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Implementing the COMP23 model in Simulink

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December 2006

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Abstract

A Simulink model equivalent to the COMP23 model of the PROPER package has been developed and tested. The work is documented in this report. A comparison of the results from both programs for a test example shows very similar results. The Simulink environment makes the model flexible, easy to use and easy to understand.

In a recent development advective transport has been added to the computational model. The new version of the program has been validated using a new test case including advection, and the results have been compared to an analytical solution with good agreement.

In an appendix a user's manual for the program can be found.

Sammanfattning

En Simulink-modell som motsvarar COMP23-modellen i PROPER har utvecklats och testats. Arbetet dokumenteras i denna rapport. En jämförelse av resultaten från de båda programmen för ett testexempel visar mycket likartade resultat. Simulink-miljön gör modellen flexibel, lätt att använda och lätt att förstå.

Beräkningsmodellen har nyligen vidareutvecklats så att advektiv transport nu finns med. Den nya versionen av programmet har validerats med hjälp av ett nytt testfall som inkluderar advektion, och resultaten har jämförts med en analytisk lösning med god överensstämmelse.

I ett appendix finns en användarmanual till programmet.

Contents

1 Introduction

The Proper package /Kjellberg 1999abc/ is a collections of computer codes that have been used by SKB for radionuclide transport calculations in previous safety assessments. The package consists of a number of modules, each used for transport modelling in distinct parts of the modelled system (commonly KBS-3 but Proper has also be used for other systems). The different modules share code used for different common tasks like generating probabilistic data or for handling of time-series. The different modules share also a scripting language. The dissolution of fuel and radionuclide transport the near-field, i.e. through the buffer and backfill system, is in the Proper package handled by the COMP23 code which is thoroughly documented in /Romero et al. 1999, Cliffe and Kelly 2004/. COMP23 is, like all other codes within the Proper framework, written in Fortran 77 and uses data generated by the probabilistic engine within Proper as in-parameters or data given in input files.

1.1 Near field modelling in SR-Can

In the near-field model, fuel dissolution and radionuclide transport are simulated for a canister having a defect that allows water to enter. The near-field model requires input data on e.g. groundwater composition, radionuclide inventory, fuel conversion data (the fraction of the inventory that is either instantly released or later dissolved), solubility limits, geometry and the physical properties of the canister, the buffer and the backfill. Some of these, like inventory and the instant release fraction are inputted directly to the code while others, like groundwater composition are used to derive other parameters used by the code. Radionuclide release from the near-field, as calculated by COMP23 in SR-Can /SKB 2006a/, occurred through three characteristic transport paths Q1–Q3, Figure 1-1, where:

- Q1, represents a fracture intersecting the deposition hole. This fracture is placed on the opposite side of the buffer to the canister defect, hence minimising the transport distance and the diffusional transport resistance.
- Q2, corresponds to the excavated damaged zone, EDZ, and is in the hydrogeology model treated as a thin conductive layer located at the bottom of the deposition tunnel.
- Q3, corresponds to a larger fracture zone intersecting the deposition tunnel. The deposition tunnel is, in the hydrogeological model, intersected by several fractures and fracture zones with different properties and the location of the Q3 fracture zone is obtained by tracking advectively transported particles released in the centre of the deposition tunnel just over the deposition hole. As the distance between the deposition hole and this fracture zone differs, the longitudinal dimensions of the modelled deposition tunnel may be different for different deposition holes.

After the particles have left the near-field model through the sinks used to represent these pathways, they are then passed to the geosphere migration code where transport calculations to the biosphere are performed.

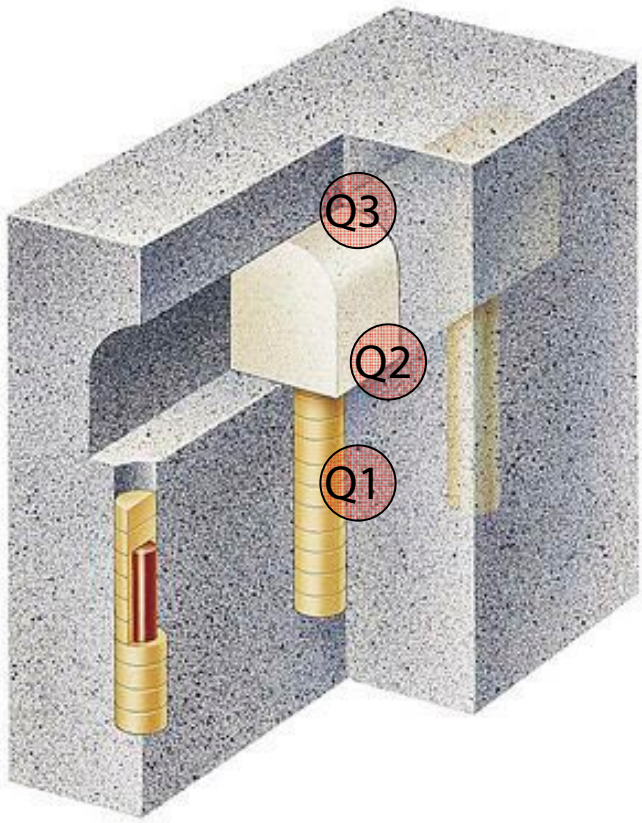

Figure 1-1. *Transport pathways implemented in the near-field model; Q1 represents that to a fracture intersecting the deposition hole located close to a canister defect, Q2 represents release through the EDZ and Q3 represents a larger fracture zone intersecting the deposition tunnel.*

1.2 Structure of the report

In the present document, an implementation of the COMP23 model in Matlab and Simulink is presented (henceforward denoted Compulink). Using Matlab in combination with Simulink to solve the near-field problem is an attractive alternative to the Fortran based COMP23 code. Besides the obvious benefits of the new environment, like a graphical interface and having access to all the tools available in Matlab and Simulink, it also provides a platform independent implementation that would simplify platform changes.

In the present document, Chapter 2 provides a brief introduction of the implemented mathematical models. This text is not intended to give a full information of the models and should be read together with the COMP23 manual where a more detailed presentation are given /Romero et al. 1999, Cliffe and Kelly 2004/. Following this, Chapter 3 presents some of the different verification tests conducted. Some have been generated during the development work the majority of the test cases are based on the COMP23 test batch /Lindgren et al. 2006/. In appendices, a short description of how to use the code is given together with listings of the code, the test batches and the implemented mathematical models.

2 The mathematical models

In Compulink, the majority of the models used in COMP23 have been implemented. Although one intention when developing Compulink has been to develop a code that is able to reproduce results of COMP23 some exceptions have although been made. This regard to some extent both the modelling strategy and the models included in the code. While COMP23 assumes solubility limiting reactions to be occurring in the whole modelled system, no solubility limiting limits have been implemented outside the canister compartment in Compulink. Another difference between the two codes concerns advection which has been fully implemented in Compulink. A brief description of the implemented models in Compulink follows below but for a full description the COMP23 manuals are suggested /Romero et al. 1999, Cliffe and Kelly 2004, Kelly and Cliffe 2006/. As apposed to the COMP23 code, Compulink is conceptually subdivided in two distinct parts, the canister compartment in which fuel dissolution and solubility calculations are handled using the graphical programming features of Simulink, Figure A-3, and a second part, which represents the buffer-backfill system of compartments with features given by a separate geometrical description file in a corresponding way as for COMP23.

2.1 The initial inventory – Bateman and Prebat

Assuming that there is no loss of radionuclides from the modelled system, the radionuclide inventory will only change due to decay and can, by using the Bateman system of equations, be determined with good accuracy at any given time. In order to speed up the execution time in probabilistic calculations it is therefore possible to use tabulated data of the inventory instead of performing these calculations at times when the canister is intact (as soon as radionuclides leave the canister the inventory must however be calculated at each time step). As transport of radionuclides out of the canister in the KBS-3 case is assumed to occur thousands of years after deposition, the amount of many short-lived radionuclides will have decayed to insignificant levels, hence reducing the number of radionuclides necessary to include in the calculations.

In Proper, two utility routines, Bateman and Prebat, handle these calculations (Bateman for the initial inventory calculations and Prebat for the table lookup). The Compulink implementation of Prebat corresponds to the Proper version and extracts inventory description from the same (big endian) binary files as used by (the SUN implementation of) COMP23. The Proper version of Bateman is however still required when generating the inventory descriptions.

An alternative to the Prebat block is to set the initial inventory using a Simulink “Constant block”. If so, the inventory in the constant block corresponds to the inventory at the starting time of the simulation.

2.2 Fuel dissolution rate

The fuel dissolution rate prescribes the rate at which the UO_2 fuel matrix dissolves and radionuclides trapped within leave (the compartment representing) the fuel matrix and enter a compartment representing solved and precipitated radionuclides (inside the canister). When the concentration of a certain element in the canister water exceeds its concentration limit a precipitate is instantaneously formed, see further discussion in Section 2.4.

In COMP23, a number of different models for fuel dissolution have been implemented. Of these, some are regarded to be obsolete and only three of the COMP23 models have been implemented in Compulink. In the first (Constant 1/yr) the fraction of the inventory dissolved per year is given. In the second, the time until the matrix is dissolved is given. (Constant yr). In the third the dissolution rate is given as the amount dissolved each year (Constant mole/yr).

2.3 Instant fuel dissolution

Part of the radionuclide inventory is not trapped inside the fuel matrix and will instead be dissolved immediately upon contact with the void water. In previous assessments, the instantly released radionuclides may either represent radionuclides in the fuel that are mobile or nuclides in metal parts pessimistically assumed to be corroded immediate upon contact with water. The ratio between the amounts of a single radionuclide that is instantly free to the total amount is the instant release fraction, IRF. In Compulink, the part of the inventory that is instantly released appears immediately at the compartment representing dissolved and precipitated radionuclides.

2.4 Solubility limits

Inside the (modelled) canister, there exist two separate compartments, one representing radionuclides in the fuel matrix and one representing radionuclides either solved or precipitated. If the calculated concentration of a radionuclide outside the fuel matrix is above the solubility limit, the remaining inventory is instantly precipitated and the concentration of the dissolved radionuclides will be kept at the solubility limit. Solubility can be treated either as a radionuclide specific property or as a property valid for a group of radionuclides using a shared solubility which is defined for each solubility group.

2.4.1 Shared solubility

In SR 97, solubility limits were assigned to each radionuclide. Provided that the solubility limits are wisely chosen, this approach may be correct and conservative. However, as radionuclides of the same element have closely related properties and that the relation between the concentration of different nuclides of the same element changes with time due to different half-lives, a more accurate approach would be to share the solubility limit between different radionuclides of the same element and to allow this to change with time. In the shared solubility implementation in Compulink, the concentration of each nuclide in a solubility group (which is defined by the user) is set proportional to the amount of each nuclide in the group that is available. The solubility limit for each nuclide i in a solubility group consisting of n radionuclides is

$$c_i = \frac{M_i}{\sum_{j=1}^{n} M_j} c$$

Where M represents the amount available for of each nuclide i and c the solubility limit for the group. Figure 2-1 shows how the concentration limits for different plutonium isotopes changes with time. Initially the solubility limit is shared by all five isotopes but as they decay only Pu-242, which has the longest half-life of the five, remains.

2.5 Chain decay

In Compulink, chain decay is modelled using a source/sink term, with the decay coefficient $\lambda = \ln(2)/T_{1/2}$, that describes the material lost and produced through radioactive decay and in-growth. In matrix form, this is

$$\begin{Bmatrix} \frac{dc_1}{dt} \\ \cdot \\ \cdot \\ \cdot \\ \frac{dc_n}{dt} \end{Bmatrix} = \begin{bmatrix} 0 & & & & \\ a_{2,1} & \cdot & & & \\ \cdot & \cdot & \cdot & & \\ \cdot & & \cdot & \cdot & \\ a_{n,1} & \cdot & \cdot & a_{n,n-1} & 0 \end{bmatrix} \begin{Bmatrix} c_1\lambda_1 \\ \cdot \\ \cdot \\ \cdot \\ c_n\lambda_n \end{Bmatrix} - \begin{Bmatrix} c_1\lambda_1 \\ \cdot \\ \cdot \\ \cdot \\ c_n\lambda_n \end{Bmatrix} \qquad 2.5.1$$

with the matrix components $a_{i,j}$ representing to what fraction decay of the mother nuclide j yields the daughter nuclide i. This formulation also enables the use of branching decay chains.

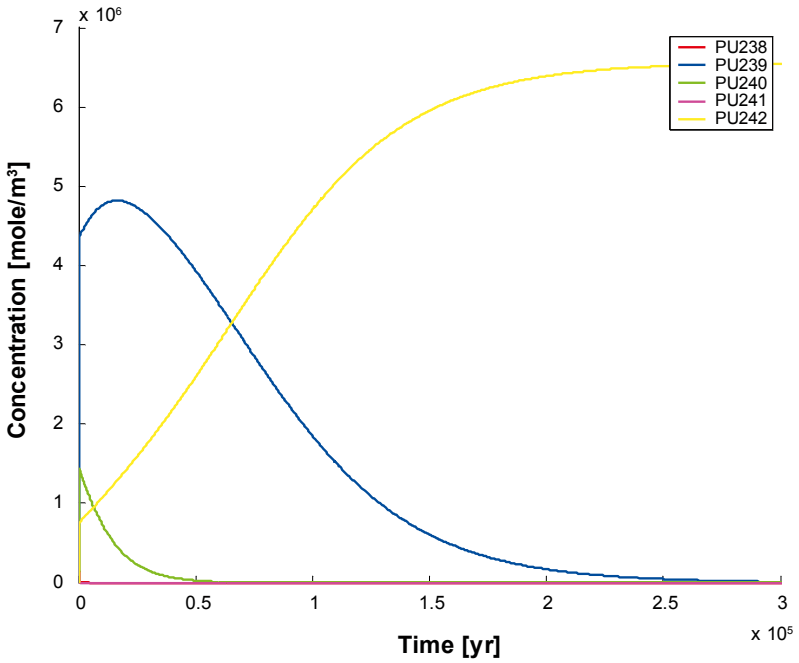

Figure 2-1. *The concentration of different plutonium isotopes as a function of time.*

2.6 Radionuclide transport

Radionuclide transport is in Compulink assumed to occur both through advection and through diffusion. In the case of having only diffusion plugs may be added to include extra resistance at geometrical features like fractures or close to the canister defect as in COMP23.

2.6.1 Diffusion

Both COMP23 and Compulink solves the transient diffusion equation for each nuclide n

$$C\frac{\partial c^n}{\partial t} = q_d + \nabla \cdot D_e \nabla c^n - C\lambda^n c^n \qquad 2.6.1$$

where c^n represents the concentration, D_e, the effective diffusivity of the different near-field materials, λ^n, the decay coefficient for each nuclide and q_d a general source term that represents nuclide in-growth or other sources that may, for different reasons, be convenient to lump in a separate term. The most important source term for the buffer-bentonite system is the canister compartment from which radionuclides are released. Integrating the transport equation over a number of finite compartments i, each having a volumes V_i, yields

$$V_i C_i^{\,n}\frac{dc_i^{\,n}}{dt} = V_i q_d - \sum_j \left(\frac{AD_e}{d}\Delta c\right)_{i,j}^{n} - V_i C_i^{\,n}\lambda^n c_i^{\,n} \qquad 2.6.2$$

with the middle term of the right hand side corresponding to nuclide transport over the boundaries of the element. Here Δc denotes the concentration difference between adjacent elements, A the area of the boundary (normal to the transport direction), and d, the distance between the centre of the element and the next element (in COMP23 terminology the terms elements and compartments are used as synonyms). In COMP23, the diffusion term in equation 2.6.2 is normally expressed using the resistance analogy where the diffusional resistance over one single element is

$$R_{diffusion} = \frac{\Delta x}{A_x D_e} \qquad 2.6.3$$

with Δx representing the length of the element in the transport direction and A_x the cross sectional area of the surface normal to the transport direction. It is important to notice that this is the diffusive transport resistance over a single element. In COMP23, nodes, where the concentration is calculated, are placed at the centre of each compartment, so the diffusive resistance from one node A to another node B will be

$$R_{A,B} = \frac{R_A}{2} + \frac{R_B}{2} \qquad 2.6.4$$

Where $\Delta x_A/2 + \Delta x_B/2 = d$. To this resistance other kinds of resistances may be added.

2.6.2 Extra transport resistances in the model

In order to reduce the number of elements in the model extra resistances are used to mimic the resistance at certain positions in the model. Presently, two different extra resistances are used, one representing the extra resistance when going from the small canister defect into a larger buffer compartment and the second the extra resistance when going from a large compartment into a small fracture. Both these are described in the COMP23 documentation /Romero et al. 1999, Cliffe and Kelly 2004, Kelly and Cliffe 2006/.

Transport from a hole in the canister into the buffer

When two compartments with very different sizes are used in COMP23, a so called plug resistance may be added to the diffusive resistance. The plug resistance, R_p, is described as

$$R_{plug} = \frac{1}{D_e\sqrt{2\pi A_{hole}}} \qquad 2.6.5$$

where D_e represent the effective diffusivity in the hole and A_{hole} the area of the hole (which in Compulink may be an arbitrary function).

Transport into a narrow fracture

Also at the interface between the fracture and the buffer backfill system, an extra resistance R_f may be used.

$$R_f = \frac{\left(F_{x,0}/\delta\right)\delta}{D_e A_f}$$

where δ is the fracture aperture De the effective diffusivity and, A_f, the area of the fracture which is denoted the plug area in the input section of the code. $(F_{x,0}/\delta)\delta$ is used direct as input and represents the plug length.

2.6.3 Diffusion into fractures

The fictitious flow rate at which water surrounding the deposition hole carries away water (and radionuclides) is described by q-equivalent, QEQ, factor. The value of this factor is different for the different transport paths and is given by the hydrogeological simulations.

2.6.4 Advection

In addition to diffusion, radionuclide transport through advection is included in the Compulink implementation. An upwind differencing scheme is used for the advective transport where the concentration at the downstream element boundary is approximated with the concentration at the centre of the element. More information about the scheme and its strengths and weaknesses may be found in most textbooks in numerical transport modelling.

2.6.5 Boundary conditions/sinks

The only possibility for nuclides to leave the computational domain is through the sinks that are implemented in the model. These represent normally fractures intersecting the deposition hole, the tunnel or the EDZ and connect the near-field to the far-field.

When advective transport is included in the model (as in Compulink) sinks representing advective transport must also be included in the model. At the upstream boundary, the concentration of the water flowing into the computational domain is in Compulink set to zero (no inflow from upstream canisters is assumed). No diffusional transport (which would occur over this boundary when the advective flow is small) is allowed over this upstream boundary. At the advective downstream boundary radionuclides are transported out of the model and further to the geosphere. Also at the downstream boundary, no diffusional transport is allowed.

2.6.6 Compulink implementation

To solve the transport problem outside the canister, represented by equation 2.6.2, a Simulink state-space block is used which solves the following equations

$$\begin{aligned} \frac{dx}{dt} &= Ax + Bu \\ y &= Cx + Du \end{aligned} \qquad 2.6.6$$

where x is the state vector, u the input vector and y the output vector. In the Compulink model, the state vector x represents the concentration of each radionuclide in each element, and the input vector u represents the influx of radionuclides into the system (from the canister). The matrix B stores the inverse of the capacity in each element hence multiplying the input vector (in moles/yr) with B yields the change in concentration. A corresponds to the system matrix which handles transport between different elements represented by Equation 2.6.2. In the present implementation, only zeros are stored in the D matrix. Multiplying the state vector x with the C matrix yields the output signal y. The matrices have the dimensions

$$\begin{aligned} &A: \left(n_{nuclides} n_{elements}, n_{nuclides} n_{elements}\right) \\ &B: \left(n_{nuclides} n_{elements}, n_{nuclides}\right) \\ &C: \left(\left(n_{sinks}+1\right) n_{nuclides}, n_{nuclides} n_{elements}\right) \\ &D: \left(\left(n_{sinks}+1\right) n_{nuclides}, n_{nuclides}\right) \end{aligned} \qquad 2.6.7$$

where $n_{elements}$ is the number of elements in the geometry description file, the canister and the hole uncounted, and n_{sinks} the number of sinks. The extra sink in the C and D matrices corresponds to the concentration in the first compartment which is used for the concentration gradient over the canister defect.

2.7 Geometric description

In COMP23, an input file is used to define all input data and to describe how the different compartments were connected. In Compulink, input data are instead defined either using the Simulink graphical interface or, mainly when scripts are used to run the simulations, by using the Matlab command set_param which assign data to the Simulink interface. Compulink uses however still the COMP23 syntax for defining the different compartments and how they are connected. The geometric model is based on a network model for diffusion through the bentonite and backfill. A network of discrete transport pathways (also called blocks) is defined, and each pathway is discretised using linear finite differences. It is possible to prescribe the dimensions of each element in the geometry definition file. As an alternative it is also possible to only specify the number of elements along a certain direction in the block. In the latter case the block will be divided into elements of equal size in that direction.

2.7.1 Element numbering

Compartments in COMP23 are normally numbered from 1 (representing the canister compartment) and 2 representing the defect and after that, sequentially as they are encountered while reading the geometry definition file. However, as these two compartments are modelled separately from the rest of the system (in the KBS-3 case representing the buffer and backfill), inside the state space block, see Section 2.6, compartment 1 in Compulink represents the first block outside the canister.

In the geometry definition file, elements may either be compartments or sub-compartments which build up a compartment. Internally there are no differences between these two.

2.8 Probabilistic simulations using Matlab scripts

One of the features of Simulink is that it is possible to run a simulation and change the values of different parameters from the Matlab prompt or from scripts running in Matlab. Hence, performing batch simulations in a probabilistic manner is straightforward. It is possible to use the probability distributions that are available in the standard Matlab version or to use distributions from the extended Statistical toolbox that provides Matlab with more advanced statistical functions.

2.9 Structure of Compulink

Compulink consists of one Simulink block (named Compulink) in which the migration calculations are performed and a number of Matlab functions that are used to generate data used by the block. Inside the Compulink block, components representing nuclides within the fuel matrix, nuclides either solved or precipitated and nuclides in the buffer-bentonite system exist. In the initial part of a simulation the geometrical description file is read and variables used in the state-space block, see subsection 2.6.6, and for other calculations are generated.

2.9.1 Input parameters used by Compulink

Table 2-1 lists the input required for the Compulink model together with a short description of each input.

Table 2-1. Input parameters for the Compulink component.

Name	size	used by	unit	Description
DEBUG				Generates extra printouts
OUTCONC		SetupCompulink.m		Unit for output of elements concentrations in the buffer – bentonite system
FDM		Matrix	–	Type of dissolution model
GEOMDEF		SetupCompulink.m		Name of geometry definition file
ADVECTIVEELEMENTS	Number of advective elements	SetupCompulink.m		List of element numbers for advective elements (if –1 is the first element number, advective conditions exists also inside the canister)
IRF	number of nuclides	InstantRelease	–	Instant release fraction
FDMC	scalar	Matrix	–	Model coefficient for fuel dissolution
SOLGROUPS	Number of solubility groups by number of nuclides	Solved/Solubility		Solubility matrix
SOLLIM	Number of solubility groups	Solved/Solubility	mole/m³	Solubility limit
RHO	Number of materials	SetupCompulink.m	kg/m³	Density

Name	size	used by	unit	Description
EPS	Number of materials by number of nuclides	SetupCompulink.m	–	Porosity
DE	Number of materials by number of nuclides	SetupCompulink.m	m²/y	Effective diffusivity
KD	Number of materials by number of nuclides	SetupCompulink.m	m³/kg	Sorption coefficient
PLUGLENGTH	Number of sinks	SetupCompulink.m	m	Plug lengths for sinks
PLUGAREA	Number of sinks	SetupCompulink.m	m²	Plug areas for sinks
QEQ	Number of sinks	SetupCompulink.m		Factor used in equivalent groundwater flow calculations
DARCYVELOC-ITY	Scalar	SetupCompulink.m	m/y	Groundwater velocity
ATOL	Scalar	Compartment/ Integrator and Solved/Integrator	mole	Lower saturation point

2.9.2 Advective elements

The parameter ADVECTIVEELEMENTS is used for specifying in which parts of the model advective transport occur. A list of element numbers should be given, and the advective flow goes from the first element in the list to the second, from the second to the third, etc. The complete advective flow path must also be connected with ordinary connections defined in the geometrical description. The advective outflow from the last element in the list can be monitored by studying the output value of the advective sink, which is the last sink in the model. If advective elements exist, the advective sink is generated automatically when the model is set up. The magnitude of the advective flow is calculated as the Darcy velocity multiplied by the area of the interface between the first and the second element in the advective flow path. The advective mass flow is kept constant along the flow path even if the area of the cross section varies.

The element number to use in the list of advective elements is the element number less 2, since only ordinary elements can be advective, and the third element is always the first ordinary element. If the list of advective elements is started by –1, advective transport out from the canister is also included in the model and the part of the inventory solved in the water are advectively transported out of the canister. In DEBUG mode the different elements are given.

2.9.3 Solubility matrix

The solubility matrix is used to link the different nuclides with the solubility limits. The number of rows in the solubility matrix corresponds to the number of solubility groups while the number of columns corresponds to the number of radionuclides. Each row in the solubility matrix represents one single solubility group, the nuclides that are part of a solubility group is represented by ones at the position of the nuclide. Table 2-2 shows one example of how the solubility matrix may be set up. Radionuclides *N1* and *N3* shares the solubility in *S1* while *N2* and *N4* are parts of the solubility groups *S2* and *S3* respectively. One nuclide may only appear in one solubility group (the sum for each column must be one). In Compulink, a utility function (GenerateSolubilityMatrix.m) may be used to generate the matrix.

Table 2-2. Solubility matrix representation.

	*N*1	*N*2	*N*3	*N*4
*S*1	1	0	1	0
*S*2	0	1	0	0
*S*3	0	0	0	1

3 Verification

The current chapter shows different verification tests conducted. Initially, a number of different test cases intended to show the capabilities of the code are presented. These are intended to give a better understanding of the models implemented. Following that, a more detailed comparison with the COMP23 code are presented where a subset of the COMP23 test batch have been used.

3.1 Demonstration of Compulink

For the different simulations values presented in Table 3-1 were used.

3.1.1 Fuel dissolution in an isolated canister without chain decay

Figure 3-1 shows the matrix inventory for a constant fuel dissolution rate of 1/10,000 moles/yr for nine different nuclides each with an initial amount of one mole. At 10,000 years, the fuel matrix will be totally dissolved and all nuclides will be free. For Ra-226 and Pu-239, the main part of the starting inventory has at the end of the simulation been lost. It is possible to see in the graph that nuclides with an instant release fraction larger than zero (I-129 and Sn-126) will not have their full initial inventory trapped in the matrix and the starting inventory of these nuclides will therefore be less than 1 mole.

As the fuel matrix dissolves the amount of the nuclides outside the fuel matrix (dissolved and precipitated) will increase as shown in Figure 3-2. Ni-59 and Nb-94 are nuclides originating from metal parts in the fuel elements and are not trapped in the fuel (has an IRF of one). Therefore, the initial amounts of these nuclides are 1 mole.

Table 3-1. Nuclide data used for simulations in Figure 3-1 to Figure 3-5.

