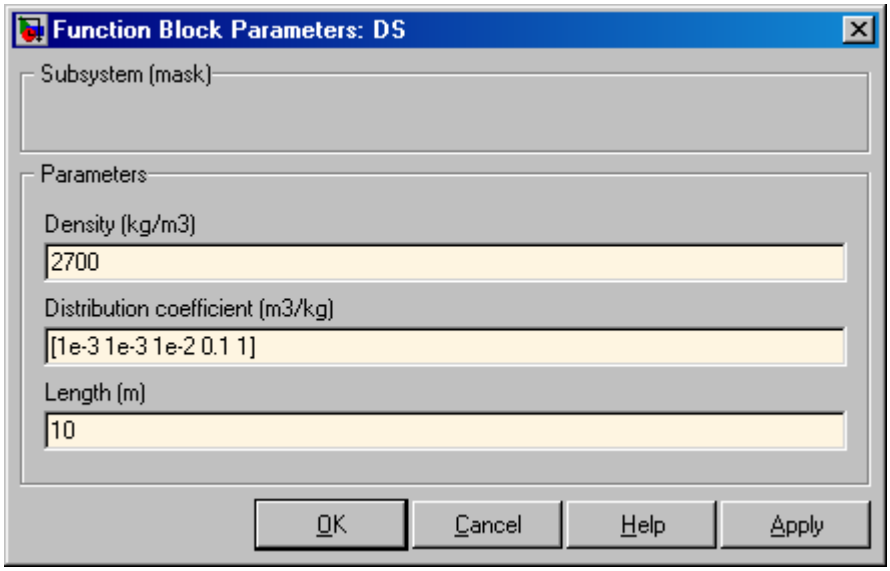


Fig. 1-6b The resulting opened mask dialog of the parameters defined according to fig. 1-6a.

1.3 Interface with MS Excel

In addition to the block-library in Ecolego Toolbox, described in section 1.2, two Matlab functions are included in the toolbox, simplifying the handling of model parameters. The two files are:

- Simulink_xls.m
- xls_simulink.m

The functions are called from the Matlab prompt and works on the currently active Ecolego Toolbox model.

The goal of these functions is to assist in editing and viewing the parameters of a model. Since a parameter in Simulink can be defined in many different ways, these files work under the assumption that the user has defined the model parameters in so called Masked Subsystems in Simulink. A Masked Subsystem is basically a set of blocks grouped together hierarchically, and having a local workspace associated with it. The Masked Subsystems workspace can be edited to include any number of parameters. Any parameter defined in a Masked Subsystem, is available for all blocks below it in the model hierarchy via references.

The function “simulink_xls.m” scans through the model for any Masked Subsystems, and extracts the data for any defined parameters. The data is summarized in a MS Excel file, containing the parameter name, location in the model, and value if specified. To use the function the user enters “simulink_xls” at the Matlab prompt, after which a dialog asks the user to enter a name of the MS Excel file to be created.

The function “xls_simulink.m” works the opposite way, by reading the data in an MS Excel file, and then for all matching parameters and Masked Subsystems in an active Ecolego Toolbox model, updates the parameters. The major benefit of this is that a user created model can have different parameter sets, stored in MS Excel files. To use the function, the user enters “xls_simulink” at the Matlab prompt, after which a dialog asks the user to select an MS Excel file.

1.4 Installation and use

To install Ecolego Toolbox, simply copy the folder containing the harddrive. Then in Matlab, add this path with subfolders to the Matlab path. This is done by selecting (in Matlab) the following menu items: File > Set Path… In the window that appears, press the button labeled “Add with Subfolders”, then locate the folder where the files were copied to and press ok. After that press the button labeled “Save” and close.

Once the Ecolego Toolbox is installed, the Simulink blockset will appear in the Simulink Library browser window the next time Simulink is started. To use a block from the library simply click-and-drag it into the model window from the library window.

1.5 Verification of the Toolbox

The Toolbox was verified by comparing the results with the results obtained from the Ecolego, for the same problem. In the test the results agreed perfectly. The problem used in the verification is taken from assessment of long-term safety for a spent nuclear fuel repository (Lindgren and Lindström, 1999) to calculate the release of radionuclide from the near field due to the leakage from a damaged canister through the bentonite buffer to the fracture. The reason for choosing this problem is that the results have been verified in a comparison of Ecolego and AMBER (Maul et al., 2003).

2. The Discretisation Block

2.1 Introduction

In many situations in compartment modelling it is the goal to model the transport of some contaminant through a medium of some sort. Since a compartment represents a unit of volume in which the contaminants entering are immediately assumed to be homogenously distributed, this gives rise to a problem when the total volume is large. This problem can be solved by using a series of connected compartments, all together representing the total volume of the medium. In this manner the dependency on the spatial variable can be obtained. Often the optimal number of compartments required to correctly approximate transport through the medium in question can be large. It can also vary depending on radionuclide properties or some other parameter in the system. Thus, the need to connect the number of compartments via the many transfer function connections can be both time-consuming and prone to error since the number of interconnections rapidly becomes large. To get around this problem a Discretisation Block was developed for Simulink.

