

The COUPLEX Test Cases : Nuclear Waste Disposal Simulation*

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Abstract

The COUPLEX models are a set of realistic test cases aimed at simulating the transport of nuclides around a nuclear waste repository. They consist in three different models :

The first test case is to compute a simplified Far Field model used in nuclear waste management simulation. From the mathematical point of view the problem is of convection diffusion type but the parameters are highly varying from one layer to another. Another particularity is the very concentrated nature of the source, both in space and in time.

The second test case is based on a Near Field computation, taking into account the glass dissolution of vitrified waste, and the congruent release of several nuclides (including filiation chains), with their transport through the geological barrier.

The aim of the third test case is to use the results of the Near Field computation (COUPLEX 2) to describe the behavior of the nuclide source term in the Far Field computation (COUPLEX 1). This test case is more open than the previous two, as the way the coupling should be effected is not a priori specified.

1 COUPLEX 1: Far Field Computation

1.1 Introduction

The repository lies at a depth of 450m (meters) inside a clay layer which has above it a layer of limestone and a layer of marl and below it is a layer of dogger limestone. Water flows slowly (creeping flow) through these porous media and convects the radioactive materials once the containers leak; there is also a dilution effect which in mathematical terms is similar to diffusion. The problem has two main difficulties:

*This version groups together the three separate documents that were submitted to the Scientific Community in January 2001, and incorporates some corrections suggested by the participants to the test cases

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1. The radioactive elements leak from the containers, into the clay, over a period that is small compared with the millions of years over which convection and diffusion are active.
2. The convection and diffusion constants are very different from one layer to another; for instance, in the clay layer there is almost no convection while, in the other layers, diffusion and convection are both important.

1.2 The Geometry

In this first test case, the computation is restricted to a 2D section of the disposal site. Thus, the computational domain is in a rectangle $\mathcal{O} = (0, 25000) \times (0, 695)$ in meters. The layers of dogger, clay, limestone, and marl are located as follows (with the origin taken at the bottom left corner of the rectangle):

- dogger $0 < z < 200$
- clay lies between the horizontal line $z = 200$ and the line from $(0, 295)$ to $(25000, 350)$
- limestone lies between the line from $(0, 295)$ to $(25000, 350)$ and the horizontal line $z = 595$
- marl $595 < z < 695$.

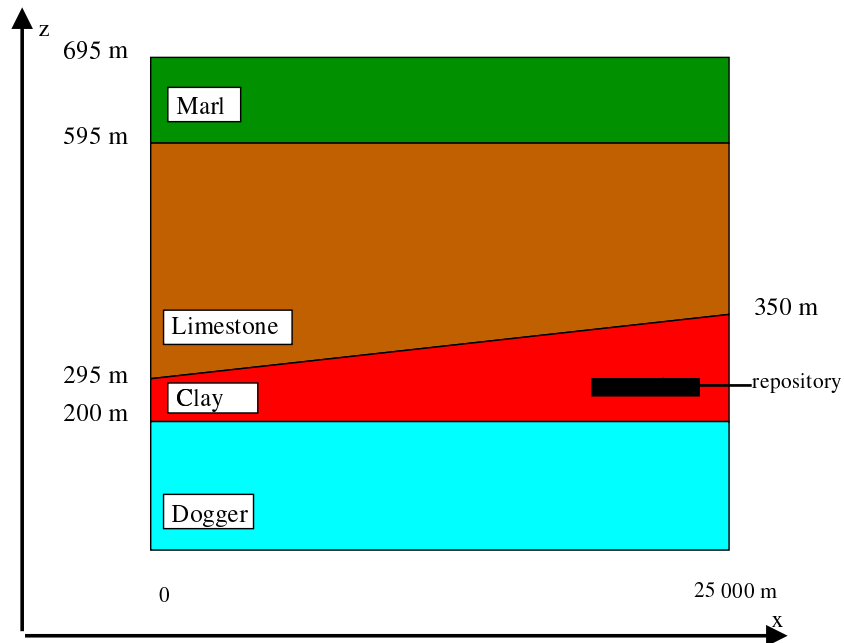


Figure 1: *Geometry of computational domain*

The repository, denoted by R , is modeled by a uniform rectangular source in the clay layer:

$$R = \{(x, z) \in (18440, 21680) \times (244, 250)\}$$

The geometry is summarized on figure 1 below. For this domain the computation should be carried for $t \in (0, T)$ with $T = 10^7$ years.