Nuclide	Half life [yr]	Instant release fraction [–]	Solubility limit [mole/m^3]	Effective diffusivity [m^2/yr]
U-238	$4.471 \cdot 10^{9}$	0	$1.28 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$
U-234	$2.447 \cdot 10^{5}$	0	0	$1.6 \cdot 10^{-2}$
Th-230	77,070	0	$1.22e \cdot 10^{-6}$	$2.2 \cdot 10^{-3}$
Ra-226	1,601	0	$2.86 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$
Pu-239	24,080	0	$6.56 \cdot 10^{-6}$	$9.5 \cdot 10^{-3}$
I-129	$1.571 \cdot 10^{7}$	0.03	10^{7}	$9.5 \cdot 10^{-5}$
Nb-94	20,310	1	1.37	$1.6 \cdot 10^{-2}$
Ni-59	80,040	1	10^{7}	$3.2 \cdot 10^{-2}$
Sn-126	$1.001 \cdot 10^{5}$	0.02	$4.49 \cdot 10^{-6}$	$2.2 \cdot 10^{-3}$

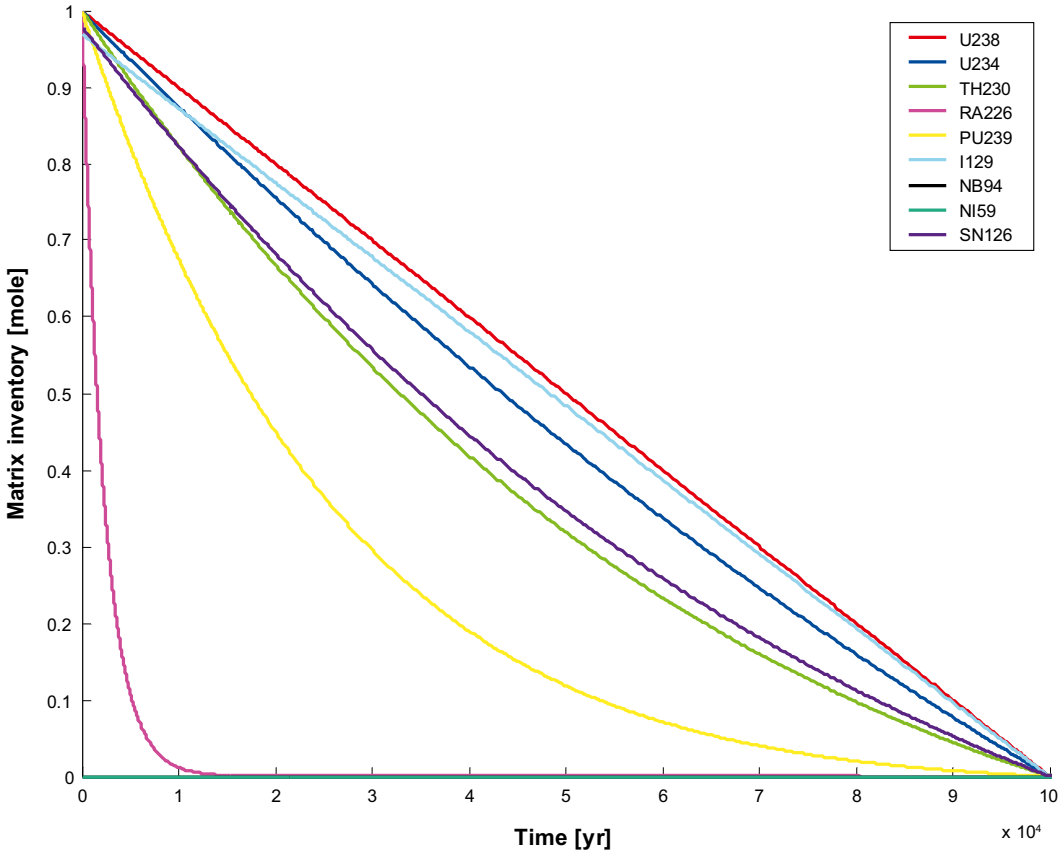

Figure 3-1. *Matrix inventory for a fuel dissolution rate of 10^5 yrs.*

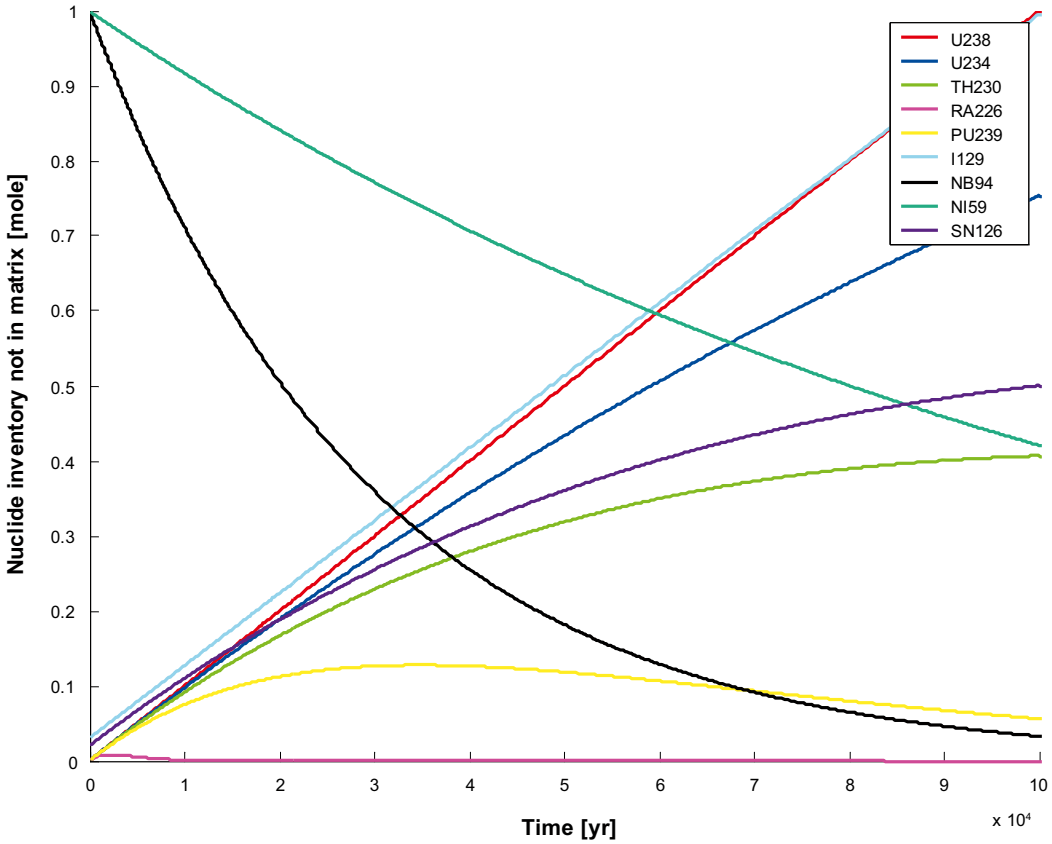

Figure 3-2. *Nuclides outside the fuel matrix.*

3.1.2 Precipitated and dissolved nuclides in an isolated canister with chain decay

As the fuel matrix dissolves, the amount of the different nuclides outside the matrix will increase. The nuclides will either be dissolved in the water surrounding the matrix or appear as a precipitate. Figure 3-3 shows the concentration of the nuclides in the water, the concentration will for most nuclides be limited by the solubility limit as seen in the graph, but for I-129, with a high solubility limit, the full inventory will be dissolved. When the solubility limit has been reached, the amount of precipitated nuclides will increase as the fuel dissolves, in the present simulation no outflow from the canister was considered and hence the only loss of nuclides will be through decay. This is also shown in Figure 3-4 where the total canister inventory is shown and the half-lives for the different nuclides can be seen.

3.1.3 Shared solubility in an isolated canister with chain decay

Figure 3-5 shows the concentration of five different plutonium isotopes for a case where shared solubility has been studied for a canister without any defect. Hence, nuclide decay is the only mechanism for changes in the inventory and as the short-lived nuclides decay, the concentration of nuclides with longer half-life increases in the canister. It can be seen that the amount of the initially dominating nuclide Pu-239 decreases after a slight increase due to the rapid decay of Pu-240. After some time, Pu-242 will be the dominating isotope and the actual solubility limit will correspond to that for a single solubility of Pu-242.

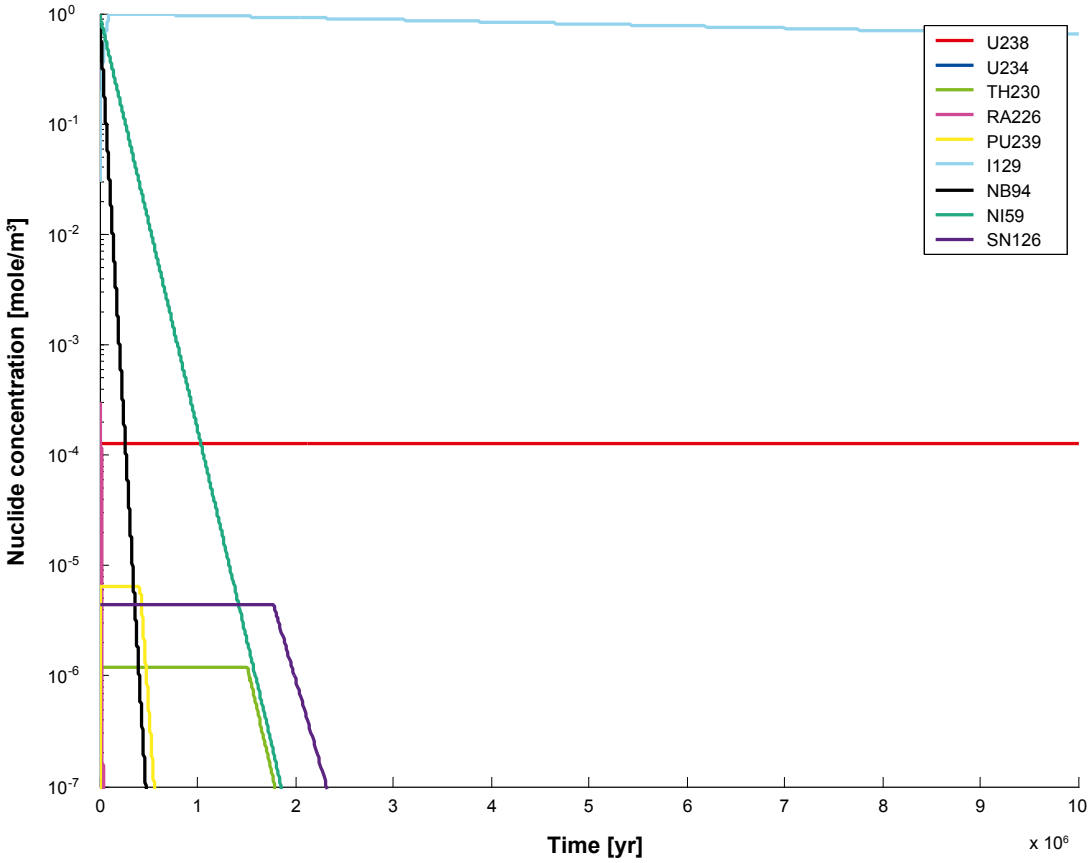

Figure 3-3. *Nuclides solved in water surrounding the matrix.*

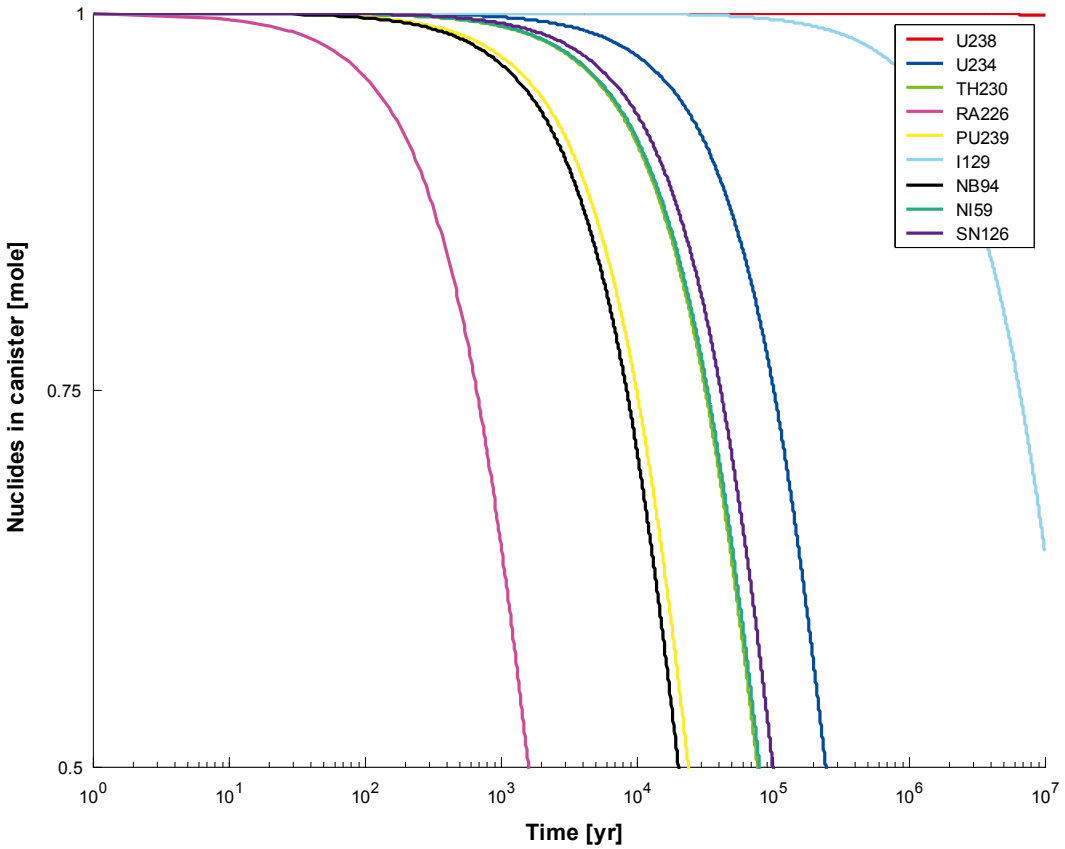

Figure 3-4. *Canister inventory.*

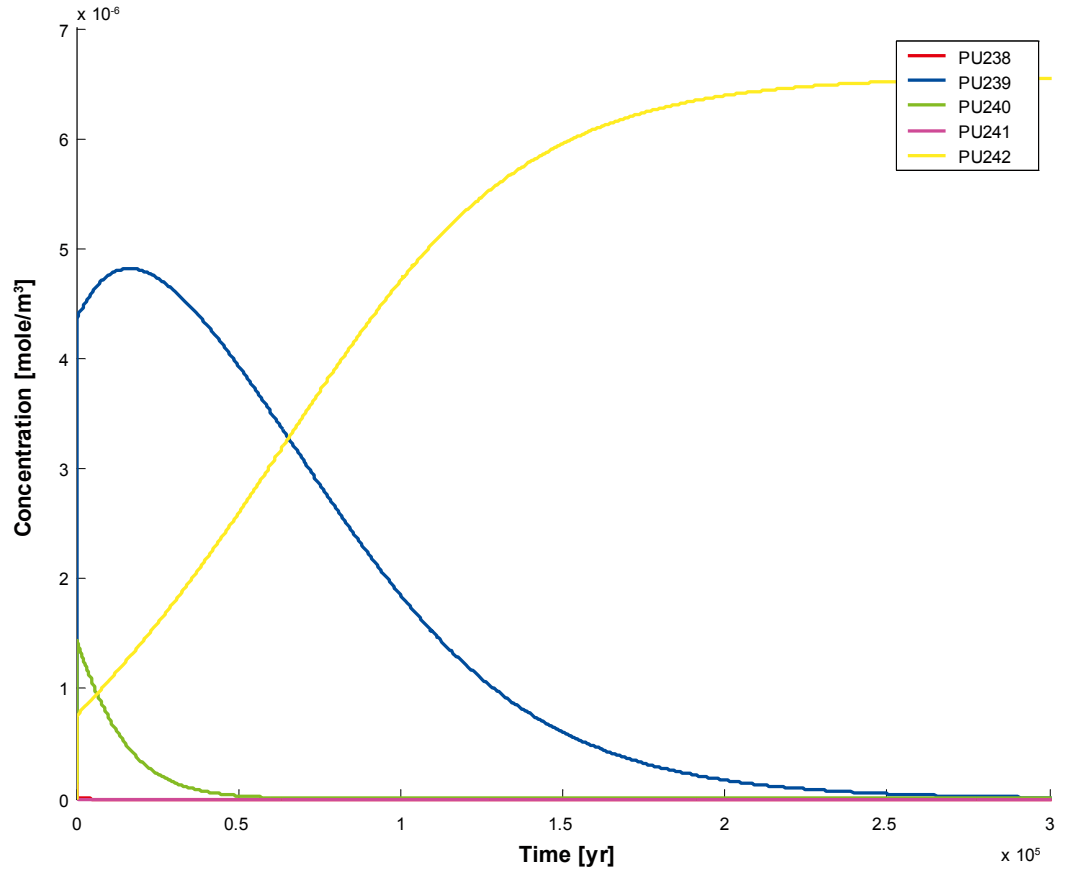

Figure 3-5. *Shared solubility.*

3.1.4 Tests using the COMP23 test batch

For COMP23 a test batch has been produces /Lindgren et al. 2006/ It can be seen that the agreement between the COMP23 runs and the Compulink runs is excellent for most nuclides. There is however an exception for some nuclides, for Se-79, there is a significant difference for the SR 97 comparison (test case 10 and test case 11). The reason for this is that the COMP23 half-lives used in SR 97 was based on other half-lives than the Bateman runs used in the Simulink simulations. If corresponding half-lives are used the agreement is excellent also for these simulations. For some of the uranium isotopes, the origin of the discrepancy is however different. In the SR 97, simulations, the solubility limit for all nuclides but U-238 was set to zero. The nuclide release for these nuclides will be non-existent in the COMP23 case while a nuclide outflow occurs for the Simulink applications.

3.2 Allocation of system resources

The memory consumption for the Simulink implementation in the runs presented above is rather low. Around 200 MB of memory is used for these standard runs. As the complexity of the calculations increases it is likely that the code will be more memory demanding as well as if an increasing number of COMP23 modules are used. The computational time for a nine nuclide probabilistic run is approximately 10 s and the corresponding time for a 32 nuclides deterministic run is 20 min on a 1,800 MHz desktop PC. This computational time corresponds to that of the Unix workstation for the original PROPER version.

4 Conclusions

A Simulink model called Compulink equivalent to the COMP23 sub model of the PROPER package has been developed. One verification example has been carefully studied, and a comparison between the codes shows very similar results for this example. The computing time needed for a deterministic run with 32 nuclides is roughly equal to that of a corresponding simulation in PROPER.

The graphical user interface of Simulink makes the model easy to understand for non-experts. At the same time it gives a great deal of flexibility and makes many of the goals behind MONITOR2000, which was intended to provide PROPER with a graphical user interface, were achieved.

5 References

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Hartley L, Hoch A, Jackson P, Joyce S, McCarthy R, Swift B, Gylling B, Marsic N, 2006b. Groundwater flow and transport modelling during the temperate period for the SR-Can assessment: Laxemar area – Version 1.2. SKB R-06-99, Svensk Kärnbränslehantering AB.

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Appendix A

Using the Compulink program

This section is intended as a user manual for the Compulink program. The reader is encouraged to have Matlab running while reading this chapter.

A1.1 The Nearfield library

The Compulink model is contained in a Simulink library called “Nearfield” together with some other useful models, Figure A-1.

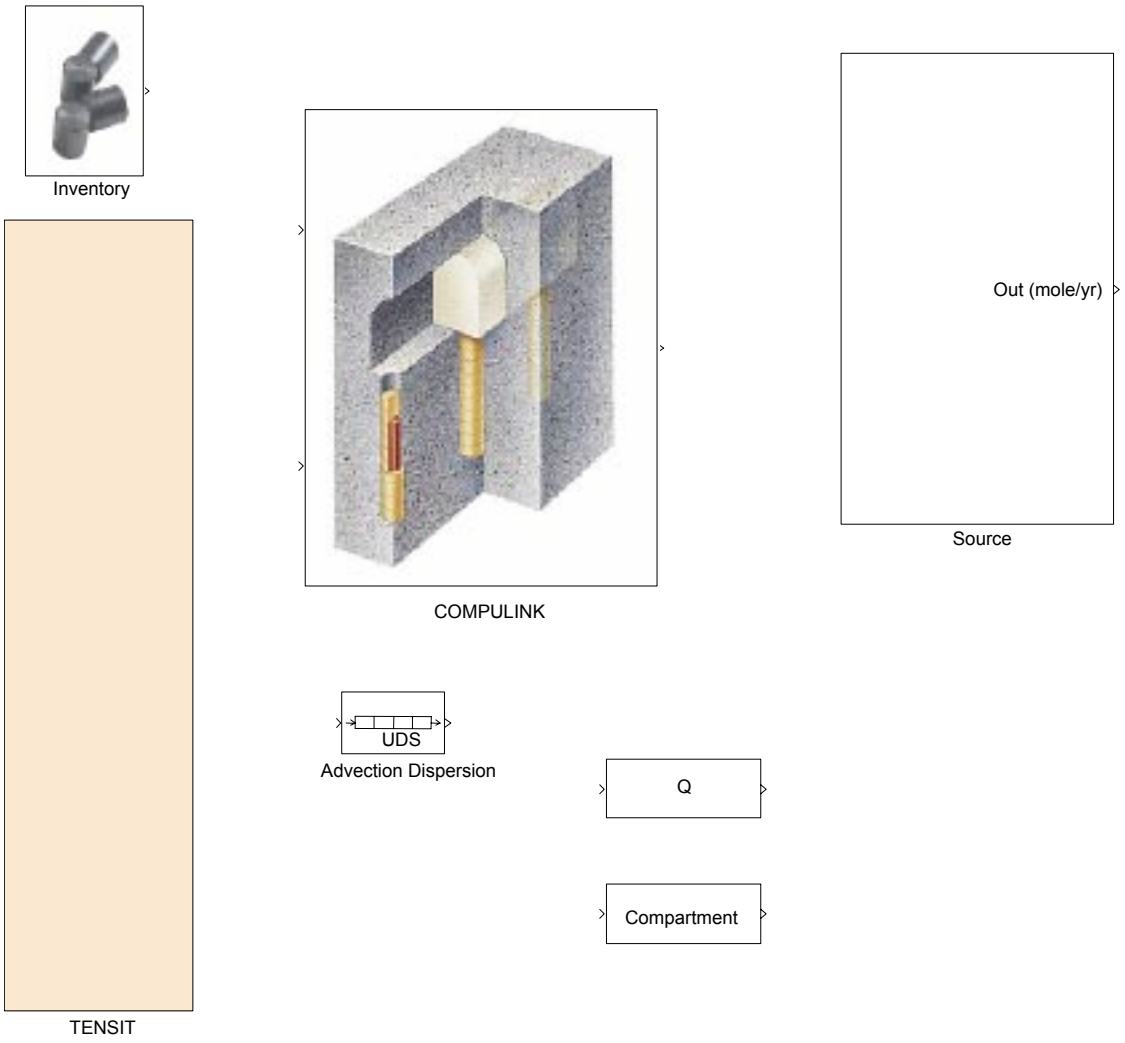

Figure A-1. *The Nearfield library.*

A1.2 Building a simple system

To build a simple system using the Compulink model, proceed as follows:

A. Create a new empty Simulink model in Matlab by choosing the menu File/New/Model.

B. Insert a Compulink block into the system.

C. Connect some block to the first input port (inventory port) of the Compulink block. A constant can be used, but there is also a special model called “Inventory” in the Nearfield library, which reads inventory files on standard PROPER format.

D. Connect some block to the second input port (defect port) of the Compulink block. A constant can be used to model a defect with an area which is constant in time.

E. Connect some kind of sink to the output port of the Compulink block, for example a scope.

F. Insert a TENSIT block into the model. NB: In every model where the Compulink block is used, there must also be a TENSIT block. The TENSIT block reads nuclide data from files on standard PROPER format.

G. Open every block and set its parameters. A block can be opened by double-clicking it. The parameters are described in section 2.12 above.

The end result might look like in Figure A-2:

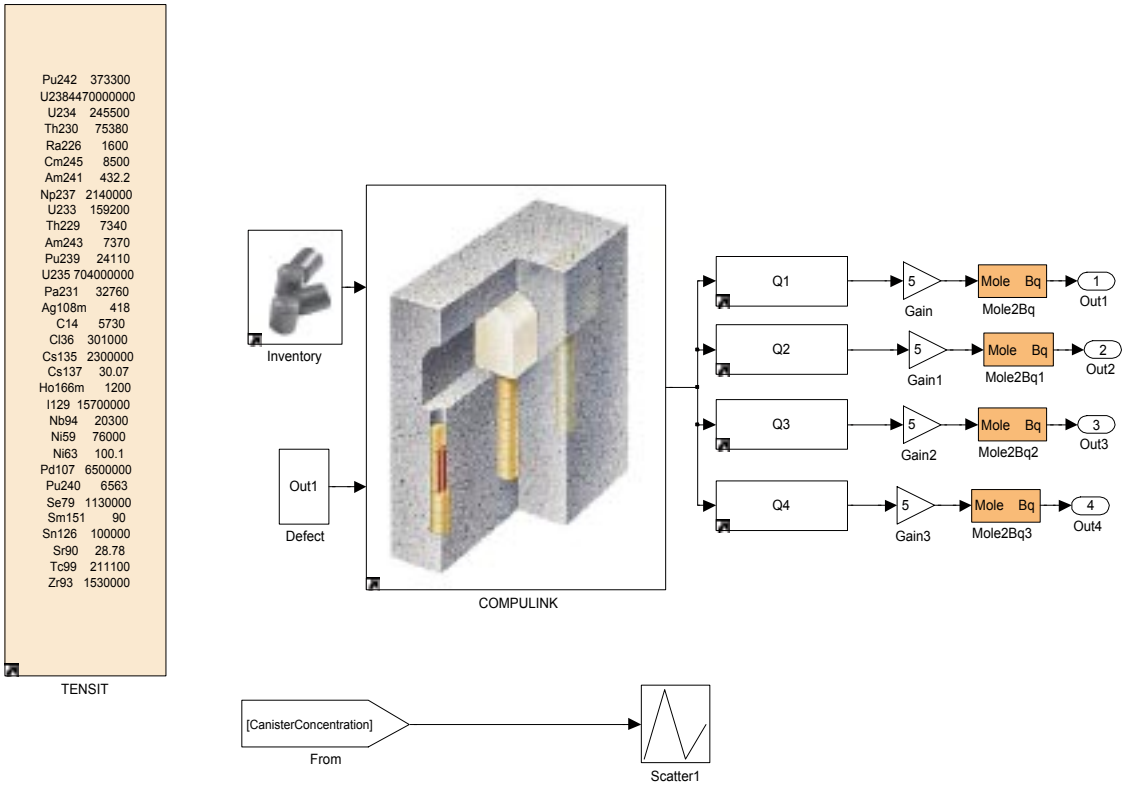

Figure A-2. *An example system using the Compulink block.*

A1.3 The Compulink block

This block is the main Compulink model. It contains four main components; an InstantRelease model, a Matrix model, a Solved model and a Transport model. It calculates the release from the near-field [moles/year] through the sinks. It takes two inputs; initial inventory (initial contents) [moles] and defect size [m²]. Initial inventory is usually taken from an Inventory module. The Compulink model must always be used together with a TENSIT model that provides nuclide data.

A1.4 Instant release

This model calculates the amount of radionuclides instantly released [moles] and the amount of radionuclides released with the fuel as it dissolves [moles] from the matrix using the parameter IRF given by the user. Input is initial inventory [moles].

A1.5 Matrix

This component models the dissolution of fuel from the matrix. It contains a sub model, which implements the fuel dissolution model chosen by the user. Output is total release rate from the matrix to the void of the canister [moles/year]. Input is initial inventory.

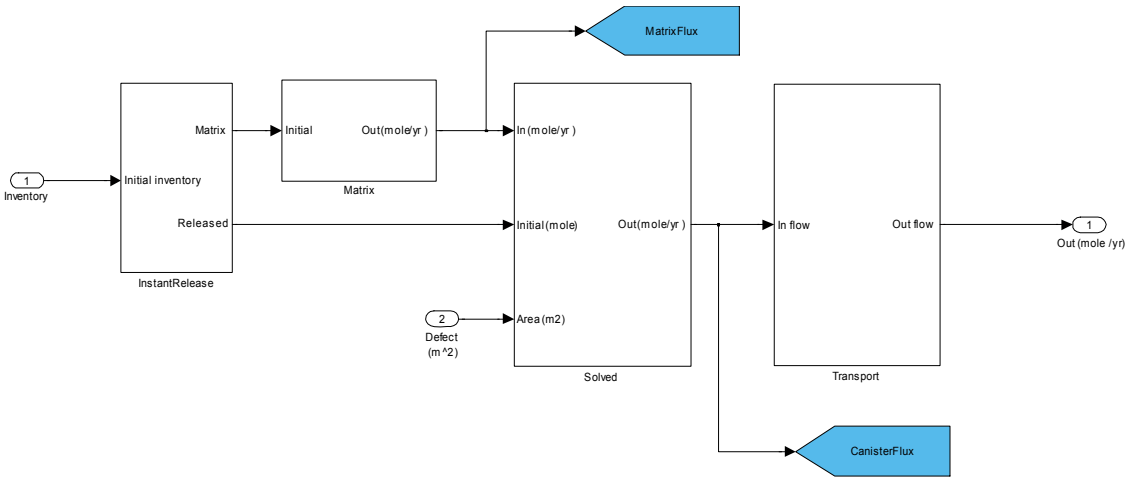

Figure A-3. *The Compulink block.*

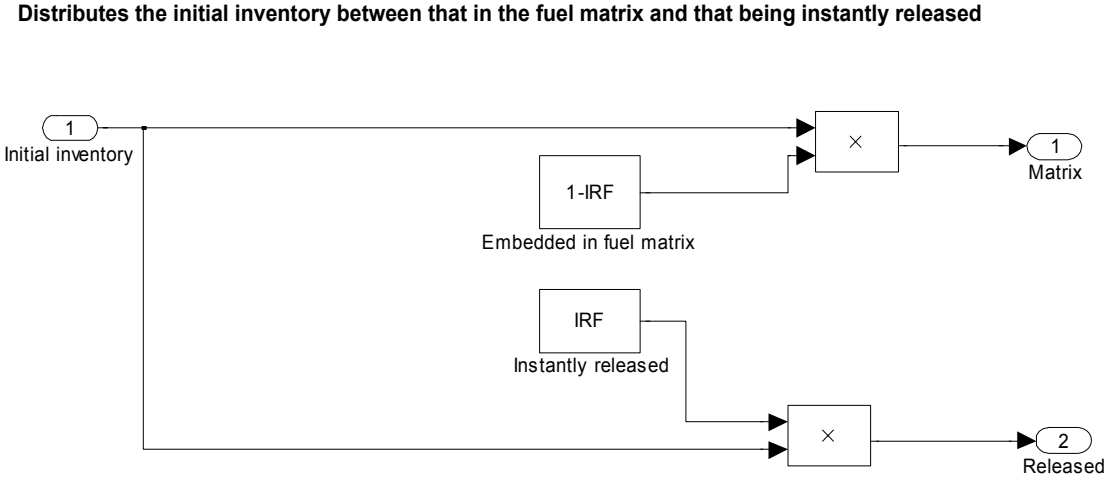

Figure A-4. *The InstantRelease block.*

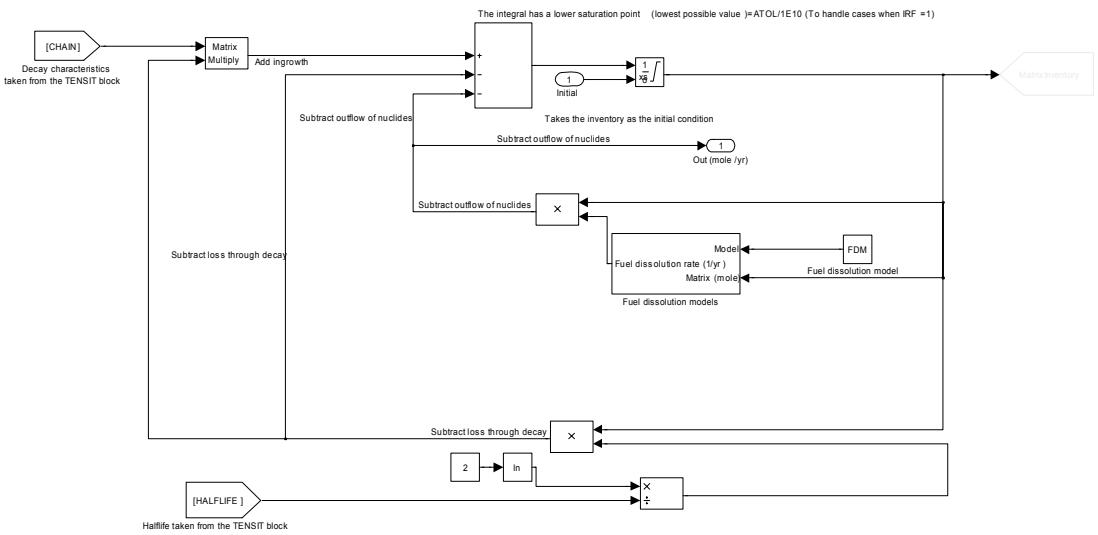

Figure A-5. *The Matrix block.*

A1.6 Solved

This component calculates the concentration of radionuclides [moles/m³] in the solute phase inside the canister, with respect to the solubility limit, and uses it to calculate the release of radionuclides from the canister through the defect (hole) [moles/year]. Its inputs are the release rate for radionuclides released with the fuel [moles/year], the initial content [moles] of instantly released nuclides and the size of the defect [m²]. It contains two low level sub models called Resistivities and Solubility_limit. The model called “Resistivities” is the plug model at the canister defect. Solubility_limit calculates the solubility limited concentration based on the solubility groups and solubility limits given by the user.