2.2 1-D Discretisation Block

This block only consists of one underlying integrator (i.e. Compartment), which is being fed the product of its output (i.e. the states) with a matrix of size N×N where N is the number of required discretisations. The matrix is set up to represent a one-dimensional and sequential transport between the discretisation nodes (states). Both forward and backward transport is allowed, as well as specifying initial conditions for any of the states. Furthermore, the block allows for multiple radionuclides, including the calculations for decay and ingrowth, in the same manner as is performed in the Compartment Block.

The transfer coefficients are fed as inputs to the block, and can thus describe any required process affecting the overall transport, for instance advection, dispersion, diffusion etc. As for the Function Block, these inputs (the transfer coefficients) can be time-varying, allowing for full time-dependency. Also, inputs can be fed to any of the given discretisation nodes.

The number of discretisations is changed by entering the required number in the blocks dialog window.

2.3 2-D Discretisation Block

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 single of the 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 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. The task is greatly simplified by just changing the values given for the number of required discretisation elements in the two dimensions (*x* and *y*) to get the required size of the system (see figure 2-1).

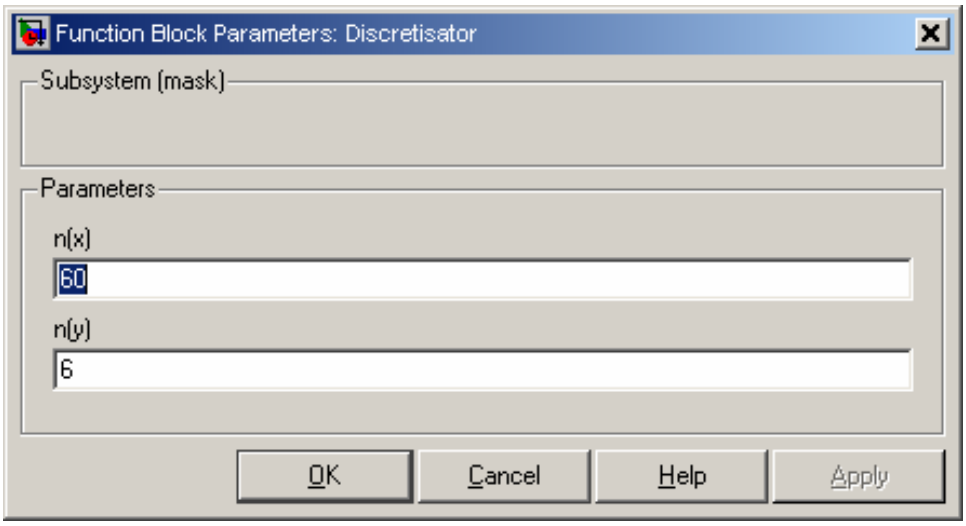


Fig. 2-1: An example of the mask dialog for the 2D Discretisation Block.

3. Application of Discretisation Block

3.1 Radionuclide transport in far field

3.1.1 A dual porosity model for radionuclide transport

Transport of radionuclide by groundwater in fractured rock is known as far field transport in assessments of the long-term safety of spent nuclear fuel repositories in crystalline bedrock. The processes involved in the transport are advection and dispersion along preferential flow paths and diffusion into the rock matrix as well as sorption on to the solid matrix. A dual porosity model for radionuclide transport along a stream tube is often used for describing radionuclide transport in far field (Norman and Kjellbert, 1990):

$$\frac{\partial C^i}{\partial t} + u\frac{\partial C^i}{\partial x} - D\frac{\partial^2 C^i}{\partial x^2} + \lambda^i C^i - \lambda^{i-1} C^{i-1} - a_w D_e^i \frac{\partial C_p^i}{\partial z}\bigg|_{z=0} = 0 \qquad (3\text{-}1)$$

$$R^i \frac{\partial C_p^i}{\partial t} - D_e^i \frac{\partial^2 C_p^i}{\partial z^2} + R^i \lambda^i C_p^i - R^{i-1}\lambda^{i-1} C_p^{i-1} = 0 \qquad (3\text{-}2)$$

where

t	=	time [y]
C_i	=	an effective stream tube average of the concentration of radionuclide i in the mobile liquid [moles m^{-3}]
C_p^i	=	a surface and stream tube averaged concentration of radionuclide *i* in the stagnant pore liquid in the impervious rock matrix [moles m^{-3}]
u	=	velocity of the mobile liquid [m y^{-1}]
D	=	longitudinal dispersion coefficient [m^2 y^{-1}]
a_w	=	total surface area of the boundary of the flow porosity per unit volume of mobile liquid [m^{-1}]
x	=	distance along stream direction [m]
z	=	penetration depth into matrix orthogonal to stream direction [m]
D_e^i	=	effective matrix diffusion coefficient for radionuclide *i* [m^2 y^{-1}]
λ^i	=	decay constant for radionuclide *i* [y^{-1}]
R^i	=	retardation factor [-] due to sorption into the rock matrix, which is defined by $R^i = \theta + K_d^i \rho$
ρ	=	bulk density of rock matrix [kg m^{-3}]
K_d^i	=	distribution coefficient for radionuclide *i* inside rock matrix [m^3 kg^{-1}]
θ	=	matrix porosity [-]