1.3 The Flow

It is assumed that all rock layers are saturated with water and that boundary loads are stationary so that the flow is independent of time. Darcy's law gives the velocity \mathbf{u} in terms of the hydrodynamic load $H = P/\rho g + z$:

$$\mathbf{u} = -K\nabla H \quad (1.1)$$

where the permeability tensor K , assumed constant in each layer is given in Table 1, P is the pressure and g is Newton's constant. Conservation of mass ($\nabla \cdot (\rho \mathbf{u}) = 0$, with the density ρ assumed constant) implies that

$$\nabla \cdot (K\nabla H) = 0 \quad \text{in } \mathcal{O} \quad (1.2)$$

	Marl	Limestone	Clay	Dogger
K (m/year)	3.1536e-5	6.3072	3.1536e-6	25.2288

Table 1: *Permeability tensor in the four rock layers*

On the boundary, conditions are:

$$\begin{aligned} H &= 289 && \text{on } \{25000\} \times (0, 200), \\ H &= 310 && \text{on } \{25000\} \times (350, 595), \\ H &= 180 + 160x/25000 && \text{on } (0, 25000) \times \{695\}, \\ H &= 200 && \text{on } \{0\} \times (295, 595), \\ H &= 286 && \text{on } \{0\} \times (0, 200), \\ \frac{\partial H}{\partial n} &= 0 && \text{elsewhere.} \end{aligned}$$

1.4 The Radioactive Elements

We are considering two species of particular interest, Iodine 129 and Plutonium 242. Both escape from the repository cave into the water and their concentrations $C_i, i = 1, 2$ is given by two independent convection-diffusion equations:

$$R_i \omega \left(\frac{\partial C_i}{\partial t} + \lambda_i C_i \right) - \nabla \cdot (\mathbf{D}_i \nabla C_i) + \mathbf{u} \cdot \nabla C_i = f_i \quad \text{in } \mathcal{O} \times (0, T) \quad i = 1, 2. \quad (1.3)$$

where

- R_i is the latency Retardation factor, with value 1 for ^{129}I , 10^5 for ^{242}Pu in the clay and 1 elsewhere for both Iodine and Plutonium;
- the effective porosity ω , is equal to 0.001 for ^{129}I , 0.2 for ^{242}Pu in the clay layer and 0.1 elsewhere for both;
- $\lambda_i = \log 2/T_i$ with T_i being the half life time of the element : $1.57 \cdot 10^7$ for ^{129}I , $3.76 \cdot 10^5$ for ^{242}Pu (in years);
- The effective diffusion/dispersion tensors \mathbf{D}_i for any species $i = 1, 2$ depend on the Darcy velocity as follows:

$$\mathbf{D}_i = d_{ei}I + |\mathbf{u}| [\alpha_{li}E(\mathbf{u}) + \alpha_{ti}(I - E(\mathbf{u}))]$$

with

$$E_{kj}(\mathbf{u}) = \frac{u_k u_j}{|\mathbf{u}|^2}.$$

and with the coefficients, assumed constant in each layer, given in Table 2 below.

	^{129}I			^{242}Pu		
	$de_1(\text{m}^2/\text{year})$	$\alpha_L(\text{m})$	$\alpha_T(\text{m})$	$de_2(\text{m}^2/\text{year})$	$\alpha_L(\text{m})$	$\alpha_T(\text{m})$
Dogger	5.0e-4	50	1	5.0e-4	50	1
Clay	9.48e-7	0	0	4.42e-4	0	0
Limestone	5.0e-4	50	1	5.0e-4	50	1
Marl	5.0e-4	0	0	5.0e-4	0	0

Table 2: Diffusion/dispersion coefficients for the radioactive elements in the 4 layers

In this test case, the values of the source terms f_i , ($i = 1, 2$) in the repository R are given in tabulated form in separately provided data files. The source terms are assumed to be spatially uniformly spread out in all the repository R . It is assumed that there is no source outside the repository (f_i , ($i = 1, 2$) in $\mathcal{O} \setminus \bar{R}$). The dependence in time is shown on figure 2, for illustrative purposes. The structure of the data file is described in appendix A.

1.5 Initial and Boundary Conditions

We call time zero the time when the containers begin to leak and the radioactive elements to spread, hence the initial values of the concentration C_i are zero at time zero.

Boundary conditions for the transport of any nuclide $i = 1, 2$ are

$$\begin{aligned} \frac{\partial C_i}{\partial n} &= 0 && \text{on } \{0\} \times (295, 595) \\ \frac{\partial C_i}{\partial n} &= 0 && \text{on } \{0\} \times (0, 200) \\ \mathbf{D}_i \nabla C_i \cdot \mathbf{n} - C_i \mathbf{u} \cdot \mathbf{n} &= 0 && \text{on } (0, 25000) \times \{0\} \\ C_i &= 0 && \text{elsewhere on the boundary.} \end{aligned}$$