A1.7 Transport

This block models the transport of radionuclide from the canister defect all the way through the sinks. The diffusion and advection through the bentonite, backfill and sinks is modelled using a state-space block. When a simulation is initiated, the program reads a standard input file for COMP23 and sets up the transport equations for diffusion and advection through the bentonite and sinks according to the geometrical specification found therein.

The output of the component is the release of radionuclides from the near-field through all sinks of the model. In addition to the sinks defined in the geometry definition file, an extra sink is added by the program to monitor the advective outflow.

One state-space block will be set up with correct parameters by the initialization script of the model. The state variables are the concentrations in all elements (compartments) outside the canister defect. The canister is always the first compartment and the defect is always the second compartment. Hence the total number of state variables will always be two less than the number of elements in the geometry definition file.

The output variables are all the state variables plus the release trough every sink including the fictitious advective sink. So the total number of output variables equals the number of state variables plus then number of sinks plus one.

The input variables are the influx radionuclide in the element to which the defect is attached.

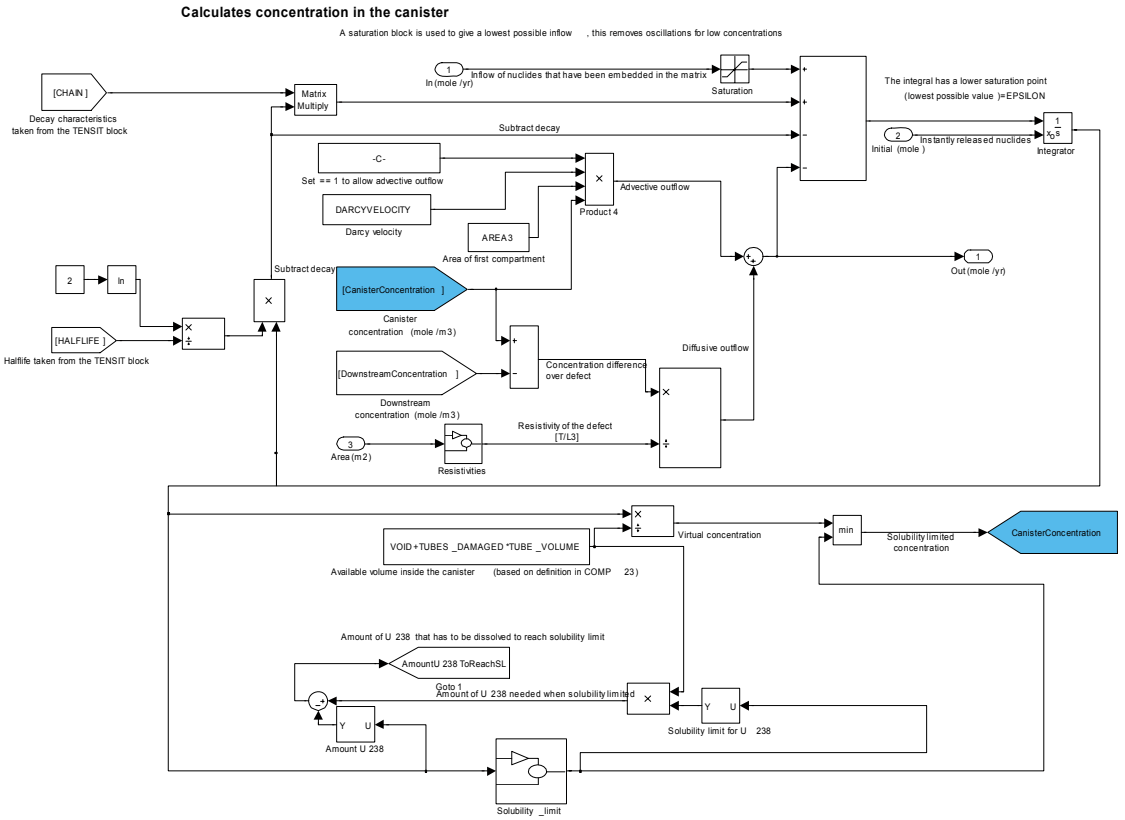

Figure A-6. *The Solved block.*

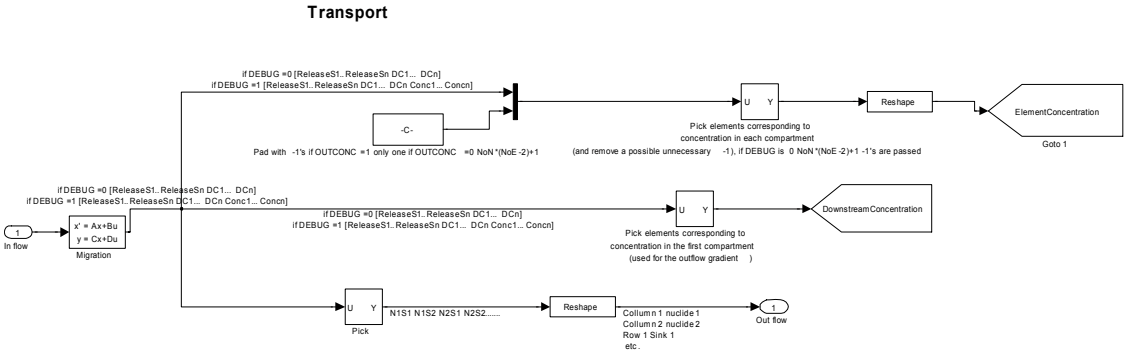

Figure A-7. *The Transport block.*

The state space matrices A, B, C and D will have the following structure:

$$A = \left(A_{res}\right)$$

$$B = \left(B_{plug}\right)$$

$$C = \begin{pmatrix} I \\ C_{sink} \end{pmatrix}$$

$$D = \left(0\right)$$

A_{res} is the resistivity matrix of the bentonite network. B_{plug} is calculated from the inlet plug model. C_{sink} is calculated from the sink parameters at all sinks.

A more detailed deduction of these can be found in Appendix D.

Appendix B

Test batch for Compulink

The test cases are based in the COMP23 test batch /Lindgren et al. 2006/ where they are deeper described. In the present section only the Compulink input files and the corresponding geometrical descriptions are presented. In the test cases the following features are tested

---

Test case 1 – Solubility limited source term

Test case 2 – Solubility limited source term, increased number of compartments

Test case 3 – Congruent dissolution from source

Test case 5 – Transport through a small hole in canister wall

Test case 6 – Transport through a large hole in canister wall

Test case 9 – One-dimensional diffusion in a medium bounded by two parallel planes (comparison with analytical solution)

Test case 10 – Calculation case from SR 97, Aberg pessimistic canister related parameters

Test case 11– Calculation case from SR 97, Aberg special case with immediate fuel dissolution, IRF=1

Test case 16 – Shared solubility

Test case 25 – Advection

B.1 Test cases for Compulink

Test case number 1, 2 and 3 builds on a geometry definition file which defines a transport network as depicted in Figure B-1.

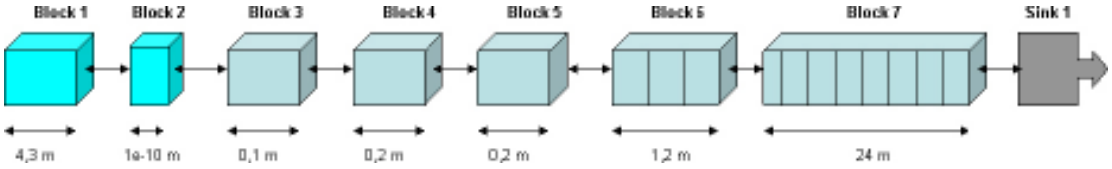

Figure B-1. *Transport network for test cases 1, 2 and 3.*

Test case number 6 uses the following geometrical configuration:

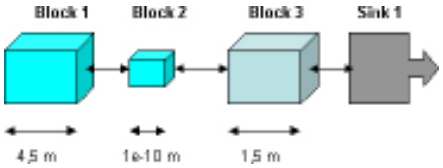

Figure B-2. *Transport network for test case 6.*

In test case number 9, the following geometrical configuration is used:

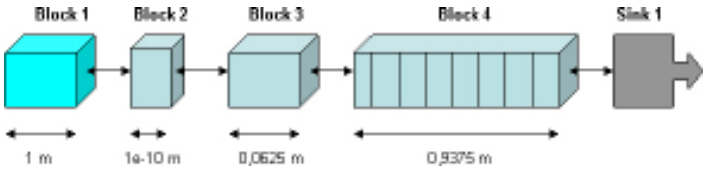

Figure B-3. *Transport network for test case 6.*

Test case number 10, 11 and 16 builds on the geometry definition file used in SR 97. The transport network used in the SR 97-studies is visualised in figure 28. In this picture B denotes a block and Q denotes a sink.

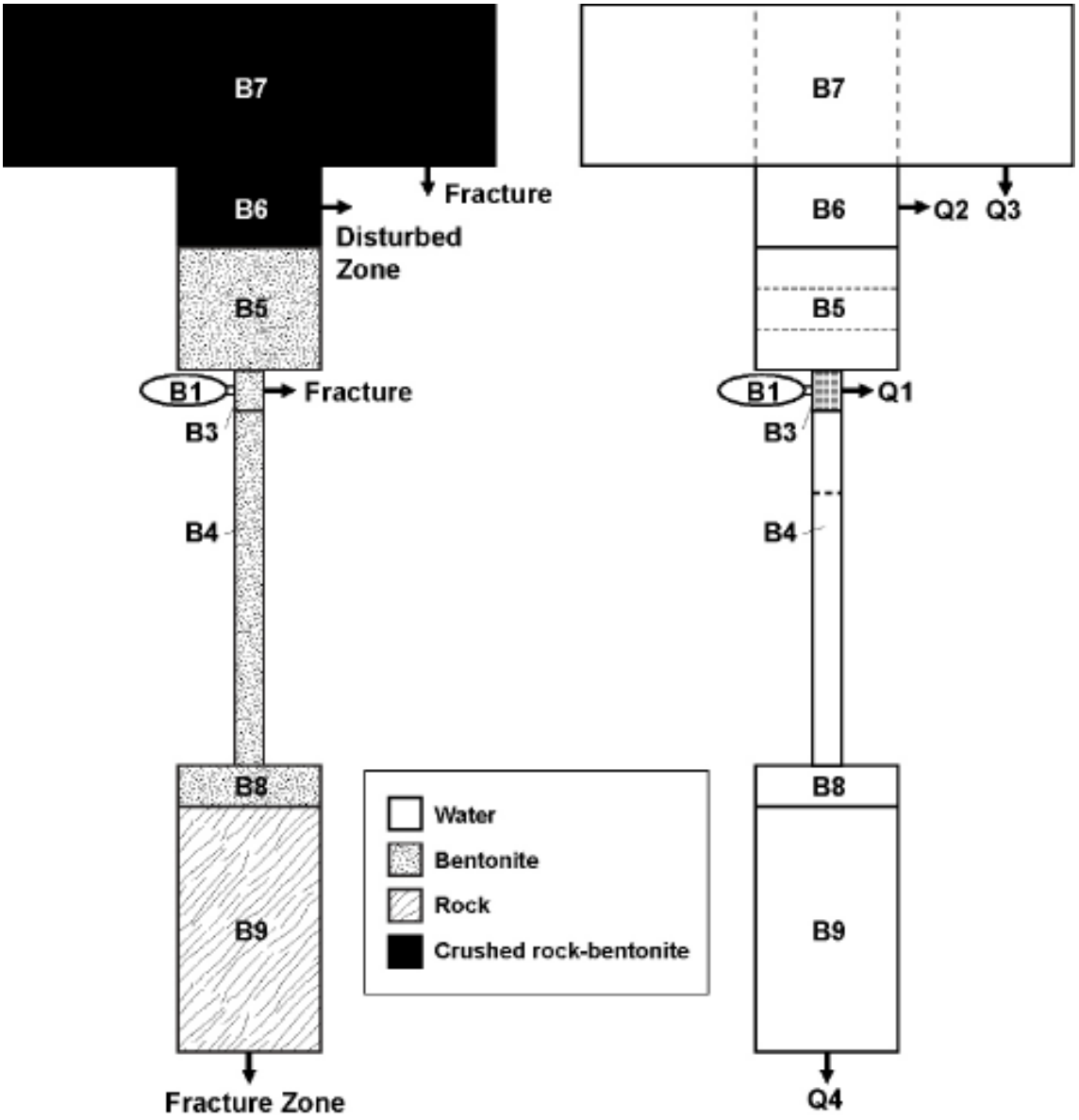

Figure B-4. *Transport network for test cases 10, 11 and 16.*

B.2 Advective transport, test case 25

In order to test the advective transport modelling, a separate test case has been constructed where an advectively travelling pulse is transported through the buffer. By setting the first of the ADVECTIVEELEMENTS to –1 advective condition will be valid also in the canister compartment. Hence, the boundary condition for the system will either be the concentration limit (if the IRF are high enough for radionuclides to precipitate) or to the release rate of the matrix (if the solubility limit is high). In the test case, the initial condition for the concentration will be zero outside the canister and the travelling pulse will be observed.

B.2.1 Geometry

The geometry consists of three blocks, the canister, the hole and one advection-diffusion block. Figure B-5 shows a schematic view of the configuration.

The canister is set up for one fictitious nuclide so that it keeps a constant concentration of 0.1 mole/m^3 at all times. The only nuclide occurring in the system is U238 with such a long half-life so that radioactive decay will be irrelevant. The area of the plug model for the hole is set to a very large value leading to a vanishing plug resistance, which is the same as an infinite concentration transfer coefficient, i.e. the wanted boundary condition for the dispersion term.

The over all length of all compartments in the advection-dispersion block is 10 m, and the porosity in the system is set to 1.

B.3 Reference and Compulink solution

The reference solution and the Compulink solutions are shown in Figure B-19. When the reference solution is a travelling wave, it is possible to se that the Compulink solution has been somewhat smoothed by numerical diffusion. One known problem with the upwind differencing scheme is numerical diffusion and these results are hence expected.

