R-04-64

COMP23 version 1.2.2 user´s manual

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Contents

1 Overview of COMP23

COMP23 is a fast, multiple-path model that calculates nuclide transport in the near field of a repository as occurring through a network of resistances and capacitances coupled together like an electrical circuit network. The model, which is a coarsely discretized, integrated finite-difference model, was designed to be fast and compact by making use of analytical solutions in sensitive zones. The code allows the user to simultaneously consider many pathways for nuclides transport, by advection and diffusion, to the flowing water in fractures surrounding the barrier system.

The nuclide dissolution may be calculated using either a solubility-limited approach or a congruent-dissolution approach. The conceptual model used in COMP23 can be represented by three bodies as shown in Figure 1-1. The bodies are the source, the barrier system, and the sinks. The source is treated as a well-mixed compartment. The barrier system is the physical medium through which the nuclides migrate to reach the sinks located in the surrounding system, or outside of the region considered as the barrier system. The sinks, considered as recipients where the water flows, are fully defined by a local equivalent flow rate.

The purpose of this document is to assist the user in managing problems with COMP23. An overview of the theory, numerical method, and the code designed to solve the problem will be presented in the following sections. Finally, an example will be described in detail.

The current version of COMP23 has been extensively revised from earlier versions of the program. The earlier standalone version of the program was called NUCTRAN. A description of the earlier version of the program can be found in reference 1.

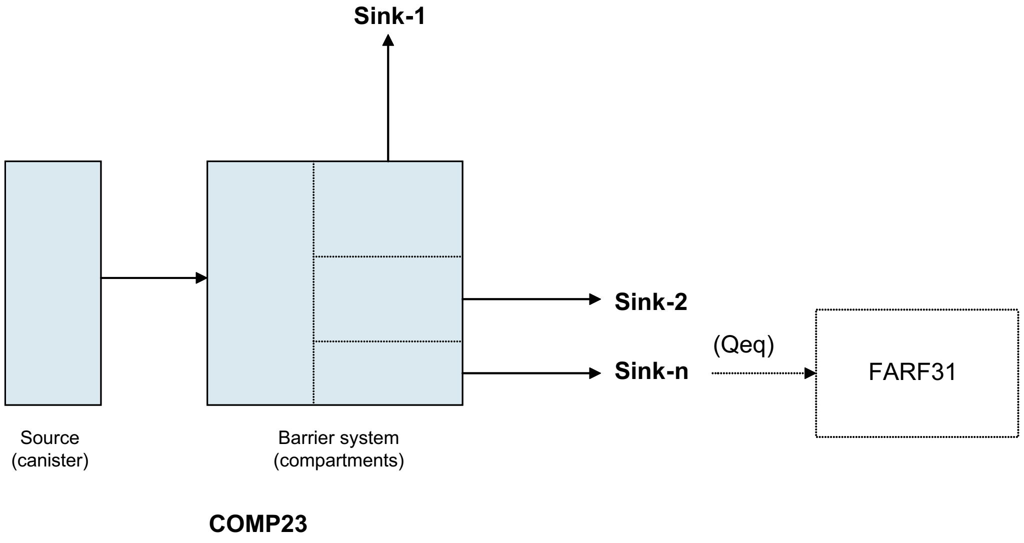


Figure 1-1. *A schematic of the conceptual model used by COMP23.*

2 Conceptual model

The presentation of the conceptual model used in COMP23 follows the definition given by Olsson et al. /2/: “a relatively general description or a definition of the way the model is constructed. This should be separated from any specific realization or application of the conceptual model.” The concepts that make up the conceptual model are: specification of the processes modelled, geometric framework, specification of the parameters, specification of the assignment of material properties and specification of boundary and initial conditions required by the model. Each of these concepts will be described for COMP23 in the following subsections.

2.1 Processes modelled

The processes modelled are radioactive decay and ingrowth, diffusion, advection, dissolution/precipitation and linear equilibrium sorption. Dissolution and precipitation are controlled either by a fixed solubility limit for each nuclide or by a solubility limit shared between nuclides in a solubility group.

The notation used for the equations described in this report is given in Appendix 1.

2.1.1 Radionuclide transport in the barrier

Radionuclides leaking from a damaged canister spread into the backfill material surrounding the canister and then migrate through different pathways into water-bearing fractures in the rock surrounding the repository. If the backfill and other materials surrounding the canister have a low permeability, the solute transport will be only by diffusion. If there is water flow through some zones of the barrier, then advection may also be a significant transport mechanism. Some solutes may be sorbed on the materials surrounding the canister along the transport paths and their migration will be retarded. Solutes may also precipitate. It is a basic assumption in the COMP23 model that the dissolution-precipitation reaction is very fast, so that, for nuclides that are solubility limited, the aqueous concentration will be at the solubility limit if there is any precipitate present. The COMP23 model allows groups of nuclides to share a solubility limit. For example, all the isotopes of a given element would be expected to share the same solubility limit.

The nuclides are labelled by consecutive integers, beginning with 1, in such a way that the parent of nuclide n, if it has one, is always nuclide n-1. Clearly nuclide 1 cannot have a parent. The fundamental equation expressing material balance for nuclide n is

$$\frac{\partial a^n}{\partial t} + \mathbf{u}_0 . \nabla c^n - \nabla \cdot D_e^n \nabla c^n = -\lambda_n a^n + \lambda_{n,.n-1} a^{n-1} \tag{1}$$

where a^n is the total amount (dissolved, sorbed and precipitated) of nuclide n per unit volume, c^n is the concentration of nuclide n in the pore water, $\mathbf{u_0}$ is the Darcy velocity, D_e^n is the effective diffusivity for nuclide n, λ_n is the decay constant for nuclide n and $\lambda_{n,n\text{-}1}$ is the decay constant for nuclide n-1 if nuclide n is the daughter of nuclide n-1 and zero if nuclide n does not have a parent. Note that the quantities a^n and c^n are functions of both position and time, and that $\mathbf{u_0}$ and D_e^n may also depend on position.

Equation (1) is to be regarded as an equation for a^n, and so c^n must be specified as a function of a^n. To do this, the assumption that the precipitation/dissolution reaction is very fast is used. Each nuclide is considered to belong to a solubility group. Normally, there will be one solubility group for each different element and a group will consist of all the nuclides that are isotopes of a particular element. Let S_E denote the solubility group for element E. Then S_E is the set of labels of the nuclides that are isotopes of element E. The total amount of element E per unit volume is denoted by a_E^T and it is clear that

$$a_E^T = \sum_{m \in S_E} a^m \tag{2}$$

The concentration c^n, where $n \in S_E$ (i.e. nuclide n is an isotope of element E), may now be related to a^n by:

$$c^n = \begin{cases} \dfrac{a^n}{K_E} & \text{if } a_E^T \le K_E c_E^S \\ \dfrac{c_E^S a^n}{a_E^T} & \text{if } a_E^T > K_E c_E^S \end{cases} \tag{3}$$

where K_E is a distribution coefficient for element E and c_E^S is the solubility limit for the solubility group, S_E, of element E. K_E is given by

$$K_E = \phi_E + (1 - \phi_E) k_E^d \rho \tag{4}$$

where ϕ_E is the porosity for element E, ρ is the density of the solid material and k_E^d is the sorption coefficient for element E. The amount of nuclide n per unit volume that is in solution is $\phi_E c^n$ and the amount that is sorbed is $(1-\phi_E)\, k_E^d\, \rho$, so that the total amount, dissolved and sorbed, per unit volume is $K_E c^n$. Note that the COMP23 model allows the porosity to depend on the element, so that effects such as anion exclusion can be treated.

Expression (3) may be derived in the following way. When the total amount of element E per unit volume, a_E^T, is less than the total amount that can be dissolved and sorbed per unit volume, $K_E c_E^S$, there will be no precipitate of any of the isotopes of E present because of the assumption that the precipitate dissolution reaction is fast. The amount of nuclide n present in solution and sorbed per unit volume will be $K_E c^n$, and this must be equal to the total amount of nuclide n present per unit volume so that:

$$K_E c^n = a^n \tag{5}$$

and the first part of equation (3) follows immediately.

When the total amount of element E per unit volume is greater than the total amount that can be dissolved and sorbed per unit volume, the aqueous concentration of E will be at the solubility limit, so that

$$\sum_{m \in S_E} c^m = c_E^S \tag{6}$$

When the system is in equilibrium, the relative proportions of the isotopes must be the same in the sorbed, dissolved and precipitated material. This means that

$$\frac{(1-\phi_E)k_E^d \rho c^n}{(1-\phi_E)k_E^d c_E^S} = \frac{\phi_E c^n}{\phi_E c_E^S} = \frac{a^n - K_E c^n}{a_E^T - K_E c_E^S} \tag{7}$$

Rearranging equation (7) gives the second part of equation (3). Note that it has been assumed that all the isotopes of E are chemically identical, so that they have the same distribution coefficient, K_E.

Parameters required

The parameters required are as follow:

- Solid density and porosity of the materials.
- Sorption coefficient and diffusivity of each radionuclide in each of the different materials.
- Solubility limit of each element in each of the different materials.
- Nuclide inventories and half lives.
- The groundwater flux.

2.1.2 Treatment of the source term

In the COMP23 model, the radionuclides in the canister may be present in three forms: in solution in the water in the canister; in the form of precipitate in the canister and embedded in the fuel matrix. It is assumed that there is no sorption in the canister and that the time taken for the nuclides to mix in the canister is very short, so that the concentration of the dissolved nuclides is uniform. It is also assumed that the volume of water in the canister is constant during the calculation. As the fuel matrix dissolves, the actual volume available for the water in the canister will increase, but since the rate of dissolution is slow, this volume change can be neglected.

COMP23 treats three types of situation:

I Solubility limited approach. All species in the canister are available for release, independently of the structure they are part of. The only limitation in the nuclide release is the solubility of the individual species.

II A particular case for nuclides initially located at the fuel surface. The handling of this situation is similar to I but only a fraction of the total nuclide inventory is available for release.

III Congruent approach for nuclides embedded in a fuel matrix. Since the matrix is mostly formed by uranium oxide, the release rate for the embedded nuclides depends on the rate at which the uranium fuel matrix is dissolving. Several models are available to treat the dissolution of the fuel matrix and the effects of alpha-radiolytically induced dissolution can be treated. These different models are described in Sections 2.1.4 and 2.1.5.

2.1.3 Source term – solubility limited

The model for cases I and II in Section 2.1.2 is essentially the same. Case I is referred to as SOL_TYPE OWNSOL and case II as SOL_TYPE FUELSURFACE. Since the dissolved nuclides in the canister are assumed to be well mixed, the amount of each nuclide in the canister is determined by a single quantity, $\hat{a}^n$, that represents the total amount of nuclide in the canister and that is a function of time. The equation for nuclide n is:

$$\frac{\partial \hat{a}^n}{\partial t} = -\lambda_n \hat{a}^n + \lambda_{n,n-1} \hat{a}^{n-1} - f^n \tag{8}$$

where f^n is the rate at which nuclide n leaves the canister by diffusion into the rest of the barrier system. If σ is the area of the canister that is breached, and so is in direct contact with the rest of the barrier system, then

$$f^n = -\int_\sigma D_e^n \mathbf{n}.\nabla c^n \tag{9}$$

where **n** is the outward pointing normal to σ, and c^n is the concentration of nuclide n in the barrier system outside the canister, as in the previous section. Again, equation (8) is to be regarded as an equation for $\hat{a}^n$. In order to determine f^n, and so complete equation (8), the concentration of nuclide n in the canister, $\hat{c}^n$, must be provided as a boundary condition on σ for the nuclide transport equation outside the canister. The relationship between $\hat{a}^n$ and $\hat{c}^n$, where nuclide n is an isotope of element E, is

$$\hat{c}^n = \begin{cases} \dfrac{\hat{a}^n}{V_C} & \text{if } \hat{a}_E^T \le V_C c_E^S \\ \dfrac{c_E^S \hat{a}^n}{\hat{a}_E^T} & \text{if } \hat{a}_E^T > V_C c_E^S \end{cases} \tag{10}$$

where V_C is the volume occupied by the water in the canister and $\hat{a}_E^T$ is the total amount of element E in the canister:

$$\hat{a}_E^T = \sum_{m \in S_E} \hat{a}^m \tag{11}$$

The derivation of equation (10) is similar to the derivation of equation (3).

Parameters required

The parameters required are as follow:

- Solubility limit of each element in the water in the canister.
- Volume of water in the canister.
- Nuclide inventories and half lives.

2.1.4 Source term – congruent release without alpha radiolysis

In case III in Section 2.1.2, which is referred to as SOL_TYPE MATRIX, the dissolution of the uranium fuel matrix, and the consequent liberation of the embedded nuclides, must be considered. In this case the quantity $\hat{a}^n$ represents the total amount of nuclide n that is in the canister, but is not embedded in the fuel matrix. In addition, it is necessary to keep track of the amount of nuclide embedded in the matrix, and this quantity is denoted by b^n. Note that both the $\hat{a}^n$ and b^n depend only on time. The equation for nuclide n becomes

$$\frac{\partial \hat{a}^n}{\partial t} = -\lambda_n \hat{a}^n + \lambda_{n,n-1} \hat{a}^{n-1} - f^n + q^n \tag{12}$$

where q^n is the rate at which nuclide n is being liberated from the fuel matrix, which is given, in terms of the rate at which the uranium matrix is dissolving, by

$$q^n = \frac{b^n}{b^M} q^M \tag{13}$$

where b^M is the amount of uranium 238 in the fuel matrix, and q^M is the rate of dissolution of the uranium 238. The basic assumption underlying equation (13) is that the nuclides are uniformly distributed within the fuel matrix, so that the ratio of the amount of nuclide n to the amount of matrix is uniform and equal to b^n/b^M. It is also assumed that all the nuclides embedded in the matrix are released when the matrix dissolves. Equation (13) follows immediately from these two assumptions.

The equation for the amount of nuclide n embedded in the matrix, b^n, is

$$\frac{\partial b^n}{\partial t} = -\lambda_n b^n + \lambda_{n,n-1} b^{n-1} - q^n \tag{14}$$

Equations (12–14) can be used to determine $\hat{a}^n$ and b^n only once q^M is known. In COMP23, the way q^M is determined depends on whether alpha radiolysis is modelled or not. The case without alpha radiolysis is considered in this section. The case with alpha radiolysis is treated in Section 2.1.5.

When alpha radioloysis is not included in the model, the rate of dissolution of the uranium matrix is determined by the solubility of the uranium in the canister. The model assumes that the rate at which the matrix dissolves is just fast enough to maintain the uranium in the water in the canister at its solubility limit without any precipitate forming. A faster rate of dissolution would obviously lead to the formation of uranium precipitate in the canister and a situation where the matrix would be dissolving rather than the precipitate, which is physically unreasonable (in the absence of effects such as alpha radiolysis) and contradicts the basic assumption that the rate of dissolution of the precipitate is very fast. On the other hand, it is possible that the matrix could dissolve at a slower rate that is not sufficient to maintain the dissolved uranium at its solubility limit. However, the current assumption is conservative and leads to a well defined and relatively simple model.

Summing equation (12) over all the isotopes of uranium and using equation (13) gives

$$\frac{\partial}{\partial t} \sum_{m \in S_U} \hat{a}^m = \sum_{m \in S_U} \left(-\lambda_m a^m + \lambda_{m,m-1} \hat{a}^{m-1} - f^m \right) + \left(\sum_{m \in S_U} b^m \right) \frac{q^M}{b^M} \tag{15}$$

Since the uranium in the water in the canister is at the solubility limit

$$\sum_{m \in S_U} \hat{a}^m = V_C \sum_{m \in S_U} \hat{c}^m = V_C c_U^S \tag{16}$$

so that

$$\frac{\partial}{\partial t} \sum_{m \in S_U} \hat{a}^m = \frac{\partial}{\partial t} V_C c_U^S = 0 \tag{17}$$

Therefore

$$q^M = b^M \frac{\sum_{m \in S_U} \left(\lambda_m a^m - \lambda_{m,m-1} \hat{a}^{m-1} + f^m \right)}{\sum_{m \in S_U} b^m} \tag{18}$$

To summarize, the model for congruent release of nuclides when there is no alpha radiolysis consists of equation (12) for each nuclide except nuclide *M* (the uranium 238 matrix), equation (14) for all nuclides and equation (16), which effectively determines the amount of uranium in the canister that is not in the matrix. To complete these equations, q^n and q^M are given by equations (13) and (18) respectively.

Parameters required

The parameters required are as follow:

- Solubility limit of each element in the water in the canister.
- Volume of water in the canister.
- Nuclide inventories and half lives.