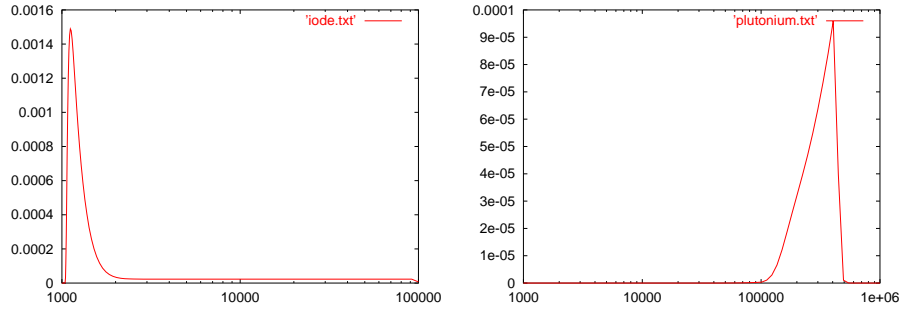


Figure 2: *Release of Iodine and Plutonium as a function of time*

where \mathbf{n} is the outward normal to the vertical line $\{0\} \times \{0, 695\}$

1.6 Output requirements

The following output quantities are expected from the simulations(both tables and graphical representations):

- Contour levels of C_i at times 200, 10110, 50110, 10^6 , 10^7 years (the following level values should be used: 10^{-12} , 10^{-10} , 10^{-8} , 10^{-6} , 10^{-4});
- Pressure field (10 values uniformly distributed between 180 and 340);
- Darcy velocity field, along the 3 vertical lines given by $x = 50$, $x = 12500$, $x = 20000$, using 100 points along each line;
- Places where the Darcy velocity is zero;
- Cumulative total flux through the top and the bottom clay layer boundaries, as a function of time;
- Cumulative total fluxes through the left boundaries of the dogger and limestone layers;
- The discretization grid of the domains and the time stepping used in the simulations should also be given.

2 COUPLEX 2: Near Field Computation

2.1 Introduction

This test case aim is to present a situation, dwelling more on numerical difficulties than on the physics itself. It still strives to stay close to real situations.

The computation is based on the Near Field modeling of 3 alveoli linked by a backfill region embedded into a homogeneous medium. The dissolution of glass, the ensuing congruent emission of radio-nuclides, and precipitation elements when several isotopes are included in the model.

2.2 Mathematical model

2.2.1 Geometry

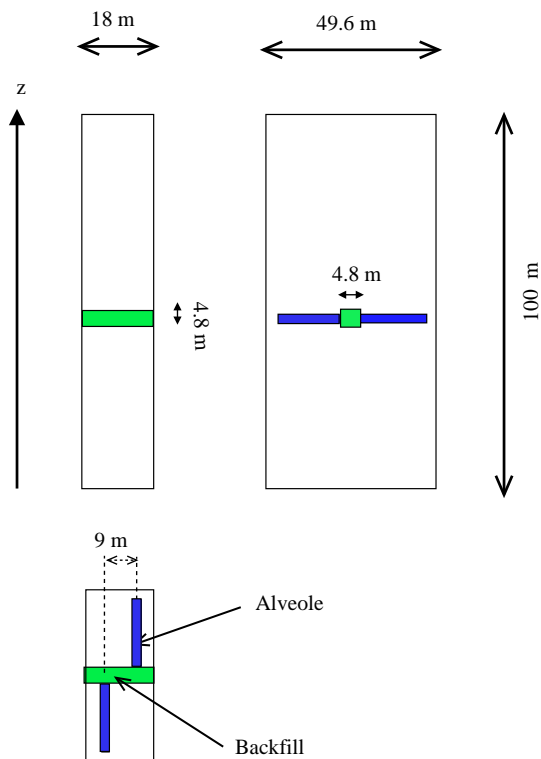


Figure 3: *Details of the simulation domain R^* , (left, front and top views) including host geological medium, backfill and alveolus*

A real repository is made up of a very large number of disposal modules, each disposal module includes a large number of alveoli, linked by backfill. Modeling all the details of such a repository still presents difficulties and we follow a usual approach in safety computations: we only consider an “elementary cell”, and we add periodicity conditions on the boundaries. This

last assumption is valid provided there is a large enough number of similar alveoli in a disposal module, and provided the module boundary layer effects are negligible.

We choose the geometry of such an elementary cell to be simple and the host geological medium to be simply made up of the clay layer into which the repository is embedded.

We describe in the following the elementary cell by successive zooms. The domain (“elementary cell”) is a parallelepiped R^* , containing 3 alveoli and a backfill. An alveolus is made up of the container (in the present case, a parallelepiped made of glass, containing the radioactive waste), a buffer and a seal.

Figure 3 shows global views of the whole domain R^* , while figure 4 shows a close-up view of the backfill with 3 alveoli, and figure 5 shows a detailed view of one alveolus.