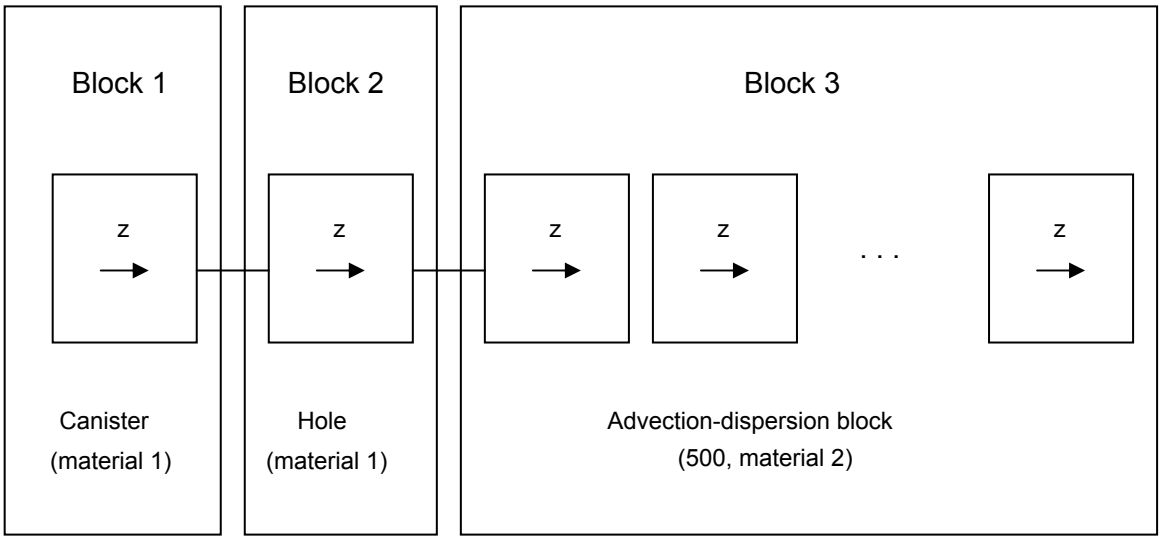

Figure B-5. *Schematic view of the geometry.*

B.4 Result for Test case 1

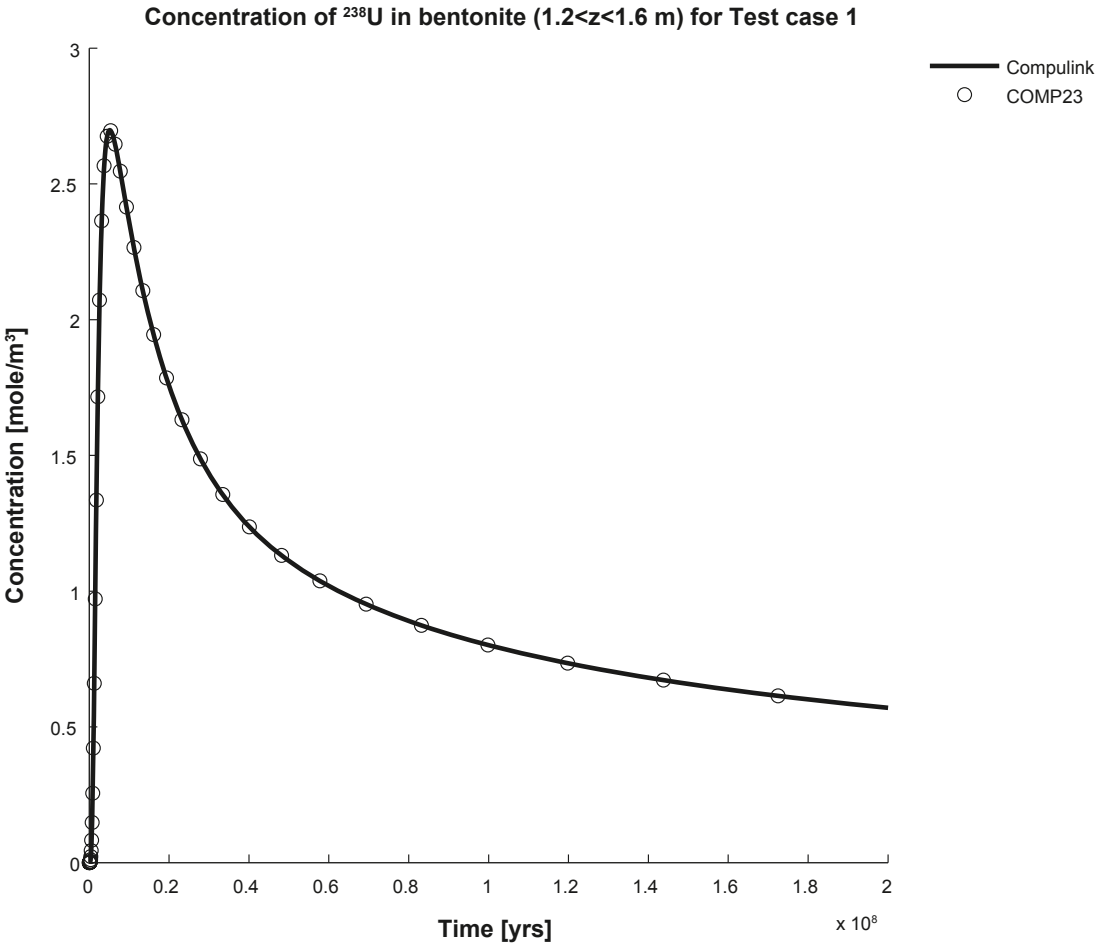

Figure B-6. *Comparison between COMP23 and Compulink results for test case 1.*

B.5 Result for Test case 2

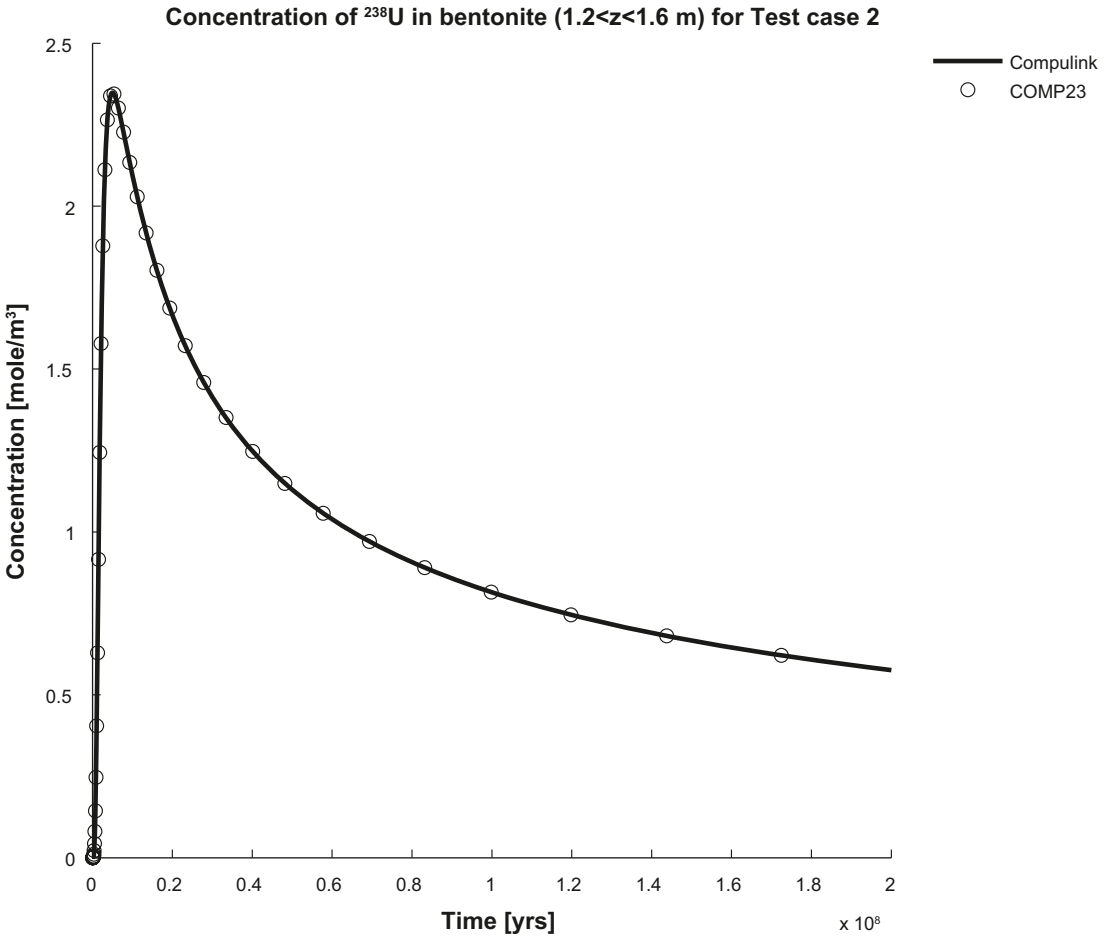

Figure B-7. *Comparison between COMP23 and Compulink results for test case 2.*

B.6 Result for Test case 3

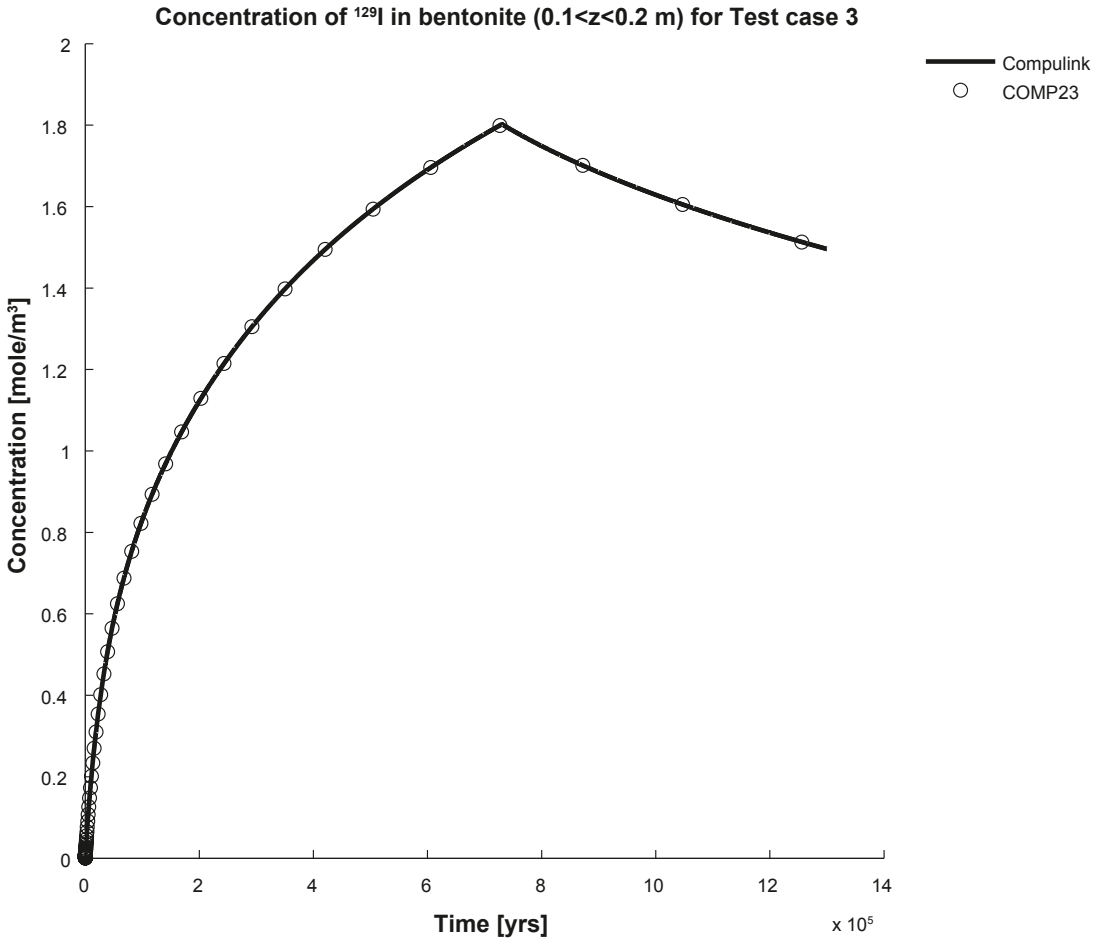

Figure B-8. *Comparison between COMP23 and Compulink results for test case 3.*

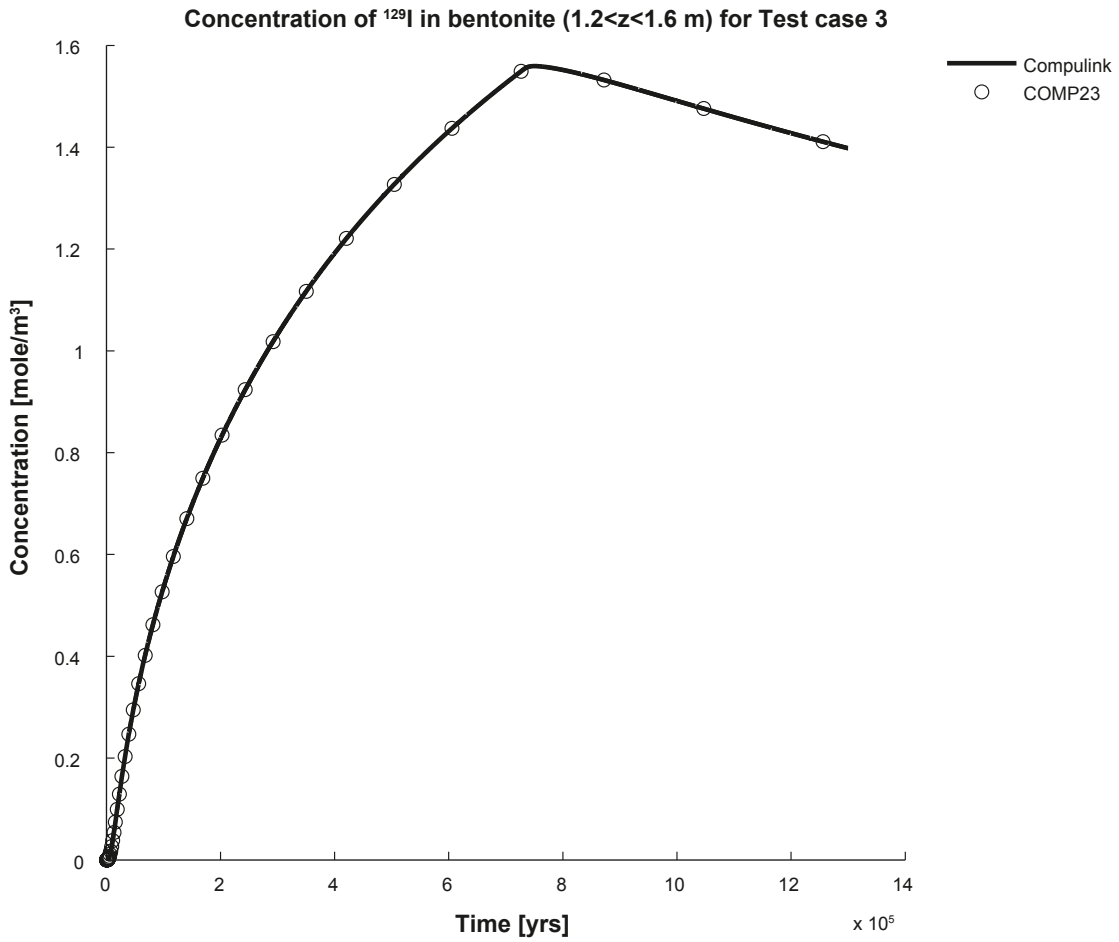

Figure B-9. *Comparison between COMP23 and Compulink results for test case 3.*

B.7 Result for Test case 5

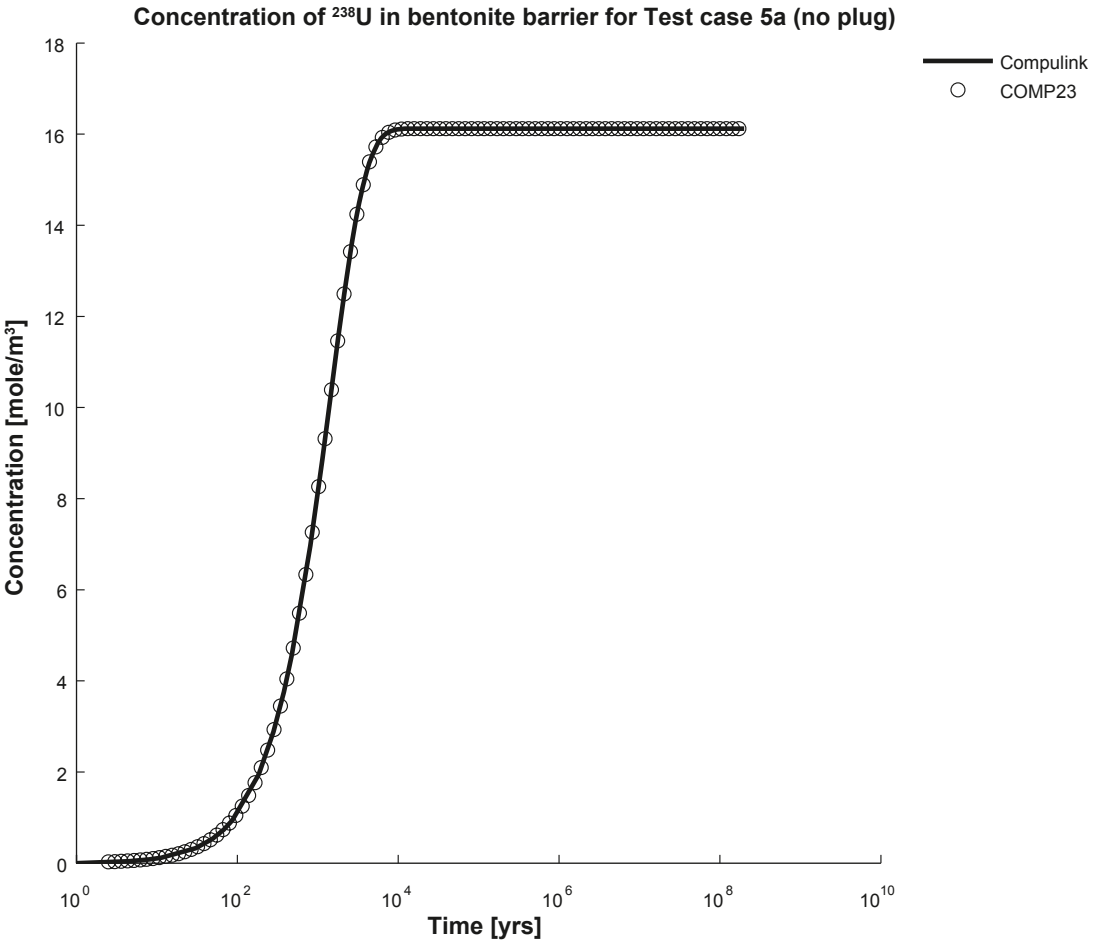

Figure B-10. *Comparison between COMP23 and Compulink results for test case 5.*

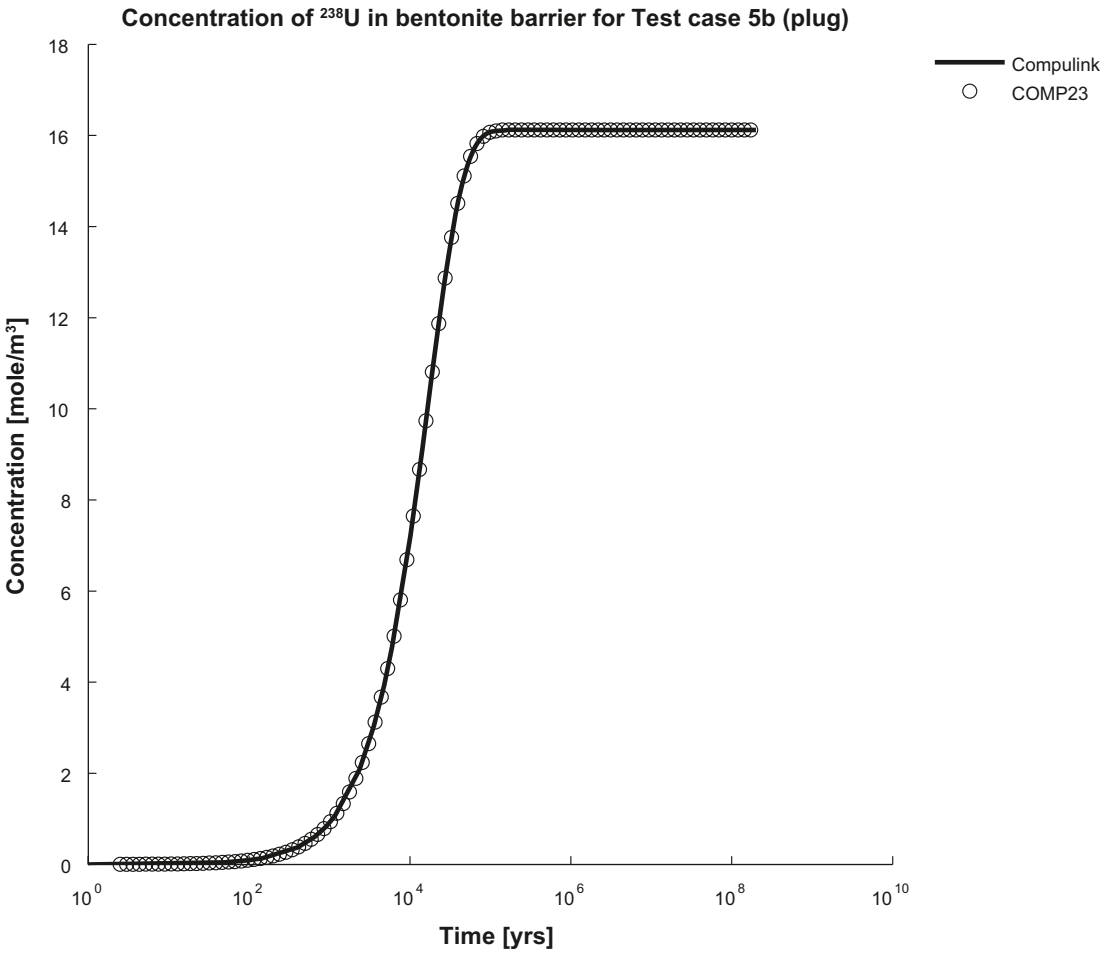

Figure B-11. *Comparison between COMP23 and Compulink results for test case 5.*

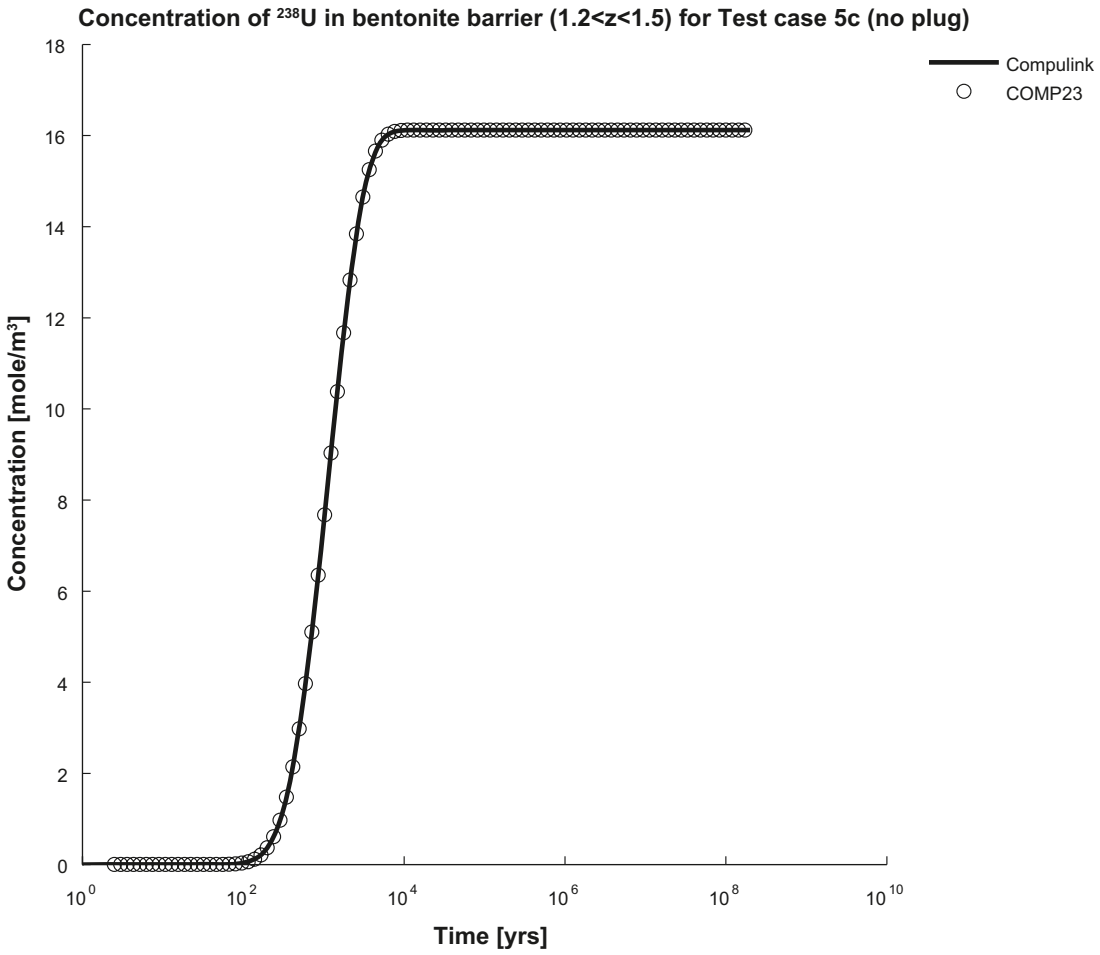

Figure B-12. *Comparison between COMP23 and Compulink results for test case 5.*

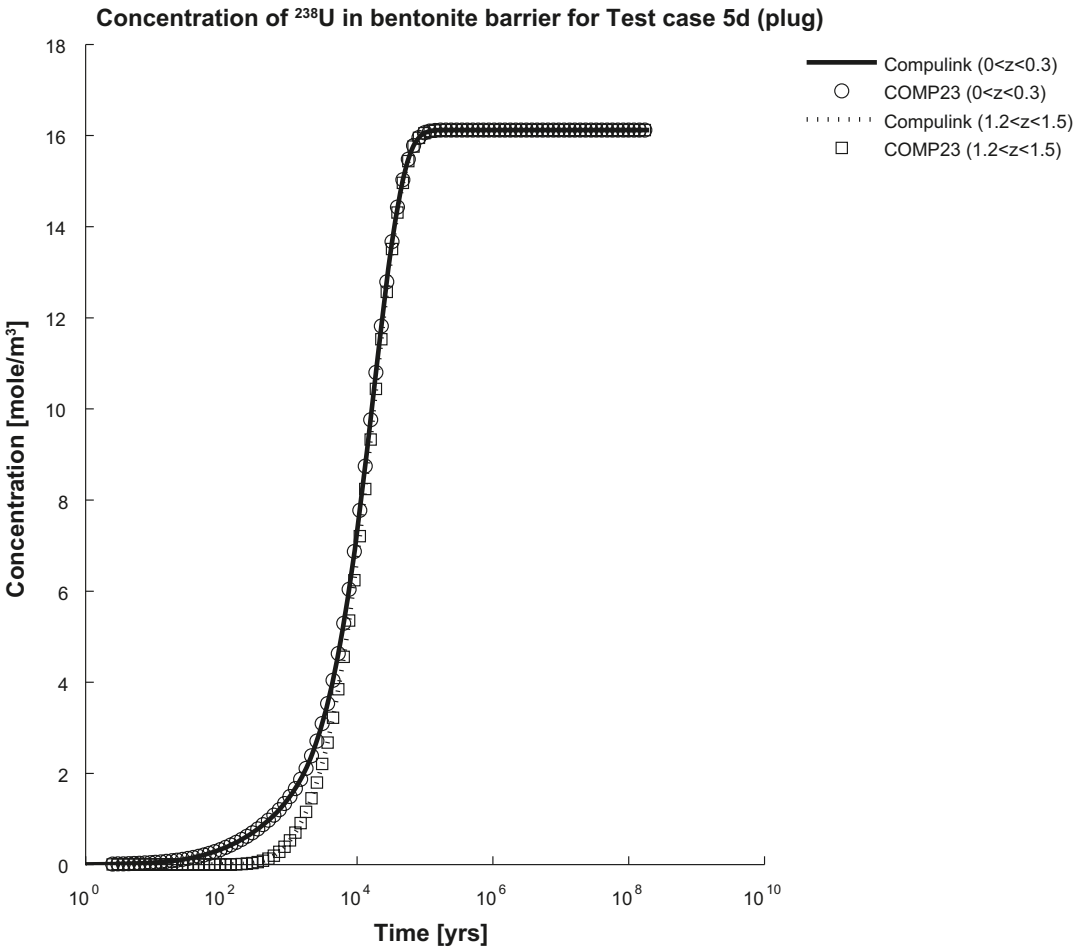

Figure B-13. *Comparison between COMP23 and Compulink results for test case 5.*

B.8 Result for Test case 6

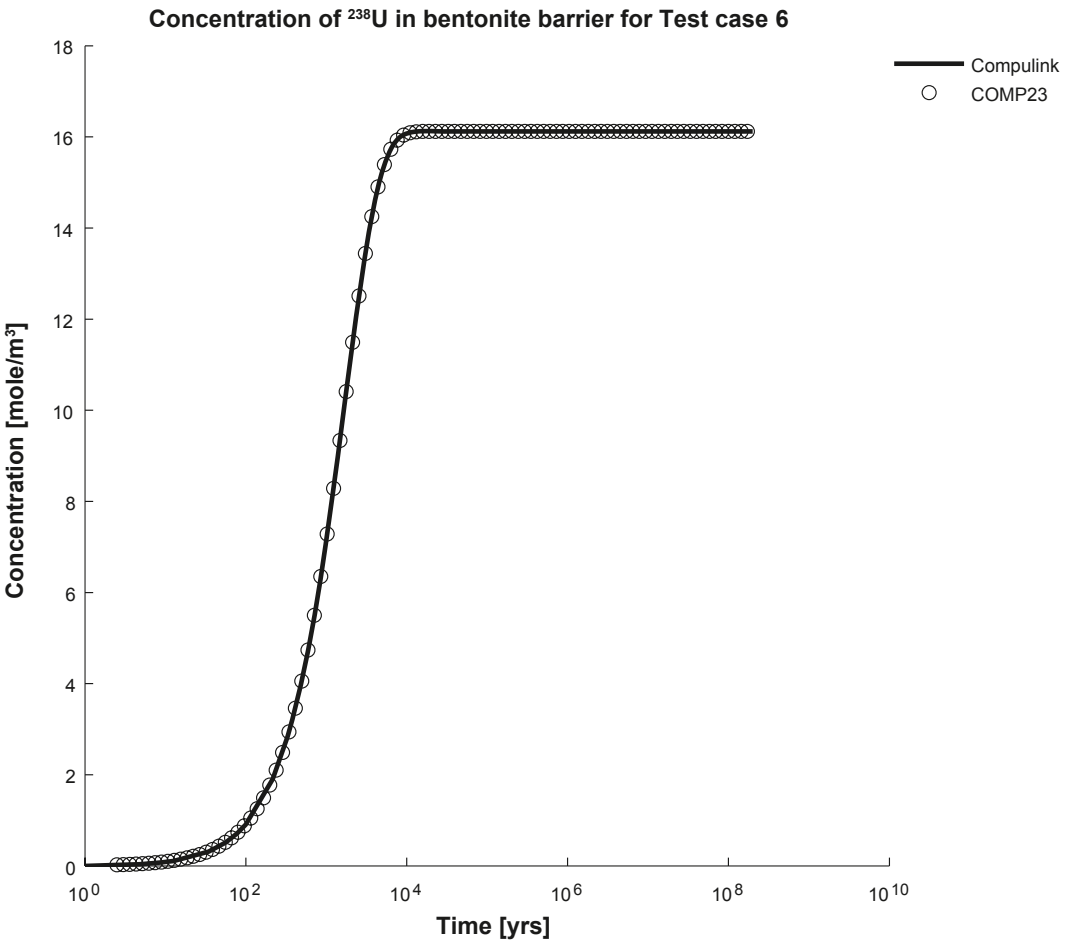

Figure B-14. *Comparison between COMP23 and Compulink results for test case 6.*

B.9 Result for Test case 9

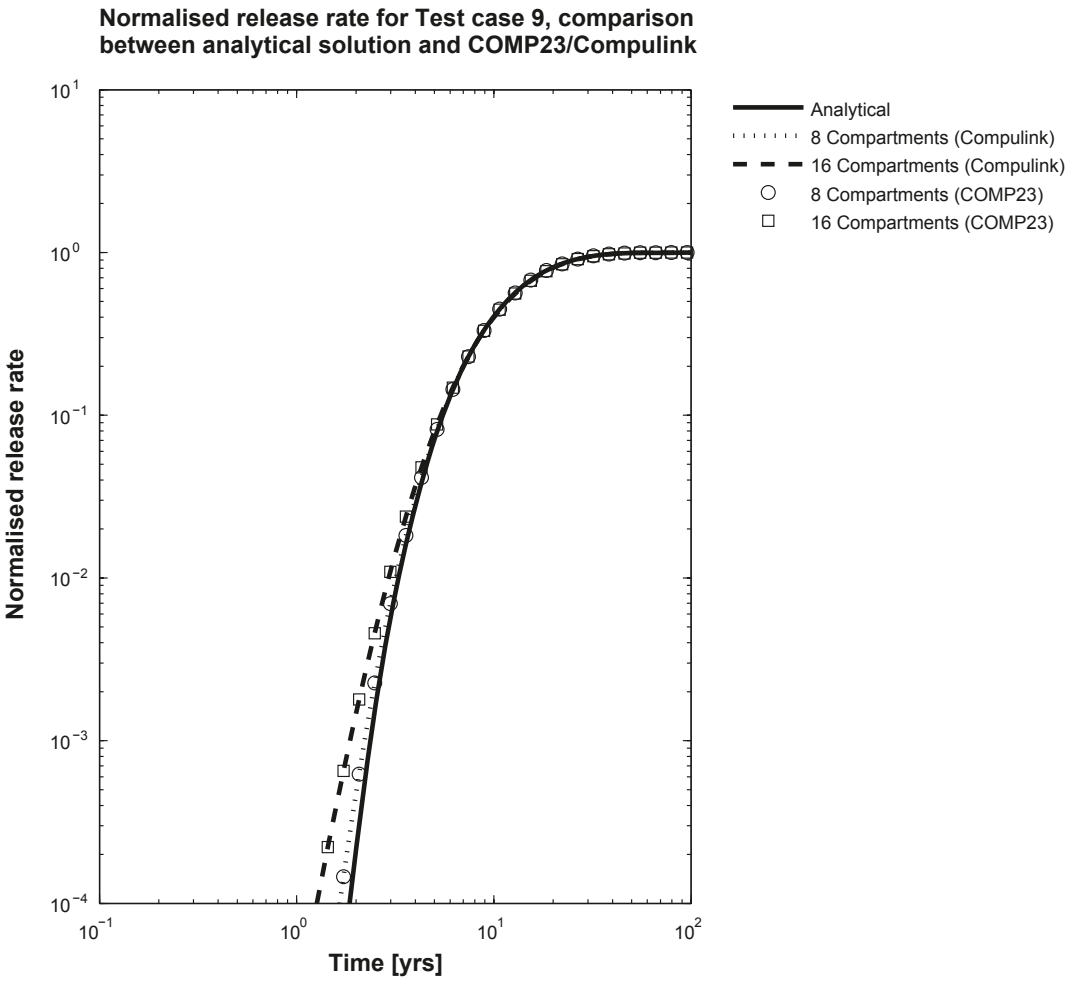

Figure B-15. *Comparison between analytical, COMP23 and Compulink results for test case 9.*

B.10 Result for Test case 10

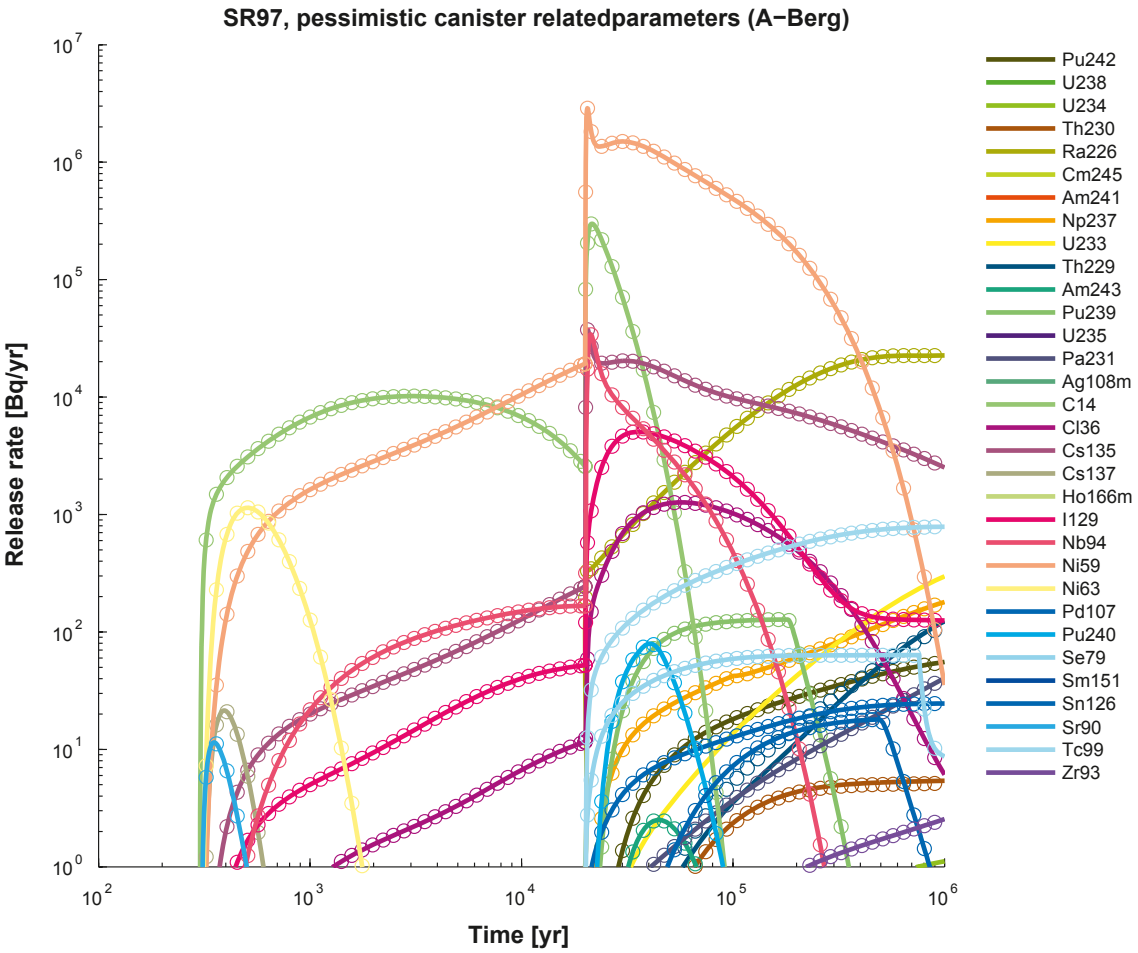

Figure B-16. *Comparison between COMP23 (circles) and Compulink (solid lines) results for test case 10.*

B.11 Result for Test case 11

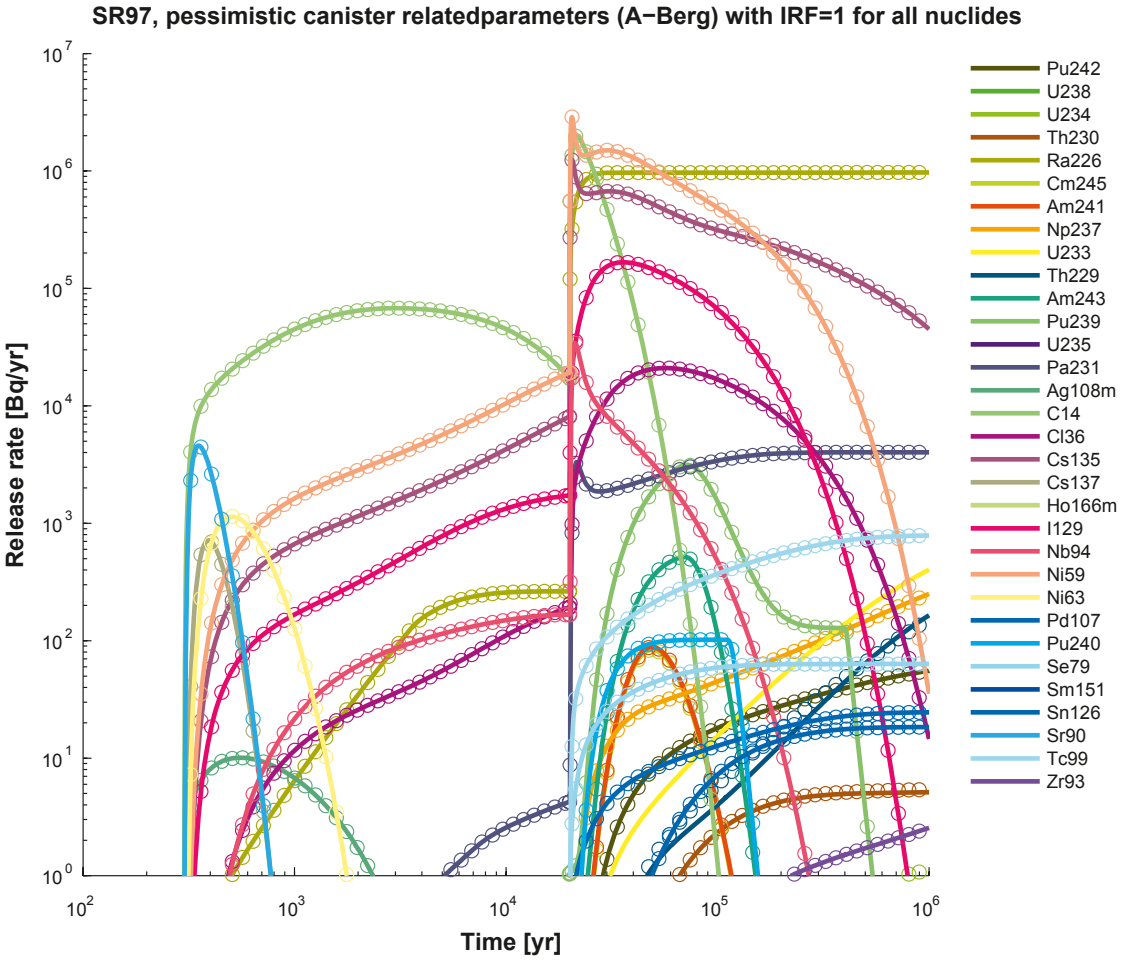

Figure B-17. *Comparison between COMP23 (circles) and Compulink (solid lines) results for test case 11.*