2.1.5 Source term – congruent release with alpha radiolysis

COMP23 can include the effects of alpha radiolysis on the spent fuel dissolution /3, 4/. The model assumes that the dissolution rate is related to the alpha-energy release of the fuel. When an alpha radiolysis model is used an instantaneous release fraction (IRF) can be specified for each embedded nuclide. This specifies the fraction of the nuclide that is assumed to dissolve instantaneously. Typically, as the matrix dissolves due to alpha radiolysis some of the uranium released will form as precipitate and the embedded nuclides will be freed to dissolve in the water.

Three different representations of the evolving alpha-energy release are included in COMP23.

a) The dissolution rate of the fuel matrix occurs at a constant rate (CONSTANT type).

b) The dissolution rate is a function of the alpha-radiolysis dose rate of the fuel, and decreases with time as a result of radioactive decay (DECAY type).

c) The dissolution rate is a function of the alpha-radiolysis dose rate of the fuel, and decreases with time as a result of radioactive decay and dissolution of alpha-emitting solids from the fuel matrix (EXPLICIT type).

The alpha radiolysis model specifies the rate at which the uranium matrix dissolves due to alpha radiolysis, denoted by q_α^M. This rate can depend on time and on the amount of various alpha-emitting nuclides in the matrix, but is independent of the rate at which the uranium is leaving the canister, which is denoted by q_d^M.

$$q_d^M = b^M \frac{\sum\limits_{m \in S_U} \left(\lambda_m \hat{a}^m - \lambda_{m,m-1} \hat{a}^m + f^m \right)}{\sum\limits_{m \in S_U} b^m} \tag{19}$$

The rate of dissolution of the uranium matrix, q^M, is specified by

$$q^M = \begin{cases} q_d^M & \text{if } \hat{a}_U^T \le V_C c_U^S \\ q_\alpha^M & \text{if } \hat{a}_U^T > V_C c_U^S \end{cases} \tag{20}$$

When the effects of alpha radiolysis are included in the model, the rate of dissolution of the uranium matrix is always at least the alpha-radiolysis rate. If there is uranium precipitate in the canister and $q_\alpha^M < q_d^M$ the amount of precipitate will decrease until such time as either $q_\alpha^M \ge q_d^M$, or else all the uranium precipitate has been dissolved. The rate of dissolution of uranium will still be q_α^M during this period because the precipitate dissolves much more readily than the matrix. Once all the uranium precipitate in the canister has been dissolved, it is assumed that the rate of matrix dissolution will be such as to keep the concentration of uranium in the water at the solubility limit, provided that $q_\alpha^M < q_d^M$ still holds. This implies that the rate of dissolution is equal to the rate at which uranium is leaving the canister, q_d^M. As was pointed out in Section 2.1.4, this particular assumption is conservative. Note that the uranium concentration in the canister cannot drop below its solubility limit until the entire uranium matrix has been dissolved (which would take a very long time in most situations).

In previous versions of COMP23 a slightly different model was used in which the uranium dissolution rate was taken to be the maximum of q_α^M and q_d^M. This earlier model would imply that in the case where there is uranium precipitate present and $q_\alpha^M < q_d^M$, the matrix would dissolve instead of the precipitate, which is both physically unrealistic and unnecessarily conservative.

If $q_\alpha^M > q_d^M$, then it is easy to show that there must be uranium precipitate in the canister (see below). So, if there is no precipitate in the canister the maximum of q_α^M and q_d^M must be q_d^M i.e. the first part of equation (20) is equivalent to the original COMP23 model. Thus, the model represented by equation (20) only differs from the original COMP23 model when there is uranium precipitate in the canister and $q_\alpha^M < q_d^M$, and then it is physically more realistic than the original COMP23 model, although it is also less conservative.

To prove the assertion made in the previous paragraph, suppose $q_\alpha^M > q_d^M$ at time t, then summing equation (12) over all the isotopes of uranium and using equation (13) gives

$$\frac{\partial}{\partial t} \sum_{m \in S_U} \hat{a}^m = \sum_{m \in S_U} \left(-\lambda_m \hat{a}^m + \lambda_{m,m-1} \hat{a}^{m-1} - f^m \right) + \left(\sum_{m \in S_U} b^m \right) \frac{q_\alpha^M}{b^M} \tag{21}$$

Using equation (19) to eliminate the first sum on the right hand side of equation (21) and rearranging gives

$$\frac{\partial}{\partial t}\sum_{m\in S_U}\hat{a}^m = \frac{1}{b^M}\left(\sum_{m\in S_U} b^m\right)\left(q_\alpha^M - q_d^M\right) \tag{22}$$

The right hand side of this equation is strictly positive since $\sum_{m\in S_U} b^m > b^M > 0$ and $q_\alpha^M > q_d^M$ by assumption. Thus

$$\frac{\partial}{\partial t}\sum_{m\in S_U}\hat{a}^m > 0 \tag{23}$$

which means that the total amount of uranium in the canister that is not embedded in the fuel matrix is strictly increasing when $q_\alpha^M > q_d^M$. It follows immediately that

$$\sum_{m\in S_U}\hat{a}^m(t) > \sum_{m\in S_U}\hat{a}^m(t-\delta t) \tag{24}$$

for all sufficiently small, positive δt. Since the concentration of uranium in the canister never drops below its solubility limit until all the fuel matrix has been dissolved

$$\sum_{m\in S_U}\hat{a}^m(t-\delta t) \ge V_C c_U^S \tag{25}$$

Combining equations (24) and (25) gives

$$a_U^T(t) = \sum_{m\in S_U}\hat{a}^m(t) > \sum_{m\in S_U}\hat{a}^m(t-\delta t) \ge V_C c_U^S \tag{26}$$

as required.

The three models for the alpha-radiolysis dissolution rate, q_α^M, are:

CONSTANT

$$q_\alpha^M = K_{CON} \tag{27}$$

where K_{CON} is a constant.

DECAY

$$q_{\alpha}^{M} = K_{DEC}\sum_{i=1}^{4} A_i \exp\left(-\frac{t\ln 2}{B_i}\right) \tag{28}$$

where K_{DEC} is a constant, t is the time, and A_i,B_i, $i = 1,\ldots,4$ are constants specific to the nuclides Am-241, Pu-239, Pu-240 and Np-237 in a particular fuel type /5/. If a different fuel to that described in reference /5/ is used, the constants will need to be changed in the program. However, it is not likely that this model will be used extensively as the CONSTANT model provides an adequate representation of dissolution. The constants, obtained from reference /5/, are given in the table below.

Nuclide	A_i	B_i
Am-241	25.3	433
Np-237	0.04	$2.1\cdot10^{6}$
Pu-239	1.1	$2.4\cdot10^{4}$
Pu-240	2.2	6,570

EXPLICIT

$$q_{\alpha}^{M} = K_{EXP}\sum_{m\in\Gamma} C_m b^m \tag{29}$$

where K_{EXP} is a constant, Γ is the set of nuclide labels for the alpha-emitting nuclides, C_m are constants corresponding to the nuclides in Γ, and b^m is the amount of nuclide m in the fuel matrix. This model is included to allow flexibility of the program. In the current version of the program the nuclides Am-241, Pu-239, Pu-240 and Np-237 are included and the values of the constants, obtained from reference /5/, are given in the table below.

Nuclide	**C**
Am-241	2.85
Np-237	$8.81\cdot10^{-3}$
Pu-239	0.0261
Pu-240	0.0992

To summarize, the form of the equations representing the model for congruent release of nuclides including alpha radiolysis depends on whether there is uranium precipitate in the canister or not. When uranium precipitate is present in the canister the model consists of equations (12) and (14) for all nuclides together with equations (13) and the second part of (20). When there is no uranium precipitate present, the model is the same as the case when there is no alpha radiolysis, described in Section 2.1.4.

Parameters required

The parameters required are as follow:

- Solubility limit of each element in the water in the canister.
- Volume of water in the canister.
- Nuclide inventories and half lives.
- Parameters for the alpha-radiolysis dissolution model.

2.2 Geometric framework

To represent the barrier system through which the species are transported, COMP23 makes use of the integrated finite-difference method /6/ and of the concept of "compartments". The barrier system is discretized into compartments. Average properties over these compartments are associated with nodes within the compartment. From the theoretical point, of view the compartments may have any shape, but consist of only one material. The material balance over a compartment is given by:

$$\frac{\partial a_i^n}{\partial t} = \sum_j g_{i,j} c_j^n - \lambda_n a_i^n + \lambda_{n,n-1} a_i^{n-1} \tag{30}$$

where a_i^n is the amount of nuclide n in compartment i, c_i^n is the concentration of nuclide n in the pore water in compartment i, λ_n and $\lambda_{n,n-1}$ are as defined in Section 2.1.1 and $g_{i,j}$ is the transport coefficient linking compartments i and j. The concentration, c_i^n, where $n \in S_E$ (i.e. nuclide n is an isotope of element E), is related to a_i^n by

$$c_i^n = \begin{cases} \dfrac{a_i^n}{V_i K_{E,i}} & \text{if } a_{E,i}^T \le V_i K_{E,i} c_E^S \\ \dfrac{c_E^S a_i^n}{a_{E,i}^T} & \text{if } a_{E,i}^T > V_i K_{E,i} c_E^S \end{cases} \tag{31}$$

where $K_{E,i}$ is the distribution coefficient for element E in compartment i, V_i is the volume of compartment i, a_E^T is the total amount of element E in compartment i and c_E^S is the solubility limit for the solubility group, S_E, of element E. $K_{E,i}$ is given by

$$K_{E,i} = \phi_{E,i} + \left(1 - \phi_{E,i}\right) k_{E,i}^d \rho_i \tag{32}$$

where $\phi_{E,i}$ is the porosity for element E in compartment i, ρ_i is the density of the solid material in compartment i and $k_{E,i}^d$ is the sorption coefficient for element E in compartment i. $a_{E,i}^T$ is given by

$$a_{E,i}^T = \sum_{m \in S_U} a_i^m \tag{33}$$

The diffusional contribution to $g_{i,j}$ is expressed in terms of diffusional resistances. Each compartment makes a contribution to this resistance. The diffusional resistance from compartment i to compartment j is $R_{i,j}$ where

$$R_{i,j} = \frac{R_i}{2} + \frac{R_j}{2} \tag{34}$$

and R_i and R_j depend on the direction of transport and the nuclide (through the diffusion coefficient). R_i takes the form

$$R_i = \frac{l_w}{A_w D^n_{e,i}} \tag{35}$$

where l_w is the length of the compartment in the transport direction (w can be either x, y or z), A_w is the cross-sectional area of the compartment normal to the direction of transport and $D^n_{\mathrm{e},i}$ is the effective diffusion coefficient for nuclide n in compartment i. Additional resistances can be added to model special situations, such as transport from a small compartment into a large one (see the following sections).

The diffusional contribution to $g_{i,j}$ may now be written in terms of $R_{i,j}$ as

$$g_{i,j} = \begin{cases} \dfrac{1}{R_{i,j}} & \text{if } i \neq j \\ -\sum\limits_{j \neq i} g_{i,j} & \text{if } i = j \end{cases} \tag{36}$$

The elements required to define the compartmentalization are the geometry of the system, dimensions of the system and the type of material. The compartments are defined by their volume, their diffusion length and cross-sectional area. Conceptually, the model uses a rather straightforward compartmentalization process. This coarse compartmentalization could yield poor or even meaningless numerical results. To avoid this, analytical or semi-analytical solutions are introduced in the model in zones where a finite-difference scheme would require a fine discretization to obtain an accurate result. Some of the approaches used by the model to describe the solute transport in these sensitive zones are shown below.

2.2.1 Analytical solutions used in the model

The approaches developed at present include transport by diffusion into the flowing water, transport of solute through a small contacting area into a large volume compartment and transport of solute into a narrow slit /7/. Other approaches could be included in the code in the future.

Transport into flowing water

For compartments in contact with water flowing in fractures in the rock, the diffusive transport is determined by an equivalent flow rate Q_{eq}. This parameter is a fictitious flow rate of water that carries with it a concentration equal to that at the compartment interface.

It has been derived by solving the equations for diffusional transport to the passing water by boundary layer theory /8/. This entity is obtained from:

$$Q_{eq} = q_o W\bar{\eta} = q_o W\sqrt{\frac{4D_w t_w}{\pi}}$$

where D_w is the diffusivity in free water, W is the width of the compartment in contact with water flowing in fractures, fracture zones or damaged zones and $\bar{\eta}$ is the mean thickness of penetration into the water by diffusion from the compartment. The residence time, t_w, is the time that the water is in contact with the compartment. This time is obtained from the flux of water q_o, the flow porosity, and the length of the pathway in contact with water.

Transport into a large compartment

Species diffusing out of a small hole into a very large volume of material spread out spherically. Very near the hole, the cross-section is still of the order of the size of the hole. Further away, the cross section increases considerably as the "sphere" grows. Thus, most of the resistance to diffusion is concentrated very near the mouth of the hole. This resistance is calculated by integrating the transport rate equation:

$$N = -2\pi r^2 D_e \frac{dc}{dr}$$

from a small hemisphere into a very large volume, between the limits of the sphere of radius r_{sph} and an outer radius r. Since the species spread over a large volume in the surrounding medium (r >> r_{sph}), the nuclide transport rate simplifies to $N = 2\pi r_{sph} D_e \Delta c$. In the model, the real situation is approximated by using an equivalent plug. This plug of a cross-sectional area equal to the hole area has a thickness Δx given by $\Delta x = r_{\text{hole}} / \sqrt{2}$.

Transport into a narrow slit

For the diffusive transport into a narrow fracture, most of the resistance to the transport will be located nearest to the fracture because of the contraction in the cross-sectional area. The transport resistance is then approximated by a plug through which the nuclides are transported. The plug has a transport area equal to the cross-sectional area of the fracture, and a diffusion length equal to a factor times the fracture aperture. Neretnieks analytically modelled the stationary transport from the bentonite surrounding a canister for spent nuclear fuel into a fracture /9/. The procedure uses the exact solution of the steady-state two-dimensional diffusion equation for a sector of the clay barrier representing half the fracture spacing that allows symmetry conditions to be used. After some simplifications, the resistance of the plug at the mouth of the fracture is expressed as:

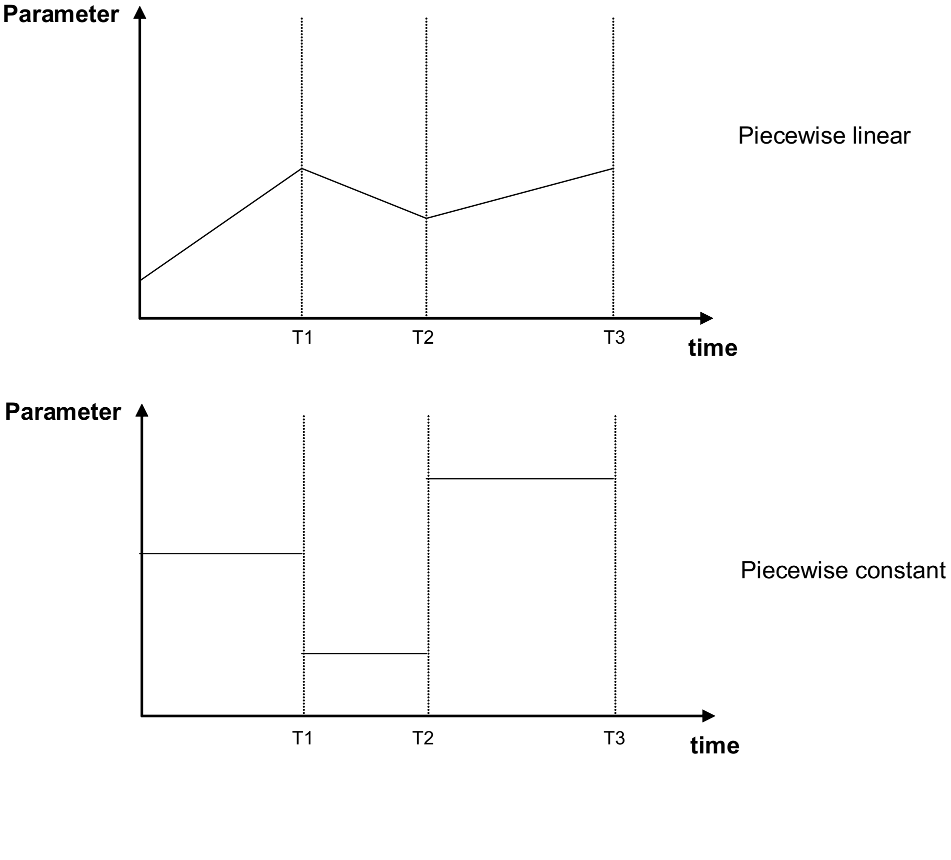
$$R_f = \left[\left(F_{x,0} / \delta\right)\delta / \left(D_e A_f\right)\right]$$

The factor ($F_{x,0}/\delta$) was calculated by Neretnieks for a number of fracture spacings, fracture apertures and barrier thicknesses. For fractures with an aperture varying between 10^{-4} and 10^{-3} m, and a backfill thickness of 0.30 to 0.35 m, the factor ranges between 3 and 7.
It can be visualized as having a plug of clay at the mouth of the slit with a thickness of ($F_{x,0}/\delta$) times the slit aperture.