For a solute pulse travelling in the fracture (a delta source), the initial and boundary conditions are:

$$C^i(x,t=0) = C_p^i(x,t=0) = 0 \tag{3-3}$$

$$C^i(x=0,t) = \delta(t)\frac{M_0}{Q} \tag{3-4}$$

$$C_p^i(z=0,t) = C^i(x,t) \tag{3-5}$$

$$\left.\frac{\partial C_p^i}{\partial z}\right|_{z=Z} = 0 \tag{3-6}$$

$$C^i(x,t=\infty) = 0 \tag{3-7}$$

in which Q is the water flux [m^3 y^{-1}], M_0 is the total mass of solute inserted into the fracture [moles], $\delta(t)$ is the Dirac delta function [y^{-1}] and Z is the maximum penetration depth [m].

3.1.2 The Representation of radionuclide transport by compartment model

There is similarity between a finite difference approximation of an advection-dispersion (A/D) type equation and compartmental models. Therefore, compartmental models can be used to obtain identical solutions to analytical solutions of A/D equations when certain criteria are fulfilled (Xu et al., 2007). The corresponding transport problem modelled by a compartmental model as a two dimensional array of compartments is schematically shown in Fig. 3-1. In the *x*-direction (along the stream flow), compartments are linked together to represent advective and dispersive fluxes both forwards and backwards. In the *y*-direction (perpendicular to the stream flow), compartments are represent the process of matrix diffusion in a stagnant liquid. The transfer rates shown in Fig. 3-1 are given below, taken from Maul and Robinson, (2002). The symbols used in the following expressions have the same definitions as in (3-1) and (3-2).

The transfer rate of advection from compartment i to i+1 is given by:

$$\lambda_{adv} = \frac{u}{X/n_x} \tag{3-8}$$

where X is length of transport domain and n_x is number of compartments in the *x*-direction.

The transfer rate for dispersion (both forward or backward) is given by:

$$\lambda_{dis\_f} = \lambda_{dis\_b} = \frac{D}{(X/n_x)^2} \tag{3-9}$$

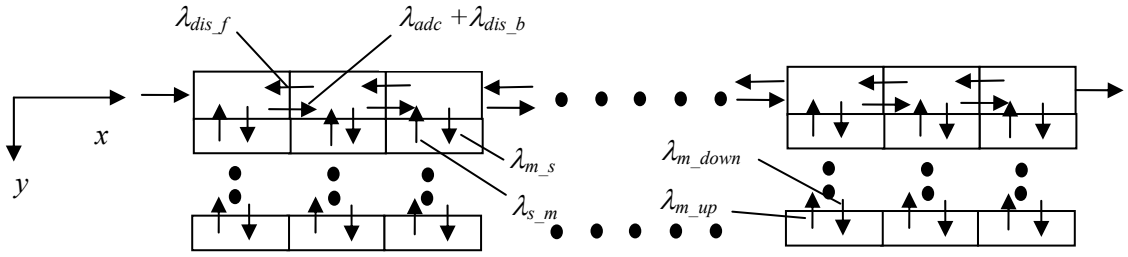


Fig. 3-1 Schematic of the compartmental model for description of transport processes in a stream tube concept.

The transfer rate from mobile to stagnant liquid is given by:

$$\lambda_{m\_s} = \frac{2a_w D_e^i}{d_1} \tag{3-10}$$

where d_1 is the length of the first layer (compartment) in y-direction.

The transfer rate from stagnant liquid (rock matrix) to mobile liquid is given by:

$$\lambda_{s\_m} = \frac{2D_e^i}{R^i d_1^2} \tag{3-11}$$

The transfer rate of diffusion from rock matrix compartment j to j+1 is given by

$$\lambda_{m\_down} = \frac{D_e^i}{R^i d_j \left(d_j + d_{j+1}\right)/2} \tag{3-12}$$

where d_j and d_{j+1} are length of the matrix compartments in the y-direction j and j+1, respectively.

The transfer rate of diffusion from rock matrix compartment j+1 to j is given by

$$\lambda_{m\_up} = \frac{D_e^i}{R^i d_{j+1} \left(d_j + d_{j+1}\right)/2} \tag{3-13}$$

3.1.3 Implementation of compartment model in the Block and comparison of the results with the semi-analytical solutions

We take as an example the pin-hole failure case in SR-Can assessment of long-term safety for a spent nuclear fuel repository (SKB, 2006) as a calculation example. Calculated release from near field due to the leakage from the damaged canister through bentonite buffer to the fracture is shown in Fig. 3-2. Details of near field transport calculation are found in (SKB, 2006) and Maul et. al., (2003). The near field release flux was used as the boundary condition for the far field transport problem. Input data to the problem are shown in Table 3-1 and 3-2. The same parameter values were used in both the dual porosity model and the compartment model calculations except the numbers of compartments, which are only used for the compartment model. The dual porosity model is solved by means of Laplace transforming of (3-1) and (3-2) (Maul et. al., 2003). Transformation back to the real domain is performed numerically by means of the series expansion algorithm of De Hoog et al., (1982) implemented in a Matlab code developed by Hollenbeck (1998). Implementation of the compartment model in the Discretisation Block simply requires that the expressions for the transfer rates in the "Function" block dialog windows are filled in (see Fig. 3-3a) together with the parameter values and the number of compartments required in both the *x*- and *y*-directions using the "Masked subsystem" dialog windows (see Fig. 3-3b and 3-3c), respectively.