B.12 Result for Test case 16

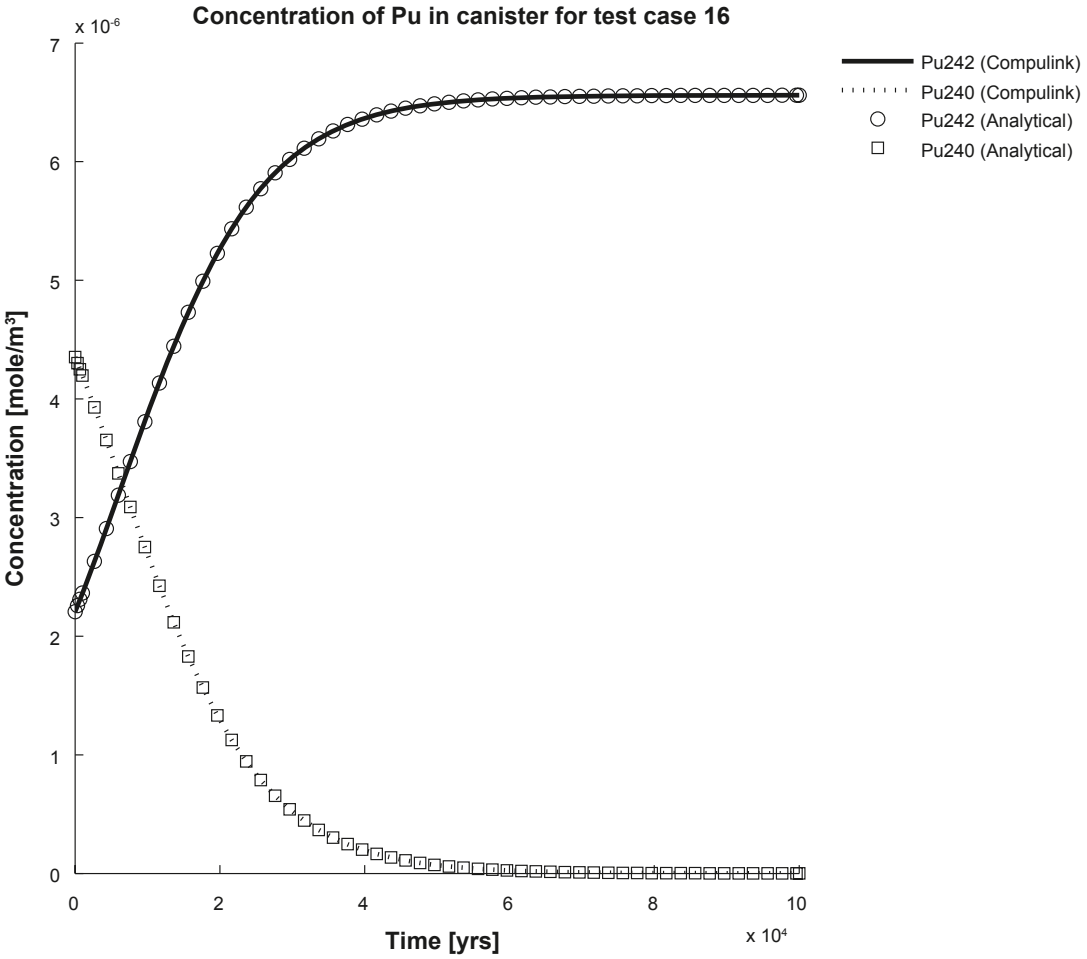

Figure B-18. *Comparison between Compulink and analytical results for test case 16.*

B.13 Result for Test case 25

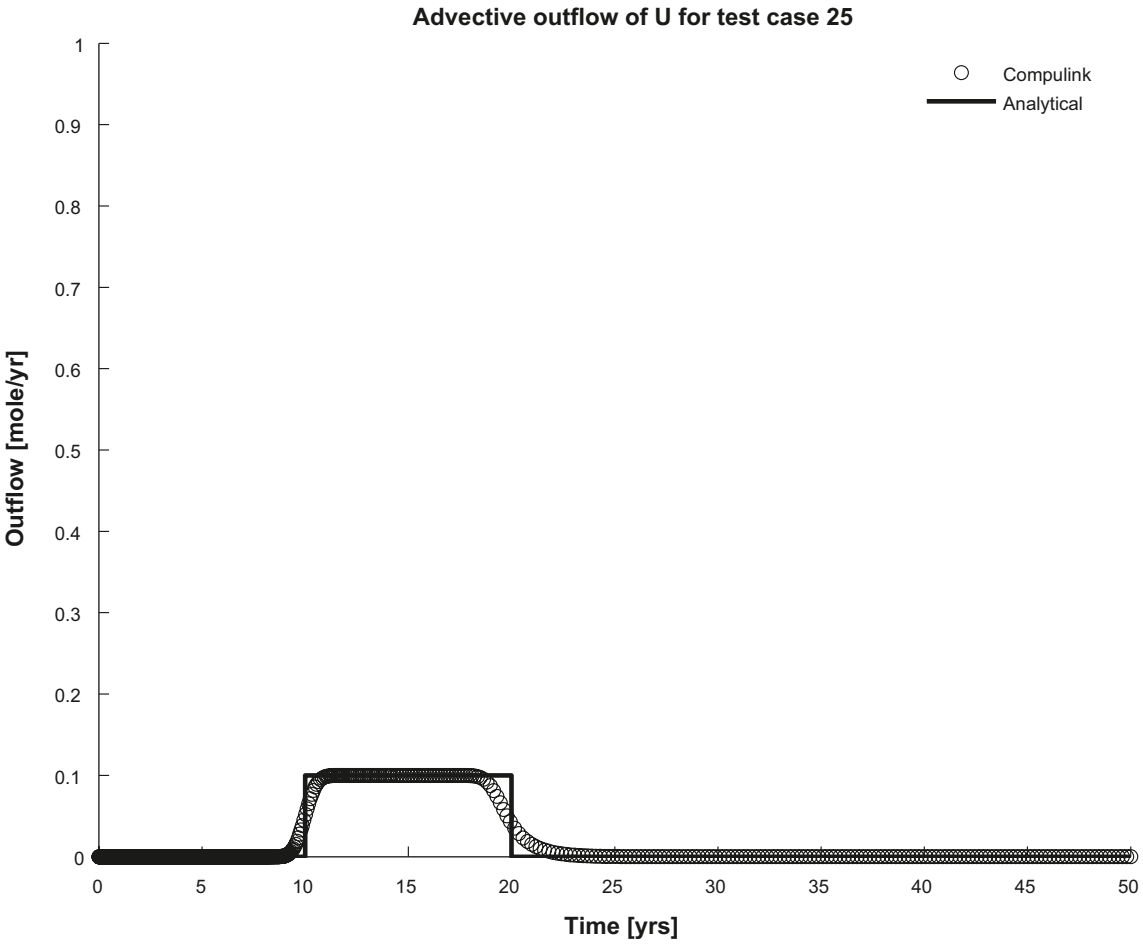

Figure B-19. *Comparison between Compulink and analytical solution for test case 25.*

B.14 Test case 1

B.14.1 Input data

```
%Load simulink file
load_system('Testcase1')


%Set parameters:
set_param( 'Testcase1/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase1/COMPULINK', 'OUTCONC', 'Concentration pore water
(mole/m3)')
set_param( 'Testcase1/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase1/COMPULINK', 'GEOMDEF', ''Block.gdf'')
set_param( 'Testcase1/COMPULINK', 'IRF', '1')
set_param( 'Testcase1/COMPULINK', 'FDMC', '1')
set_param( 'Testcase1/COMPULINK', 'SOLLIM', '16.12')
set_param( 'Testcase1/COMPULINK', 'RHO', '[1000;2000]')
set_param( 'Testcase1/COMPULINK', 'EPS', '[1;0.25]')
set_param( 'Testcase1/COMPULINK', 'DE', '[0.123;7.885E-4]')
set_param( 'Testcase1/COMPULINK', 'KD', '[0;3]')
set_param( 'Testcase1/COMPULINK', 'SOLGROUPS','{''U238''}')
set_param( 'Testcase1/COMPULINK', 'PLUGLENGTH', '0')
set_param( 'Testcase1/COMPULINK', 'PLUGAREA', '1')
set_param( 'Testcase1/COMPULINK', 'QEQ', '[0 ]')
set_param( 'Testcase1/COMPULINK', 'ATOL', '1e-20')
set_param( 'Testcase1/Pick compartment', 'COMPARTMENT', '6')

set_param( 'Testcase1/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase1/TENSIT', 'NUCLIDES', '{''U238''}')
set_param( 'Testcase1/TENSIT', 'HALFLIFE', '4.47E+09')
set_param( 'Testcase1/TENSIT', 'CHAIN', '0')

%Start simulation
[tout,X,C1] = sim('Testcase1',[1 2e8]);

%Load COMP23 data (for comparison)
load COMP23

%Print results
figure('Name','Testcase 1','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite (1.2<z<1.6 m) for Test
case 1')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
leg(2)=plot(COMP23(:,1),COMP23(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)
```

B.14.2 Geometry

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
```

```
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 1
        MATERIAL_NAME WATER
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   4.3E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 2
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME WATER
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.0E-10
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.10E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 4
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
```

```
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.10E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
       END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 5
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.20E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 6
        NUM_Z_COMP  3
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.20E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 7
        NUM_Z_COMP  8
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE

        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   24.0E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
```

```
        END_DEF

        END_DEF
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        FROM_COMP  1
        TO_BLOCK  2
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE FALSE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  2
        TO_BLOCK  3
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  3
        TO_BLOCK  4
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  4
        TO_BLOCK  5
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
```

```
        END_DEF
        BEGIN_DEF CONNECTION
                FROM_BLOCK  5
                TO_BLOCK  6
                FROM_COMP  1
                TO_COMP  1
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF CONNECTION
                FROM_BLOCK  6
                TO_BLOCK  7
                FROM_COMP  3
                TO_COMP  1
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF SINK
                FROM_BLOCK         7
                FROM_COMP          8
                DIRECTION          Z
                PLUG_AT_INLET      YES
                PLUG_LENGTH        0.000
                PLUG_AREA          1.000
                QEQ_FACTOR         1.000
                QEQ_EXPONENT       0.500
        END_DEF
        TUBE_VOLUME     4.655E-5
        NUM_TUBE        1440
        TUBES_DAMAGED    1440
        VOID   1.1487644
        NUM_STEP_NODES        2
END_BLOCK
```

B.15 Input data for Test case 2

B.15.1 Input data

```
%Load simulink file
load_system('Testcase2')


%Set parameters:
set_param( 'Testcase2/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase2/COMPULINK', 'OUTCONC', 'Concentration pore water
(mole/m3)')
set_param( 'Testcase2/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase2/COMPULINK', 'GEOMDEF', ''Block.gdf'')
set_param( 'Testcase2/COMPULINK', 'IRF', '1')
set_param( 'Testcase2/COMPULINK', 'FDMC', '1')
set_param( 'Testcase2/COMPULINK', 'SOLLIM', '16.12')
set_param( 'Testcase2/COMPULINK', 'RHO', '[1000;2000]')
set_param( 'Testcase2/COMPULINK', 'EPS', '[1;0.25]')
set_param( 'Testcase2/COMPULINK', 'DE', '[0.123;7.885E-4]')
set_param( 'Testcase2/COMPULINK', 'KD', '[0;3]')
set_param( 'Testcase2/COMPULINK', 'SOLGROUPS', '{''U238''}')
set_param( 'Testcase2/COMPULINK', 'PLUGLENGTH', '0')
set_param( 'Testcase2/COMPULINK', 'PLUGAREA', '1')
set_param( 'Testcase2/COMPULINK', 'QEQ', '[0 ]')
set_param( 'Testcase2/COMPULINK', 'ATOL', '1e-23')
set_param( 'Testcase2/Pick compartment', 'COMPARTMENT', '6')

set_param( 'Testcase2/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase2/TENSIT', 'NUCLIDES', '{''U238''}')
set_param( 'Testcase2/TENSIT', 'HALFLIFE', '4.47E+09')
set_param( 'Testcase2/TENSIT', 'CHAIN', '0')

%Start simulation
[tout,X,C1] = sim('Testcase2',[1 2e8]);

%Load COMP23 data (Comparmtent 7 taken from the COMP23/comp32
load COMP23

%Print results
figure('Name','Testcase 2','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite (1.2<z<1.6 m) for Test
case 2')

xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
leg(2)=plot(COMP23(:,1),COMP23(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)
```

B.15.2 Geometry

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
```

```
END_DEF
BEGIN_DEF MATERIAL
        MATERIAL_NAME BENTONITE
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 1
        MATERIAL_NAME WATER
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   4.3E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 2
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME WATER
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.0E-10
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.10E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 4
        NUM_Z_COMP  1
        NUM_X_COMP  1
```

```
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.10E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
       END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 5
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.20E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 6
        NUM_Z_COMP  3
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.20E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 7
        NUM_Z_COMP  16
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   24.0E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
```

```
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF

        END_DEF
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        FROM_COMP  1
        TO_BLOCK  2
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE FALSE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  2
        TO_BLOCK  3
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  3
        TO_BLOCK  4
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  4
        TO_BLOCK  5
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
```

```
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF CONNECTION
                FROM_BLOCK  5
                TO_BLOCK  6
                FROM_COMP  1
                TO_COMP  1
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF CONNECTION
                FROM_BLOCK  6
                TO_BLOCK  7
                FROM_COMP  3
                TO_COMP  1
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF SINK
                FROM_BLOCK         7
                FROM_COMP          8
                DIRECTION          Z
                PLUG_AT_INLET      YES
                PLUG_LENGTH        0.000
                PLUG_AREA          1.000
                QEQ_FACTOR         1.000
                QEQ_EXPONENT       0.500
        END_DEF
        TUBE_VOLUME     4.655E-5
        NUM_TUBE        1440
        TUBES_DAMAGED    1440
        VOID   1.1487644
        NUM_STEP_NODES        2
END_BLOCK
```

B.16 Input data for Test case 3

B.16.1 Input data

```
%Load simulink file
load_system('Testcase3')


%Set parameters:
set_param( 'Testcase3/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase3/COMPULINK', 'OUTCONC', 'Concentration pore water
(mole/m3)')
set_param( 'Testcase3/COMPULINK', 'FDM', 'Constant (mole/yr)')
set_param( 'Testcase3/COMPULINK', 'GEOMDEF', ''Block.gdf'')
set_param( 'Testcase3/COMPULINK', 'IRF', '[0;0]')
set_param( 'Testcase3/COMPULINK', 'FDMC', '0')
set_param( 'Testcase3/COMPULINK', 'SOLLIM', '[16.12;8.05E10]')
set_param( 'Testcase3/COMPULINK', 'RHO', '[1000;2000]')
set_param( 'Testcase3/COMPULINK', 'EPS', '[1 1;0.25 0.25]')
set_param( 'Testcase3/COMPULINK', 'DE', '[0.123 0.123;7.885E-4 1.972e-
5]')
set_param( 'Testcase3/COMPULINK', 'KD', '[0 0;3 0]')
set_param( 'Testcase3/COMPULINK', 'SOLGROUPS', '{''U238'';''I129''}')
set_param( 'Testcase3/COMPULINK', 'PLUGLENGTH', '0')
set_param( 'Testcase3/COMPULINK', 'PLUGAREA', '1')
set_param( 'Testcase3/COMPULINK', 'QEQ', '[0 ]')
set_param( 'Testcase3/COMPULINK', 'ATOL', '1e-23')

set_param( 'Testcase3/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase3/TENSIT', 'NUCLIDES', '{''U238'';''I129''}')
set_param( 'Testcase3/TENSIT', 'HALFLIFE', '[4.47E+09;1.57E+07]')
set_param( 'Testcase3/TENSIT', 'CHAIN', '[0 0;0 0]')
%Start simulation
[tout,X,C1,C2] = sim('Testcase3',[1 1.3e6]);

%Load COMP23 data (for comparison)
load COMP23

%Print results
figure('Name','Testcase 3-1','NumberTitle','off')
hold on
title('Concentration of ^1^2^9I in bentonite (0.1<z<0.2 m) for Test
case 3')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,2),'Color','k','LineWidth',2);
leg(2)=plot(COMP23(:,1),COMP23(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)

figure('Name','Testcase 3-2','NumberTitle','off')
hold on
title('Concentration of ^1^2^9I in bentonite (1.2<z<1.6 m) for Test
case 3')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C2(:,2),'Color','k','LineWidth',2);
leg(2)=plot(COMP23(:,1),COMP23(:,3),'ok');
legend(leg,'Compulink','COMP23',-1)
```

B.16.2 Geometry

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 1
                MATERIAL_NAME WATER
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   4.3E+0
                        Z_AREA     0.28274334E+0
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
        END_DEF
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 2
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                MATERIAL_NAME WATER
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   1.0E-10
                        Z_AREA     0.28274334E+0
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
        END_DEF
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 3
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP   1
                AREA_CHANGE NO
                MATERIAL_NAME BENTONITE
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   0.10E+0
                        Z_AREA     0.28274334E+0
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
```

```
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 4
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.10E+0
                Z_AREA     0.28274334E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
       END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 5
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.20E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 6
        NUM_Z_COMP  3
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.20E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
BEGIN_DEF BLOCK
        BLOCK_NUMBER 7
        NUM_Z_COMP  8
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
```

```
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   24.0E+0
                Z_AREA     0.28274334E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF

        END_DEF
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        FROM_COMP  1
        TO_BLOCK  2
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE FALSE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  2
        TO_BLOCK  3
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  3
        TO_BLOCK  4
        FROM_COMP  1
        TO_COMP  1
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
END_DEF
BEGIN_DEF CONNECTION
        FROM_BLOCK  4
        TO_BLOCK  5
        FROM_COMP  1
        TO_COMP  1
```

```
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF CONNECTION
                FROM_BLOCK  5
                TO_BLOCK  6
                FROM_COMP  1
                TO_COMP  1
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF CONNECTION
                FROM_BLOCK  6
                TO_BLOCK  7
                FROM_COMP  3
                TO_COMP  1
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
        END_DEF
        BEGIN_DEF SINK
                FROM_BLOCK         7
                FROM_COMP          8
                DIRECTION          Z
                PLUG_AT_INLET      YES
                PLUG_LENGTH        0.000
                PLUG_AREA          1.000
                QEQ_FACTOR         1.000
                QEQ_EXPONENT       0.500
        END_DEF
        TUBE_VOLUME     4.655E-5
        NUM_TUBE        1440
        TUBES_DAMAGED    1440
        VOID   1.1487644
        NUM_STEP_NODES        2
END_BLOCK
```

B.17 Input data for Test case 5

B.17.1 Input data

```
%Load simulink file
load_system('Testcase5')

%Set parameters:
set_param( 'Testcase5/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase5/COMPULINK', 'OUTCONC', 'Concentration pore water
(mole/m3)')
set_param( 'Testcase5/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase5/COMPULINK', 'GEOMDEF', ''Testcase5a.gdf'')
set_param( 'Testcase5/COMPULINK', 'IRF', '1')
set_param( 'Testcase5/COMPULINK', 'FDMC', '1')
set_param( 'Testcase5/COMPULINK', 'SOLLIM', '16.12')
set_param( 'Testcase5/COMPULINK', 'RHO', '[1000;2000]')
set_param( 'Testcase5/COMPULINK', 'EPS', '[1;1]')
set_param( 'Testcase5/COMPULINK', 'DE', '[0.123;7.885E-4]')
set_param( 'Testcase5/COMPULINK', 'KD', '[0;0]')
set_param( 'Testcase5/COMPULINK', 'SOLGROUPS', '{''U238''}')
set_param( 'Testcase5/COMPULINK', 'PLUGLENGTH', '0')
set_param( 'Testcase5/COMPULINK', 'PLUGAREA', '1')
set_param( 'Testcase5/COMPULINK', 'QEQ', '[0 ]')
set_param( 'Testcase5/COMPULINK', 'ATOL', '1e-23')
set_param( 'Testcase5/Pick compartment', 'COMPARTMENT', '1')

set_param( 'Testcase5/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase5/TENSIT', 'NUCLIDES', '{''U238''}')
set_param( 'Testcase5/TENSIT', 'HALFLIFE', '4.47E+09')
set_param( 'Testcase5/TENSIT', 'CHAIN', '0')
set_param( 'Testcase5/DEFECT', 'Value', '5e-4')

%Start simulation
[tout,X,C1] = sim('Testcase5',[1 2e8]);

%Load COMP23 data (for comparison)
load COMP23

%Print results
figure('Name','Testcase 5a','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite barrier for Test case 5a
(no plug)')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
hold on
leg(2)=plot(COMP23a(:,1),COMP23a(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)
set(gca,'XScale','log','YScale','lin')

%Change to case b
set_param( 'Testcase5/COMPULINK', 'GEOMDEF', ''Testcase5b.gdf'')

%Start simulation
[tout,X,C1] = sim('Testcase5',[1 2e8]);
```

```
%Print results
figure('Name','Testcase 5b','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite barrier for Test case 5b
(plug)')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
hold on
leg(2)=plot(COMP23b(:,1),COMP23b(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)
set(gca,'XScale','log','YScale','lin')

%Change to case c
set_param( 'Testcase5/COMPULINK', 'GEOMDEF', ''Testcase5c.gdf''')
set_param( 'Testcase5/Pick compartment', 'COMPARTMENT', '5')

%Start simulation
[tout,X,C1] = sim('Testcase5',[1 2e8]);

%Print results
figure('Name','Testcase 5c','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite barrier (1.2<z<1.5) for
Test case 5c (no plug)')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
hold on
leg(2)=plot(COMP23c(:,1),COMP23c(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)
set(gca,'XScale','log','YScale','lin')
%
%Change to case d
set_param( 'Testcase5/COMPULINK', 'GEOMDEF', ''Testcase5d.gdf''')
set_param( 'Testcase5/Pick compartment', 'COMPARTMENT', '[1 5]')

%Start simulation
[tout,X,C1] = sim('Testcase5',[1 2e8]);

%Print results
figure('Name','Testcase 5d','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite barrier for Test case 5d
(plug)')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
hold on
leg(2)=plot(COMP23d(:,1),COMP23d(:,2),'ok');
leg(3)=plot(tout,C1(:,2),'Color','k','LineStyle',':','LineWidth',2);
leg(4)=plot(COMP23d(:,1),COMP23d(:,3),'sk');
legend(leg,'Compulink (0<z<0.3)','COMP23 (0<z<0.3)','Compulink
(1.2<z<1.5)','COMP23 (1.2<z<1.5)',-1)
set(gca,'XScale','log','YScale','lin')
```

B.17.2 Geometry 5a

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        #
        # Blocks definition
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 1
                MATERIAL_NAME WATER
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   4.5E+0
                        Z_AREA     0.50265E+0
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
        END_DEF
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 2
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                MATERIAL_NAME BENTONITE
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   1.0E-10
                        Z_AREA     5.0E-2
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
        END_DEF
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 3
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP   1
                AREA_CHANGE NO
                MATERIAL_NAME BENTONITE
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   1.5+0
                        Z_AREA     0.50265E+0
                        X_LENGTH   0.0E+0
```

```
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF

#
# Connection definition
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        TO_BLOCK  2
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
        FROM_COMP  1
        TO_COMP  1
END_DEF
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  2
        TO_BLOCK  3
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE TRUE
        TO_RESISTANCE FALSE
        PLUG_POSITION TO_BLOCK
        EXTERNAL_RESIST FALSE
        FROM_COMP  1
        TO_COMP  1
END_DEF
BEGIN_DEF SINK
                        FROM_BLOCK         3
                        FROM_COMP          1
                        DIRECTION          Z
                        PLUG_AT_INLET      YES
END_DEF
#
VOID 1.2158
END_BLOCK
```

B.17.3 Geometry 5b

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        #
```

```
# Blocks definition
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 1
        MATERIAL_NAME WATER
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   4.5E+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 2
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.0E-10
                Z_AREA     5.0E-2
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.5+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF

#
# Connection definition
#
```

```
        BEGIN_DEF CONNECTION
                FROM_BLOCK  1
                TO_BLOCK  2
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE FALSE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        #
        BEGIN_DEF CONNECTION
                FROM_BLOCK  2
                TO_BLOCK  3
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE FALSE
                PLUG_POSITION TO_BLOCK
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        BEGIN_DEF SINK
                                FROM_BLOCK         3
                                FROM_COMP          1
                                DIRECTION          Z
                                PLUG_AT_INLET      YES
        END_DEF
        #
        VOID 1.2158
END_BLOCK
```

B.17.4 Geometry 5c

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        #
        # Blocks definition
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 1
                MATERIAL_NAME WATER
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
```

```
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   4.5E+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 2
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.0E-10
                Z_AREA     5.0E-2
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  5
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.5+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF

#
# Connection definition
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        TO_BLOCK  2
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
```

```
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        #
        BEGIN_DEF CONNECTION
                FROM_BLOCK  2
                TO_BLOCK  3
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1

                TO_COMP  1
        END_DEF
        BEGIN_DEF SINK
                                FROM_BLOCK          3
                                FROM_COMP           1
                                DIRECTION           Z
                                PLUG_AT_INLET       YES
        END_DEF
        #
        VOID 1.2158
END_BLOCK
```

B.17.5 Geometry 5d

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        #
        # Blocks definition
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 1
                MATERIAL_NAME WATER
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   4.5E+0
                        Z_AREA     0.50265E+0
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
```

```
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 2
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.0E-10
                Z_AREA     5.0E-2
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  5
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.5+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF

#
# Connection definition
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        TO_BLOCK  2
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE TRUE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
        FROM_COMP  1
        TO_COMP  1
END_DEF
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  2
        TO_BLOCK  3
```

```
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE FALSE
                PLUG_POSITION TO_BLOCK
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        BEGIN_DEF SINK
                                FROM_BLOCK         3
                                FROM_COMP          1
                                DIRECTION          Z
                                PLUG_AT_INLET      YES
        END_DEF
        #
        VOID 1.2158
END_BLOCK
```

B.18 Input data for Test case 6

B.18.1 Input data

```
%Load simulink file
load_system('Testcase6')

%Set parameters:
set_param( 'Testcase6/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase6/COMPULINK', 'OUTCONC', 'Concentration pore water
(mole/m3)')
set_param( 'Testcase6/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase6/COMPULINK', 'GEOMDEF', ''Testcase6.gdf'')
set_param( 'Testcase6/COMPULINK', 'IRF', '1')
set_param( 'Testcase6/COMPULINK', 'FDMC', '1')
set_param( 'Testcase6/COMPULINK', 'SOLLIM', '16.12')
set_param( 'Testcase6/COMPULINK', 'RHO', '[1000;2000]')
set_param( 'Testcase6/COMPULINK', 'EPS', '[1;1]')
set_param( 'Testcase6/COMPULINK', 'DE', '[0.123;7.885E-4]')
set_param( 'Testcase6/COMPULINK', 'KD', '[0;3]')
set_param( 'Testcase6/COMPULINK', 'SOLGROUPS', '{''U238''}')
set_param( 'Testcase6/COMPULINK', 'PLUGLENGTH', '0')
set_param( 'Testcase6/COMPULINK', 'PLUGAREA', '1')
set_param( 'Testcase6/COMPULINK', 'QEQ', '[0 ]')
set_param( 'Testcase6/COMPULINK', 'ATOL', '1e-23')
set_param( 'Testcase6/Pick compartment', 'COMPARTMENT', '1')

set_param( 'Testcase6/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase6/TENSIT', 'NUCLIDES', '{''U238''}')
set_param( 'Testcase6/TENSIT', 'HALFLIFE', '4.47E+09')
set_param( 'Testcase6/TENSIT', 'CHAIN', '0')

%Start simulation
[tout,X,C1] = sim('Testcase6',[1 2e8]);

%Load COMP23 data (for comparison)
load COMP23

%Print results
figure('Name','Testcase 6','NumberTitle','off')
hold on
title('Concentration of ^2^3^8U in bentonite barrier for Test case 6')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C1(:,1),'Color','k','LineWidth',2);
hold on
leg(2)=plot(COMP23(:,1),COMP23(:,2),'ok');
legend(leg,'Compulink','COMP23',-1)
set(gca,'XScale','log','YScale','lin')
```

B.18.2 Geometry

```
BEGIN_BLOCK GEOMETRY
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
```

```
        MATERIAL_NAME BENTONITE
END_DEF
#
# Blocks definition
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 1
        MATERIAL_NAME WATER
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   4.5E+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 2
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.0E-10
                Z_AREA     5.0E-2
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   1.5+0
                Z_AREA     0.50265E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
```