2.3 Assignment of material properties

In the standalone version of COMP23, the physical parameters defining the transport in a repository are specified as constant. In the version to be used as a module in the PROPER package /10/, the transport parameters, as sorption, diffusion, and equivalent flow rates may be specified as constant or as functional correlations.

Porosity, sorption coefficient, diffusion coefficient and solubility limit can also be made time dependent in version 1.2.2 of COMP23. The time dependence can be in the form of piecewise constant (step) or piecewise-linear (ramp) variations. These are illustrated in the figure below.



2.4 Initial conditions

COMP23 solves an initial value problem, comprising a system of differential and possibly algebraic equations. The solution of this system is straightforward once the initial conditions have been defined. The variables defining these conditions are determined by the amount of the species dissolved, the amount of the species as solid inventory in the compartments and the amounts of nuclides embedded in the fuel matrix when a congruent dissolution model is used. The default initial condition is zero for all compartments, except for the compartment acting as the source where the initial condition is determined by the inventory and the solubility of the species.

3 Numerical methods

3.1 Spatial discretization

The compartment model COMP23 formulates the near-field transport in terms of integrated finite differences, introducing the concept of "compartments" to define the discretization of the system. This concept is very useful when the transport is through materials with different properties and the geometry of the whole system is complex. The compartment is fully defined by its capacity and the resistances defining a two-dimensional nuclide transport. The capacity is determined by the volume and the sorption coefficient, and will also depend on the porosity and density of the material. The diffusion length(s), cross sectional area(s), and the diffusion coefficient define the resistance. The compartmentalization of the system is rather straightforward. The system to be modelled is subdivided into compartments taking into consideration the different geometric shapes and the various materials found in the system. COMP23 uses a coarse discretization.

3.2 Temporal discretization

Once the spatial discretisation has been carried out, the equations to be solved consist of a set of ordinary differential equations for the amounts of each nuclide in each compartment, a_i^n, in the form of equation (30). In the congruent dissolution model, equation (14) for the amount of each nuclide in the matrix, b^n, must also be solved, together with the algebraic equation (19) for the rate at which uranium is leaving the canister. These equations may be written in the general form

$$F(\dot{y}, y, t) = 0 \tag{37}$$

where y is a vector comprising all the a_i^n (and b^n and q_d^M when congruent dissolution is being treated), and $\dot{y}$ is the time derivative of y. These equations are stiff, due to the wide range of timescales in the problem. COMP23 uses the package DDASKR to solve this system of implicit differential-algebraic equations (DAES). The package uses backward difference methods of varying order of accuracy[1], and chooses the order and the size of the time-step to maintain a specified level of accuracy whilst minimizing the computational time /11/. DDASKR can produce results at intermediate time very efficiently. The user of COMP23 specifies points at which output is needed. DDASKR also has a facility for monitoring user defined functions and finding the time at which any of these functions becomes zero.

The methods used in DDASKR rely on the solution to the equations (37) being sufficiently smooth. The degree of smoothness required depends on the highest order of method to be used, which is typically 5. The main technical difficulty with the equations arising in COMP23 is that the smoothness assumption breaks down at various points in time, such as when the amount of nuclide in a compartment exceeds the solubility limit, or when the size of the hole in the canister changes abruptly, or when the rate of uranium dissolution changes type in the congruent release model. This is dealt with in COMP23 by monitoring various

[1] A method of order *n* has an error that is proportional to the *n*th power of the size of the timestep.

quantities that mark these changes. The root finding capabilities in DDASKR are used to identify the precise time at which the change takes place. The computation is then restarted from that time using the appropriate new set of equations. The essential point here is that DDASKR is only ever solving smooth systems of equations, and so its methods work well and the program is reasonably robust.

The conditions that are monitored by the code will now be described. When the OWNSOL or FUELSURFACE models are used the following quantities are monitored:

- $\sum_{m \in S_E} a_i^m - V_i K_{E,i} c_E^S$ for each compartment *i* and each element *E*. When this quantity passes through zero and is increasing, the element E is changing from being not solubility limited to being solubility limited (and the other way round if the quantity is decreasing). When the quantity changes sign, the calculation is restarted using the appropriate form of equation (31) to compute c_i^n in terms of a_i^n.
- Times at which the size of the hole in the canister changes abruptly. In these cases some of the coefficients in the equations change. When COMP23 detects an abrupt change in the hole size, it recalculates the relevant coefficients and restarts the calculation.

When the MATRIX model is used the following quantities are monitored:

- $\sum_{m \in S_E} a_i^m - V_i K_{E,i} c_E^S$ for each compartment *i*, and each element *E* except for uranium in the canister. When this quantity passes through zero and is increasing, the element E is changing from being not solubility limited to being solubility limited (and the other way round if the quantity is decreasing). When the quantity changes sign, the calculation is restarted using the appropriate form of equation (31) to compute c_i^n in terms of a_i^n.
- b^M – the amount of uranium 238 in the fuel matrix. When this quantity becomes zero the calculation is restarted without fuel dissolution. The model becomes the same as the OWNSOL or FUELSURFACE models.
- Times at which the size of the hole in the canister changes abruptly. In this cases some of the coefficients in the equations change. When COMP23 detects an abrupt change in the hole size, it recalculates the relevant coefficients and restarts the calculation.

The other quantity to be monitored depends on whether uranium precipitate is present in the canister or not. If uranium precipitate is present, then the following quantity is monitored:

- $\sum_{m \in S_U} a_1^m - V_C c_U^S$ where by convention, compartment 1 is the canister. This quantity should only pass through zero in the decreasing direction (otherwise there cannot be uranium precipitate in the canister). When this quantity passes through zero, the rate of dissolution due to alpha radiolysis is not sufficiently high to keep the uranium in the canister at the solubility limit, so the fuel matrix dissolution rate will be controlled by rate at which uranium is leaving the canister. The calculation is restarted with the amount of uranium 238 in the canister that is not in the matrix being calculated from equation (16).

If there is no uranium precipitate present in the canister, then the following quantity is monitored:

- $q_{\alpha}^{M} - q_{d}^{M}$. Initially, this quantity must be negative (otherwise there would be uranium precipitate present – see the discussion in Section 2.1.5). When this quantity goes through zero uranium is about to be precipitated in the canister. The calculation is restarted using q_{α}^{M} as the fuel matrix dissolution rate and solving equations for all the nuclide amounts, including the uranium 238. It can be shown that when the calculation is restarted, the rate of increase of uranium precipitate in the canister is initially zero, but that the second derivative of the total amount of uranium in the canister is positive. So, although uranium will be precipitated, the initial amount precipitated will be small. This can cause numerical problems if the accuracy of the solution is not sufficiently high.

Finally, note that the case when there is no alpha radiolysis can be considered as a special instance of the case with alpha radiolysis with $q_{\alpha}^{M} = 0$ as far as the quantities monitored is concerned.

4 Description of the COMP23 code

The COMP23 code is written in FORTRAN. There are two versions depending on the environment it works in: a standalone version and a special version to be used as a submodel of the PROPER code. The code consists mainly of three parts that are:

MAIN PROGRAM:	CMP23
SOLVER:	DDASKR
INPUT FILES:	system.dsc, *casename*.inv, *casename*.nam and submod.lib

The main program CMP23 makes use of several subroutines that will be described later. The INPUT files are described in detail in the next sections.

The code solves three types of specific situations:

I Solubility limited approach. All species in the canister are available for release, independently of the structure they are part of. The only limitation on the nuclide release is the solubility of the individual species.

II A particular case for nuclides initially located at the fuel surface. The handling of this situation is similar to I but considers that only a fraction of the total nuclide inventory is available for release.

III Congruent approach for nuclides embedded in a fuel matrix. Since the matrix is mostly formed by uranium oxide, the escape rate for the embedded nuclides will depend on the escape rate of the uranium. Thus, to calculate the release of these nuclides, the U-238 is simultaneously run with the nuclides of interest.

The solubility limits may be either fixed or calculated from a shared solubility limit for a group of nuclides.

There are also special uses of the code that are easy to manage. They are:

a) Addition of a transport resistance between two compartments. The code needs know only the value and where the resistance will be placed.

b) The damage in the canister wall is handled as a special compartment where the user has the alternative of choosing a growing hole or a hole of stationary size. For the situation of a growing hole, the user may choose a linear function or a step function for the growth.

c) Addition of a plug at the outlet of the source in order to approximate the mass transport between a small compartment and a large one. This is applied to the nuclide transport from the small hole in the canister wall into the bentonite outside the hole.

d) Addition of a plug situated inside the canister (source) when the backfill material is granulated. This is a special use for copper/iron canister as source, where the nuclide transport into the damage in the canister wall is approximated by a plug at the inlet of the damage. This plug has the same dimensions as the plug at the outlet of the damage. The effective diffusion coefficient (D_e) is established beforehand and is 10^{-10} m^2/s.

Note:

The dimensions of both plugs (inlet and outlet) depend on the size of the hole at the canister wall. So if the size of the hole varies, the dimensions of both plugs vary too.

4.1 Subroutines and functions used by COMP23

4.1.1 Key variables used by the subroutines

AREA: variable that defines the cross-sectional area for a compartment whose size changes with time.

AGQ: partial matrix of constant coefficients.

AINV: vector storing the input amount (inventory) of the species.

EPS: requested relative accuracy in all solution components.

EWT: problem zero, i.e. the smallest physically meaningful value for the solution.

ICALL: index controlling the recall of the solver from the main program or the stopping of the program execution.

ICH: index identifying the decay chain number.

INABS absolute index identifying a nuclide without reference to a chain.

INUC: index identifying the nuclide in a chain.

IPRINT: position index in the time series.

ISPSOL: shared solubility flag: = 0 if no shared solubility, = 1 if shared solubility is required.

NEQ: the number of differential equations.

NROOT: the number of equations whose roots are desired. If NROOT is zero, the root search is not active. This option is useful for obtaining output at points that are not known in advance, but depend upon the solution.

QDURAN: dissolution rate of the fuel matrix.

ADURAN: dissolution rate of the fuel matrix due to alpha radiolysis.

T: independent variable in the ODEs/DAEs.

TIME: independent variable in the ODEs/DAEs.

TOUT: the point (time) at which the solution is desired.

Y: vector of nuclide amounts – solution of ODEs/DAEs.

YPRIME: vector of derivatives of the solution to the ODEs /DAEs.

4.1.2 Description of key subroutines

ALPH23 (TIME, Y, ADURAN)

This subroutine calculates the dissolution rate of the fuel matrix (U238), ADURAN, due to alpha radiolysis.

CONC23 (Y, IPRINT, ICALL)

This subroutine stores the output data, such as concentrations for all compartments and time at which they were calculated. The main program CMP23 calls CONC23.

CSTO23 (IPRINT, ICALL, T, Y)

This subroutine called by CMP23 if DDASKR indicates that a zero has been found in one of the conditions being monitored. It sets LSOLIM and IMFLAG do indicate the change in the equations to be solved. It also sets the flag ICALL to indicate whether initialisation needs to be carried out or if a fatal error has occurred.

DDASKR (SSRES, NEQ, T, Y, YPRIME, TOUT, INFO, RTOL, ATOL, IDID, RWORK, LRW, IWORK, LIW, RPAR, IPAR, SSJAC, PSOL, SSRT, MROOT, JRTSS)

This subroutine solves the implicit differential-algebraic equations (DAEs) of the form $F(\dot{y}, y, t) = 0$, given the initial conditions $y_0 = y(t = 0)$ which must be used to supply consistent initial values for $\dot{y}_0$. DDASKR is called once for each output point of T. The subroutines SSRES, SSJAC and SSRT are part of COMP23 and their functions are described below. The main program CMP23 calls DDASRT.

FLOW23 (IFSTOP, IPRINT, MULTI)

This subroutine calculates the release, by molar flow rate, from the source and into the various sinks. These data are written to the PROPER database via a call to PUTS. The time series at which the molar flow rates are calculated is determined beforehand by the user. The main program CMP23 calls FLOW23.

FMCO23 (ICH)

This subroutine defines the coupling resistances between compartments, including the external coupling with the flowing water surrounding the barrier system. FMCO23 is called by IMAT23.

FMDE23 (ICH)

This subroutine defines the capacity and individual resistances to transport of all compartments. FMDE23 is called by IMAT23.

MAT23 (TIME)

This subroutine computes the coefficients that appear the governing equations. MAT23 is called by IMAT23.

PRIN23 (IPRINT, NAMES)

This subroutine prints out results of the execution such as concentrations in the various compartments, release into the various sinks and solid inventory in the canister. The results are printed at times determined by TIME23. It also prints out the variation with time of the hole size in the canister wall. The main program CMP23 calls PRIN23.

READ23 (NAMES, EPS, EWT, NLOOP, NPREPAR, LSTALON, U0, CASE)

This subroutine reads the data from the INPUT files with help of an auxiliary subroutine HUIM23 created specially to operate in the PROPER environment. The main program CMP23 calls READ23.

SET23 (NAMES, Y, CASE)

This subroutine sets the initial conditions for the problem and the flags (IFLAG) for the material balance control in the various compartments. The main program CMP23 calls SET23.

SSJAC (NEQ, TIME, Y, YPRIME, PD, CJ, RPAR, IPAR)

This subroutine computes the Jacobian matrix for $F(\dot{y}, y, t)$, the equations defining the DAE at time, to be evaluated at Y, YRPIME and TIME. A return from this function passes control back to DDASKR.

SSRES (TIME, Y, YPRIME, CJ, DELTA, IRES, RPAR, IPAR)

This subroutine computes $F(\dot{y}, y, t)$, the equations defining the DAEs. When this subroutine is called, the entries in Y are intermediate approximations to the solution components and the entries in YPRIME are intermediate approximations to their derivatives. A return from this function passes control back to DDASKR.

SSRT (NEQ, TIME, Y, YPRIME, NRT, RVAL, RPAR, IPAR)

This subroutine computes the values of the various functions being monitored by DDASKR. A return from this function passes control back to DDASKR.

SSINI (TIME, Y, YPRIME)

Calculates the values of $\dot{y}$ (YPRIME) based on the values of y (Y) at time t (TIME).

TIME23 (TINIT, ICALL)

This subroutine determines the time series at which the user wishes to obtain results. The time step is determined by a geometric progression. The main program CMP23 calls TIME23.

URC23 (TIME)

This subroutine updates the coupling resistances between compartments, including the external coupling with the flowing water surrounding the barrier system to taking into account the effect changes in the size of the hole in the canister. URC23 is called by IMAT23.

WRIT23 (NAMES)

This subroutine gives information on capacities and resistances of the various compartments. It also gives information on the matrix of the coefficients “F” initially executed. WRIT23 is called by FMAT23.

4.1.3 Additional subroutines

A description of these subroutines is found in the Proper Monitor User’s Manual /12/ and Proper Submodel Designer’s Manual /10/. These subroutines are implemented and of use only in the PROPER version of the code COMP23. Some of them are part of the PROPER package. “They are service routines for setting up communications with the database, for acquiring values of sampled parameters, for handling time series and for handling data from external submodel-specific files” /10/.

INVEN (FILNAM, IUNAM, FILINV, IUINV, NNUCL, NAMES, TBREAK, AINV)
This subroutine gives information on the inventory in the canister. SET23 calls INVEN.

PRELUD (FILE)
Set up communication with the internal database.

POSLUD

Closing down communication with the internal database.

GETP (INDEX)
Used to obtain sampled parameters from the internal database.

PUTS (IDD, TSERIE, VALUE)
Used to send output time series to the internal database.

To avoid conflict, service routines are used to obtain an unused unit number and the unique name of a data file when opening. They are:

IGETUN (IDUM)	to get the unit number.
GETDAT (IDUM)	to get the unique name of a data file.

and when closing the file

PUTUN (IUDAT)	to return the unit number to the monitor.

4.2 General description of the input requrements

The physical geometry of the system is simplified by dividing it into blocks. The blocks are numbered in ascending order. The discretization in blocks considers the geometry and the various materials by which the nuclides migrate. Not all blocks have the same geometry and orientation, so each block has its own axes of references. So far there are only two transport directions defined for the block (horizontal (x or y) direction and z-direction).

The transport in a block is completely defined by the physical properties of the material, the nuclide transport properties and the geometrical dimensions of the block. These properties are used by the code to calculate the capacity of the block and its resistance to transport for each of the two defined transport directions. These data are the input data for the problem to be solved. The capacity and the resistance are determined by the following expressions:

$$\text{Capacity} = V\left[\phi + (1-\phi)k_d\rho\right]$$

$$\text{Resistance} = \frac{x}{AD_e}$$

where x is the diffusion length of the block (in the direction of transport), A is the cross-sectional area of the block (perpendicular to the direction of transport) and D_e is the effective diffusion coefficient. The porosity and the density of the material solid are denoted by ϕ and ρ respectively, k_d is the sorption coefficient and V is the volume of the block.