The numbers of compartments for both *x*- and *y*-directions in the compartment model were tuned until the solution convergence. This was done in two steps. Firstly, we kept number of compartments in the *y*-direction constant and tuned number of compartments in the *x*-direction until the solution no longer changed with the number of compartments. Secondly, we set number of compartments in *x*-direction as obtained in the first step and tuned the number of compartments in y-direction until the solution became stable. The simulated breakthrough curve remains unchanged when the number of compartments in the *x*-direction was tuned to be more than 40 while the number of compartments in the *y*-direction was kept constant (see Fig. 3-4). The length of the compartments in both directions was equally divided. We used 60 compartments for the discretisation of rock matrix in the *x*-direction and then tuned the number of compartments in the *y*-direction. As can be seen from Fig. 3-5 when the number of compartments is more than 12 the solution converges, i.e., the breakthrough curves obtained with 10 and 12 compartments are almost overlapped.

Fig. 3-6 shows the far field release fluxes calculated from both models for five radionuclides in pin-hole failure case. It can be seen that the agreement between two model solutions is excellent.

Table 3-1 Parameter values used in far field transport calculation (Hedin, 2007)

Symbols	*Definitions*	*Units*	*Values*
$X^{[I]}$	length of transport domain	[m]	500
$u^{[I]}$	velocity of the mobile liquid	[m y^{-1}]	12.5
$D^{[I]}$	longitudinal dispersion coefficient	[m^2 y^{-1}]	625
a_w	half width of fracture	[m]	1×10^{4}
ρ	bulk density of rock matrix	[kg m^{-3}]	2700
θ	matrix porosity	[-]	0.001
Z	the maximum penetration depth	[m]	0.03

[I] In Hedin (2007) the values of the transport time (t_w) and Peclet (Pe) number are given as t_w =40 [y] and Pe=10. t_w and Pe have been interpreted into corresponding parameters u and D in our calculation based on assuming X=500 [m] and the relationship of $t_w = X/u$ and $D/u^2 = t_w/Pe$ (Norman and Kjellbert, 1990).

Table 3-2 Distribution and diffusivity coefficients used in calculations (Hedin, 2007).

	^{14}C	^{36}Cl	^{135}Cs	^{129}I	^{59}Ni
K_d [kg m^{-3}]	1×10^{-3}	0	4.2×10^{-2}	0	1×10^{-2}
D_e [m^2 y^{-1}]	8.138×10^{-8}	1.356×10^{-7}	1.424×10^{-6}	5.629×10^{-8}	4.611×10^{-7}

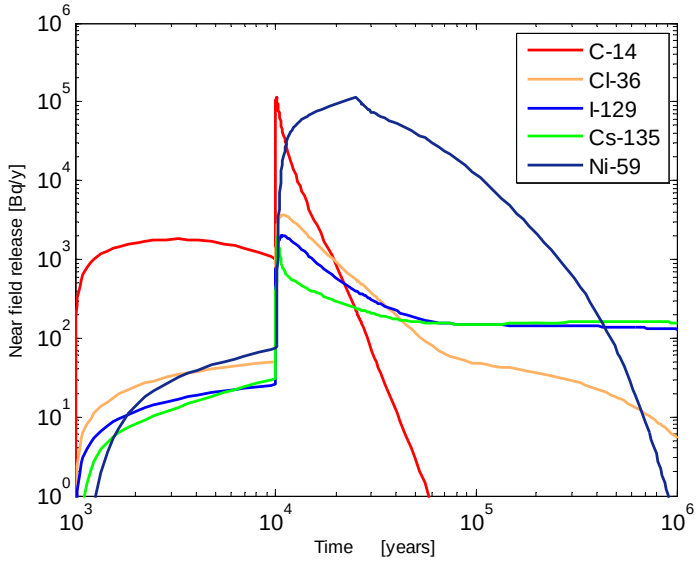
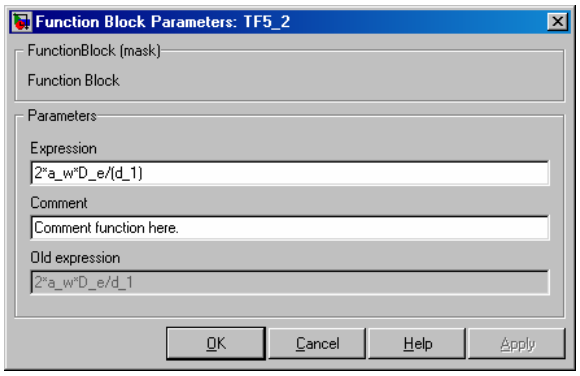
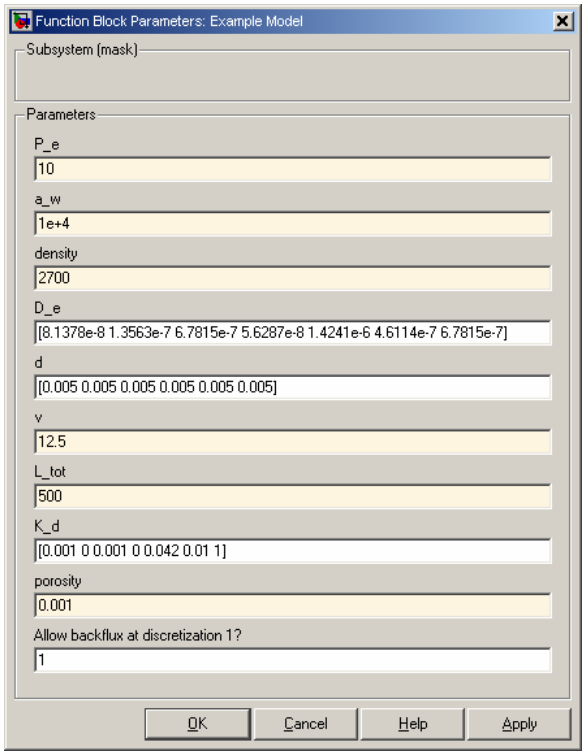