```
        #
        # Connection definition
        #
        BEGIN_DEF CONNECTION
                FROM_BLOCK  1
                TO_BLOCK  2
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE FALSE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        #
        BEGIN_DEF CONNECTION
                FROM_BLOCK  2
                TO_BLOCK  3
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE FALSE
                PLUG_POSITION TO_BLOCK
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        BEGIN_DEF SINK
                                FROM_BLOCK         3
                                FROM_COMP          1
                                DIRECTION          Z
                                PLUG_AT_INLET      YES
        END_DEF
        #
        VOID 1.2158
END_BLOCK
```

B.19 Input data for Test case 9

B.19.1 Input data

```
%Load simulink file
load_system('Testcase9')


%Set parameters:
set_param( 'Testcase9/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase9/COMPULINK', 'OUTCONC', 'Concentration pore water
(mole/m3)')
set_param( 'Testcase9/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase9/COMPULINK', 'GEOMDEF', ''Testcase9a.gdf'')
set_param( 'Testcase9/COMPULINK', 'IRF', '1')
set_param( 'Testcase9/COMPULINK', 'FDMC', '1')
set_param( 'Testcase9/COMPULINK', 'SOLLIM', '1')
set_param( 'Testcase9/COMPULINK', 'RHO', '[1000;2000]')
set_param( 'Testcase9/COMPULINK', 'EPS', '[1;0.25]')
set_param( 'Testcase9/COMPULINK', 'DE', '[0.123; 3.E-3]')
set_param( 'Testcase9/COMPULINK', 'KD', '[0;0]')
set_param( 'Testcase9/COMPULINK', 'SOLGROUPS', '{''U238''}')
set_param( 'Testcase9/COMPULINK', 'PLUGLENGTH', '0')
set_param( 'Testcase9/COMPULINK', 'PLUGAREA', '1')
set_param( 'Testcase9/COMPULINK', 'QEQ', '100')
set_param( 'Testcase9/COMPULINK', 'ATOL', '1e-23')

set_param( 'Testcase9/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase9/TENSIT', 'NUCLIDES', '{''U238''}')
set_param( 'Testcase9/TENSIT', 'HALFLIFE', '4.47E+09')
set_param( 'Testcase9/TENSIT', 'CHAIN', '0')
set_param( 'Testcase9/TENSIT', 'ITERATION', '1')

%Start simulation
[tout1,X,C1] = sim('Testcase9',[0 100]);
set_param( 'Testcase9/COMPULINK', 'GEOMDEF', ''Testcase9b.gdf'')
[tout2,X,C2] = sim('Testcase9',[0 100]);

%Analytical solution
De=3.E-3;
A=0.7854;
c0=1;
L=1;
Dp=De/0.25;
tout=logspace(0,2,100);

for n=1:length(tout)

   N(n)=analytical(De,A,c0,L,Dp,tout(n));
end

%Load COMP23 data (for comparison)
load COMP23

%Print results
figure('Name','Testcase 9','NumberTitle','off')
leg(1)=loglog(tout,N,'Color','k','LineWidth',2,'LineStyle','-');
```

```
hold on
title({'Normalised release rate for Test case 9, comparison ';'between
analytical solution and COMP23/Compulink'})
xlabel('Time [yrs]')
ylabel('Normalised release rate')
leg(2)=loglog(tout1,C1(:,1),'Color','k','LineWidth',2,'LineStyle',':')
;
leg(3)=loglog(tout2,C2(:,1),'Color','k','LineWidth',2,'LineStyle','--
');


leg(4)=loglog(COMP23a(:,1),COMP23a(:,2)/2.36e-3,'ok');
leg(5)=loglog(COMP23b(:,1),COMP23b(:,2)/2.36e-3,'sk');



legend(leg,'Analytical','8 Compartments (Compulink)','16 Compartments
(Compulink)','8 Compartments (COMP23)','16 Compartments (COMP23)',-1)

axis([0.1 100 0.0001 10])
```

B.19.2 Geometry

```
BEGIN_BLOCK GEOMETRY
        #
        # Materials definition
        #
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        #
        # Blocks definition
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 1
                MATERIAL_NAME WATER
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   1.0
                        Z_AREA     .7854
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
        END_DEF
        #
        BEGIN_DEF BLOCK
                        BLOCK_NUMBER 2
                        NUM_Z_COMP  1
```

```
                NUM_X_COMP  1
                NUM_Y_COMP   1
                AREA_CHANGE YES
                MATERIAL_NAME BENTONITE
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   1.0E-10
                        Z_AREA     0.7854E+0
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 3
        NUM_Z_COMP  1
        NUM_X_COMP  1
        NUM_Y_COMP   1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.0625E+0
                Z_AREA     0.7854E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 4
        NUM_Z_COMP  15
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.9375E+0
                Z_AREA     0.7854E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
# Connection definition
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        TO_BLOCK  2
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
```

```
                FROM_RESISTANCE FALSE
                TO_RESISTANCE FALSE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        #
        BEGIN_DEF CONNECTION
                        FROM_BLOCK  2
                        TO_BLOCK  3
                        COUPLES   1
                        FROM_DIRECTION Z
                        TO_DIRECTION   Z
                        FROM_RESISTANCE FALSE
                        TO_RESISTANCE TRUE
                        PLUG_POSITION NONE
                        EXTERNAL_RESIST FALSE
                        FROM_COMP  1
                        TO_COMP  1
        END_DEF
        #
        BEGIN_DEF CONNECTION
                FROM_BLOCK  3
                TO_BLOCK  4
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        #
        #
        BEGIN_DEF SINK
                FROM_BLOCK 4
                FROM_COMP 15
                DIRECTION Z
                PLUG_AT_INLET YES
                PLUG_LENGTH 0.0
                PLUG_AREA  1.0
                QEQ_FACTOR 1.0
                QEQ_EXPONENT 1.0
        END_DEF
#
        VOID           1E-5
        TUBE_VOLUME    2E-5
        NUM_TUBE      1
        TUBES_DAMAGED    1

END_BLOCK
```

B.19.3 Geometry 9b

```
BEGIN_BLOCK GEOMETRY
        #
        # Materials definition
        #
        BEGIN_DEF MATERIAL
                MATERIAL_NAME WATER
        END_DEF
        BEGIN_DEF MATERIAL
                MATERIAL_NAME BENTONITE
        END_DEF
        #
        # Blocks definition
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 1
                MATERIAL_NAME WATER
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP  1
                AREA_CHANGE NO
                BEGIN_DEF DISCRETIZATION
                        Z_LENGTH   1.0
                        Z_AREA     .7854
                        X_LENGTH   0.0E+0
                        X_AREA     1.0E+0
                        Y_LENGTH   0.0E+0
                        Y_AREA     1.0E+0
                END_DEF
        END_DEF
        #
        BEGIN_DEF BLOCK
                        BLOCK_NUMBER 2
                        NUM_Z_COMP  1
                        NUM_X_COMP  1
                        NUM_Y_COMP   1
                        AREA_CHANGE YES
                        MATERIAL_NAME BENTONITE
                        BEGIN_DEF DISCRETIZATION
                                Z_LENGTH   1.0E-10
                                Z_AREA     0.7854E+0
                                X_LENGTH   0.0E+0
                                X_AREA     1.0E+0
                                Y_LENGTH   0.0E+0
                                Y_AREA     1.0E+0
                        END_DEF
        END_DEF
        #
        BEGIN_DEF BLOCK
                BLOCK_NUMBER 3
                NUM_Z_COMP  1
                NUM_X_COMP  1
                NUM_Y_COMP   1
                AREA_CHANGE NO
                MATERIAL_NAME BENTONITE
```

```
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.125E+0
                Z_AREA     0.7854E+0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
BEGIN_DEF BLOCK
        BLOCK_NUMBER 4
        NUM_Z_COMP  7
        NUM_X_COMP  1
        NUM_Y_COMP  1
        AREA_CHANGE NO
        MATERIAL_NAME BENTONITE
        BEGIN_DEF DISCRETIZATION
                Z_LENGTH   0.8750E+0
                Z_AREA     0.7854E0
                X_LENGTH   0.0E+0
                X_AREA     1.0E+0
                Y_LENGTH   0.0E+0
                Y_AREA     1.0E+0
        END_DEF
END_DEF
#
# Connection definition
#
BEGIN_DEF CONNECTION
        FROM_BLOCK  1
        TO_BLOCK  2
        COUPLES   1
        FROM_DIRECTION Z
        TO_DIRECTION   Z
        FROM_RESISTANCE FALSE
        TO_RESISTANCE FALSE
        PLUG_POSITION NONE
        EXTERNAL_RESIST FALSE
        FROM_COMP  1
        TO_COMP  1
END_DEF
#
BEGIN_DEF CONNECTION
                FROM_BLOCK  2
                TO_BLOCK  3
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE FALSE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
END_DEF
```

```
        #
        BEGIN_DEF CONNECTION
                FROM_BLOCK  3
                TO_BLOCK  4
                COUPLES   1
                FROM_DIRECTION Z
                TO_DIRECTION   Z
                FROM_RESISTANCE TRUE
                TO_RESISTANCE TRUE
                PLUG_POSITION NONE
                EXTERNAL_RESIST FALSE
                FROM_COMP  1
                TO_COMP  1
        END_DEF
        #
        #
        BEGIN_DEF SINK
                FROM_BLOCK 4
                FROM_COMP 7
                DIRECTION Z
                PLUG_AT_INLET YES
                PLUG_LENGTH 0.0
                PLUG_AREA  1.0
                QEQ_FACTOR 1.0
                QEQ_EXPONENT 1.0
        END_DEF
#
        VOID           1E-5
        TUBE_VOLUME    2E-5
        NUM_TUBE      1
        TUBES_DAMAGED    1

END_BLOCK
```

B.20 Input data for Test case 10

B.20.1 Input data

```
%Load simulink file
load_system('Testcase10')


%Set parameters:
set_param( 'Testcase10/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase10/COMPULINK', 'FDM', 'Constant (mole/yr)')
set_param( 'Testcase10/COMPULINK', 'OUTCONC', 'off')
set_param( 'Testcase10/COMPULINK', 'GEOMDEF', ''SR97.gdf'')
set_param( 'Testcase10/COMPULINK', 'IRF', '[0;0;0;0;0;0;0;0;0;0;0;0;0;
0;0.03;0.15;0.06;0.03;0.03;0;0.03;1;1;1;0.002;0;0.03;0;0.02;0.0025;0.0
02;1e-006]')
set_param( 'Testcase10/COMPULINK', 'FDMC', '8.06e-005')
set_param( 'Testcase10/COMPULINK', 'SOLGROUPS', '{''Pu242'';''U238'';'
'U234'';''Th230'';''Ra226'';''Cm245'';''Am241'';''Np237'';''U233'';''T
h229'';''Am243'';''Pu239'';''U235'';''Pa231'';''Ag108m'';''C14'';''Cl3
6'';''Cs135'';''Cs137'';''Ho166m'';''I129'';''Nb94'';''Ni59'';''Ni63'
';''Pd107'';''Pu240'';''Se79'';''Sm151'';''Sn126'';''Sr90'';''Tc99'';
''Zr93''}')
set_param( 'Testcase10/COMPULINK', 'SOLLIM', '[6.56e-006;0.000128;3.2e-
8;1.22e-006;0.000286;0.000222;0.000687;5.87e-005;1e-010;1.22e-
006;0.000687;6.56e-006;1e-010;0.000316;0.0296;10000000;10000000;10000
000;10000000;0.00627;10000000;1.37;10000000;10000000;4.21e-006;6.56e-
006;2.59e-006;0.00213;4.49e-006;6.88;7.67e-006;2.5e-006]')
set_param( 'Testcase10/COMPULINK', 'RHO', '[1000;2695;2714;2700]')
set_param( 'Testcase10/COMPULINK', 'EPS', '[1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1;0.41 0.41 0.41 0.41 0.41 0.41
0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41
0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41;0.3 0.3
0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3
0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3;0.005 0.005 0.005
0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005
0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005
0.005 0.005 0.005 0.005 0.005 0.005 0.005]')
set_param( 'Testcase10/COMPULINK', 'DE', '[0.032 0.032 0.032 0.032
0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032
0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032
0.032 0.032 0.032 0.032 0.032 0.032;0.0095 0.016 0.016 0.0022 0.016
0.0022 0.0022 0.032 0.016 0.0022 0.0022 0.0095 0.016 0.022 0.0063
0.00095 3.2e-005 0.019 0.019 0.0063 9.5e-005 0.016 0.032 0.032 0.0032
0.0095 0.0022 0.0063 0.0022 0.016 0.016 0.0016;0.0032 0.0032 0.0032
0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032
0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032
0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032;1.3e-
006 1.3e-006 1.3e-006 2e-007 1.2e-006 1.3e-006 1.3e-006 1.3e-006
1.3e-006 2e-007 1.3e-006 1.3e-006 1.3e-006 1.3e-006 2.2e-006 1.6e-006
2.6e-006 2.8e-006 2.8e-006 1.3e-006 2.6e-006 1.3e-006 8.8e-007 8.8e-
007 1.3e-006 1.3e-006 1.3e-006 1.3e-006 1.3e-006 1e-006 1.3e-006 1.3e-
006]')
set_param( 'Testcase10/COMPULINK', 'KD', '[0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;3 1 1 3 0.01 3 3 3 1 3 3 3 1 0.3 0
0 0 0.05 0.05 1 0 0.2 0.1 0.1 0.01 3 0.003 1 3 0.01 0.1 2;5 4 4 5 0.02
3 3 5 4 5 3 5 4 0.9 0.05 0.0009 0 0.05 0.05 2 0 0.9 0.03 0.03 0.01 5
```

```
0.001 2 0.5 0.002 0.9 1;5 5 5 5 0.02 3 3 5 5 5 3 5 5 1 0.05 0.001 0
0.05 0.05 2 0 1 0.02 0.02 0.01 5 0.001 2 0.001 0.0002 1 1]’)
set_param( ‘Testcase10/COMPULINK’, ‘PLUGLENGTH’, ‘[0.0005 0 0.002 0]’)
set_param( ‘Testcase10/COMPULINK’, ‘PLUGAREA’, ‘[0.00055 1 0.006 1]’)
set_param( ‘Testcase10/COMPULINK’, ‘QEQ’, ‘[0.00134164078649987
0.00447213595499958 0.0447213595499958 0.0447213595499958]’)
set_param( ‘Testcase10/COMPULINK’, ‘ATOL’, ‘1e-23’)
set_param( ‘Testcase10/Defect’, ‘TDELAY’, ‘300’)
set_param( ‘Testcase10/Defect’, ‘ADELAY’, ‘1e-6’)
set_param( ‘Testcase10/Defect’, ‘TLARGE’, ‘20000’)
set_param( ‘Testcase10/Defect’, ‘ALARGE’, ‘1e-2’)
set_param( ‘Testcase10/Inventory’, ‘DEBUG’, ‘off’)
set_param( ‘Testcase10/Inventory’, ‘FILEINV’, ‘’’SR97.inv’’’)
set_param( ‘Testcase10/Inventory’, ‘FILENAM’, ‘’’SR97.nam’’’)
set_param( ‘Testcase10/Pick sink’, ‘Q’, ‘1’)
set_param( ‘Testcase10/Pick sink1’, ‘Q’, ‘2’)
set_param( ‘Testcase10/Pick sink2’, ‘Q’, ‘3’)
set_param( ‘Testcase10/Pick sink3’, ‘Q’, ‘4’)

set_param( ‘Testcase10/TENSIT’, ‘DEBUG’, ‘off’)
set_param( ‘Testcase10/TENSIT’, ‘NUCLIDES’, ‘{’’Pu242’’;’’U238’’;’’U2
34’’;’’Th230’’;’’Ra226’’;’’Cm245’’;’’Am241’’;’’Np237’’;’’U233’’;’’Th2
29’’;’’Am243’’;’’Pu239’’;’’U235’’;’’Pa231’’;’’Ag108m’’;’’C14’’;’’Cl36
’’;’’Cs135’’;’’Cs137’’;’’Ho166m’’;’’I129’’;’’Nb94’’;’’Ni59’’;’’Ni63’
’;’’Pd107’’;’’Pu240’’;’’Se79’’;’’Sm151’’;’’Sn126’’;’’Sr90’’;’’Tc99’’;
’’Zr93’’}’)
set_param( ‘Testcase10/TENSIT’, ‘HALFLIFE’, ‘[373300;4.47E+09;245500;7
5380;1600;8500;432.2;2.14E+06;159200;7340;7370;24110;7.04E+08;32760;41
8;5730;301000;2.30E+06;30.07;1200;1.57E+07;20300;76000;100.1;6.50E+06;
6563;1.13E+06;90;100000;28.78;211100;1.53E+06]’)
set_param( ‘Testcase10/TENSIT’, ‘CHAIN’, ‘[0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0;0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0;0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0;0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0
0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 1 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]')

%Start simulation
[tout1,X,C1,C2,C3,C4] = sim('Testcase10',[300 1e6]);

%Load COMP23 data (for comparison)
load COMP23

%Print results
NUCLIDES=['Pu242 ';'U238  ';'U234  ';'Th230 ';'Ra226 ';'Cm245 ';'Am241
';'Np237 ';'U233  ';'Th229 ';'Am243 ';'Pu239 ';'U235  ';'Pa231
';'Ag108m';'C14   ';'Cl36  ';'Cs135 ';'Cs137 ';'Ho166m';'I129  ';'Nb94
';'Ni59  ';'Ni63  ';'Pd107 ';'Pu240 ';'Se79  ';'Sm151 ';'Sn126 ';'Sr90
';'Tc99  ';'Zr93  '];
figure('Name','Testcase 10 / TR99-23 Comparison total','NumberTitle','
off')
hold on
cc=ColorCube  ;

for a=1:32
    leg(a)=plot(tout1,C1(:,a)+C2(:,a)+C3(:,a)+C4(:,a),'LineWidth',2,'C
olor',cc(a,:),'Tag',NUCLIDES(a,:));
    plot(COMP23(1,:),COMP23(a+1,:),'o','Color',cc(a,:),'Tag',NUCLIDES(
a,:))
end
legend(leg,NUCLIDES,-1)
set(legend,'FontSize',8.0)

xlabel('Time [yr]')
ylabel('Release rate [Bq/yr]')
title('SR97, pessimistic canister relatedparameters (A-Berg)')
set(gca,'XScale','log','YScale','log','XLim',[100 1e6],'YLim',[1
1e7])
```

B.20.2 Geometry

```
 BEGIN_BLOCK GEOMETRY
    BEGIN_DEF MATERIAL
          MATERIAL_NAME      WATER
          DENSITY              1000.000
          POROSITY                1.000
        END_DEF
        BEGIN_DEF MATERIAL
          MATERIAL_NAME      BENTONITE
          DENSITY              2695.000
          POROSITY                0.410
        END_DEF
        BEGIN_DEF MATERIAL
          MATERIAL_NAME      SAND-BENTONITE
          DENSITY              2714.000
          POROSITY                0.300
        END_DEF
        BEGIN_DEF MATERIAL
```

```
      MATERIAL_NAME      ROCK
      DENSITY              2700.000
      POROSITY                0.005
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       1
  MATERIAL_NAME      WATER
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.000
    Z_AREA                1.000
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       2
  MATERIAL_NAME      WATER
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  AREA_CHANGE        YES
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.050
    Z_AREA             1.000E-06
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       3
  MATERIAL_NAME      BENTONITE
  NUM_Z_COMP         1
  NUM_X_COMP         6
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                0.203
    X_LENGTH              0.058
    X_AREA                1.741
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                0.224
    X_LENGTH              0.058
    X_AREA                1.924
    Y_LENGTH              0.0
    Y_AREA                1.0
```

```
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                0.246
    X_LENGTH              0.058
    X_AREA                2.107
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                0.267
    X_LENGTH              0.058
    X_AREA                2.291
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                0.289
    X_LENGTH              0.058
    X_AREA                2.474
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                0.310
    X_LENGTH              0.058
    X_AREA                2.657
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       4
  MATERIAL_NAME      BENTONITE
  NUM_Z_COMP         2
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              1.000
    Z_AREA                1.539
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              3.330
    Z_AREA                1.539
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
```

```
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       5
  MATERIAL_NAME      BENTONITE
  NUM_Z_COMP         3
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                2.405
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                2.405
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                2.405
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       6
  MATERIAL_NAME      SAND-BENTONITE
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              1.000
    Z_AREA                2.405
    X_LENGTH              1.750
    X_AREA                5.500
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       7
  MATERIAL_NAME      SAND-BENTONITE
  NUM_Z_COMP         3
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              2.125
    Z_AREA               12.566
```

```
    X_LENGTH              2.000
    X_AREA               26.700
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              1.750
    Z_AREA               12.566
    X_LENGTH              2.000
    X_AREA               22.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              2.125
    Z_AREA               12.566
    X_LENGTH              2.000
    X_AREA               26.700
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       8
  MATERIAL_NAME      BENTONITE
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.500
    Z_AREA                2.405
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       9
  MATERIAL_NAME      ROCK
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              3.000
    Z_AREA                2.405
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         1
  TO_BLOCK           2
  COUPLES            1
```

```
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    FALSE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        1
    TO_COMP          1
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         2
  TO_BLOCK           3
  COUPLES            1
  FROM_DIRECTION     Z
  TO_DIRECTION       X
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      FALSE
  PLUG_POSITION      TO_BLOCK
  EXTERNAL_RESIST    FALSE
    FROM_COMP        1
    TO_COMP          1
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         3
  TO_BLOCK           4
  COUPLES            6
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        1
    TO_COMP          1
    FROM_COMP        2
    TO_COMP          1
    FROM_COMP        3
    TO_COMP          1
    FROM_COMP        4
    TO_COMP          1
    FROM_COMP        5
    TO_COMP          1
    FROM_COMP        6
    TO_COMP          1
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         3
  TO_BLOCK           5
  COUPLES            6
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        1
    TO_COMP          1
    FROM_COMP        2
    TO_COMP          1
```

```
    FROM_COMP        3
    TO_COMP          1
    FROM_COMP        4
    TO_COMP          1
    FROM_COMP        5
    TO_COMP          1
    FROM_COMP        6
    TO_COMP          1
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         4
  TO_BLOCK           8
  COUPLES            1
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        2
    TO_COMP          1
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         5
  TO_BLOCK           6
  COUPLES            1
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        3
    TO_COMP          1
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         6
  TO_BLOCK           7
  COUPLES            1
  FROM_DIRECTION     Z
  TO_DIRECTION       X
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        1
    TO_COMP          2
END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         8
  TO_BLOCK           9
  COUPLES            1
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    TRUE
  TO_RESISTANCE      TRUE
  EXTERNAL_RESIST    FALSE
    FROM_COMP        1
    TO_COMP          1
```

```
 END_DEF
 BEGIN_DEF SINK
   FROM_BLOCK         3
   FROM_COMP          6
   DIRECTION          X
   PLUG_AT_INLET      NO
   PLUG_LENGTH         5.000E-04
   PLUG_AREA           5.500E-04
   QEQ_FACTOR              0.030
   QEQ_EXPONENT            0.500
 END_DEF
 BEGIN_DEF SINK
   FROM_BLOCK         6
   FROM_COMP          1
   DIRECTION          X
   PLUG_AT_INLET      YES
   PLUG_LENGTH             0.000
   PLUG_AREA               1.000
   QEQ_FACTOR              0.100
   QEQ_EXPONENT            0.500
 END_DEF
 BEGIN_DEF SINK
   FROM_BLOCK         7
   FROM_COMP          3
   DIRECTION          X
   PLUG_AT_INLET      NO
   PLUG_LENGTH             0.002
   PLUG_AREA               0.006
   QEQ_FACTOR              1.000
   QEQ_EXPONENT            0.500
 END_DEF
 BEGIN_DEF SINK
   FROM_BLOCK         9
   FROM_COMP          1
   DIRECTION          Z
   PLUG_AT_INLET      YES
   PLUG_LENGTH             0.000
   PLUG_AREA               1.000
   QEQ_FACTOR              1.000
   QEQ_EXPONENT            0.500
 END_DEF
 TUBE_VOLUME          4.500E-05
 NUM_TUBE            1440
 TUBES_DAMAGED       1440
 VOID                     1.000
NUM_STEP_NODES       2
END_BLOCK
```

B.21 Input data for Test case 11

B.21.1 Input data

```
%Load simulink file
load_system('Testcase11')


%Set parameters:
set_param( 'Testcase11/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase11/COMPULINK', 'OUTCONC', 'off')
set_param( 'Testcase11/COMPULINK', 'FDM', 'Constant (mole/yr)')
set_param( 'Testcase11/COMPULINK', 'GEOMDEF', ''SR97.gdf'')
set_param( 'Testcase11/COMPULINK', 'IRF', '[1;1;1;1;1;1;1;1;1;1;1;1;1;
1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1]')
set_param( 'Testcase11/COMPULINK', 'FDMC', '8.06e-005')
set_param( 'Testcase11/COMPULINK', 'SOLGROUPS', '{''Pu242'';''U238'';'
''U234'';''Th230'';''Ra226'';''Cm245'';''Am241'';''Np237'';''U233'';''T
h229'';''Am243'';''Pu239'';''U235'';''Pa231'';''Ag108m'';''C14'';''Cl3
6'';''Cs135'';''Cs137'';''Ho166m'';''I129'';''Nb94'';''Ni59'';''Ni63'
';''Pd107'';''Pu240'';''Se79'';''Sm151'';''Sn126'';''Sr90'';''Tc99'';
''Zr93''}')
set_param( 'Testcase11/COMPULINK', 'SOLLIM', '[6.56e-006;0.000128;1e-
020;1.22e-006;0.000286;0.000222;0.000687;5.87e-005;1e-010*0;1.22e-
006;0.000687;6.56e-006;1e-010;0.000316;0.0296;10000000;10000000;10000
000;10000000;0.00627;10000000;1.37;10000000;10000000;4.21e-006;6.56e-
006;2.59e-006;0.00213;4.49e-006;6.88;7.67e-006;2.5e-006]')
set_param( 'Testcase11/COMPULINK', 'RHO', '[1000;2695;2714;2700]')
set_param( 'Testcase11/COMPULINK', 'EPS', '[1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1;0.41 0.41 0.41 0.41 0.41 0.41
0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41
0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41 0.41;0.3 0.3
0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3
0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3 0.3;0.005 0.005 0.005
0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005
0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005 0.005
0.005 0.005 0.005 0.005 0.005 0.005 0.005]')
set_param( 'Testcase11/COMPULINK', 'DE', '[0.032 0.032 0.032 0.032
0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032
0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032 0.032
0.032 0.032 0.032 0.032 0.032 0.032 0.032;0.0095 0.016 0.016 0.0022 0.016
0.0022 0.0022 0.032 0.016 0.0022 0.0022 0.0095 0.016 0.022 0.0063
0.00095 3.2e-005 0.019 0.019 0.0063 9.5e-005 0.016 0.032 0.032 0.0032
0.0095 0.0022 0.0063 0.0022 0.016 0.016 0.0016;0.0032 0.0032 0.0032
0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032
0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032
0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032 0.0032;1.3e-
006 1.3e-006 1.3e-006 2e-007 1.2e-006 1.3e-006 1.3e-006 1.3e-006
1.3e-006 2e-007 1.3e-006 1.3e-006 1.3e-006 1.3e-006 2.2e-006 1.6e-006
2.6e-006 2.8e-006 2.8e-006 1.3e-006 2.6e-006 1.3e-006 8.8e-007 8.8e-
007 1.3e-006 1.3e-006 1.3e-006 1.3e-006 1.3e-006 1e-006 1.3e-006 1.3e-
006]')
set_param( 'Testcase11/COMPULINK', 'KD', '[0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;3 1 1 3 0.01 3 3 3 1 3 3 3 1 0.3 0
0 0 0.05 0.05 1 0 0.2 0.1 0.1 0.01 3 0.003 1 3 0.01 0.1 2;5 4 4 5 0.02
3 3 5 4 5 3 5 4 0.9 0.05 0.0009 0 0.05 0.05 2 0 0.9 0.03 0.03 0.01 5
0.001 2 0.5 0.002 0.9 1;5 5 5 5 0.02 3 3 5 5 5 3 5 5 1 0.05 0.001 0
```

```
0.05 0.05 2 0 1 0.02 0.02 0.01 5 0.001 2 0.001 0.0002 1 1]’)
set_param( ‘Testcase11/COMPULINK’, ‘PLUGLENGTH’, ‘[0.0005 0 0.002 0]’)
set_param( ‘Testcase11/COMPULINK’, ‘PLUGAREA’, ‘[0.00055 1 0.006 1]’)
set_param( ‘Testcase11/COMPULINK’, ‘QEQ’, ‘[0.00134164078649987
0.00447213595499958 0.0447213595499958 0.0447213595499958]’)
set_param( ‘Testcase11/COMPULINK’, ‘ATOL’, ‘1e-23’)
set_param( ‘Testcase11/Defect’, ‘TDELAY’, ‘300’)
set_param( ‘Testcase11/Defect’, ‘ADELAY’, ‘1e-6’)
set_param( ‘Testcase11/Defect’, ‘TLARGE’, ‘20000’)
set_param( ‘Testcase11/Defect’, ‘ALARGE’, ‘1e-2’)
set_param( ‘Testcase11/Inventory’, ‘DEBUG’, ‘off’)
set_param( ‘Testcase11/Inventory’, ‘FILEINV’, ‘’’SR97.inv’’’)
set_param( ‘Testcase11/Inventory’, ‘FILENAM’, ‘’’SR97.nam’’’)
set_param( ‘Testcase11/Pick sink’, ‘Q’, ‘1’)
set_param( ‘Testcase11/Pick sink1’, ‘Q’, ‘2’)
set_param( ‘Testcase11/Pick sink2’, ‘Q’, ‘3’)
set_param( ‘Testcase11/Pick sink3’, ‘Q’, ‘4’)

set_param( ‘Testcase11/TENSIT’, ‘DEBUG’, ‘off’)
set_param( ‘Testcase11/TENSIT’, ‘NUCLIDES’, ‘{‘’Pu242’’;’’U238’’;’’U2
34’’;’’Th230’’;’’Ra226’’;’’Cm245’’;’’Am241’’;’’Np237’’;’’U233’’;’’Th2
29’’;’’Am243’’;’’Pu239’’;’’U235’’;’’Pa231’’;’’Ag108m’’;’’C14’’;’’Cl36
’’;’’Cs135’’;’’Cs137’’;’’Ho166m’’;’’I129’’;’’Nb94’’;’’Ni59’’;’’Ni63’’
;’’Pd107’’;’’Pu240’’;’’Se79’’;’’Sm151’’;’’Sn126’’;’’Sr90’’;’’Tc99’’;
’’Zr93’’}’)
set_param( ‘Testcase11/TENSIT’, ‘HALFLIFE’, ‘[373300;4.47E+09;245500;7
5380;1600;8500;432.2;2.14E+06;159200;7340;7370;24110;7.04E+08;32760;41
8;5730;301000;2.30E+06;30.07;1200;1.57E+07;20300;76000;100.1;6.50E+06;
6563;1.13E+06;90;100000;28.78;211100;1.53E+06]’)
set_param( ‘Testcase11/TENSIT’, ‘CHAIN’, ‘[0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0;0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0;0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0;0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0
0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 1
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 1 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
0 0 0 0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0;0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]')