As two transport directions have been defined, the code needs to know the geometrical dimensions of the block for both directions to define the transport. Such geometrical dimensions are diffusion length and cross-sectional area for each direction. The volume of the block is calculated by the code from the given dimensions for transport in the z-direction.

Any block, except the source, may be subdivided into compartments in any of the two directions named above. The block itself is a compartment if it is not subdivided. A simple subdivision is that by discretization in the z-direction the code makes the block into compartments of equal capacities. The code needs only to know the desired number of subdivisions in the z-direction NZ, so that NX = NY = 1, which means no subdivision in the x or y directions. For any other subdivision, all compartments have to be defined in the INPUT file. The compartments are numbered by the code following the z-axis for the block, while the other direction is kept constant.

The first block defined in the INPUT data is the source (interior of the canister) followed by the block describing the damage of the source (hole in the canister wall).

Each block may be connected to one or more than one block, except the source. At present, the source can only be connected to one compartment. Each couple of connected blocks (A and B) is specified by the user in the INPUT file. Several control numbers define the connection. Such numbers are used to define: the position of each block (A and B), the numbers of the couples of compartments involved in the connection of block A and B, the direction (z-axis or x or y-axis) of each block and the contribution of each block to the coupling resistance. After the connection of the two blocks is specified, the code needs to know the position of the couples of compartments involved in each connection. All this information is used to calculate the coupling resistance $R_{i,j}$:

$$R_{i,j} = \frac{R_i}{2} + \frac{R_j}{2}$$

where R_i and R_j are the individual resistances of the compartment "i" and the adjacent compartment "j" respectively.

External resistances specified in the input data may be added between two blocks.
For resistances added in the form of a plug, these are codified by IPLUG = index (block number A or B). This index block is used by the code to obtain the diffusion coefficient. This plug concept is very useful when the transport is between a block of very small volume (block A) and a block of large volume (block B). The plug resistance value is:

$$\text{plug resistance} = \frac{\sqrt{A_{hole}/(2\pi)}}{D_e A_{hole}} = \frac{1}{D_e\sqrt{2\pi A_{hole}}}$$

where A_{hole} is the cross-sectional area of the block of small capacity. Suppose that for some A-B connection, IPLUG = block B number (block of large capacity). Then, the coupling resistance calculated by the code is:

$$\text{Coupling resistance } R_{ab} = \frac{R_a}{2} + \text{plug resistance}$$

The size of the block of small capacity may vary with time. If this is the case, the plug resistance will also vary. The existence of other types of resistances added to the connection are indicated by IRADD = 1, whose values are given following the description for such effects in the input file. Suppose that for some A-B connection, IRADD = 1. If the user specifies the resistance value as RADD, the calculated coupling resistance is:

$$\text{Coupling resistance } R_{ab} = \frac{R_a}{2} + RADD + \frac{R_b}{2}$$

The connections of the various sinks to the system (repository) are defined by identifying the position of the block and compartment connected to each sink. In addition, the user has to codify the direction of the nuclide transport (IRZ) and the contribution of the compartment to the coupling resistance (ICRS). For the situation of one fracture intersecting the system, a plug approximates the nuclide transport into the fracture. The dimension of this plug have to be defined by the user. For this situation ICRS = 0.

As the code for COMP23 exists in two different operative versions, there are two input data files. The differences between them are in the structure of the subroutines to read the input data, to process the output data, and to get information of the initial nuclide inventory. The variable definition is the same for both versions. In the standalone version of COMP23, the nuclide inventory has to be given in the INPUT file. In the PROPER version of COMP23, the nuclide inventory is implicitly obtained by the code; it needs only to know the names of the nuclides and the break-time (TINIT) for the canister. In the next section, the INPUT file for the PROPER version will be presented. The standalone version is described in a separate manual.

5 Simulation setup using Proper

5.1 Overview

COMP23 can be run as a submodel of the PROPER package. A User Guide for the PROPER package is given in reference /12/. This section gives details specific to running COMP23 as a submodel of PROPER.

Section 5.2 describes the input files that are required by the PROPER package when COMP23 is included as a submodel.

The PROPER version of COMP23 uses the HYDRASTAR User Interface (HUI) /13/. HUI is a preprocessing facility incorporated into the HYDRASTAR code and the COMP23 code. The main objectives of the HUI are:

- Free-format input in a single input file.
- Input data validity testing.
- Input data consistency checking.

A general description of the HUI input file is given in Section 5.3 of this report. A detailed description of the COMP23 input required is given in Section 5.4.

Details of the output produced by the HUI interface are discussed in Section 5.5.

5.2 Input files required

The following input files are required to run COMP23 as a submodel of PROPER:

Name	Description
system.dsc	The system description file that is used for all PROPER simulations. The input requirements for this file are described in more detail below.
casename.inv, *casename*.nam	These two files hold the information on the radionuclide inventories for one canister. The inventory files used by COMP23 are identical to the files used by TULLGARN /14/, so these two files should preferably be links if TULLGARN is used in the same simulation. *casename* is read in from the CONTROL block of the system.dsc file.
submod.lib	Lists the modules that are used by PROPER. The module name for COMP23 is COMP23 and it is connected as an internal submodel /12/.

5.3 HUI input

The following notational conventions are used to describe the format of the input data for this model. In general the definition follows that of INFERENS /15/. A detailed description of the input required when running the PROPER version of COMP23 is given in Section 5.4.

5.3.1 Typefaces

CAPITAL	Keywords
lowercase italics	Variable name or variable text.
CAPITAL ITALICS	Object name or name of variable in the code.
underlined	Fixed text.
bold underline	Program validity check.

5.3.2 Separators

#	Beginning of comment.
{}	List of items.
[]	Enclosed list of optional items.
|	Optional items separator.
@	Zero or more occurrences of preceding expression.
+	One or more occurrences of preceding expression.
<>	Keystrokes or special characters.

5.3.3 Format specifiers

A*	Free-format string.
A*:wordlist	Free-format string; must be member of wordlist.
F*	Free-format floating point number.
I*	Free-format integer.
wordlist	List of alternative keywords [word1|...|wordN] which are allowed for the specified context.

5.3.4 Program validity check

V	Validity
C	Consistency
E	Existence
W	Warning

5.3.5 Format syntax

```
{input_file} =
    [system_commands]@
    [{a_block} | {comments} ]+

{a_block} =
    BEGIN_BLOCK block_id
        {block_definition}
    END_BLOCK

{block_definition} =
    [{keywords} |
    {lists}|
    {definition_block} |
    {switchcommands} |
    {comments} ]+

{keywords} =
    KEYWORD [I*|F*|A*|A*:wordlist| ]+ [{comments}]
```

```
{lists} =
    KEYWORD
        [I*|F*|A*|A*:wordlist| ]+ [{comments}]
    END_LIST

{definition_block} =
    BEGIN_DEF def_id
        [ [{keywords} | {comments} ]+ | [I*|F*|A*|A*:wordlist| ]+  ]
    END_DEF

{switch_command} =
switch (switch_var)
    case VALUE1:
        {keywords}
    ...
    case VALUEn:
        {keywords}
endswitch

{comments} =
    ’ #’ {any_text} {end_of_line}

system_commands =
    SYSTEM KEYWORD
```

5.4 The system description file

5.4.1 Overview

The system description file, system.dsc, is used to specify for PROPER the module intercommunication, sampled parameters etc. The general format of the system description file is (only the parts relevant to this manual have been included):

PROPER_KEYWORDS
MACROS definitions
PARAMETERS section
MODULE definitions

each **MODULE** definition has the general format:

MODULE module (Input_Timeseries; Output_Timeseries)

INPAR section
DATA section

END module

Note: the order of the INPAR and DATA sections is not significant.

Any lines beginning with the ’#’-character are handled as a comment line.

5.4.2 Parameters

The PARAMETERS section in the system description file defines the sampled parameters and their distributions. The general syntax for the PARAMETERS section is:

PARAMETERS
Parameter_name distribution_type [(arg1[,arg2[...]])]
END PARAMETERS

The order in which the parameters are passed to COMP23 is defined within the INPAR section within the MODULE definition. The general syntax for the INPAR section is:

INPAR
parameter_name1 [parameter_name2 ...]
END INPAR

No Time-dependent Parameters

The following parameters need to be defined in the PARAMETERS section for COMP23. A detailed description of the parameters is given below.

Suggested name(s)	Description
CSYNC	Random number seed.
MULT	The number of canisters the calculation segment (normally from HYDRASTAR).
PROB	Probability for initial damage to canister.
PITFAQ, QS, CONHS, DEFFS	Corrosion data (not used by present version of the model).
DENS	Density of different barrier materials (if not defined in BLOCK data).
POR	Porosity of different barrier materials (if not defined in BLOCK data).
T_HOLE, A_HOLE	Hole growth data for chosen growth model.
CSOL	Solubility of the nuclides.
DIF	Effective diffusion coefficient in the different barrier materials for all nuclides.
KD	K_d-value in the different barrier materials for all nuclides.
VTUBE, NTUBES, NTDAM, VHEMA	Tube volume, number of tubes, tubes damaged and void (if not defined in BLOCK data).
AER	Alpha-radiolysis parameter *K* for chosen model (if required).
ZRFRA, APFRA, QFAC, QEXP	Data for each sink (if not defined in BLOCK data).
IRF	Instantaneous Release Fraction (IRF) values (only required for nuclides that use a FUELSURFACE or alpha-radiolysis model).

The order that these are listed above is the order that the parameters must be specified within the INPAR section. When COMP23 is used as a standalone model two extra parameters are given as the first parameters. These are NCAN and UC.

Suggested name	Units	Description
NCAN	(–)	Number of canisters to be modelled (recommended value 1). (Only used for standalone version)
UC	($m^3/m^2/yr$)	Water flow rate outside canister. (Only used for standalone version)
CSYNC	(–)	Random number seed.
MULT	(–)	Number of (assumed identical) canisters in region.
PROB	(–)	Probability of a single canister being penetrated at time of emplacement.

If COMP23 finds that there is a single canister that has been penetrated at time of emplacement, it ignores the other canisters and calculates the rate using one initially damaged canister. If no canister is initially damaged, no release calculations are performed in the present version.

The next parameters define the densities of the barrier materials. They must be present if this data is not defined in the MATERIAL section of the GEOMETRY block but will be overridden by that data if it is present.

Suggested name	Units	Description
DENS *m*	(kg/m^3)	Density of barrier material *m*.

The next parameters define the porosities of the barrier materials. They must be present if this data is not defined in the MATERIAL section of the GEOMETRY block but will be overridden by that data if it is present. If the System Command USE_NUCLIDE_DEPENDENT_POROSITIES is present, then the porosity data **must** be entered here and **must not** be entered in the MATERIAL section of the GEOMETRY block. In this case the porosity for each nuclide, in each material must be entered.

If the System Command USE_NUCLIDE_DEPENDENT_POROSITIES is not present:

Suggested name	Units	Description
POR *m*	(–)	Porosity of barrier material *m*.

If the System Command USE_NUCLIDE_DEPENDENT_POROSITIES is present:

Suggested name	Units	Description
POR *nm*	(–)	Porosity of barrier for nuclide *n* in material *m*.

The next group of parameters defines the hole growth depending on the hole growth model chosen. For each step in the hole growth model a time and area must be given including the initial and final times.

Suggested name	Units	Description
T_HOLE *n*	(y)	Time at which following are is attained.
A_HOLE *n*	(m^2)	Area of hole.

For example if the hole growth model is a linear ramp from the initial size to the final size the following data would be given:

T_HOLE0 CONST (1.0E+3)
A_HOLE0 CONST(1.0E–6)
T_HOLE1 CONST(1.0E+6)
A_HOLE1 CONST(2.0E–3)

The next parameter defines the solubility of the nuclides:. If the system command USE_MATERIAL_DEPENDENT_SOLUBILITY_LIMITS is not present:

Suggested name	Units	Description
CSOL	(mol/m^3)	Solubility for the nuclides, one parameter for each nuclide *n*.

For example, if two nuclides (A and B) are used the definition would look like:

```
CSOLA CONST (2.0E–4)
CSOLB CONST (2.0E–5)
```

If the system command USE_MATERIAL_DEPENDENT_SOLUBILITY_LIMITS is present, then a solubility limit is required for each material. For example, if two materials, M1 and M2 are present, then the definition would look like:

```
CSOLAM1 CONST (2.0E–4)
CSOLBM1 CONST (2.0E–5)
CSOLAM2 CONST (2.0E–3)
CSOLBM2 CONST (2.0E–3)
```

The next parameters are repeated in the order stated below, for each material type in the model. Usually there are four materials used, *water*, *bentonite*, *sand-bentonite* and *rock*. For every material type, the data for every nuclide must be defined. Note that the order of nuclides as defined within the DATA section must be followed.

Suggested name	**Units**	**Description**
DIF *nm*	(m^2/year)	Effective diffusivity for nuclide *n* in material *m*.
KD *nm*	(m^3/kg)	K$_d$ for nuclide *n* in material *m*.

For example, if two nuclides (A and B) and four materials (1 to 4) are used the definition would look like:

```
# Specific to material 1
DIFA1 CONST (0.123E0)
DIFB1 CONST (0.123E0)
KDA1 CONST (0.0E0)
KDB1 CONST (0.0E0)
#
# Specific to material 2
DIFA2 CONST (0.3154E–2)
DIFB2 CONST (0.3154E–2)
KDA2 CONST (3.0E0)
KDB2 CONST (3.0E0)
#
# Specific to material 3
DIFA3 CONST (0.3154E–2)
DIFB3 CONST (0.3154E–2)
KDA3 CONST (0.1E0)
KDB3 CONST (0.1E0)
#
# Specific to material 4
DIFA4 CONST (3.1536E–6)
DIFB4 CONST (3.1536E–6)
KDA4 CONST (3.0E0)
KDB4 CONST (3.0E0)
```

Time-dependent Parameters

When it is necessary to incorporate time-dependent parameters into a system model, extra parameters must be specified that define the times at which ramp or step changes occur (see Section 2.3), and also the values of the various parameters in each of the different time regimes. Sorption coefficient, porosity, diffusion coefficient and solubility limit can all be made time dependent.

In order to explain the procedure for setting up time-dependent parameters in COMP23, it is easier to proceed with an example. Suppose, in the examples given above, it is desired to make the diffusion coefficient for nuclide A in material 1 piecewise-constant as shown in the figure in Section 2.3. It is first necessary to define the times T1, T2 and T3 in system. dsc. For example, this could be done as follows:

```
TIME_T1 CONST(1.0E2)
TIME_T2 CONST(1.0E4)
TIME_T3 CONST(1.0E5)
```

Next, it is necessary to define the values of the diffusion coefficient for the various time regimes. For example:

```
DIFA1T1 CONST (0.123E–2)
DIFA1T2 CONST (0.123E–1)
DIFA1T3 CONST (0.123E0)
```

For the non-time-dependent case described in the previous subsection, the INPAR section would contain the following lines in the appropriate place:

```
DIFA1      KDA1
DIFB1      KDB1
DIFA2      KDA2
DIFB2      KDB2
DIFA3      KDA3
DIFB3      KDB3
DIFA4      KDA4
DIFB4      KDB4
```

In the time-dependent example we are considering, the INPAR section would look as follows:

```
TIME_T1

DIFA1T1    KDA1
DIFB1      KDB1
DIFA2      KDA2
DIFB2      KDB2
DIFA3      KDA3
DIFB3      KDB3
DIFA4      KDA4
DIFB4      KDB4
```

```
TIME_T2
DIFA1T2     KDA1
DIFB1       KDB1
DIFA2       KDA2
DIFB2       KDB2
DIFA3       KDA3
DIFB3       KDB3
DIFA4       KDA4
DIFB4       KDB4
```

```
TIME_T3
DIFA1T3     KDA1
DIFB1       KDB1
DIFA2       KDA2
DIFB2       KDB2
DIFA3       KDA3
DIFB3       KDB3
DIFA4       KDA4
DIFB4       KDB4
```

It should be noted that it is necessary to define all of the parameters for all of the time regimes. In words, this INPAR section states that for times between 0 and T1, the diffusion coefficient takes a value DIFA1T1. Between times T1 and T2, it takes the value DIFA1T2. Between times T2 and T3 it takes the value DIFA1T3.

Time dependence for the porosity and solubility limits are set up in a very similar way, and the corresponding parts of the INPAR section of system.dsc must be written in the form shown above.

It is also necessary to specify, in the control block, the details of the form of the time dependence that is to be modelled (see Section 5.4.4, subtitle Control block definition).