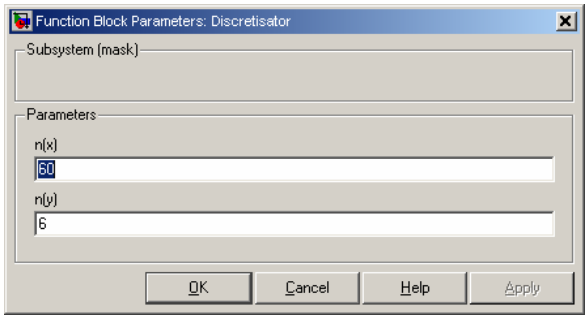
Fig. 3-2 Calculated near-field releases from pathway Q1 for the deterministic pin-hole failure case, which are used as boundary condition for far field release calculations.



a)



b)



c)

Fig. 3-3 Implementation of compartmental model representing far field transport in the discretisation Block, a) an example of transfer rate, Eq. (3-10), is filled in "Function" block window, b) parameter values are filled in "Masked subsystem" dialog window, c) the number of compartments in the *x*- and *y*-directions is filled in "Masked subsystem" dialog window.

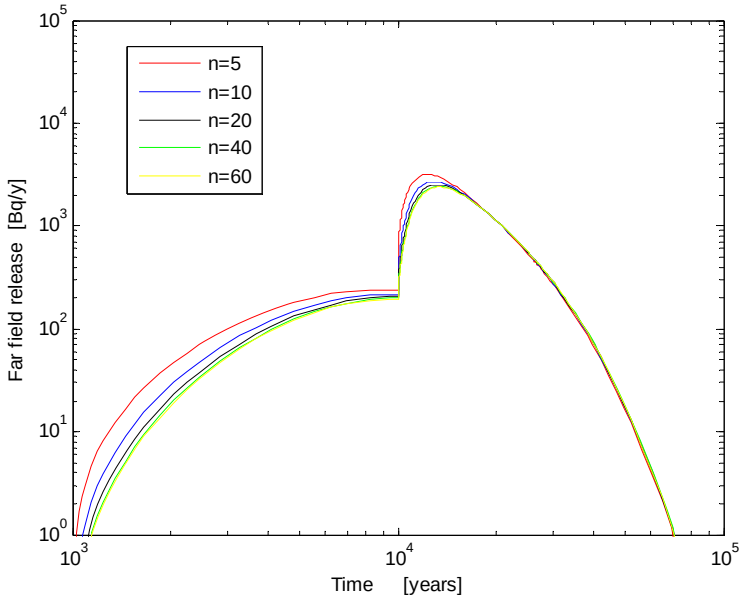


Fig. 3-4 Comparison of calculated far field release by using different number of compartments in the *x*-direction representing mobile liquid in compartment model. The number of compartments in the *y*-direction representing rock matrix is set to be constant (6 compartments in this case).