%Start simulation
[tout1,X,C1] = sim('Testcase11',[300 1e6]);

%Load COMP23 data (for comparison)
load COMP23

%Print results
NUCLIDES=['Pu242 ';'U238  ';'U234  ';'Th230 ';'Ra226 ';'Cm245 ';'Am241
';'Np237 ';'U233  ';'Th229 ';'Am243 ';'Pu239 ';'U235  ';'Pa231
';'Ag108m';'C14   ';'Cl36  ';'Cs135 ';'Cs137 ';'Ho166m';'I129  ';'Nb94
';'Ni59  ';'Ni63  ';'Pd107 ';'Pu240 ';'Se79  ';'Sm151 ';'Sn126 ';'Sr90
';'Tc99  ';'Zr93  '];
figure('Name','Testcase 11 Comparison','NumberTitle','off')
hold on
cc=ColorCube  ;


for a=1:32
leg(a)=plot(tout1,C1(:,a),'LineWidth',2,'Color',cc(a,:),'Tag',NUCLIDES
(a,:));
plot(COMP23(1,:),COMP23(a+1,:),'o','Color',cc(a,:),'Tag',NUCLIDES(a,:)
)
end
legend(leg,NUCLIDES,-1)
set(legend,'FontSize',8.0)

xlabel('Time [yr]')
ylabel('Release rate [Bq/yr]')
title('SR97, pessimistic canister relatedparameters (A-Berg) with
IRF=1 for all nuclides')
set(gca,'XScale','log','YScale','log','XLim',[100 1e6],'YLim',[1
1e7])
```

B.21.2 Geometry

See corresponding file for test case 10

B.22 Input data for Test case 16

B.22.1 Input data

```
%Load simulink file
load_system('Testcase16')

m0=[6.026 8061 11.89];
Halflife=[387200;4.47E+09;6542];
cShared=[1.28E-04;6.56E-06];

%Set parameters:
set_param( 'Testcase16/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase16/COMPULINK', 'OUTCONC', 'off')
set_param( 'Testcase16/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase16/COMPULINK', 'GEOMDEF', ''SR97.gdf'')
set_param( 'Testcase16/COMPULINK', 'IRF', '[1;1;1]')
set_param( 'Testcase16/COMPULINK', 'FDMC', '1')
set_param( 'Testcase16/COMPULINK', 'SOLGROUPS', '{''U2'';''Pu''}')
set_param( 'Testcase16/COMPULINK', 'SOLLIM',mat2str(cShared) )
set_param( 'Testcase16/COMPULINK', 'RHO', '[1000;2695;2714;2700]')
set_param( 'Testcase16/COMPULINK', 'EPS', '[1 1 1 ; 0.41 0.41 0.41;
0.3 0.3 0.3; 0.005 0.005 0.005]')
set_param( 'Testcase16/COMPULINK', 'DE', '[3.2E-02 3.2E-02 3.2E-02 ;
9.5E-03 1.6E-02 9.5E-03 ; 3.2E-03 3.2E-03 3.2E-03; 1.3E-06 1.3E-06
1.3E-06]')
set_param( 'Testcase16/COMPULINK', 'KD', '[0 0 0 ; 3 1 3; 5 4 5 ; 5 5
5]')
set_param( 'Testcase16/COMPULINK', 'PLUGLENGTH', '[0.0005 0 0.002 0]')
set_param( 'Testcase16/COMPULINK', 'PLUGAREA', '[0.00055 1 0.006 1]')
set_param( 'Testcase16/COMPULINK', 'QEQ', '[0.00134164078649987
0.00447213595499958 0.0447213595499958 0.0447213595499958]')
set_param( 'Testcase16/COMPULINK', 'ATOL', '1e-23')

set_param( 'Testcase16/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase16/TENSIT', 'NUCLIDES', '{''Pu242'';''U238'';''Pu2
40''}')
set_param( 'Testcase16/TENSIT', 'HALFLIFE', mat2str(Halflife))
set_param( 'Testcase16/TENSIT', 'CHAIN', '[0 0 0; 1 0 0 ; 0 0 0]')
set_param( 'Testcase16/Inventory', 'Value', mat2str(m0))

%Start simulation
[tout,X,C] = sim('Testcase16',[0 1e5]);

%Print results
figure('Name','Testcase 16','NumberTitle','off')
hold on
title('Concentration of Pu in canister for test case 16')
xlabel('Time [yrs]')
ylabel('Concentration [mole/m^3]')
leg(1)=plot(tout,C(:,1),'Color','k','LineWidth',2,'LineStyle','-');
leg(2)=plot(tout,C(:,3),'Color','k','LineWidth',2,'LineStyle',':');
leg(3)=plot(tout,cShared(2)*m0(1)*exp(-log(2)/Halflife(1)*tout)./
(m0(1)*exp(-log(2)/Halflife(1)*tout)+m0(3)*exp(-log(2)/Halflife(3)*tou
t)),'ok');
leg(4)=plot(tout,cShared(2)*m0(3)*exp(-log(2)/Halflife(3)*tout)./
(m0(1)*exp(-log(2)/Halflife(1)*tout)+m0(3)*exp(-log(2)/Halflife(3)*tou
t)),'sk');
legend(leg,'Pu242 (Compulink)','Pu240 (Compulink)','Pu242
(Analytical)','Pu240 (Analytical)',-1)
```

B.23 Input data for Test case 25

B.23.1 Input data

```
%Load simulink file
load_system('Testcase25')

%Set parameters:
set_param( 'Testcase25/COMPULINK', 'DEBUG', 'off')
set_param( 'Testcase25/COMPULINK', 'OUTCONC', 'off')
set_param( 'Testcase25/COMPULINK', 'FDM', 'Constant (yr)')
set_param( 'Testcase25/COMPULINK', 'GEOMDEF', ''advective.gdf'')
set_param( 'Testcase25/COMPULINK', 'ADVECTIVE', '[-1 1:500]')
set_param( 'Testcase25/COMPULINK', 'IRF', '[1]')
set_param( 'Testcase25/COMPULINK', 'FDMC', '1')
set_param( 'Testcase25/COMPULINK', 'SOLGROUPS', '{''U2''}')
set_param( 'Testcase25/COMPULINK', 'SOLLIM', '[0.1]')
set_param( 'Testcase25/COMPULINK', 'RHO', '[1000;2695]')
set_param( 'Testcase25/COMPULINK', 'EPS', '[1;1]')
set_param( 'Testcase25/COMPULINK', 'DE', '[1e-9;1e-9]')
set_param( 'Testcase25/COMPULINK', 'KD', '[0;0 ]')
set_param( 'Testcase25/COMPULINK', 'PLUGLENGTH', '[ 0]')
set_param( 'Testcase25/COMPULINK', 'PLUGAREA', '[ 1]')
set_param( 'Testcase25/COMPULINK', 'QEQ', '[1]')
set_param( 'Testcase25/COMPULINK', 'DARCYVELOCITY', '1')
set_param( 'Testcase25/COMPULINK', 'ATOL', '1e-23')

set_param( 'Testcase25/TENSIT', 'DEBUG', 'off')
set_param( 'Testcase25/TENSIT', 'NUCLIDES', '{''U238''}')
set_param( 'Testcase25/TENSIT', 'HALFLIFE', '[4470000000]')
set_param( 'Testcase25/TENSIT', 'CHAIN', '[0]')

%Start simulation
[tout,X,C] = sim('Testcase25',[0 50]);
C=squeeze(C);

%Print results
figure('Name','Testcase 25','NumberTitle','off')
hold on
title('Advective outflow of U for test case 25')
xlabel('Time [yrs]')
ylabel('Outflow [mole/yr]')
leg(1)=plot(tout,C(:,1),'ok');
leg(2)=plot([0 10 10 20 20 50],[0 0 0.1 0.1 0 0],'Color','k','LineWidt
h',2,'LineStyle','-');
legend(leg,'Compulink','Analytical')

axis([0 50 0 1])
```

B.23.2 Geometry

```
BEGIN_BLOCK GEOMETRY
    BEGIN_DEF MATERIAL
          MATERIAL_NAME      WATER
        END_DEF
        BEGIN_DEF MATERIAL
          MATERIAL_NAME      BENTONITE
```

```
    END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       1
  MATERIAL_NAME      WATER
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              0.000
    Z_AREA                1.000
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       2
  MATERIAL_NAME      WATER
  NUM_Z_COMP         1
  NUM_X_COMP         1
  NUM_Y_COMP         1
  AREA_CHANGE        NO
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              1.0e-9
    Z_AREA                1.0
    X_LENGTH              0.000
    X_AREA                1.000
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
END_DEF
BEGIN_DEF BLOCK
  BLOCK_NUMBER       3
  MATERIAL_NAME      BENTONITE
  NUM_Z_COMP         500
  NUM_X_COMP         1
  NUM_Y_COMP         1
  BEGIN_DEF DISCRETIZATION
    Z_LENGTH              10.0
    Z_AREA                1.0
    X_LENGTH              0.0
    X_AREA                1.0
    Y_LENGTH              0.0
    Y_AREA                1.0
  END_DEF
      END_DEF
BEGIN_DEF CONNECTION
  FROM_BLOCK         1
  TO_BLOCK           2
  COUPLES            1
  FROM_DIRECTION     Z
  TO_DIRECTION       Z
  FROM_RESISTANCE    FALSE
  TO_RESISTANCE      FALSE
  EXTERNAL_RESIST    FALSE
```

```
    FROM_COMP        1
    TO_COMP          1
 END_DEF
 BEGIN_DEF CONNECTION
   FROM_BLOCK        2
   TO_BLOCK          3
   COUPLES           1
   FROM_DIRECTION    Z
   TO_DIRECTION      Z
   FROM_RESISTANCE   FALSE
   TO_RESISTANCE     FALSE
   PLUG_POSITION     TO_BLOCK
   EXTERNAL_RESIST   FALSE
     FROM_COMP       1
     TO_COMP         1
 END_DEF
 TUBE_VOLUME          4.500E-05
 NUM_TUBE            1440
 TUBES_DAMAGED       0
 VOID                     1.000
END_BLOCK
```

Appendix C

Code listing

The following function sets up the Compulink model from data contained in the geometry definition file. It is called by the initialisation function of the Simulink block. It uses some lower level functions, which are not all listed below.

C.1 SetupCompulink.m

```
function [A,B,C,D,LENGTH1,LENGTH2,LENGTH3,DE1,DE2,DE3,AREA1,AREA3,PLUG
23,VOID,TUBES_DAMAGED,TUBE_VOLUME,NoN,NoC,NoS,NoE]= ...
    SetupCompulink(NUCLIDES,HALFLIFE,CHAIN,GEOMDEF,IRF,SOLLIM,RHO,EPS,
DE,KD,SOLMATRIX,PLUGLENGTH,PLUGAREA,QEQ,CURRENTBLOCK,DEBUG,OUTCONC,var
argin)
%SetupCompulink10 Function to setup COMPULINK
%
% SetupCompulink This function sets up a COMPULINK problem based on a
number of parameters
% provided by the user. The geometry definition is taken from a file
in the
% same format as that used by COMP23. The file name of the geometry
definition
% file should be supplied in the GEOMDEF parameter. The variables
NUCLIDES,
% HALFLIFE and CHAIN comes from a TENSIT block which must always be
present
% in the same model as this COMPULINK block.
%
% Input parameters:
% NUCLIDES - Names of nuclides
% HALFLIFE - Halflife of nuclides
% CHAIN - Decay chain definition
% GEOMDEF - Name of geometry definition file
% IRF - Instant release fractions
% KCON - Dissolution rate
% SOLLIM - Solubility limit
% RHO - Density
% EPS - Porosity
% DE - Effective diffusivity
% KD - Distribution coefficient
% SOLGROUPS - Solubility matrix
% PLUGLENGTH - Plug lengths for sinks
% PLUGAREA - Plug areas for sinks
% U - Groundwater velocity vector
% QEQFAC - Plug factor for sinks
% QEQEXP - Plug exponent for sinks
% CURRENTBLOCK - This COMPULINK block itself
% DEBUG - Debug flag
%

if DEBUG
    disp('Entering setup')
end
%
```

```
% The matrix model must know what nuclide it consists of.
% The fuel matrix is always assumed to consist of U238 (unless changed
% here).
%
MATRIXNUCLIDE=strmatch('U238  ',NUCLIDES);

if DEBUG
    disp('Matrix')
    disp(['   NUCLIDES(' num2str(MATRIXNUCLIDE) ')=U238'])
end


if DEBUG
    for j1=1:size(SOLMATRIX,1)
        disp(['Solubility group ' num2str(j1) ':'])
        disp(    NUCLIDES(find(SOLMATRIX(j1,:)>0),:));
    end
end

%
% Here we read the complete geometry definition from the geometry
% definition file and extract all needed parameters. The matrices A,
B, C
% and D are needed for the state-space blocks, which decribes the
bentonite
% diffusion process and the release into the sinks.
%
if length(varargin) == 0
    [A,B,C,D,LENGTH1,AREA1,MATERIAL1,LENGTH2,MATERIAL2,PLUG23,LENGTH3,
AREA3,MATERIAL3,TUBE_VOLUME,NUM_TUBE,TUBES_DAMAGED,VOID,NoN,NoC,NoS,No
E]= ...
    DefineComp(DE,KD,EPS,RHO,PLUGLENGTH,PLUGAREA,QEQ,HALFLIFE,CHAIN,GE
OMDEF,DEBUG,OUTCONC);
else
    [A,B,C,D,LENGTH1,AREA1,MATERIAL1,LENGTH2,MATERIAL2,PLUG23,LENGTH3,
AREA3,MATERIAL3,TUBE_VOLUME,NUM_TUBE,TUBES_DAMAGED,VOID,NoN,NoC,NoS,No
E]= ...
        DefineComp(DE,KD,EPS,RHO,PLUGLENGTH,PLUGAREA,QEQ,HALFLIFE,CHAI
N,GEOMDEF,DEBUG,OUTCONC,varargin);
end


%
% Propagate resistivity data extracted from the geometry definition
file to

% the plug model of the canister
%
if DEBUG
    disp(['Propagating LENGTH1:' num2str(LENGTH1) ' To canister
resistivity'])
    disp(['Propagating AREA1:' num2str(AREA1) ' To canister
resistivity'])
    disp(['Propagating LENGTH2:' num2str(LENGTH2) ' To canister
resistivity'])
    disp(['Propagating LENGTH3:' num2str(LENGTH3) ' To canister
```

```
resistivity'])
    disp(['Propagating AREA3:' num2str(AREA3) ' To canister
resistivity'])
end

DE1=DE(MATERIAL1,:);
DE2=DE(MATERIAL2,:);
DE3=DE(MATERIAL3,:);



%
% end of function SetupCompulink
%
```

C.2 DefineComp.m

```
function [A,B,C,D,LENGTH1,AREA1,MATERIAL1,LENGTH2,MATERIAL2,PLUG23,LEN
GTH3,AREA3,MATERIAL3,TUBE_VOLUME,NUM_TUBE,TUBES_DAMAGED,VOID,NoN,NoC,N
oS,NoE]= ...
    DefineComp(DE,KD,EPS,RHO,PLUGLENGTH,PLUGAREA,QEQ,HALFLIFE,CHAIN,BL
OCKDEF,DEBUG,OUTCONC,varargin)
%DefineComp Function to set up data structures needed by COMPULINK
%
% DefineComp This function sets up the data structures needed by
COMPULINK
% based on data read from a geometry definition file on COMP23 format.
% The file name of the geometry definition file should be supplied in
the
% BLOCKDEF parameter. The variable HALFLIFE comes from a TENSIT block
which
% must always be present in the same model as this COMPULINK block.
%
% Input parameters:
% DE - Effective diffusivity
% KD - Distribution coefficient
% EPS - Porosity
% RHO - Density
% PLUGLENGTH - Plug lengths for sinks
% PLUGAREA - Plug areas for sinks
% QEQFAC - Plug factor for sinks
% QEQEXP - Plug exponent for sinks
% U - Groundwater velocity vector
% HALFLIFE - Halflife of nuclides
% BLOCKDEF - Name of geometry definition file
%
% varargin arguments: DARCYVELOCITY,ADVECTIVEELEMENTS
% DARCYVELOCITY - Darcy velocity
% ADVECTIVEELEMENTS - Information about where in the model advection
should be active
%
% Output parameters:
% A,B,C,D - Matrices for the state-space block
% LENGTH1,AREA1,LENGTH2,LENGTH3,AREA3 - Resistivity data for the
defect plug model
% MATERIAL1 - Material of the void of the canister (usually water)
```

```
% MATERIAL2 - Material of the defect (usually water)

% MATERIAL3 - Material outside the defect (usually bentonite)
% TUBE_VOLUME,NUM_TUBE,TUBES_DAMAGED,VOID - Internal geometry data for
the canister
%

%
% Extract varargin arguments
%
if length(varargin) == 0
    DARCYVELOCITY=[];
    ADVECTIVEELEMENTS=[];
    UPSTREAMCONCENTRATION=0;
    NoAS=0; %Number of advective sinks
else
    DARCYVELOCITY=varargin{1}{1};
    ADVECTIVEELEMENTS=varargin{1}{2};
    if size(varargin{1},2) > 2
        UPSTREAMCONCENTRATION=varargin{1}{3};
    else
        UPSTREAMCONCENTRATION=0;
    end
    %Test version that includes advection
    disp('Testversion of DefineComp.m, advection included')
    NoAS=1; %Number of advective sinks
end

%
% Read the geometry definition file
%
[MATERIALS,ELEMENTS,CONNECTIONS,SINKS,TUBE_VOLUME,NUM_TUBE,TUBES_DAMAG
ED,VOID,COMP,CONN]=ReadBlockFile(BLOCKDEF,DEBUG);



if DEBUG
    save BLOCKDEFINITION.mat MATERIALS ELEMENTS CONNECTIONS SINKS
TUBE_VOLUME NUM_TUBE TUBES_DAMAGED VOID COMP CONN
end

%
% Calculate the volume of all elements. The first element is always
the
% canister itself.
%
% Define Number of Nuclides, Number of Connections, Number of Sinks
and
% Number of Elements
NoN=length(HALFLIFE);
NoC=size(CONNECTIONS,2);
NoS=size(SINKS,2)+NoAS;
NoE=size(ELEMENTS,2);
A=zeros(NoN*(NoE-2),NoN*(NoE-2));
B=zeros(NoN*(NoE-2),NoN);
```

```
switch OUTCONC
    case 'off'
        C=zeros((NoS+1)*NoN,NoN*(NoE-2));
        D=zeros((NoS+1)*NoN,NoN);
    otherwise
        % If the concentration is sent as output it is necessary to
rescale the D matrix
        C=zeros((NoS+1)*NoN+(NoN*(NoE-2)),NoN*(NoE-2));
        D=zeros((NoS+1)*NoN+(NoN*(NoE-2)),NoN);
end
CB=zeros(size(ELEMENTS,2),NoN);

XLAMBDA=log(2)./HALFLIFE;



VOLUME(1)=VOID+TUBES_DAMAGED*TUBE_VOLUME;
for a=2:size(ELEMENTS,2)
    VOLUME(a)=ELEMENTS(a).DZ*ELEMENTS(a).AZ ;
end

%
% Calculate the capacity of all elements for each nuclide
%
for NUCL=1:NoN
    for a=1:NoE
        CAPACITY(a,NUCL)=VOLUME(a)*(EPS(ELEMENTS(a).MATERIAL,NUCL)+(1-
EPS(ELEMENTS(a).MATERIAL,NUCL))*KD(ELEMENTS(a).MATERIAL,NUCL)*RHO(ELEM
ENTS(a).MATERIAL));
    end
end

%
% Set up the resistivity matrix
%
for NUCL=1:NoN

    % Based on the connection definition set up the RESC matrix
    % For COMP23, the corresponding definition is performed in the
FMCO23 and in the FMMA23
    % subroutines

    %Note that the resistance between element 1-2 and 2-3 are treated
    %explicitly in the simulink sheet
    for a=1:NoC
        %All elements
        if CONNECTIONS(a).FROMRESISTANCE
            switch CONNECTIONS(a).FROMDIRECTION
                case 'X'
                    RA=ELEMENTS(CONNECTIONS(a).FROM).DX/
ELEMENTS(CONNECTIONS(a).FROM).AX/DE(ELEMENTS(CONNECTIONS(a).FROM).
MATERIAL,NUCL)/2;
                case 'Y'
                    RA=ELEMENTS(CONNECTIONS(a).FROM).DY/
ELEMENTS(CONNECTIONS(a).FROM).AY/DE(ELEMENTS(CONNECTIONS(a).FROM).
MATERIAL,NUCL)/2;
```

```
                case 'Z'
                    RA=ELEMENTS(CONNECTIONS(a).FROM).DZ/
ELEMENTS(CONNECTIONS(a).FROM).AZ/DE(ELEMENTS(CONNECTIONS(a).FROM).
MATERIAL,NUCL)/2;
            end
        else
            RA=0;
        end
        if CONNECTIONS(a).TORESISTANCE
            switch CONNECTIONS(a).TODIRECTION
                case 'X'
                    RB=ELEMENTS(CONNECTIONS(a).TO).DX/
ELEMENTS(CONNECTIONS(a).TO).AX/DE(ELEMENTS(CONNECTIONS(a).TO).
MATERIAL,NUCL)/2;
                case 'Y'
                    RB=ELEMENTS(CONNECTIONS(a).TO).DY/
ELEMENTS(CONNECTIONS(a).TO).AY/DE(ELEMENTS(CONNECTIONS(a).TO).
MATERIAL,NUCL)/2;
                case 'Z'
                    RB=ELEMENTS(CONNECTIONS(a).TO).DZ/
ELEMENTS(CONNECTIONS(a).TO).AZ/DE(ELEMENTS(CONNECTIONS(a).TO).
MATERIAL,NUCL)/2;
            end
        else
            RB=0;
        end
        RESC(CONNECTIONS(a).FROM,CONNECTIONS(a).TO,NUCL)=RA+RB;


    end

end



% for NUCL=1:NoN
%     for a=1:NoC
%         %Define the system matrix AG corresponds to GMAS23
%         %This is done for the different connections, hence
connections
%         %between element 1 & 2 may be includes (due to an arbitrary
order
%         %of the connection definition)
%         %Define the system matrix AG corresponds to GMAS23
%         AG(CONNECTIONS(a).FROM,CONNECTIONS(a).
TO,NUCL)=1/RESC(CONNECTIONS(a).FROM,CONNECTIONS(a).TO,NUCL)/
CAPACITY(CONNECTIONS(a).FROM,NUCL);
%         AG(CONNECTIONS(a).TO,CONNECTIONS(a).FROM,NUCL)=1/
RESC(CONNECTIONS(a).FROM,CONNECTIONS(a).TO,NUCL)/
CAPACITY(CONNECTIONS(a).TO,NUCL);
%     end
% end

% Explicit treatment for connections between 1-2 and 2-3

%
```

```
% Set up data for the inlet plug models. The second element is always
the
% hole (canister defect).
%
%From element 1-2
if CONNECTIONS(CONN(1,2)).FROMRESISTANCE

    switch CONNECTIONS(CONN(1,2)).FROMDIRECTION
        case 'X'
            LENGTH1=ELEMENTS(1).DX;
            AREA1=ELEMENTS(1).AX;
        case 'Y'
            LENGTH1=ELEMENTS(1).DY;
            AREA1=ELEMENTS(1).AY;
        case 'Z'
            LENGTH1=ELEMENTS(1).DZ;
            AREA1=ELEMENTS(1).AZ;
    end

else
    AREA1=1;
    LENGTH1=0;
end

if CONNECTIONS(CONN(1,2)).TORESISTANCE
    switch CONNECTIONS(CONN(1,2)).TODIRECTION
        case 'X'
            LENGTH2=ELEMENTS(2).DX/2;
        case 'Y'
            LENGTH2=ELEMENTS(2).DY/2;
        case 'Z'
            LENGTH2=ELEMENTS(2).DZ/2;
    end
else
    LENGTH2=0;
end

%From element 2-3
if CONNECTIONS(CONN(2,3)).FROMRESISTANCE
    switch CONNECTIONS(CONN(2,3)).FROMDIRECTION
        case 'X'
            LENGTH2=LENGTH2+ELEMENTS(2).DX/2;
            % AREA2 is the hole
        case 'Y'
            LENGTH2=LENGTH2+ELEMENTS(2).DY/2;
        case 'Z'
            LENGTH2=LENGTH2+ELEMENTS(2).DZ/2;
    end
else
    LENGTH2=LENGTH2+0;
end

if CONNECTIONS(CONN(2,3)).TORESISTANCE
    switch CONNECTIONS(CONN(2,3)).TODIRECTION
        case 'X'
            LENGTH3=ELEMENTS(3).DX;
```

```
            AREA3=ELEMENTS(3).AX;
        case 'Y'
            LENGTH3=ELEMENTS(3).DY;
            AREA3=ELEMENTS(3).AY;
        case 'Z'
            LENGTH3=ELEMENTS(3).DZ;
            AREA3=ELEMENTS(3).AZ;

    end
else
    AREA3=1;
    LENGTH3=0;
end

if CONNECTIONS(CONN(2,3)).PLUGPOSITION
    switch CONNECTIONS(CONN(2,3)).PLUGPOSITION
        case 'NONE'
            PLUG23=0;
        case 'TO_BLOCK'
            PLUG23=1;
        case 'FROM_BLOCK'
            disp('Plug position: FROM_BLOCK not implemented for the
canister defect')

    end
else
    disp('No Plug defined between canister defect and exteriour,
assume no plug (likely to be very conservative')
    PLUG23=0;
end




%
% Now we must define calculate sink data for all nuclides and all
sinks
% This is where the A, B, C and D matrices of the state-space blocks
are defined
%
%
%Define sinks
%
for NUCL=1:NoN

    for a=1:NoS-NoAS
        %QEQ according to READ23
        %QEQ=QEQFAC(a)*sqrt(sum(U.^2)).^QEQEXP(a);
        RSB1=0;
        RSB2=0;
        switch SINKS(a).DIRECTION
            case 'X'
                RSB1=SINKS(a).PLUGATINLET*ELEMENTS(SINKS(a).
FROM).DX/ELEMENTS(SINKS(a).FROM).AX/DE(ELEMENTS(SINKS(a).FROM).
MATERIAL,NUCL)/2;
            case 'Y'
```

```
                RSB1=SINKS(a).PLUGATINLET*ELEMENTS(SINKS(a).
FROM).DY/ELEMENTS(SINKS(a).FROM).AY/DE(ELEMENTS(SINKS(a).FROM).
MATERIAL,NUCL)/2;
            case 'Z'
                RSB1=SINKS(a).PLUGATINLET*ELEMENTS(SINKS(a).
FROM).DZ/ELEMENTS(SINKS(a).FROM).AZ/DE(ELEMENTS(SINKS(a).FROM).
MATERIAL,NUCL)/2;
        end
        %Definition of QEW READ23
        QEW=1/(PLUGLENGTH(a)/PLUGAREA(a)/DE(ELEMENTS(SINKS(a).FROM).
MATERIAL,NUCL)+1/QEQ(a));
        RSB2 = 1.0D0/QEW;
        CB(SINKS(a).FROM,NUCL)=1/(RSB1+RSB2)/CAPACITY(SINKS(a).
FROM,NUCL);
        % Set the matrix element of C related to this sink
        %
        C((NUCL-1)*NoS+a,(NoE-2)*(NUCL-1)+SINKS(a).FROM-
2)=1/(RSB1+RSB2);
    end
end



for NUCL=1:NoN




    %
    % Set submatrices of A related to nuclide for all elements
    %

    for a=1:NoC

        %Define the system matrix A
        %This is done for the different connections, hence connections
        %between element 1 & 2 may be includes (due to an arbitrary
order
        %of the connection definition)
        if ~((CONNECTIONS(a).FROM==1) | (CONNECTIONS(a).FROM==2))