Remaining Parameters

The next parameters give details of the modelled canister comprising a number of tubes surrounded by void space. The number of damaged tubes is specified here. They must be present if this data is not defined in the GEOMETRY block but will be overridden by that data if it is present.

Suggested name	Units	Description
VTUBE	(m^3)	Volume of water in one tube in the canister.
NTUBES	(–)	Total number of tubes in the canister.
NTDAM	(–)	Number of damaged tubes in the canister.
VOID	(m^3)	Water volume inside the canister.

The next parameter is the constant in the alpha-radiolysis model. It's exact meaning and units will depend on the model chosen, see Section 2.1.5. It is optional but must be present if alpha-radiolysis is modelled.

Suggested name	Units	Description
AER	(depends on model)	Alpha-radiolysis parameter *K* for chosen model (if required).

The next parameters define the sink data and must be present if this data is not defined in the SINK section of the GEOMETRY block but will be overridden by that data if it is present.

Suggested name	Units	Description
PLUG_LEN *n*	(m)	Length of the plug (extra resistance) added to the connection between compartment and sink *n*.
PLUG_AREA *n*	(m^2)	Cross-sectional area of the plug added to the connection between compartment and sink *n*. **This parameter must be positive.**
QFAC *n*	(–)	See below.
QEXP *n*	(–)	See below.

The QFAC and QEXP values are used to calculate the equivalent groundwater flow at the sink according to the formula:

$$Qeq = QFAC.\ \boldsymbol{q}^{QEXP}$$

where $\boldsymbol{q}$ is the groundwater flux at the canister position obtained from HYDRASTAR.

For example, if two sinks are used the definition would be as follows:

```
# Sink 1
PLUG_LEN1        CONST (5.0E–4)
PLUG_AREA1       CONST (5.5E–4)
QFAC1            CONST (0.03)
EQXP1            CONST (0.5)
#
# Sink 2
PLUG_LEN2        CONST (0.002)
PLUG_AREA2       CONST (0.006)
QFAC2            CONST (1.0)
EQXP2            CONST (0.5)
```

The next parameter defines the IRF for the nuclides in the model. Note that the order of nuclides as defined within the DATA section must be followed.

Suggested name	Units	Description
IRF *n*	(–)	Instantaneous Release Fraction for nuclide *n*. One value for each nuclide that uses a FUELSURFACE or alpha-radiolysis model.

For example, if two nuclides (A and B) are used the definition would look like:

```
# IRF values (only for FUELSURFACE or alpha-radiolysis models)
IRFA CONST (0.1E0)
IRFB CONST (0.1E0)
```

5.4.3 Input timeseries

As with the TULLGARN code, COMP23 needs to obtain the Darcy groundwater velocities outside the canister(s) as an input timeseries from another model.

There are three pseudo-timeseries that are to be supplied to COMP23. The pseudo-timeseries must be specified in the order below within the MODULE definition.

Suggested name	Units	Description
U0X	($m^3/m^2/yr$)	Darcy velocity of groundwater in first horizontal direction outside canister.
U0Y	($m^3/m^2/yr$)	Darcy velocity of groundwater in second horizontal direction outside canister.
U0Z	($m^3/m^2/yr$)	Vertical Darcy velocity of groundwater outside canister.

Note that the number of entries in the input time series is not equal to the sampled parameter MULTI. Normally when using HYDRASTAR to generate the input pseudo-timeseries, there is only one entry in the input pseudo-timeseries.

The input timeseries are defined in the MODULE definition in the system description file. The general syntax for the MODULE definition is:

MODULE [mod:]sub([pm1:ts1 [ts2 ...][, pm2: ...]];[tso1 [tso2 ...]])

END sub/mod

For example the module definition for a segment can look like:

```
MODULE COMP231:COMP23 (HYDR11: TS1HYDR11; TS1COMP23)
```

when the Macros:

```
MACRO TS1HYDR11 = UxC1 UyC1 UzC1
MACRO TS1COMP23 = QAC1 QBC1
```

have been defined earlier. In this example, water flow rates are taken as input timeseries from HYDRASTAR and output mass flow for the two nuclides are sent as output timeseries to a subsequent submodel, e.g. FARF31. The unit of mass flux is moles/year or Bq/year depending on the value of the keyword RELEASE_TYPE in the CONTROL BLOCK described below.

5.4.4 Module specific input data

COMP23 also needs a number of non-sampled parameters specified in the module specific DATA section within the module definition. The general syntax for the DATA section is:

DATA
GEOMETRY BLOCK
CONTROL BLOCK
END DATA

The DATA section for COMP23 is read in free format using the HUI input format, very similar to the input structure used for HYDRASTAR in *casename*.hyd.

The input in the DATA section to the COMP23 submodel is supplied as module-specific data and consists of two input data blocks. The input data blocks may appear in any order. Between the input data blocks, comment lines and system commands may be inserted in any order. The lines in the input file <u>must not exceed 71 characters</u>. The program ignores multiple white space. That is two or more consecutive occurrences of white-space characters. White space is defined as <blank> or <tab>. The general format of a block is described in Section 5.3.

The *block_id* identifies the current input data block. Valid input data block names are:

GEOMETRY	<u>Required</u> block. Contains definitions of compartments, sinks, materials, etc.
CONTROL	<u>Required</u> block. General description of calculation control parameters and nuclide definitions.

The {*block_definition*} holds data for the current input data block. It is constructed from a set of keywords with optional values assigned or special keyword constructs. The input data is case-insensitive regarding keywords. Filenames input may be case-sensitive depending on computer system requirements and is always case sensitive on UNIX systems.

Sub-blocks can also be included between blocks, for example the SINK sub-block is used within the GEOMETRY block.

CONTROL block definition

The general structure/syntax of the CONTROL block is given below. A description of each keyword is given.

Keyword	**Variable type**	**Comment**	
BEGIN_BLOCK CONTROL			
{*nuclidedef*}+			
RELEASE_TYPE	A*:itype	# ITYPE = [MOL|BQ]	
{*chaindef*}+			
TSTART	F*	# AGEO	>–SMALL
INCREMENT_FACTOR	F*	# RAT	>–SMALL
NUM_STEP	I*	# NTERM	>–SMALL
CONV_EPS	F*	# EPS	>–SMALL
EWT	F*	# EWT	>–SMALL
NLOOP	I*	# NLOOP	>–SMALL
CASENAME	A*	# CASE	
[ADVECTION]		# IWFLOW	
[SHARED_SOLUBILITY]		# ISPSOL	
[SOL_GROUPS]	A* itype	# ITYPE = [AUTO | MANUAL]	
{*solgroupdef*}+		# If SOL_GROUPS defined as MANUAL	
[AER_CONSTANT]		# }Only one AER keyword may be used	
[AER_DECAY]		# }for each problem	
[AER_EXPLICIT]		# }K1AER	
[NUM_SOL_LIMIT_STEP_NODES]	I*		
[NUM_SOL_LIMIT_RAMP_NODES]	I*		
[NUM_DIFF_KD_STEP_NODES]	I*		
[NUM_DIFF_KD__RAMP_NODES]	I*		

```
    [NUM_POROSITY_STEP_        I*
    NODES]
    [NUM_POROSITY_RAMP_        I*
    NODES]
END_BLOCK
#
nuclidedef = {
BEGIN_DEF NUCLIDE
    NAME                       A*           #  NAMES, for example I129
    HALF_LIFE                  F*           #  TAU                              > 0
    SOL_TYPE                   A*:ispec     #  ISPEC = [OWNSOL| FUELSURFACE | MATRIX]
    switch (SOL_TYPE)
    case (FUELSURFACE)
    case (MATRIX and one of the
    AER_ keywords used)
    IRF                        F*           #  CIRF
    endswitch
END_DEF
}
#
    {chaindef} = {
                               CHAIN MOTHER DAUGHTER+ END_CHAIN
}
    {solgroupdef} = {
                               SOLUBILITY_GROUP NUCLIDE+ END_SOLUBILITY_GROUP
}
```

RELEASE_TYPE	Units in which the results will be given. It is specified as MOL for molar units and Bq for activity units.
TSTART	Time for the first printed results.
INCREMENT_FACTOR	Ratio between two successive times in output timeseries.
NUM_STEP	Number of printouts required. For different reasons, the code sometimes needs to take smaller time increments than defined by INCREMENT_FACTOR. This can often create output time series with more time steps than defined by NUM_STEP.
CONV_EPS	On input, the requested relative accuracy in the calculations of the solver. EPS = 0 is allowed. On output, the adjusted relative accuracy if the input value was too small.
EWT	Problem zero, i.e. the smallest physically meaningful value for the solution.Setting EWT to zero provides pure relative error control.
NLOOP	Number of times the solver is called if there is no satisfactory solution.
CASENAME	Name for identifying model case. Used to define the names of input and output files.
ADVECTION	Optional keyword indicating if advection should be modelled. Not fully developed.
SHARED_SOLUBILITY	Optional keyword for shared solubilities.
SOL_GROUPS	[AUTO | MANUAL] How the shared solubility groups will be defined. AUTO means the groups are generated by COMP23 based on nuclide name. MANUAL means the used will specify them in the input file with the SOLUBILITY_GROUP keyword.

Three different models of alpha-radiolytically-induced spent fuel dissolution are available in COMP23. The models are described in Section 4 of this report. The models are selected by including a keyword-value pair in the CONTROL block of the system.dsc file; a different keyword is used to select each of the models and the AER parameter in the INPAR section must be set to the appropriate value of K. Only one of the keywords can be used for each simulation. If two or more of the keywords are found, an error message will be given and the code will stop.

AER_CONSTANT	The CONSTANT model is used (see Section 2.1.5)
AER_DECAY	The DECAY model is used (see Section 2.1.5)
AER_EXPLICIT	The EXPLICIT model is used (see Section 2.1.5)

For each of the three alpha-radiolysis models, U-238 must be defined as SOL_TYPE MATRIX and must be in the first group defined in the CONTROL block. Any nuclides that are assumed to dissolve congruently from the fuel matrix should also be defined as SOL_TYPE MATRIX. An IRF value must be included for each nuclide that is defined as SOL_TYPE MATRIX when an alpha-radiolysis model is used. When MATRIX is used without an alpha-radiolysis model, IRF values must not be specified. The alpha radiolysis model underestimates ingrowth of U-238. This is unlikely to introduce a significant error since the amount of U-238 will usually be much greater than the amount of the U-238 parent nuclide.

The final six parameters define the nature of any time dependences that are to be modelled.

NUM_SOL_LIMIT_STEP_NODES	Defines the number of piecewise-constant regions for modelling time-dependent solubility limits
NUM_SOL_LIMIT_RAMP_NODES	Defines the number of piecewise-linear regions for modelling time-dependent solubility limits
NUM_DIFF_KD_STEP_NODES	Defines the number of piecewise-constant regions for modelling time-dependent diffusion and sorption coefficients
NUM_DIFF_KD_RAMP_NODES	Defines the number of piecewise-linear regions for modelling time-dependent diffusion and sorption coefficients
NUM_POROSITY_STEP_NODES	Defines the number of piecewise-constant regions for modelling time-dependent porosities
NUM_POROSITY_RAMP_NODES	Defines the number of piecewise-linear regions for modelling time-dependent porosities

It should be noted that a parameter can be modelled as either piecewise constant or piecewise linear, but not both simultaneously. Therefore, for example, one cannot set both the NUM_SOL_LIMIT_STEP_NODES and NUM_SOL_LIMIT_RAMP_NODES in the same model simulation. The time dependence is either one or the other.

NUCLIDE DEFINITION

NAME	Name of the nuclide.
HALF_LIFE	Nuclide half-life.
SOL_TYPE	[OWNSOL| FUELSURFACE| MATRIX]. Dissolution model to use within the canisters. Use OWNSOL for nuclides that are not embedded in the fuel matrix, FUELSURFACE when only a fraction of the nuclide is available for release and MATRIX when nuclides are embedded in the fuel matrix. *All nuclides in a CHAIN-definition must have the same SOL_TYPE.* When MATRIX is used for any of the nuclides, the chain that contains U-238 must be the first chain defined in the CONTROL block.
IRF	Instantaneous release fraction for this nuclide. Only used when: (i) SOL_TYPE is set to FUELSURFACE or (ii) SOL_TYPE is set to MATRIX and an alpha-radiolysis model is used. Note: for the FUELSURFACE model, the IRF specified for the first nuclide in the chain is used for all nuclides in the chain.

Summary of data required for each dissolution model

Description	SOL_TYPE (note 1)	IRF	AER keyword
Dissolution rate controlled by the solubility of each radionuclide.	OWNSOL	No	No
Dissolution rate controlled by the solubility of each radionuclide. Only a fraction of the nuclide inventory is available for release.	FUELSURFACE	Yes (note 2)	No
Radionuclides dissolve congruently with the fuel.	MATRIX (note 3)	No	No
The fuel dissolution rate is controlled by a constant rate of alpha radiolysis. Radionuclides dissolve congruently with the fuel.	MATRIX (note 3)	Yes	AER_ CONSTANT
The fuel dissolution rate is controlled by a variable rate of alpha radiolysis. Decay of alpha emitters is represented in the model. Radionuclides dissolve congruently with the fuel. (note 4)	MATRIX (note 3)	Yes	AER_DECAY
The fuel dissolution rate is controlled by a variable rate of alpha radiolysis. Decay and transport of alpha emitters are represented in the model. Radionuclides dissolve congruently with the fuel. (notes 4 and 5)	MATRIX [note 3)	Yes	AER_ EXPLICIT

Notes:

1. All nuclides in a chain must have the same SOL_TYPE.
2. The IRF value specified by the user for the first nuclide in a chain will be used for all nuclides in that chain when the FUELSURFACE model is used.
3. The chain containing U238 must be the first chain defined. The U238 chain must be defined as SOL_TYPE MATRIX.
4. The expression used for this model is only valid for a specific fuel. See reference /5/ for more details.
5. One or more of the following nuclides must be included as SOL_TYPE MATRIX when this option is used: Am-241, Np-237, Pu-239, Pu-240.

CHAIN DEFINITION

CHAIN	Keyword indicating start of a decay chain.
MOTHER	The first modelled nuclide in a decay chain.
DAUGHTER	The nuclide(s) following in the decay chain. The list of the daughter nuclide must be given in the correct decay order for example:

For example, "CHAIN Am241 Np237 U233 Th229 END_CHAIN"

Where Am241 is modelled as the mother nuclide and Np237, U233 and Th229 are the daughter nuclides in the given order. The maximum number of nuclides in a chain is defined by parameter NUN (currently 6) and no nuclide can be defined in more than one CHAIN definition.

Limitations

A group is either a CHAIN or a single nuclide defined by BEGIN_DEF NUCLIDE but not used in any CHAIN definition. For example, defining the nuclides C14, I129 and the CHAIN:

"CHAIN Am241 Np237 U233 Th229 END_CHAIN" corresponds to 3 groups. C14 is one group, I129 is the second group and the CHAIN is the third group. It is very important to notice that every nuclide in a group *must* have the same SOL_TYPE.

SOLUBILITY GROUP DEFINITION

SOLUBILITY_GROUP	Keyword indicating start of a solubility group.
NUCLIDE	The nuclide(s) in a solubility group.

For example, "SOLUBILITY_GROUP Pu242 Pu240 END_ SOLUBILITY_GROUP"

The maximum number of nuclides in a group is defined by parameter NSGR (currently 25) and no nuclide can be defined in more than one SOLUBILITY_GROUP definition.

GEOMETRY block definition

The general structure/syntax of the GEOMETRY block is given below. A description of each keyword is given. The contents of the GEOMETRY block define which materials are included in the simulation, typically water, bentonite, sand-bentonite and rock. There are also keywords for describing the canister and its properties.

The basic entities for building a model with COMP23 are the model block. The use of the term "block" should not be confused with the input data blocks CONTROL and GEOMETRY. The model block consists of one or more connected compartments of the same material with identical properties. For example, the bentonite barrier around the canister can be divided in to several blocks, where each block can be compartmentalized or subdivided into compartments. Every model block is given an identification number that is later used to define the connections between the model blocks.

The connections between the model blocks are also given inside the GEOMETRY block. This defines which model blocks are connected to each other and can thus exchange nuclides. The final part of the GEOMETRY block is the SINK DEFINITIONs. This section defines the locations in the model where nuclides can escape from the near-field and the flow rates that the individual sinks should have.