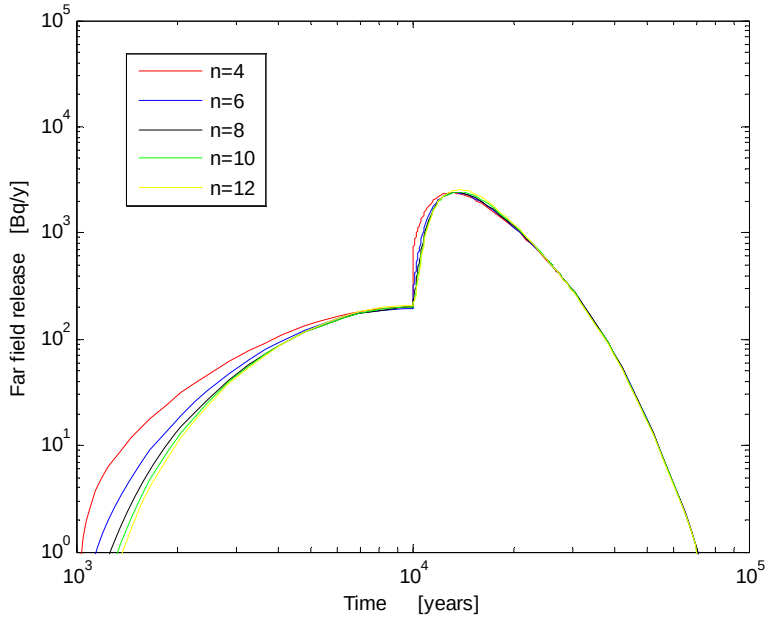


Fig. 3-5 Comparison of calculated far field release by using different number of compartments in y-direction representing rock matrix in compartment model. The number of compartments in x-direction representing mobile liquid is set to be constant (60 compartments in this case).

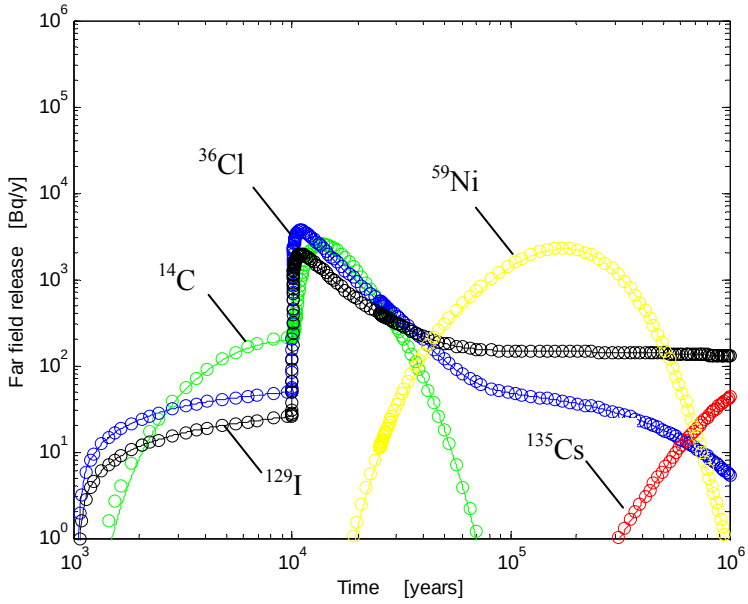


Fig. 3-6 Comparison of the semi-analytical (solid line) and compartment (circles) models for far field release.

3.2 Radionuclide transport in streams

3.2.1 Description of the stream model

Radionuclide transport in streams can be described by processes such as advection, dispersion and exchange with hyporheic zones as well as adsorption (e.g., Bencala and Walters, 1983; Elliott and Brooks, 1997). Over the last two decades different models describing transport processes in streams have been developed, such as the first-order mass transfer model (FOT model), the impermeable model (IS model), the water infiltration model (WI model) and advective-storage-path model (ASP model). By using the method of temporal moments of the residence time the relationships between parameters of the different models can be determined (Wörman, 2000), resulting in identical model predictions up to the first three temporal moments. Thus, selection of any of these models is not critical for predictability. We use the ASP model to describe radionuclide transport in streams. The governing equations of the ASP model (Wörman et al., 2002) is written as:

$$\frac{\partial C}{\partial t}+\frac{1}{A_T}\frac{\partial(AUC)}{\partial x}-D\frac{\partial^2 C}{\partial x^2}=J_S \qquad (3\text{-}14)$$

where C is the activity concentration in stream water [Bq m^{-3}], A_T [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 [m s^{-1}], Q(= UA) is the discharge [m^3 s^{-1}], and D is the main stream dispersion coefficient [m^2 s^{-1}]. The effective flow velocity in the main stream channel corrected for side pockets with stagnant water is given by $U_e=Q/A_T$ (Wörman, 1998).

The net solute mass flux [Bq/(m^3s)] in the dissolved phase in the stream water can be written, integrating over the distribution of transport pathways:

$$J_S = \frac{1}{2}\int_0^\infty f(T)\frac{P}{A}\xi\left(-V_Z(\tau,T)\big|_{\tau=0}c_d + \left(V_Z(\tau,T)\right)\big|_{\tau=T}g_d\right)dT \qquad (3\text{-}15)$$

where g_d is solute mass per unit volume of water in the hyporheic zone [Bq m^{-3}], V_z is the infiltration velocity [m s^{-1}] into the bed in the direction of the streamlines denoted by $V_Z(\tau,T)\big|_{\tau=0}$ and exfiltration velocity out of the bed in the direction of the streamlines by $V_Z(\tau,T)\big|_{\tau=T}$, $f(T)$ 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], τ is the exfiltration residence time [s] ($0<\tau<T$), P is the wetted perimeter [m], A is the cross-sectional area of the stream [m^2], and ξ 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.