            A(CONNECTIONS(a).FROM-2+(NoE-2)*(NUCL-1),CONNECTIONS(a).
TO-2+(NoE-2)*(NUCL-1))  =A(CONNECTIONS(a).FROM-2+(NoE-2)*(NUCL-
1),CONNECTIONS(a).TO-2+(NoE-2)*(NUCL-1))  +1/RESC(CONNECTIONS(a).
FROM,CONNECTIONS(a).TO,NUCL)/CAPACITY(CONNECTIONS(a).FROM,NUCL);
            A(CONNECTIONS(a).FROM-2+(NoE-2)*(NUCL-1),CONNECTIONS(a).
FROM-2+(NoE-2)*(NUCL-1))=A(CONNECTIONS(a).FROM-2+(NoE-2)*(NUCL-
1),CONNECTIONS(a).FROM-2+(NoE-2)*(NUCL-1))-1/RESC(CONNECTIONS(a).
FROM,CONNECTIONS(a).TO,NUCL)/CAPACITY(CONNECTIONS(a).FROM,NUCL);

            A(CONNECTIONS(a).TO-2+(NoE-2)*(NUCL-1),CONNECTIONS(a).
FROM-2+(NoE-2)*(NUCL-1))=A(CONNECTIONS(a).TO-2+(NoE-2)*(NUCL-
1),CONNECTIONS(a).FROM-2+(NoE-2)*(NUCL-1))+1/RESC(CONNECTIONS(a).
FROM,CONNECTIONS(a).TO,NUCL)/CAPACITY(CONNECTIONS(a).TO,NUCL);
            A(CONNECTIONS(a).TO-2+(NoE-2)*(NUCL-1),CONNECTIONS(a).
TO-2+(NoE-2)*(NUCL-1))=  A(CONNECTIONS(a).TO-2+(NoE-2)*(NUCL-
```

```
1),CONNECTIONS(a).TO-2+(NoE-2)*(NUCL-1))  -1/RESC(CONNECTIONS(a).
FROM,CONNECTIONS(a).TO,NUCL)/CAPACITY(CONNECTIONS(a).TO,NUCL);

        end
    end

    %
    %Define the diagonal (GMAS23)
    %
    for a=3:NoE
        A(a-2+(NoE-2)*(NUCL-1),a-2+(NoE-2)*(NUCL-1))=A(a-2+(NoE-
2)*(NUCL-1),a-2+(NoE-2)*(NUCL-1))-CB(a,NUCL)-XLAMBDA(NUCL);
    end


    %Assume inflow to element #3 (#1 canister & #2 defect) for each
nuclide
    B(1+(NoE-2)*(NUCL-1),NUCL)=1/CAPACITY(3,NUCL);

    %
    % Set the matrix element of C related to the concentration in the
first
    % element for nuclide NUCL
    %
    C(NoN*NoS+NUCL,1+(NoE-2)*(NUCL-1))=1;

    if ~strcmp(OUTCONC,'No')
        for a=3:NoE
            switch OUTCONC
                case 'off'
                    %No special operation for this case (the keyword
no is
                    %included to prevent the error message for case
                    %otherwise
                case 'Concentration pore water (mole/m3)'
                    C(NoN*(NoS+1)+(NoE-2)*(NUCL-1)+a-2,(NoE-2)*(NUCL-
1)+a-2)=1;
                case 'Concentration sorbed (mole/kg)'
                    C(NoN*(NoS+1)+(NoE-2)*(NUCL-1)+a-2,(NoE-2)*(NUCL-
1)+a-2)=KD(ELEMENTS(a).MATERIAL,NUCL);
                case 'Amount (mole)'
                    C(NoN*(NoS+1)+(NoE-2)*(NUCL-1)+a-2,(NoE-2)*(NUCL-
1)+a-2)=VOLUME(a)*(EPS(ELEMENTS(a).MATERIAL,NUCL)+(1-EPS(ELEMENTS(a).
MATERIAL,NUCL))*KD(ELEMENTS(a).MATERIAL,NUCL)*RHO(ELEMENTS(a).
MATERIAL));
                case 'Amount sorbed (mole)'
                    C(NoN*(NoS+1)+(NoE-2)*(NUCL-1)+a-2,(NoE-2)*(NUCL-
1)+a-2)=VOLUME(a)*(1-EPS(ELEMENTS(a).MATERIAL,NUCL))*KD(ELEMENTS(a).
MATERIAL,NUCL)*RHO(ELEMENTS(a).MATERIAL);
                case 'Amount solution (mole)'
                    C(NoN*(NoS+1)+(NoE-2)*(NUCL-1)+a-2,(NoE-2)*(NUCL-
1)+a-2)=VOLUME(a)*EPS(ELEMENTS(a).MATERIAL,NUCL);
                otherwise
                    error([OUTCONC ' unknown'])
            end
        end
```

```
    end

    %Add ingrowth to the A matrix
    %Nuclides with ingrowth to NUCL will be stored in MNUCL
    MNUCL=find(CHAIN(NUCL,:));



    for L=MNUCL
        %Loop over MNUCL
        %disp([num2str(L) '->' num2str(NUCL)])
        for a=1:NoE-2
            A((NoE-2)*(NUCL-1)+a,(NoE-2)*(L-1)+a)=A((NoE-2)*(NUCL-
1)+a,(NoE-2)*(L-1)+a)+XLAMBDA(L)*CAPACITY(a+2,L)/CAPACITY(a+2,NUCL)*CH
AIN(NUCL,L);
        end
    end




end



MATERIAL1=ELEMENTS(1).MATERIAL;
MATERIAL2=ELEMENTS(2).MATERIAL;
MATERIAL3=ELEMENTS(3).MATERIAL;

if DEBUG
    disp('COMP23 notation                          COMPULINK notation')
    disp('Compartment   Subcompartment          Element      Material')
    disp(['          1                 1           Void      '    MATE
RIALS(ELEMENTS(COMP(1,1)).MATERIAL).NAME ])
    disp(['          2                 1           Hole      '    MATE
RIALS(ELEMENTS(COMP(1,1)).MATERIAL).NAME])

    for a=3:size(COMP,1)

        for b=1:length(find(COMP(a,:)))
            disp(sprintf('%11d %16d %16d %16s', [a b COMP(a,b)-2
MATERIALS(ELEMENTS(COMP(a,b)).MATERIAL).NAME]))
        end
    end


    disp('Properties of the compartments')
    disp('   I     VOL         dz          dy          dx       AREAZ
AREAY      AREAX')
    disp(sprintf('VOID %11.4e %11.4e %11.4e %11.4e %11.4e %11.4e
%11.4e %11.4e %11.4e %11.4e %11.4e %11.4e %11.4e', [VOLUME(1) ELEMENTS(1).
DZ ELEMENTS(1).DY ELEMENTS(1).DX ELEMENTS(1).AZ ELEMENTS(1).AY
ELEMENTS(1).AX]))

    disp(sprintf('HOLE %11.4e %11.4e %11.4e %11.4e %11.4e %11.4e
%11.4e %11.4e %11.4e %11.4e %11.4e %11.4e %11.4e', [VOLUME(2) ELEMENTS(2).
```

```
DZ ELEMENTS(2).DY ELEMENTS(2).DX ELEMENTS(2).AZ ELEMENTS(2).AY
ELEMENTS(2).AX]))

    for a=3:NoE
        disp(sprintf('%4d %11.4e %11.4e %11.4e %11.4e %11.4e
%11.4e %11.4e %11.4e %11.4e %11.4e %11.4e %11.4e %11.4e', [a-2 VOLUME(a)
ELEMENTS(a).DZ ELEMENTS(a).DY ELEMENTS(a).DX ELEMENTS(a).AZ
ELEMENTS(a).AY ELEMENTS(a).AX]))

    end

    for NUCL=1:NoN
        disp(num2str(NUCL))
        disp('   I   CAPACITY     RZ          RY          RX')
        disp(sprintf('VOID %11.4e %11.4e %11.4e %11.4e',
[CAPACITY(1,NUCL) ELEMENTS(1).DZ/ELEMENTS(1).AZ/DE(ELEMENTS(1).
MATERIAL,NUCL) ELEMENTS(1).DY/ELEMENTS(1).AY/DE(ELEMENTS(1).
MATERIAL,NUCL) ELEMENTS(1).DX/ELEMENTS(1).AX/DE(ELEMENTS(1).
MATERIAL,NUCL)]))
        disp(sprintf('HOLE %11.4e %11.4e %11.4e %11.4e',
[CAPACITY(2,NUCL) ELEMENTS(2).DZ/ELEMENTS(2).AZ/DE(ELEMENTS(2).
MATERIAL,NUCL) ELEMENTS(2).DY/ELEMENTS(2).AY/DE(ELEMENTS(2).
MATERIAL,NUCL) ELEMENTS(2).DX/ELEMENTS(2).AX/DE(ELEMENTS(2).
MATERIAL,NUCL)]))

        for a=3:NoE
            disp(sprintf('%4d %11.4e %11.4e %11.4e %11.4e', [a-
2 CAPACITY(a,NUCL) ELEMENTS(a).DZ/ELEMENTS(a).AZ/DE(ELEMENTS(a).
MATERIAL,NUCL) ELEMENTS(a).DY/ELEMENTS(a).AY/DE(ELEMENTS(a).
MATERIAL,NUCL) ELEMENTS(a).DX/ELEMENTS(a).AX/DE(ELEMENTS(a).
MATERIAL,NUCL)]))
        end
        disp('  I    J   RESISTANCE')
        [dummy,b]=sort([CONNECTIONS.FROM]);
        for a=b
            disp(strrep(strrep(sprintf('%4d %4d
%11.4e',[CONNECTIONS(a).FROM-2 CONNECTIONS(a).TO-2 RESC(CONNECTIONS(a).
FROM,CONNECTIONS(a).TO,NUCL)]),'  -1','VOID'),'   0','HOLE'))
        end


    end

    for a=1:NoS-NoAS
        disp(['Sink: ' num2str(a) ' From element:' num2str(SINKS(a).
FROM)])

    end

end

if DEBUG
    save Transport.mat A B C RESC VOLUME CAPACITY
end

if ~isempty(DARCYVELOCITY) & ~isempty(ADVECTIVEELEMENTS)
```

```
    U=DARCYVELOCITY;

    %
    % Make a sanity check of ADVECTIVEELEMENTS
    %
    P=max(ADVECTIVEELEMENTS);
    if P+2 > length(ELEMENTS)
        error 'Error in ADVECTIVEELEMENTS! Element number exceeds
number of elements in the model.'
    end
    P=min(ADVECTIVEELEMENTS);
    if P+2 < 3
        error 'Error in ADVECTIVEELEMENTS! Only transport element may
be advective.'
    end

    %
    % Calculate the flow in all advective elements, taking area
changes
    % into account so that mass continuity is maintained.
    %
    advectiveflow=zeros(size(ELEMENTS));
    for i=1:length(ADVECTIVEELEMENTS)-1

        element1=ADVECTIVEELEMENTS(i);
        element2=ADVECTIVEELEMENTS(i+1);
        %
        % Find the connection between these elements, and then the
flow
        % direction and area. Check for errors in the definition.
        % Rememer that CONN and ELEMENTS are numbered according to the
COMP23 element definition where
        % the canister and the defect are numbered as 1 and 2, hence
the
        % elements in numbered using the COMPULINK numbering system
must be
        % added
        currconn=CONN(element1+2,element2+2);
        if currconn == 0
            error 'Error in ADVECTIVEELEMENTS. Connection missing.'
        end

        flowdir=CONNECTIONS(currconn).FROMDIRECTION;
        switch flowdir
            case 'X'
                flowarea=ELEMENTS(element1+2).AX;
            case 'Y'
                flowarea=ELEMENTS(element1+2).AY;
            case 'Z'
                flowarea=ELEMENTS(element1+2).AZ;
            otherwise
                error 'Error in direction for advective flow.'
        end
        %
        % If this is the first advective element we set the reference
mass
```

```
        % flow, which should be kept constant through the model.
        %
        if i == 1
            referenceflow=U*flowarea;
        elseif U*flowarea ~= referenceflow
            disp 'Warning: The cross section area varies along the
flow path.'
        end
        advectiveflow(element1)=referenceflow;
        advectiveflow(element2)=referenceflow;
    end

    for NUCL=1:NoN
        %Advective elements are given in element notation not
        %compartment/sumcompartment
        for i=1:length(ADVECTIVEELEMENTS)
            %Upwind differencing scheme
            if i == 1
                %First advective element
                %Assume no advective inflow to the first advective
element, only outflow
                P=ADVECTIVEELEMENTS(i);
                A(P+(NoE-2)*(NUCL-1),P+(NoE-2)*(NUCL-1))=A(P+(NoE-
2)*(NUCL-1),P+(NoE-2)*(NUCL-1))-advectiveflow(P)/CAPACITY(P+2,NUCL);
            else
                %Internal advective elements, assume advective inflow
and
                %outflow
                W=ADVECTIVEELEMENTS(i-1);
                P=ADVECTIVEELEMENTS(i);
                A(P+(NoE-2)*(NUCL-1),P+(NoE-2)*(NUCL-1))=A(P+(NoE-
2)*(NUCL-1),P+(NoE-2)*(NUCL-1))-advectiveflow(P)/CAPACITY(P+2,NUCL);
                A(P+(NoE-2)*(NUCL-1),W+(NoE-2)*(NUCL-1))=A(P+(NoE-
2)*(NUCL-1),W+(NoE-2)*(NUCL-1))+advectiveflow(P)/CAPACITY(P+2,NUCL);
            end
        end
        % Outflow is calculated, and output in the only advective sink
        P=ADVECTIVEELEMENTS(length(ADVECTIVEELEMENTS));
        C((NUCL-1)*NoS+NoS,P+(NoE-2)*(NUCL-1))=C((NUCL-
1)*NoS+NoS,P+(NoE-2)*(NUCL-1))+advectiveflow(P);
    end
end


%
% end of function DefineComp
%
if DEBUG
    save A.mat A
end
```

Appendix D

Numerical method

D.1 Discretisation

The geometric model is based on a network model for the diffusion through the bentonite and backfill. A network of discrete transport pathways (also called blocks) is defined, and each pathway is discretized using linear finite differences. The model has no sense of directions, although the geometry can be specified in terms of global Cartesian coordinates in the geometry definition file.

D.1.1 Nuclide diffusion without decay

In the Simulink model all material transport is by diffusion, and all elements can have arbitrary dimensions but in the example below only 1-D diffusion is considered.

Start with the diffusion equation for a sorbing material

$$R^i \frac{\partial C_f{}^i}{\partial t} = D_e \frac{\partial^2 C_f{}^i}{\partial x^2}$$

where

$R^i = \varepsilon + (1-\varepsilon)Kd\rho$

is called the retardation coefficient for nuclide i. Rewrite and integrate over an arbitrary volume dV

$$\frac{\partial c}{\partial t} = \frac{D_e}{R^i} \nabla^2 C_f{}^i$$

$$\int \frac{\partial c}{\partial t} dV = \frac{D_e}{R^i} \oint \nabla C_f{}^i \cdot \hat{n} dS$$

1D diffusion in the east-west direction yields

$$\frac{\partial c}{\partial t} \Delta x_P \Delta y_P = \Delta y_P \frac{D_e}{R} \left(\left. \frac{\partial c}{\partial x} \right|_e - \left. \frac{\partial c}{\partial x} \right|_w \right)$$

Use a central differencing scheme to estimate the differentials

$$\left. \frac{\partial c}{\partial x} \right|_e = \frac{c_e - c_P}{\left(\frac{\Delta x_P + \Delta x_E}{2} \right)}$$

$$\left. \frac{\partial c}{\partial x} \right|_w = \frac{c_P - c_W}{\left(\frac{\Delta x_P + \Delta x_W}{2} \right)}$$

and write the system of equations, so that

$$\frac{\partial}{\partial t} \begin{Bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n-1} \\ c_n \end{Bmatrix} = \begin{bmatrix} A_P & A_E & & & \\ A_W & A_P & A_E & & \\ & \ddots & \ddots & \ddots & \\ & & A_W & A_P & A_E \\ & & & A_W & A_P \end{bmatrix} \begin{Bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{n-1} \\ c_n \end{Bmatrix}$$

with the coefficients

$$A_P = -\frac{D_e}{R}\frac{1}{\Delta x_P}\left(\frac{2}{\Delta x_P + \Delta x_E} + \frac{2}{\Delta x_P + \Delta x_W}\right)$$

$$A_E = \frac{D_e}{R}\frac{1}{\Delta x_P}\frac{2}{\Delta x_P + \Delta x_E}$$

$$A_W = \frac{D_e}{R}\frac{1}{\Delta x_P}\frac{2}{\Delta x_P + \Delta x_W}$$

Inflow boundary, Neumann BC, is given by

$$\left.\frac{\partial c}{\partial x}\right|_e = In$$

$$A_P = -\frac{D_e}{R}\frac{1}{\Delta x_P}\left(\frac{2}{\Delta x_P + \Delta x_E}\right)$$

$$A_W = \frac{D_e}{R}\frac{1}{\Delta x_P}\frac{2}{\Delta x_P + \Delta x_W}$$

$$B(1) = \frac{D_e}{R}\frac{1}{\Delta x_P}In$$

Inflow boundary, Dirichlet BC, is given by

$$\left.\frac{\partial c}{\partial x}\right|_e \approx \frac{c_P - c|_e}{\frac{\Delta x_P}{2}}$$

$$A_P = -\frac{D_e}{R}\frac{1}{\Delta x_P}\left(\frac{2}{\Delta x_P + \Delta x_E} + \frac{2}{\Delta x_P}\right)$$

$$A_W = \frac{D_e}{R}\frac{1}{\Delta x_P}\frac{2}{\Delta x_P + \Delta x_W}$$

$$B(1) = \frac{2c|_e}{\Delta x_P}\frac{D_e}{R}\frac{1}{\Delta x_P}$$

Outflow boundary, free BC, is given by

$$\left.\frac{\partial c}{\partial x}\right|_e = \left.\frac{\partial c}{\partial x}\right|_w + \frac{\left.\frac{\partial c}{\partial x}\right|_w - \left.\frac{\partial c}{\partial x}\right|_{ww}}{\Delta x_W}\Delta x_P = \left(1 + \frac{\Delta x_P}{\Delta x_W}\right)\left.\frac{\partial c}{\partial x}\right|_w - \frac{\Delta x_P}{\Delta x_W}\left.\frac{\partial c}{\partial x}\right|_{ww}$$

$$\frac{\partial c}{\partial t}\Delta x_P \Delta y_P = \Delta y_P \frac{D_e}{R}\frac{\Delta x_P}{\Delta x_W}\left(\left.\frac{\partial c}{\partial x}\right|_w - \left.\frac{\partial c}{\partial x}\right|_{ww}\right)$$

$$A_P = \frac{D_e}{R}\frac{1}{\Delta x_P}\frac{\Delta x_P}{\Delta x_W}\left(\frac{2}{\Delta x_P + \Delta x_W}\right)$$

$$A_W = -\frac{D_e}{R}\frac{1}{\Delta x_P}\frac{\Delta x_P}{\Delta x_W}\left(\frac{2}{\Delta x_P + \Delta x_W} + \frac{2}{\Delta x_W + \Delta x_{WW}}\right)$$

$$A_{WW} = \frac{D_e}{R}\frac{1}{\Delta x_P}\frac{\Delta x_P}{\Delta x_W}\left(\frac{2}{\Delta x_W + \Delta x_{WW}}\right)$$

$$B(1) = \frac{2c|_e}{\Delta x_P}\frac{D_e}{R}\frac{1}{\Delta x_P}$$

D.1.2 Using concentration or amount

One has to be careful about the use of concentration or amount for representing the nuclide content of an element

$$V_i K_i^{\,n} \frac{dc_i^{\,n}}{dt} = q_d + V_i K_i^{\,n-1} c_i^{\,n-1} \lambda^{n-1} - V_i K_i^{\,n} c_i^{\,n} \lambda^n - \sum_j \left(\frac{AD_e}{d} \Delta c \right)_{i,j}^n$$

$$\frac{dc_i^{\,n}}{dt} = \frac{q_d}{V_i K_i^{\,n}} + \frac{K_i^{\,n-1}}{K_i^{\,n}} c_i^{\,n-1} \lambda^{n-1} - c_i^{\,n} \lambda^n - \sum_j \left(\frac{\Delta c}{R V_i K_i^{\,n}} \right)_{i,j}^n$$

Note: If the intention is to solve for concentration, an influx must be divided with *VK*.

$$\frac{dM_i^{\,n}}{dt} = q_d + M_i^{\,n-1} \lambda^{n-1} - M_i^{\,n} \lambda^n - \sum_j \left(\frac{AD_e}{d} \Delta c \right)_{i,j}^n$$

$$\frac{dM_i^{\,n}}{dt} = q_d + M_i^{\,n-1} \lambda^{n-1} - M_i^{\,n} \lambda^n - \sum_j \left(\frac{\Delta c}{R} \right)_{i,j}^n$$

$$\begin{Bmatrix} \frac{dM_1^{\,n}}{dt} \\ \frac{dM_2^{\,n}}{dt} \\ \\ \frac{dM_{n-1}^{\,n}}{dt} \\ \frac{dM_n^{\,n}}{dt} \end{Bmatrix} = \begin{bmatrix} -\frac{1}{CR} - \lambda^n & \frac{1}{CR} & & & \\ \frac{1}{CR} & -\frac{2}{CR} - \lambda^n & \frac{1}{CR} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{CR} & -\frac{2}{CR} - \lambda^n & \frac{1}{CR} \\ & & & \frac{1}{CR} & -\frac{1}{CR} - \lambda^n \end{bmatrix} \begin{Bmatrix} M_1^{\,n} \\ M_2^{\,n} \\ \\ M_{n-1}^{\,n} \\ M_n^{\,n} \end{Bmatrix} + \begin{Bmatrix} \dot{x}_{in} + M_1^{\,n-1} \lambda^{n-1} \\ M_2^{\,n-1} \lambda^{n-1} \\ \\ M_{n-1}^{\,n-1} \lambda^{n-1} \\ M_n^{\,n-1} \lambda^{n-1} - \dot{x}_{out} \end{Bmatrix}$$

This system of equations can also be represented by a state-space component in Simulink, that is a component solving following system of equations

$$\frac{dx}{dt} = Ax + Bu$$

$$y = Cx + Du$$

where u is called the input vector, x the state vector and y the output vector.

D.1.3 Outflow from the bentonite

An equivalent flow rate is calculated (in a corresponding way as in the COMP23 function READ23) from the equations

$$Q_{eq} = Q_{fac}\, U_0^{\mathrm{Qexp}}$$

$$Q_{ew} = \frac{1}{\frac{1}{Q_{eq}} + \frac{L_{frac}}{A_{frac} D_e}}$$

with a transport resistance for the outflow represented by

$$R = \frac{1}{Q_{eq}} + \frac{L_{frac}}{A_{frac} D_e} + \frac{Element}{2}$$

and

$$Q_{out} = \frac{1}{\frac{1}{Q_{eq}} + \frac{L_{frac}}{A_{frac} D_e} + \frac{Element}{2}}$$

The model described above is called a sink in COMP23. An arbitrary number of sinks can be connected to the bentonite diffusion network.

Appendix E

Advective transport

In the assessment project SR-Can, hydraulic simulations was used to generate the data for the Compulink simulation /Hartley et al. 2006ab, SKB 2006b/. In these simulations, particle tracking of advectively transported particles were performed for particles released in a fracture intersecting the deposition hole (Q1), the EDZ (Q2) and at a position above the deposition hole (Q3). The transport lengths and times in the tunnel for particles released over the canister were used to determine the advective flow rate in the deposition tunnel. In addition, the length from the canister to the fracture through which the particles leave the model was used to determine the longitudinal extension of the discretised tunnel.

Appendix F

Discretisation of the near field, SR-Can

The present section describes the geometrical discretisation used in the SR-Can assessment. The geometry is based on the SR 97 discretisation with two major exceptions:

- In SR 97, a fourth exit-path was used for diffusive transport through the rock matrix. The release through this exit-path was small and hence judged to be of no importance.
- In the SR-Can assessment, also advective flow through the backfill is included. Hence a sink through which matter may exit advectively must be added.

F.1 Geometry

The geometry used is shown in Figure F-1.

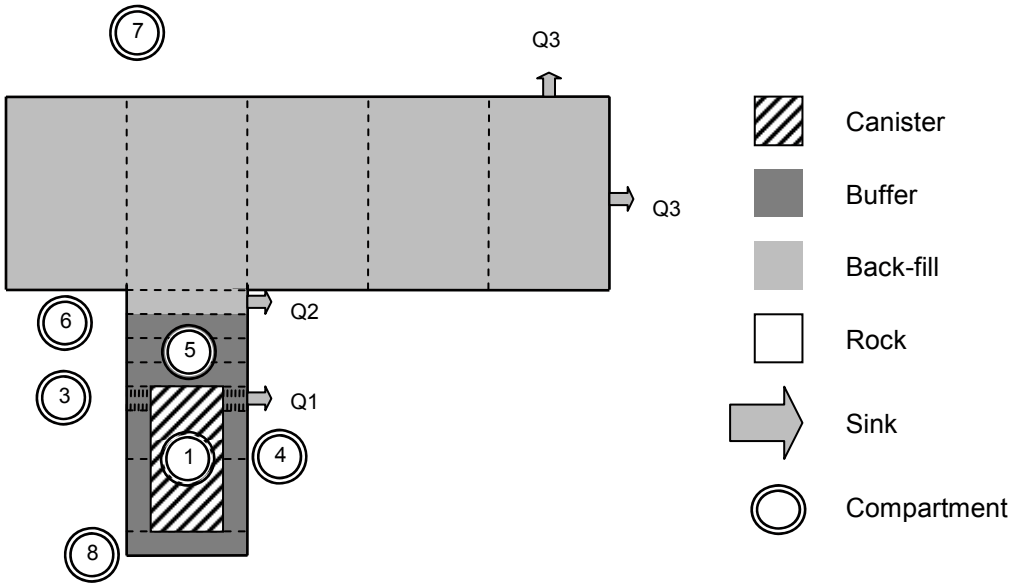

Figure F-1. *Discretisation of the near-field. Sink Q3 has two components, one advective and one diffusional (horisontal and vertical pointer respectively in figure). The deposition hole has a cylindrical symmetry.*

F.2 Compartments

Table F-1 and Table F-2 show the different compartments used in the analysis.

Table F-1. Compartments in the analysis, conceptual representation.

Compartment, number of sub-compartments		Description
1	–	Canister
2	–	Defect
3	6	Bentonite between defect and sink Q1.
4	2	Bentonite below Q1 sink
5	3	Bentonite above canister
6	–	Backfill above canister, connected to Q2 (EDZ).
7	Depending on distance to Q3	Tunnel, ending at Q3.
8	–	Bentonite below canister

Table F-2. Compartments used in the analysis, geometry.

Compartment	Sub-compartment	Dimensions			
1		Volume			
		1 m^3			
2					
3		$Length_z$	$Area_R$	R	
	1	0.5	0.203	0.058	1.741
	2	0.5	0.224	0.058	1.924
	3	0.5	0.246	0.058	2.107
	4	0.5	0.267	0.058	2.291
	5	0.5	0.289	0.058	2.474
	6	0.5	0.31	0.058	2.657
4		$Length_z$	$Area_z$		
	1	1	1.539		
	2	3.33	1.539		
5		$Length_z$	$Area_z$		
	1	0.5	2.405		
	2	0.5	2.405		
	3	0.5	2.405		
6		$Length_z$	$Area_z$	$Length_r$	$Area_r$
	1	1	2.405	1.75	5.5
7		$Length_z$	$Area_z$	$Length_r$	$Area_r$
	1	2.125	12.566	2	26.7
	2	1.75	12.566	2	22
	3..n[1]	2.125	12.566	2	26.7
8	–	$Length_z$	$Area_z$		
		0.5	2.405		

[1] Depending on length to Q3.

F.3 Connections

How the different compartments are connected is shown in Table F-3.

Table F-3. Connections between the different compartments, 2 downstream compartments are used in tunnel.

From compartment-subcompartment	To compartment-subcompartment	From direction	To direction
3-1	3-2	X	X
3-2	3-3	X	X
3-3	3-4	X	X
3-4	3-5	X	X
3-5	3-6	X	X
4-1	4-2	Z	Z
5-1	5-2	Z	Z
5-2	5-3	Z	Z
7-1	7-2	Z	Z
7-2	7-3	Z	Z
7-3	7-4	Z	Z
1-1	2-1	Z	Z
2-1	3-1	Z	X
3-1	4-1	Z	Z
3-2	4-1	Z	Z
3-3	4-1	Z	Z
3-4	4-1	Z	Z
3-5	4-1	Z	Z
3-6	4-1	Z	Z
3-1	5-1	Z	Z
3-2	5-1	Z	Z
3-3	5-1	Z	Z
3-4	5-1	Z	Z
3-5	5-1	Z	Z
3-6	5-1	Z	Z
4-2	8	Z	Z
5-3	6	Z	Z
6	7-2	Z	X

F.4 Plugs used in the analysis

In addition to the resistances used in the model, plug resistances are also uses, the values of the plug lengths and plug areas for the different exit paths are shown in Table F-4. If the effect of spalling is included in the analysis, the plugs are assumed to have no limiting effect on the transport resistance.

Table F-4. Plug lengths and plug areas used in the analysis.

	Plug length	Plug area
Q1	$5 \cdot 10^{-4}$/0*	$5.5 \cdot 10^{-4}$
Q2	0	1
Q3	0.002	0.006

* A plug length of 0 is used to create a negligible transport resistance for the Q1 plug in the case of having a spalled deposition hole (the Base case in the assessment calculations).