Keyword	**Variable type**		**Comment**	
BEGIN_BLOCK GEOMETRY				
{*materialdef*}+				
{*blockdef*}+				
{*connectiondef*}+				
{*sinkdef*}+				
[TUBE_VOLUME]	F*	#	VTUBE	> 0
[NUM_ TUBE]	I*	#	NTUBES	> 0
[TUBES_DAMAGED]	I*	#	NTDAM	> –1
[VOID]	F*	#	VHEMA	> –SMALL
[NUM_RAMP_NODES]	I*	#	NNODE	
[NUM_STEP_NODES]		#	NNODE	
END_BLOCK				
#				
materialdef = {				
BEGIN_DEF MATERIAL		#	NMAT	
MATERIAL_NAME	A*:*mater*	#	MATNAM = [WATER; BENTONITE; SAND-BENTONITE; ROCK]	
[DENSITY]	F*	#	DENSM	> 0
[POROSITY]	F*	#	PORM	1> PORM > 0
END_DEF				
}				

```
#
Blockdef = {
BEGIN_DEF BLOCK                          #  NBLOCK
      BLOCK_NUMBER          I*           #  BLOCK
      MATERIAL_NAME         A*:mater     #  MATNAM = [WATER; BENTONITE;.
                                            SAND-BENTONITE; ROCK]
      NUM_Z_COMP            I*           #  NZ
      NUM_Y_COMP            I*           #  NY
      NUM_X_COMP            I*           #  NX
      [AREA_CHANGE]         A*:nbtd      #  NBTD = [NO| YES]
      {discretizationdef}+               #  Either 1 or NZ*NY*NX times
      [ADVECTION]                        #  IQFLOW
      Switch (IQFLOW)
      Case (TRUE):
      FLOW_RATE             F*           #  QFLOW
      INIT_CONC             F*           #  CINPUT
      INLET_NODE            I*           #  NWIN
      OUTLET_NODE           I*           #  NWOUT
      endswitch
Discretizationdef = {
      BEGIN_DEF DISCRETIZATION
          Z_LENGTH              F*             ZBLEN                 > 0
          Z_AREA                F*             ZBAR                  > 0
          Y_LENGTH              F*             YBLEN                 > 0
          Y_AREA                F*             YBAR                  > 0
          X_LENGTH              F*             XBLEN                 > 0
          X_AREA                F*             XBAR                  > 0
      END_DEF
END_DEF
}
#
Connectiondef = {–
BEGIN_DEF CONNECTION                     #  NCB
      FROM_BLOCK            I*           #  IBA                    > 0
         TO_BLOCK           I*           #  IBB                    > 0
      COUPLES               I*           #  NCON                   > 0
      FROM_DIRECTION        A*:irza      #  IRZA = [Z | Y | X]
         TO_DIRECTION       A*:irzb      #  IRZB = [Z | Y | X]
      FROM_RESISTANCE       A*:icra      #  ICRA = [FALSE| TRUE]
         TO_RESISTANCE      A*:icrb      #  ICRB = [FALSE| TRUE]
      [PLUG_POSITION]       A*:nplug     #  IPLUG, NPLUG = [NONE|
                                         FROM_BLOCK | TO_BLOCK]
      [EXTERNAL_RESIST]     A*:iradd     #  IRADD = [FALSE| TRUE]
      switch (IRADD)
      case TRUE:

      EXTERNAL_VALUE        F*           #  List of real values, one for each nuclide in the same order
                                            as in BEGIN_DEF NUCLIDE section END_LIST
      endswitch
      FROM_COMP             I*           #  IDCA
         TO_COMP            I*           #  IDCB
END_DEF
}

sinkdef = {
BEGIN_DEF SINK                           #  NSINKS
      FROM_BLOCK            I*           #  IBS
      FROM_COMP             I*           #  ICS
      DIRECTION             A*:irz       #  IRZ = [Z | Y | X]
      PLUG_AT_INLET         A*:icrs
                                         #  ICRS = [NO| YES]
```

```
    [PLUG_LENGTH]          F*          #  ZPFRA
    [PLUG_AREA]            F*          #  APFRA                         > 0.0
    [QEQ_FACTOR]           F*          #  QFAC                          > 0.0
    [QEQ_EXPONENT]         F*          #  QEXP                          > 0.0
END_DEF
}
outputdef = {
BEGIN_DEF OUTPUT                       #
    FROM_SINK              I*          #                                >0
END_DEF
}
#
```

GEOMETRY DEFINITION

TUBE_VOLUME	Water volume in one zircaloy tube.
NUM_TUBE	Number of tubes in the canister (source).
TUBES_DAMAGED	Number of tubes damaged in the canister (source).
VOID	Water volume inside the canister.

If these data are given they will override any data set in the INPAR block (see Section 5.4.2).

Note: The volume of the source is calculated by:

Volume = TUBE_VOLUME*TUBES_DAMAGED + VOID

[NUM_RAMP_NODES]	Hole grows linearly with this many defining points.
[NUM_STEP_NODES]	Hole grows as step functions with this many defining points.

If neither of these keywords are given then there is no hole growth and the appearance time and hole area are the first T_HOLE and A_HOLE data in the INPAR block (see Section 5.4.2).

Hole growth may be defined using only one of these keywords and its value must be set to 2 at present.

The start time and area and end time and area are given by data in the INPAR block.

MATERIAL DEFINITION

The MATERIAL definition is repeated once for each material used in the model.

MATERIAL_NAME	Defines the material type. Available options are [WATER| BENTONITE| SAND-BENTONITE| ROCK]
DENSITY	Density of the material.
POROSITY	Porosity of the material.

If density and porosity data are given they will override any data set in the INPAR block (see Section 5.4.2).

BLOCK DEFINITION

The BLOCK definition is repeated once for each block used in the model.

BLOCK_NUMBER	Block identity number, a unique integer number for each model block.
MATERIAL_NAME	Define the material in the present model block.
NUM_Z_COMP	Number of subdivisions in the z-axis directions. That is, the number of compartments vertically in this model block.
NUM_Y_COMP	Number of subdivisions in the y-axis. That is, the number of compartments in one horizontal direction in this model block. Usually, only one of NUM_Z_COMP, NUM_Y_COMP, NUM_X_COMP is greater than 1[1].
NUM_X_COMP	Number of subdivisions in the x-axis. That is, the number of compartments in one horizontal direction in this model block. Usually, only one of NUM_Z_COMP, NUM_Y_COMP, NUM_X_COMP is greater than 1[1].
[AREA_CHANGE	Optional keyword indicating the contact area of this model block will change size. Used to model increased hole size for the damage in the canister.
[ADVECTION]	Optional. Default is no advection.
[FLOW_RATE]	If ADVECTION selected, defines the flow of water through the block.
[INIT_CONC]	If ADVECTION selected, concentration in incoming water, usually zero. Can only be non-zero if only one nuclide is modelled.
[INLET_NODE]	If ADVECTION selected, node number for inlet.
[OUTLET_NODE]	If ADVECTION selected, node number for outlet.
Z_LENGTH	Diffusion length in the z-axis. The vertical length of the model block.
Z_AREA	Cross-sectional area for transport in the z-direction.
Y_LENGTH	Diffusion length for transport in the y-direction. One horizontal length of the model block.
Y_AREA	Cross-sectional area for transport in the y-direction.
X_LENGTH	Diffusion length for transport in the x-direction. One horizontal length of the model block.
X_AREA	Cross-sectional area for transport in the x-direction.

[1] If NUM_Z_COMP and one of NUM_X_COMP or NUM_Y_COMP are > 1 then compartment numbers loop fastest in the z-direction moving in the other direction once one lot of compartments have been numbered in the z-direction.

CONNECTION DEFINITION

FROM_BLOCK	Number (BLOCK_NUMBER) of the first model block in this connection.
TO_BLOCK	Number (BLOCK_NUMBER) of the second model block in this connection.
COUPLES	Number of connections or couples of compartments involved in the connection between two blocks. FROM_COMP and TO_COMP have to be repeated COUPLES times.
FROM_DIRECTION	Direction in which the transport of the species occurs from first block in connection. [Z | Y | X].
TO_DIRECTION	Direction in which the transport of the species occurs to second block in connection. [Z | Y | X].
FROM_RESISTANCE	Set to TRUE if the resistance from the first block is to be included in the coupling resistance and to FALSE otherwise.
TO_RESISTANCE	Set to TRUE if the resistance from the second block is to be included in the coupling resistance and to FALSE otherwise.

[PLUG_POSITION]	Addition of a plug (an extra transport resistance between the model blocks) between two blocks is indicated by an index block. A particular case is a small hole connected to a large compartment. For example, the couple formed by the hole in the canister wall and the bentonite compartment outside the canister. This keyword must give the number of the block with the largest capacity associated to the plug.
[EXTERNAL_RESIST]	Set to TRUE if there exist resistances added by the user and not defined by the code [FALSE| TRUE]. Normally set to FALSE.
[EXTERNAL_VALUE]	If EXTERNAL_RESIST is set to TRUE this keyword defines the list of values (one value for each nuclide) for resistances added by the user and not defined in the system.
FROM_COMP	The number for the compartment inside the first model block that is part of the connection. This and the next keyword have to be repeated as many times as defined by COUPLES.
TO_COMP	The number for the compartment inside the second model block that is part of the connection.

SINK DEFINITION

FROM_BLOCK	Number (BLOCK_NUMBER) of the model block in contact with the sink.
FROM_COMP	Number of the compartment in contact with the sink.
DIRECTION	Direction in which the transport of the species occurs. [Z | Y | X].
PLUG_AT_INLET	Contribution to the coupling resistance R_{SW} of the compartment in contact with the sink [NO| YES].
[PLUG_LENGTH]	Length of the plug (extra resistance) added to the connection between IDCS and the sink.
[PLUG_AREA]	Cross-sectional area of the plug added to the connection between compartment and the sink. **If this parameter is present it must be positive.**
[QEQ_FACTOR]	See below.
[QEQ_EXPONENT]	See below.

The QEQ_FACTOR and QEQ_EXPONENT values are used to calculate the equivalent groundwater flow at the sink according to the formula:

$Qeq = QFactor.\ \mathbf{q}Qexponent$

where ***q*** is the groundwater flux at the canister position obtained from HYDRASTAR.

If the PLUG_LENGTH, PLUG_AREA, QEQ_FACTOR and QEQ_EXPONENT data are given they will override any data set in the INPAR block (see Section 5.4.2).

OUTPUT DEFINITION

It is possible to produce more than one set of output time series from COMP23. If there are no OUTPUT BLOCKS present then the output from all the sinks is summed to give the total output for each nuclide. If one or more OUTPUT BLOCKS are present, then an output time series for each nuclide is produced for each BLOCK and the sinks contributing to the output are specifed in the OUTPUT BLOCK, as shown below.

FROM_SINK n	List of sinks connected to this output, one line per sink.

Limitations

The maximum number of material definitions that can appear in the system.dsc file is defined by the parameter MATER in file nvol23.inc. MATER is set to 4 in the latest version of COMP23.

The maximum number of block definitions that can appear in the system.dsc file is defined by the parameter NBOX in file nvol23.inc. NBOX is set to 10 in the latest version of COMP23.

The maximum number of connection definitions that can appear in the system.dsc file is defined by the parameter NVOL*2 in file nvol23.inc. NVOL is set to 20 in the latest version of COMP23.

The maximum number of sink definitions that can appear in the system.dsc file is defined by the parameter NPATH in file nvol23.inc. NPATH is set to 7 in the latest version of COMP23.

System commands

The SYSTEM_COMMANDS may be inserted in the input data at any point outside a block. The format of a SYSTEM_COMMAND is:

SYSTEM KEYWORD

The SYSTEM keywords available in the latest version of COMP23 are:

LIST_DICTIONARY	This command toggles the flag that controls listing of a dictionary[1] and the accompanying wordlists whenever a dictionary is loaded. A subsequent LIST_DICTIONARY command will turn the listing off. This option is off by default.
LIST_ALL_DICTIONARIES	At the instant the LIST_ALL_DICTIONARIES command is encountered, all dictionaries with accompanying wordlists will be listed.
IGNORE_FATAL_ERRORS	This command toggles the IFATDO flag. If a fatal error is encountered the program will stop if the flag is off. If the flag is on the program stops after reading all input data. The flag is off by default.
SAVE_SCRATCH_FILES	This command toggles the ISAVSC switch. It allows temporary files used by the code to be retained (they are normally deleted when the code finishes executing).
IGNORE_ERRORS	This command toggles the IGNERR flag. If an error is encountered (validity, consistency, syntax or existence) in the input data the program will stop after reading all input if the flag is off. If the flag is on the program continues. The flag is off by default.
SKIP_USER_INTERFACE	This command sets IGNERR flag to 1.
WRITE_INPUT_FILE	This flag is intended for debugging purposes. If turned on the code will generate a COMP23 input file of the old format (via routine WOFC23). That is a FORTRAN formatted data file. The flag is off by default.
NO_SIMULATION	This command sets the INOSIM flag to 1. This is not used in the latest version of COMP23.
READ_INVENTORY_IN_EACH_LOOP	This command causes the *casename*.inv file to be read for each simulation. When this flag is not set, the file will be read only once.

OUTPUT_DEBUG_FILES	This flag is intended for debugging purposes. If turned on, the code will generate four files that give the following information: a summary of the properties of the compartments, including capacitances and resistances; the release rate of each nuclide; the aqueous and solid amount of each nuclide; and, flow rate fractions for each nuclide. The flag will also cause debug information to be written to standard output.
SKIP_USER_INTERFACE	If this command is found the rest of the input data block is skipped and the code continues with the main COMP23 code.
USE_NUCLIDE_DEPENDENT_ POROSITIES	This command indicates that the porosities depend on the nuclides as well as the materials. When this command is present the porosities **must** be entered as parameters in the INPAR section of the input, one value for each nuclide in each material. They **must not** be entered in the geometry block.
USE_MATERIAL_DEPENDENT_ SOLUBILITY_LIMITS	This command indicates that the solubility limits depend on the materials as well as the nuclides. When this command is present the solubility limits **must** be entered as parameters in the INPAR section of the input, one value for each nuclide in each material.

[1] Whenever a new block is to be read, the dictionary for that block is loaded. The dictionary consists of the keywords and associated wordlists that are valid in the current block.

5.5 HUI output

All output is sent through the routine WLIN11. This means that currently all output is sent to the standard output. A description of the output format used by HUI is given in Appendix 2.

6 Example

6.1 Desription of problem

Release of U-238 and Pu-239 from the KBS-3 repository type will be calculated. A view of this repository is showed in Figure 6-1, including a view of the canister and the small hole in the canister wall. These nuclides escape from a copper/iron canister through a small hole into the bentonite by diffusion. In the bentonite, they migrate through various pathways into the water flowing in the rock. As this repository has been well described in several SKB-reports, details on this repository will not be given here.

6.2 Compartmentalization of the KBS-3 repository

The compartmentalization of the barrier system in the KBS-3 repository is made considering the geometry of the system and the materials through which the species are transported. The material, the transport properties and the dimensions of the compartment define the transport in a compartment. They are used by COMP23 to calculate the capacity of the compartment and the transport resistance in each transport direction. The capacity of a compartment includes the nuclide either in its water volume or sorbed in/on the solid. The volume of the compartment and the distribution coefficient K in the compartment determines this term. The diffusion coefficient, diffusion length(s) and cross-sectional area(s) of the compartment determine the transport resistance. These resistances are used to determine the nuclide flow rate between coupled compartments.

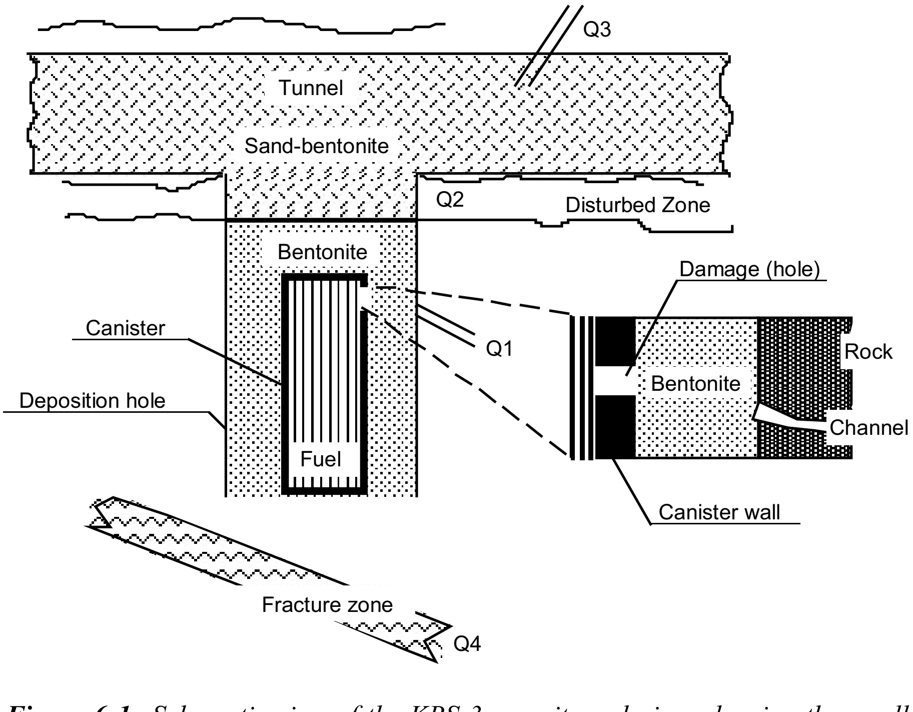


Figure 6-1. Schematic view of the KBS-3 repository design, showing the small hole in the canister and the location of the various escape routes.