3.2.2 Derivation of compartment model for description of radionuclide transport in streams

Similar to the APS model the mass balance for the compartments in the stream and the sediment based on the conceptual description in Fig. 3-7 can be written as:

$$\frac{dM_i}{dt} = -\underbrace{\frac{U}{L/n_{riv}}}_{TR_{adv}}M_i - \underbrace{\frac{D}{(L/n_{riv})^2}}_{TR_{dis}}M_i + \underbrace{\frac{D}{(L/n_{riv})^2}}_{TR_{dis}}M_{i+1} - \underbrace{\frac{\xi V_z}{2h}}_{TR_{wat\_sed}}M_i + \underbrace{\frac{\xi V_Z}{2(Z/n_{sed})}}_{TR_{sed\_wat}}\frac{m_j}{R_j} - \lambda M_i \qquad (3\text{-}16)$$

$$\frac{dm_j}{dt} = -\underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{up\_down}}\frac{m_j}{R_j} + \underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{down\_up}}\frac{m_{j+1}}{R_{j+1}} - \underbrace{\frac{\xi V_z}{2(Z/n_{sed})}}_{TR_{sed\_wat}}\frac{m_j}{R_j} + \underbrace{\frac{\xi V_Z}{2h}}_{TR_{wat\_sed}}M_i - \lambda m_j \qquad (3\text{-}17)$$

Where M_i is the total inventory in stream compartment i [Bq] or [kg], m_j is the total inventory in sediment compartment j [Bq] or [kg], U is the advective velocity, D is dispersion coefficient, V_Z is the infiltration velocity, ξ is the area reduction factor as described previously for ASP model, h is the depth of the river [m] and equivalent to A/P in ASP model, λ 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

$$R_j = 1 + k_{d,j}\rho / \varepsilon_j \tag{3-18}$$

Where ε_j is the porosity of the sediment compartment j, $k_{d,j}$ is the distribution coefficient in the compartment j, ρ is the bulk density of the sediment in compartment j.

Further, the total inventories in stream and sediment compartments are expressed as:

$$M_i = C_i V_i \tag{3-19}$$

$$m_j = g_j \left(\varepsilon_j v_j + k_{d,j} \rho \right) \tag{3-20}$$

Where C_i is the dissolved activity concentration in the stream compartment i [Bq m^{-3}], V_i is the volume of compartment i [m^3], g_j is the solute concentration in the sediment pore water in the compartment j [Bq m^{-3}], v_j is the volume of the sediment compartment j [m^3].

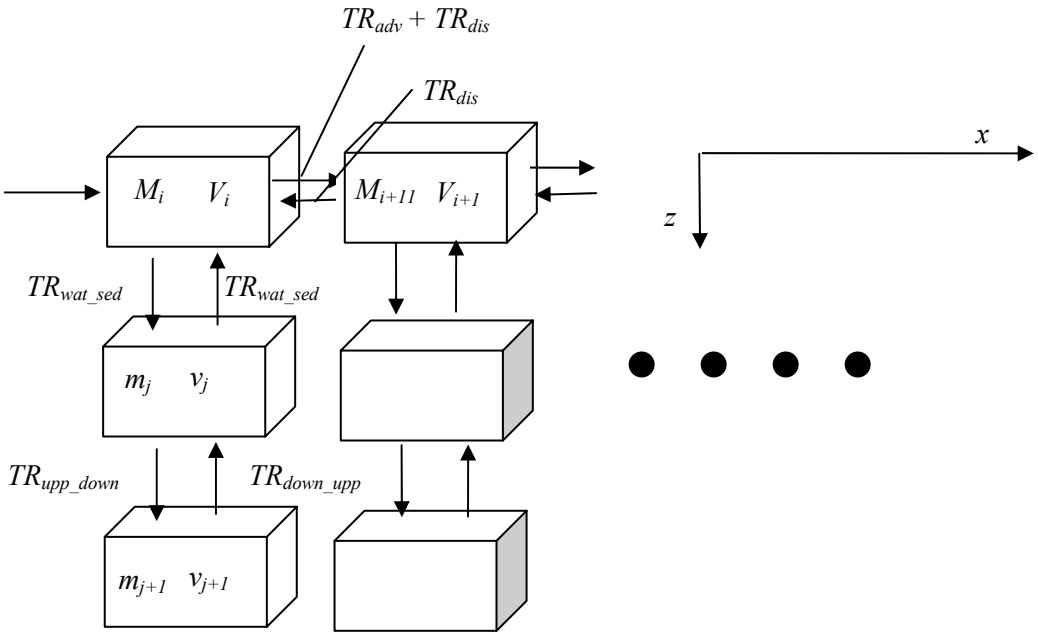


Fig. 3-7 Schematic of the compartmental model for conceptual description of transport processes in a stream.

3.2.3 Model implementation and discretisation

Table 3-3 summarises the expressions of those transfer rates derived from the previous section. Data obtained from a tracer experiment performed in Säva Brook in Uppland County (Johansson et al., 2001) was used to verify the compartment model of the stream. In the experiment, moderately sorbing ^{51}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 data are shown in Table 3-4, in which some parameter values are obtained from model fitting (Wörman et. al., 2002).

Following a similar procedure to that described in the previous section the model was implemented in the Discretisation Block. First, we tuned the number of compartments in the *x*-direction. Fig. 3-8 shows 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. 3-8). The calibrated lumped parameter value of TR_{wat_sed} is 0.033 [$hour^{-1}$] 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.

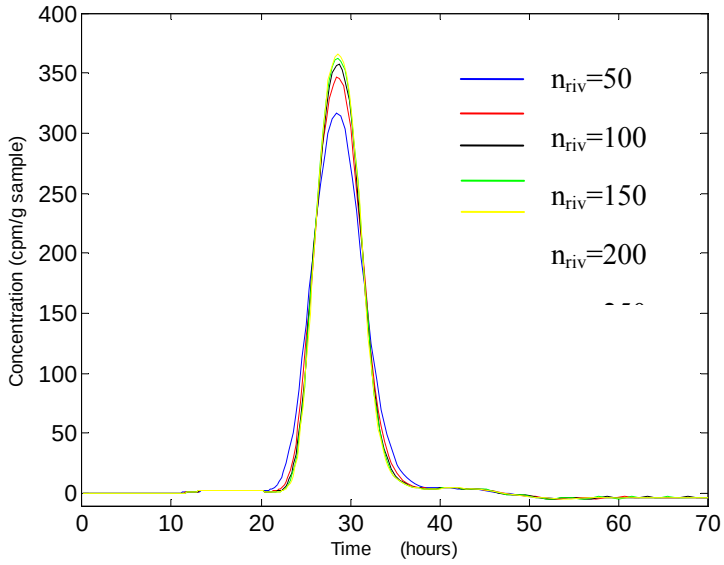


Fig. 3-8 Comparison of calculated concentration-time distribution for ^{51}Cr at station D by using different number of compartments in representing stream water in the compartment model.

Table 3-3 Description of transfer rates in compartmental models (definitions and values of the parameters in the descriptions are found in Table 3-4).

Transfer rate	Description of transfer rate
TR_{adv}	$\frac{U}{L/n_{riv}}$
TR_{dis}	$\frac{D}{(L/n_{riv})^2}$
TR_{wat_sed}	$\frac{V_Z \xi}{2h}$
TR_{sed_wat}	$\frac{(V_Z \xi/2)}{R(z/n_{sed})}$, where $R = 1 + k_d \rho/\varepsilon$
TR_{upp_down}	$\frac{(V_Z \xi/2)}{R(Z/n_{sed})}$
TR_{down_upp}	$\frac{(V_Z \xi/2)}{R(Z/n_{sed})}$

Table 3-4 Parameter values used to evaluate the breakthrough curve of ^{51}Cr in the Säva Brook experiment 1998 (after Johansson et al., 2000; Wörman et. al., 2002).

Symbol	Definitions	unit	values
U	The effective flow velocity	[m s^{-1}]	0.088
D	The longitudinal dispersion coefficient	[m s^{-2}]	0.8
L	The length of the river	[m]	3980
$\xi<V_z>/2$	The advective velocity into the bed sediment	[m/s]	3.96×10^{-6}
h	The hydraulic radius (ratio of cross section area and wetted perimeter)	[m]	0.77
R	The retardation factor in bed sediment for ^{51}Cr	[-]	20 000
Z	The penetration depth in the bed sediment	[m]	0.4
n_{riv}	Number of compartments in stream	[-]	250
n_{sed}	Number of compartments in sediments	[-]	4

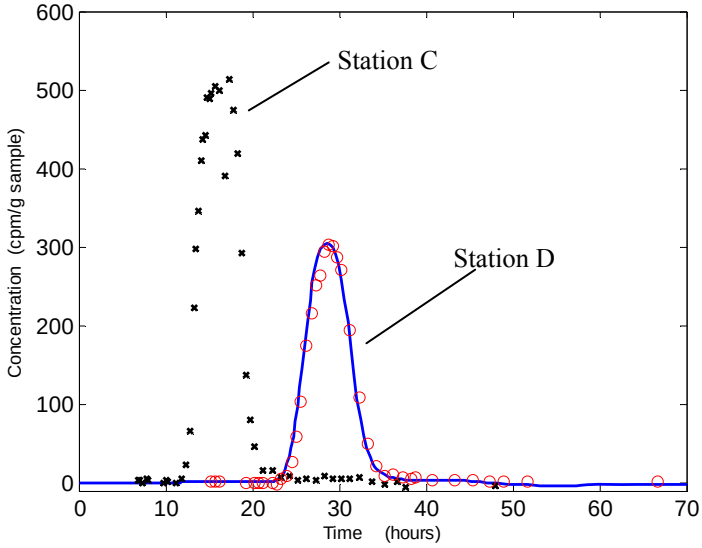


Fig. 3-9. Measured concentration-time distribution for ^{51}Cr at station D (marked with '○') in Säva Brook experiment (Johansson et al., 2001) and predicted curve (solid line) at station D using compartmental river model with 250 compartments and TR_{wat_sed} as 0.033 [$hour^{-1}$].

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