In the compartmentalization, the geometry of the repository is simplified as shown in Figure 6-2 for the bentonite surrounding the canister. It is clear that errors are introduced in the solution given by COMP23, but these errors are minimized by an additional subdivision into a few compartments as is the case when the transport is controlled by sensitive points such as at the small hole in the canister wall for the KBS-3 repository.

Figure 6-3 shows the coarse discretization of the whole repository. A finer compartmentalization next to the hole in the canister wall (bentonite surrounding the canister) may be made in order to get a better accuracy in the calculations of the early release. This finer subdivision into two to four compartments is important for the short-lived nuclides /2/.

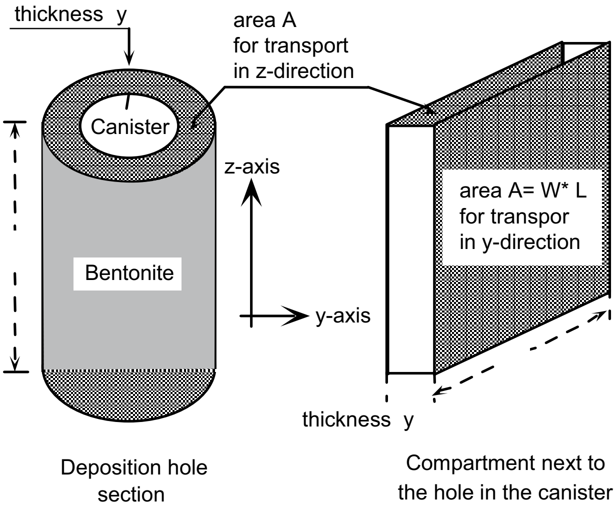


Figure 6-2. A schematic view of the simplification process of the volume of bentonite surrounding the canister into a compartment. W is an average dimension (width).

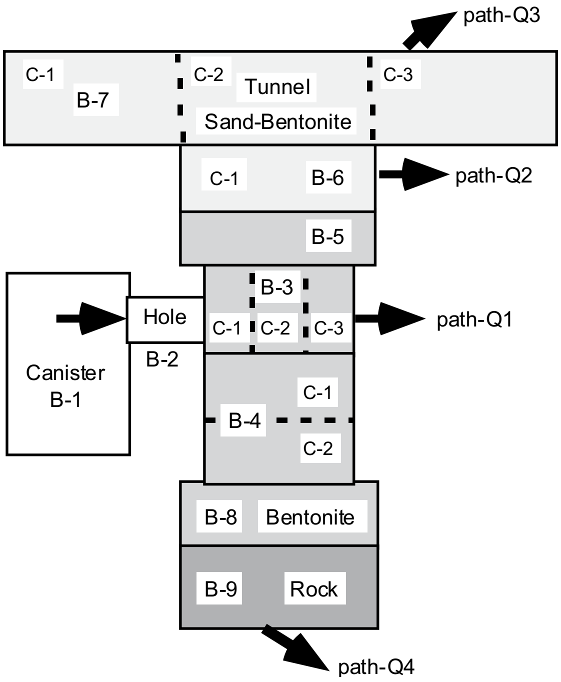


Figure 6-3. The coarse compartmentalization of the KBS-3 repository, where each rectangle is a compartment and the dash lines are finer divisions of the blocks. The arrows show the various pathways followed by the species from the canister to the flowing water. (Not to scale.)

6.3 Input file used for problem

The INPUT file to execute this sample problem is shown below; the results are shown in Figure 6-4 and 6-5.

This format of the INPUT file is valid for running COMP23 as a submodel of the PROPER package. The characteristic of this system is “to provide a module-type code package where submodels describing radionuclide transport, etc., are linked by the user and not by the programmer. The PROPER Monitor controls the execution given to the interconnected system of submodels”. Only the parts that belong to COMP23 are included in this example. The data used in the calculations are tabulated in Table 6-1.

System Description File system.dsc (applied to the PROPER system)

```
#  Input file in the PROPER system
#  U-238 and Pu-239, copper/iron canister, KBS-3.
BATCHES 1,1
SEED 930311
CPUTIME 00:15:00
VRMETHOD CMC:1
MACRO TS1HYDR11 = UxC1 UyC1 UzC1
#  ---------------------------------------------------
#  PARAMETERS
#  A and B... Denote nuclides;
#  1, 2, 3 , and 4....denote different materials
#  S1, S2, S3, and S4....denote Qeqs for the various sinks
#  Number of canisters (Standalone only)
     NCAN CONST ( 1 )
#  NUMBER OF IDENTICAL CANISTERS IN THIS STREAM TUBE
     CSYNC1  UNIF (0.  1.)
     MULTIS1 COMPUTED
#  Groundwater flux for NCAN canisters (standalone only)
     UC CONST( 1.0E-3 )
#  PROBABILITY FOR AN INITIALLY DAMAGED CANISTER
#  Probability that a canister is penetrated at emplacement
     PROB      CONST(1.E-3)
     PITFAQ    CONST(1.)
     QS        CONST(1.)
     CONHS     CONST(1.)
     DEFFS     CONST(1.)
#
#  Nuclide solubility, mol/m3
     CSOLA     CONST (2.0E-4)
     CSOLB     CONST (2.0E-5)
#
#  Specific data to Material. Dif m2/yr; kd m3/kg
#  1  WATER
#  2  BENTONITE
#  3  BENTONITE-SAND
#  4  ROCK
#
#  Specific to material 1
     DIFA1     CONST ( 0.123 )
     DIFB1     CONST ( 0.123 )
     KDA1      CONST ( 0.0 )
     KDB1      CONST ( 0.0 )
```

```
#
#  Specific to material 2
      DIFA2     CONST ( 0.003154 )
      DIFB2     CONST ( 0.003154 )
      KDA2      CONST ( 3.0 )
      KDB2      CONST ( 3.0 )
#
#  Specific to material 3
      DIFA3     CONST ( 0.003154 )
      DIFB3     CONST ( 0.003154 )
      KDA3      CONST ( 0.1 )
      KDB3      CONST ( 0.1 )
#
#  Specific to material 4
      DIFA4     CONST ( 3.1536E-6 )
      DIFB4     CONST ( 3.1536E-6 )
      KDA4      CONST ( 3.0 )
      KDB4      CONST ( 3.0 )
#
#  Hole growth data
   T_ZERO       CONST( 0.0 )
   A_ZERO       CONST( 5.0E-6 )
   T_LIMIT      CONST( 5.0E+3 )
   A_LIMIT      CONST( 0.1E-0 )

#  If any of the nuclides require IRF values,
#  they should specified here:
#  For example
#     IRFC14    CONST (0.5)
END PARAMETERS

# --------------------------------------------------------
MODULE COMP23 (HYDR11: TS1HYDR11 ; UB1 UB2)
INPAR
#  The parameters are numbered following the order indicated
   below
#  For instance:DIFA1 corresponds to GETP(5)
      NCAN
      CSYNC1
      MULTIS1
      UC
      PROB
#     PITFAQ    QS              CONHS           DEFFS
      T_ZERO    A_ZERO          T_LIMIT         A_LIMIT
      CSOLA     CSOLB
      DIFA1     DIFB1           KDA1            KDB1
      DIFA2     DIFB2           KDA2            KDB2
      DIFA3     DIFB3           KDA3            KDB3
      DIFA4     DIFB4           KDA4            KDB4
#
#  Any nuclides with an IRF must have one parameter for the
   IRF value.
#  These should be the last items in the INPAR section
END INPAR
```

```
#
#  DATA
#
#  Input file for COMP23 with HUI
#  U-238 and Pu-239, copper/iron canister, KBS-3.
#
SYSTEM WRITE_INPUT_FILE
#
BEGIN_BLOCK GEOMETRY
   VOID                        1.0
   TUBE_VOLUME                 4.655E-5
   NUM_TUBE                    1440
   TUBES_DAMAGED               1440
   NUM_STEP_NODES              2
#
#   ------ Materials definition
   BEGIN_DEF MATERIAL
     MATERIAL_NAME             WATER
     DENSITY                   1000.0
     POROSITY                  1.0
   END_DEF
   BEGIN_DEF MATERIAL
     MATERIAL_NAME             BENTONITE
     DENSITY                   2700.0
     POROSITY                  0.25
   END_DEF
   BEGIN_DEF MATERIAL
     MATERIAL_NAME             SAND-BENTONITE
     DENSITY                   2280.0
     POROSITY                  0.24
   END_DEF
   BEGIN_DEF MATERIAL
     MATERIAL_NAME             ROCK
     DENSITY                   2700.0
     POROSITY                  0.005
   END_DEF
#
#   ------ Blocks definition
   BEGIN_DEF BLOCK
     BLOCK_NUMBER              1
     MATERIAL_NAME             WATER
     NUM_Z_COMP                1
     NUM_Y_COMP                1
     NUM_Y_COMP                1
     AREA_CHANGE               NO
     BEGIN_DEF DISCRETIZATION
       Z_LENGTH                0.0E+0
       Z_AREA                  1.0E+0
       Y_LENGTH                0.0E+0
       Y_AREA                  1.0E+0
       X_LENGTH                0.0E+0
       X_AREA                  1.0E+0
     END_DEF
   END_DEF
```

```
BEGIN_DEF BLOCK
   BLOCK_NUMBER                 2
   NUM_Z_COMP                   1
   NUM_Y_COMP                   1
   NUM_X_COMP                   1
   AREA_CHANGE                  YES
   MATERIAL_NAME                WATER
   BEGIN_DEF DISCRETIZATION
     Z_LENGTH                   5.0E-2
     Z_AREA                     5.0E-6
     Y_LENGTH                   0.0E+0
     Y_AREA                     1.0E+0
     X_LENGTH                   0.0E+0
     X_AREA                     1.0E+0
   END_DEF
END_DEF
BEGIN_DEF BLOCK
   BLOCK_NUMBER                 3
   NUM_Z_COMP                   1
   NUM_Y_COMP                   3
   NUM_X_COMP                   1
   AREA_CHANGE                  NO
   MATERIAL_NAME                BENTONITE
   BEGIN_DEF DISCRETIZATION
     Z_LENGTH                   0.5E+0
     Z_AREA                     5.13E-1
     Y_LENGTH                   1.17E-1
     Y_AREA                     1.8E+0
     X_LENGTH                   0.0E+0
     X_AREA                     1.0E+0
   END_DEF
   BEGIN_DEF DISCRETIZATION
     Z_LENGTH                   0.5E+0
     Z_AREA                     5.13E-1
     Y_LENGTH                   1.17E-1
     Y_AREA                     2.2E+0
     X_LENGTH                   0.0E+0
     X_AREA                     1.0E+0
   END_DEF
   BEGIN_DEF DISCRETIZATION
     Z_LENGTH                   0.5E+0
     Z_AREA                     5.13E-1
     Y_LENGTH                   1.17E-1
     Y_AREA                     2.6E+0
     X_LENGTH                   0.0E+0
     X_AREA                     1.0E+0
   END_DEF
END_DEF
BEGIN_DEF BLOCK
   BLOCK_NUMBER                 4
   NUM_Z_COMP                   2
   NUM_Y_COMP                   1
   NUM_X_COMP                   1
   AREA_CHANGE                  NO
   MATERIAL_NAME            BENTONITE
   BEGIN_DEF DISCRETIZATION
      Z_LENGTH              4.333E+0
      Z_AREA                1.539E+0
      Y_LENGTH              0.0E+0
      Y_AREA                1.0E+0
      X_LENGTH              0.0E+0
      X_AREA                1.0E+0
   END_DEF
END_DEF
BEGIN_DEF BLOCK
   BLOCK_NUMBER             5
   NUM_Z_COMP               1
   NUM_Y_COMP               1
   NUM_X_COMP               1
   AREA_CHANGE              NO
   MATERIAL_NAME            BENTONITE
   BEGIN_DEF DISCRETIZATION
      Z_LENGTH              1.5E+0
      Z_AREA                2.405E+0
      Y_LENGTH              0.0E+0
      Y_AREA                1.0E+0
      X_LENGTH              0.0E+0
      X_AREA                1.0E+0
   END_DEF
END_DEF
BEGIN_DEF BLOCK
   BLOCK_NUMBER             6
   NUM_Z_COMP               1
   NUM_Y_COMP               1
   NUM_X_COMP               1
   AREA_CHANGE              NO
   MATERIAL_NAME            SAND-BENTONITE
   BEGIN_DEF DISCRETIZATION
      Z_LENGTH              1.0
      Z_AREA                2.405E+0
      Y_LENGTH              0.875E+0
      Y_AREA                4.95E+0
      X_LENGTH              0.0E+0
      X_AREA                1.0E+0
   END_DEF
END_DEF
BEGIN_DEF BLOCK
   BLOCK_NUMBER             7
   NUM_Z_COMP               3
   NUM_Y_COMP               1
   NUM_X_COMP               1
   AREA_CHANGE              NO
   MATERIAL_NAME            SAND-BENTONITE
   BEGIN_DEF DISCRETIZATION
      Z_LENGTH              2.125E+0
      Z_AREA                1.224E+1
      Y_LENGTH              1.97E+0
      Y_AREA                2.64E+01
```

```
        X_LENGTH               0.0E+0
        X_AREA                 1.0E+0
     END_DEF
     BEGIN_DEF DISCRETIZATION
        Z_LENGTH               1.75E+0
        Z_AREA                 1.224E+1
        Y_LENGTH               1.97E+0
        Y_AREA                 2.17E+01
        X_LENGTH               0.0E+0
        X_AREA                 1.0E+0
     END_DEF
     BEGIN_DEF DISCRETIZATION
        Z_LENGTH               2.125E+0
        Z_AREA                 1.224E+1
        Y_LENGTH               1.97E+0
        Y_AREA                 2.64E+01
        X_LENGTH               0.0E+0
        X_AREA                 1.0E+0
     END_DEF
  END_DEF
  BEGIN_DEF BLOCK
        BLOCK_NUMBER           8
        NUM_Z_COMP             1
        NUM_Y_COMP             1
        NUM_X_COMP             1
     AREA_CHANGE               NO
     MATERIAL_NAME             BENTONITE
     BEGIN_DEF DISCRETIZATION
        Z_LENGTH               0.5E+0
        Z_AREA                 2.405E+0
        Y_LENGTH               0.0E+0
        Y_AREA                 1.0E+0
        X_LENGTH               0.0E+0
        X_AREA                 1.0E+0
     END_DEF
  END_DEF
  BEGIN_DEF BLOCK
        BLOCK_NUMBER           9
        NUM_Z_COMP             1
        NUM_Y_COMP             1
        NUM_X_COMP             1
     AREA_CHANGE               NO
     MATERIAL_NAME             ROCK
     BEGIN_DEF DISCRETIZATION
        Z_LENGTH               3.0
        Z_AREA                 2.405E+0
        Y_LENGTH               0.0E+0
        Y_AREA                 1.0E+0
        X_LENGTH               0.0E+0
        X_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             Y
      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                     3
      FROM_DIRECTION              Z
         TO_DIRECTION             Z
      FROM_RESISTANCE             TRUE
         TO_RESISTANCE            TRUE
      PLUG_POSITION               NONE
      EXTERNAL_RESIST             FALSE
      FROM_COMP                   1
         TO_COMP                  1
      FROM_COMP                   2
         TO_COMP                  1
      FROM_COMP                   3
         TO_COMP                  1
   END_DEF
   BEGIN_DEF CONNECTION
      FROM_BLOCK                  3
         TO_BLOCK                 5
      COUPLES                     3
      FROM_DIRECTION              Z
         TO_DIRECTION             Z
      FROM_RESISTANCE             TRUE
         TO_RESISTANCE            TRUE
      PLUG_POSITION               NONE
   EXTERNAL_RESIST          FALSE
   FROM_COMP                1
      TO_COMP               1
   FROM_COMP                2
      TO_COMP               1
   FROM_COMP                3
      TO_COMP               1
END_DEF
BEGIN_DEF CONNECTION
   FROM_BLOCK               5
      TO_BLOCK              6
   COUPLES                  1
   FROM_DIRECTION           Z
      TO_DIRECTION          Y
   FROM_RESISTANCE          TRUE
      TO_RESISTANCE         TRUE
   PLUG_POSITION            NONE
   EXTERNAL_RESIST          FALSE
   FROM_COMP                1
      TO_COMP               1
END_DEF
BEGIN_DEF CONNECTION
   FROM_BLOCK               6
      TO_BLOCK              7
   COUPLES                  1
   FROM_DIRECTION           Z
      TO_DIRECTION          Y
   FROM_RESISTANCE          TRUE
      TO_RESISTANCE         TRUE
   PLUG_POSITION            NONE
   EXTERNAL_RESIST          FALSE
   FROM_COMP                1
      TO_COMP               2
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
   PLUG_POSITION            NONE
   EXTERNAL_RESIST          FALSE
   FROM_COMP                2
      TO_COMP               1
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
      PLUG_POSITION            NONE
      EXTERNAL_RESIST          FALSE
      FROM_COMP                1
         TO_COMP               1
   END_DEF
#
#   ------ Sink definition
#
   BEGIN_DEF SINK
      FROM_BLOCK               3
      FROM_COMP                3
      DIRECTION                Y
      PLUG_AT_INLET            NO
      PLUG_LENGTH              5.0E-4
      PLUG_AREA                5.5E-4
      QEQ_FACTOR               0.25
      QEQ_EXPONENT             1.0
   END_DEF
   BEGIN_DEF SINK
      FROM_BLOCK               6
      FROM_COMP                1
      DIRECTION                Y
      PLUG_AT_INLET            YES
      PLUG_LENGTH              0.0
      PLUG_AREA                1.0
      QEQ_FACTOR               4.0
      QEQ_EXPONENT             1.0
   END_DEF
   BEGIN_DEF SINK
      FROM_BLOCK               7
      FROM_COMP                3
      DIRECTION                Y
      PLUG_AT_INLET            NO
      PLUG_LENGTH              5.0E-4
      PLUG_AREA                5.97E-3
      QEQ_FACTOR               0.5
      QEQ_EXPONENT             1.0
   END_DEF
   BEGIN_DEF SINK
      FROM_BLOCK               9
      FROM_COMP                1
      DIRECTION                Z
      PLUG_AT_INLET            YES
      PLUG_LENGTH              0.0
      PLUG_AREA                1.0
      QEQ_FACTOR               6.0
      QEQ_EXPONENT             1.0
   END_DEF
END_BLOCK
#
BEGIN_BLOCK CONTROL
   CASENAME                    sr95test
   RELEASE_TYPE                Bq
   TSTART                      5.0
   INCREMENT_FACTOR            2.5
   NUM_STEP                    50
   CONV_EPS                    1.0E-6
   EWT                         1.0E-18
   NLOOP                       3
#  An AER_keyword would appear in this block.
   BEGIN_DEF NUCLIDE
      NAME                     U238
      HALF_LIFE                4.47E9
      SOL_TYPE                 OWNSOL
   END_DEF
   BEGIN_DEF NUCLIDE
      NAME                     PU239
      HALF_LIFE                2.41E4
      SOL_TYPE                 OWNSOL
   END_DEF
END_BLOCK
#
END DATA

   STATISTICS
#
   END STATISTICS
#
END COMP23
```

6.4 Results

The predicted release by COMP23 for U-238 and Pu-239 are shown in Figures 6-4 and 6-5 respectively. These releases were calculated assuming that the only limitation for the nuclides to be released is the solubility, i.e. the solubility limit approach (OWNSOL type).

Table 6-1. Data used in the calculations of the release.

Data on the KBS-3 repository design		
Deposition hole	Diameter (mm)	1,750
	Length (mm)	7,833
Canister	Diameter (mm)	1,050
	Thickness (mm)	50
	Length (mm)	4,833
Tunnel	Width (mm)	3,400
	Height (mm)	4,000
Distance between canister centres (mm)		6,000
Canister bottom to deposition hole bottom (mm)		500
Thickness of the disturbed zone (mm)		1,000
Deposition hole bottom to fracture zone (mm)		3,000

Hydraulic properties				
Gradient (m/m)			$3\cdot10^{-3}$	
Fracture aperture (mm)			0.1	
	path-Q1	path-Q2	path-Q3	path-Q4
Flow porosity	$2\cdot10^{-5}$	10^{-3}	$1.7\cdot10^{-5}10^{-3}$	10^{-3}
Conductivity (m/s)	10^{-9}	10^{-7}	10^{-9}	10^{-6}
Flux (m3/m2, year)	$9.5\cdot10^{-5}$	$9.5\cdot10^{-3}$	$9.5\cdot10^{-5}$	$9.5\cdot10^{-2}$
Qeq (l/year)	0.25	4	0.5	6

Material properties			
	Bentonite	Sand-bentonite	Rock
Density (kg/m^3)	2,700	2,280	2,700
Porosity (%)	25	24	0.5

Data on transport properties								
			Bentonite		Sand-bentonite		Rock	
Nuclide	Solubility	Half-life	D_e	K_d	D_e	K_d	D_e	K_d
	(mol/l)	(yr)	(m^2/s)	(m^3/kg)	(m^2/s)	(m^3/kg)	(m^2/s)	(m^3/kg)
U-238	10^{-4}	$4.47\cdot10^{9}$	10^{-10}	3.0	10^{-10}	0.1	10^{-13}	3.0
Pu-239	10^{-5}	24,100	10^{-10}	3.0	10^{-10}	0.1	10^{-13}	3.0

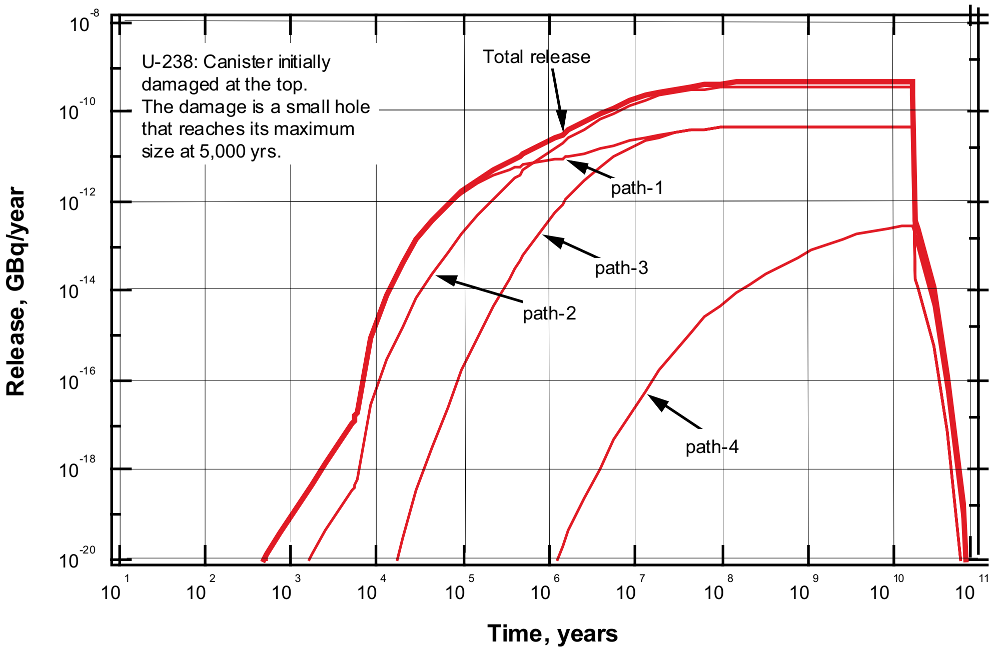


Figure 6-4. *Release of U-238 from the repository for a copper/iron canister with a suddenly rupture of the canister at 10^3 years after deposition. See Figure 6-1 or 6-3 for the location of the various paths.*

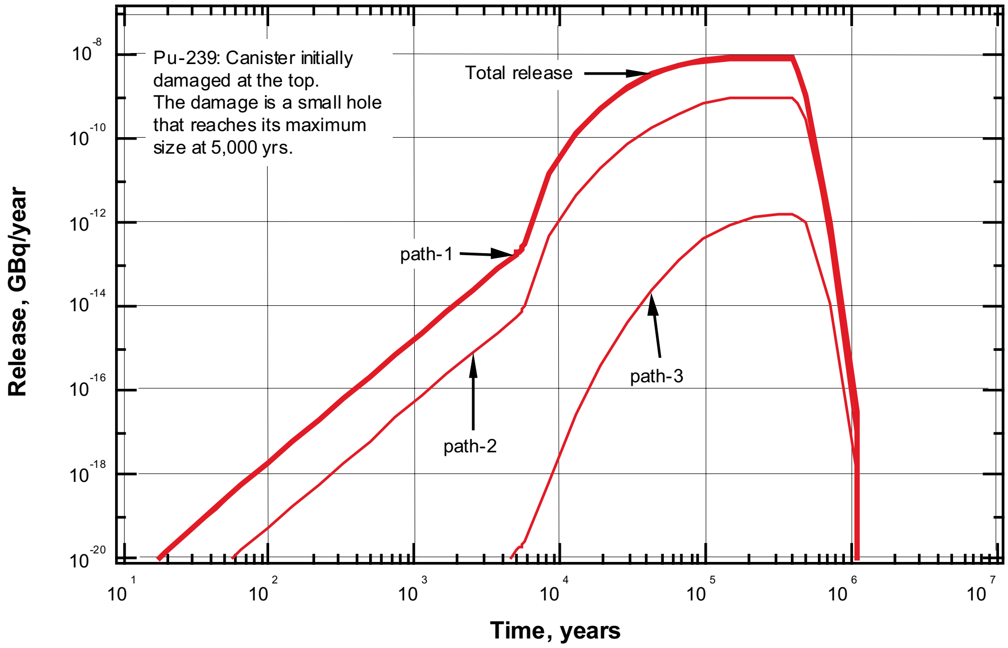


Figure 6-5. *Release of Pu-239 from the repository for a copper/iron canister with a suddenly rupture of the canister at 10^3 years after deposition. See Figure 6-2 or 6-3 for the location of the various paths.*

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/14/ "TULLGARN User's Guide".

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Appendix 1

Notation

a^n	amount of nuclide *n* per unit volume	mol/m^3
$\hat{a}^n$	amount of nuclide *n* in the canister not embedded in matrix	mol
a_E^T	total amount of element *E* per unit volume	mol/m^3
$\hat{a}_E^T$	total amount of element E in the canister not embedded	mol
A_w	area	m^2
b^n	amount of nuclide *n* embedded in the fuel matrix	mol
c	concentration	mol/m^3
c^n	concentration of nuclide *n*	mol/m^3
$\hat{c}^n$	concentration of nuclide *n* in the water in the canister	mol/m^3
c_E^S	solubility limit for element *E*	mol/m^3
D_e^n	effective diffusivity for nuclide *n*	m^2/year
D_w	diffusivity in free water	m^2/year
f^n	rate at which nuclide *n* is leaving the canister by diffusion	mol/year
$g_{i,j}$	transport coefficient linking compartments *i* and *j*	m^3/year
k_E^d	sorption coefficient for element *E*	m^3/kg
K_E	distribution coefficient for element *E*	–
l_w	diffusion length	m
N	dissolution rate or molar flow rate	mol/year
q^M	dissolution rate of fuel matrix	mol/year
q_α^M	dissolution rate of fuel matrix due to alpha radiolysis	mol/year
q_d^M	rate at which uranium leaves the canister	mol/year
Q_{eq}	equivalent flow rate	m^3/year
R	resistance to transport	years/m^3
r	radius	m
S_E	set of nuclides in solubility group for element *E*	–
S_U	set of nuclides that are isotopes of uranium	–
t	time	year
t_w	residence time	year
$\mathbf{u}_0$	flux of water	m^3/m^2/year
W	width	m
V	volume	m^3

Greek

ϕ_E	porosity for element *E*	–
λ	decay constant	year^{-1}
δ	fracture aperture	m
$\bar{\eta}$	mean penetration thickness	m
ρ	density	kg/m^3

Appendix 2

HUI output

The HUI output starts with the following lines of output:

```
==========================================================================
HYDRASTAR User Interface - Initialize
Opened unit nn as file:
filename
==========================================================================
```

and ends with the following lines of output:

```
==========================================================================
HYDRASTAR User Interface Error Report
    Number of validity          errors : nv
    Number of consistency       errors : nc
    Number of existence         errors : ne
    Number of syntax            errors : nv
Input data is correct. Continuing ...
==========================================================================
```

Output from the various input BLOCKs read are initiated by the following lines:

```
==========================================================================
=  Start of block : block_identifier       =
============================================================
```

and ended by:

```
============================================================
=  End of block : block_identifier         =
============================================================
```

Between these two sets there exists four types of output:

- Input line echoing.
- Input data echoing.
- Error messages.
- Definition block IO**.**

Definition block IO are initiated by the following lines:

```
---------------------------------------------------------------------------
-  Start of definition : definition_identifier      -
----------------------------------------------------------------------------
```

and ended by:

```
---------------------------------------------------------------------------
-  End of definition : definition_identifier        -
---------------------------------------------------------------------------
```

Between these two sets there exists three types of output:

- Input line echoing.
- Input data echoing.
- Error messages.

Input data echoing and error messages are explained in the following section

Input line echoing has the form of:

```
Line nnn: The comment stripped left-justified valid input line
```

where nnn is the line number of the line read in the input file. The line numbers include blank lines and comment lines.

Input data echoing

Input data echoing takes the form:

```
================ Keyword assignments are :

Keyword <KEYWORD1> assigned value(s) : value1 value2 ...
Keyword <KEYWORDn> assigned value(s) : value1 value2 ...

================ End of Keyword assignments
```

The value list may continue over several lines. For keywords assigned filenames, the filenames are just listed in the order they were read separated by one blank.

Error messages

There are five types of error reports and one warning report.

Validity errors: If the values read for a specific keyword do not lie within the specified limits, the following message will be displayed:

```
******* VALIDITY error has occurred in routine ROUTINE

after reading line HUINL.
Check failed for CBOUN keyword <KEYWORD>.
Upper bound  Lower Bound    Input value
u.uuuuE+ee  l.llllE+ee      r.rrrrE+ee/iiiiiii

******* End of Error
```

where

- ROUTINE is the name of the routine that read the data.
- HUINL is the number of lines, including blank and comment lines, that have been read.
- CBOUN may be ”upper bound in”, ”lower bound in” or ”” (empty string)
- KEYWORD is the name of the keyword.
- Upper bound is the specified upper limit.
- Lower bound is the specified lower limit.
- REAL is the real value that has been read for the keyword.
- INT is the integer value that has been read for the keyword.

The last line is repeated for all values that have been read for the particular keyword.

Consistency errors: If a required keyword, or an optional keyword that depends on the value assigned to a required keyword, has not been found in the input file, the following message will be displayed:

******** CONSISTENCY error has occurred in routine ROUTINE after reading line HUINL.*
These are:
Keyword <KEYWORD> Not set. Tok :TOKEN
Keyword <KEYWORD> Not set. Tok :TOKEN
depend on <KEYWORD=WORD> which has been set. Tok:TOKEN
Setting keyword <KEYWORD> has no effect
it depend on <KEYWORD=WORD> which has not been set.

******** End of Error*

where

- ROUTINE is the name of the routine that read the data.
- HUINL is the number of lines, including blank and comment lines, that have been read.
- KEYWORD is the name of a keyword.
- TOKEN is the token value for the keyword, see ”HYDRASTAR USER INTERFACE – Programmers reference”.
- WORD is the word in a wordlist applicable to the keyword (see the Input Data Chapter).

Existence errors: If any of the files in a list of files specified for a specific keyword does not exist the following message will be displayed:

******** EXISTENCE error has occurred in routine ROUTINE after reading line HUINL.*
Check failed for keyword <KEYWORD>.
File:(filename) Exist:YON

******** End of Error*

where

- ROUTINE is the name of the routine that read the data.
- HUINL is the number of lines, including blank and comment lines, that have been read.
- KEYWORD is the name of the keyword.
- filename is the name of a file specified.
- YON may be either ”YES” or ”NO” (It may be YES since all files are listed if one or more files do not exist).

The last line is repeated for all files specified in the file list for the particular keyword.

Syntax errors: If a syntax error has occurred the following message will be displayed:

******** SYNTAX error has occurred in routine ROUTINE after reading line HUINL.*

where

- ROUTINE is the name of the routine that read the data.
- HUINL is the number of lines, including blank and comment lines, that have been read.

System errors: A system error may be over-indexed arrays, etc. This type of error should not be very common to the normal user. If a system error has occurred the following message will be displayed:

******** SYSTEM error has occurred in routine ROUTINE after reading line HUINL.*

where

- ROUTINE is the name of the routine that read the data.
- HUINL is the number of lines, including blank and comment lines, that have been read.

Warnings: A warning is a note to the user that there may something wrong in the input.
A warning does not terminate the program. If a warning has occurred the following message will be displayed:

******* *WARNING in routine ROUTINE after reading line HUINL.*

where

- ROUTINE is the name of the routine that read the data.
- HUINL is the number of lines, including blank and comment lines, that have been read.