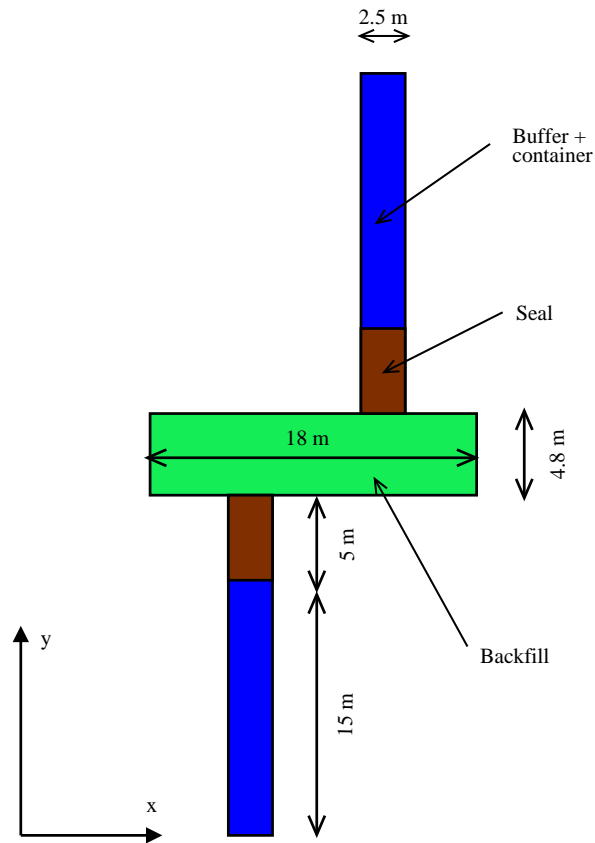


Figure 4: *Backfill and 3 alveoli included in the host geological medium*

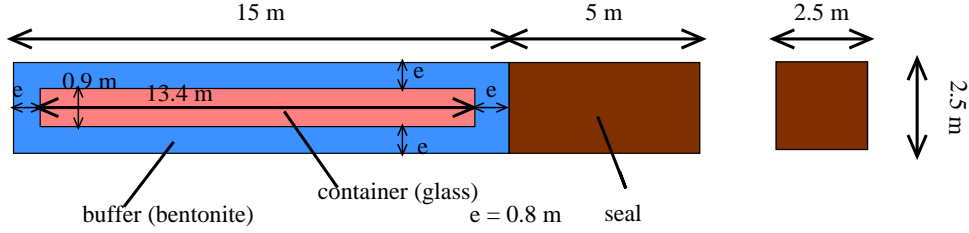


Figure 5: *Dimensions of an alveolus*

2.2.2 Flow model

We consider a saturated porous medium, such that Darcy's law holds. The piezometric charge H (m), (with $H = \frac{P}{\rho g} + z$, P is the pressure) solves the equation

$$-\nabla \cdot (K \nabla H) = 0 \quad \text{in the cell domain } R^* \quad (2.1)$$

where K (m/s) is the permeability tensor.

The boundary conditions are

- H is given on the 2 horizontal sides of R^* . The difference in piezometric head is taken equal to 50 m;
- The container is impervious, thus the boundary condition on the container boundary is no-flow: $\frac{\partial H}{\partial n} = 0$ there;
- H is supposed to be periodic on the 4 vertical sides of R^* (so as to simulate a whole disposal module).

According to Darcy's law in R^* , the flow velocity is given by:

$$\mathbf{u} = -K \nabla H. \quad (2.2)$$

2.2.3 The general transport operator

We are making use of the following notations later on. First we associate to any element species or isotope an index k , that will take the values $k = s, 0, 1, 2, -1, -2$ according to the convention in table 4 below. Then we define the transport operator in the cell domain R^* except the container \bar{C} by:

$$L_k(C_k) = -\nabla \cdot (\mathbf{D}_k \nabla C_k - \mathbf{u} C_k) \quad \text{in } R^* \setminus \bar{C}, \quad (2.3)$$

where \mathbf{D}_k is the diffusion–dispersion tensor, given by:

$$\mathbf{D}_k = d_k I + |\mathbf{u}| [\alpha_{lk} E(\mathbf{u}) + \alpha_{tk} (I - E(\mathbf{u}))] \quad (2.4)$$

with

$$E_{ij}(\mathbf{u}) = \frac{u_i u_j}{|\mathbf{u}|^2}. \quad (2.5)$$

For any species or isotope k , d_k (m²/s) is the effective diffusion coefficient, α_{lk} and α_{tk} are the longitudinal and transverse dispersion coefficients (both in meters).

2.2.4 Transport of silica

Transport of silica is described by a convection–diffusion–reaction type equation:

$$\phi R_s \frac{\partial C_s}{\partial t} + L_s(C_s) = \rho_p \frac{\nu_p}{\lambda_p} \left(1 - \frac{C_s}{S_p}\right) \quad \text{in } R^* \setminus \bar{\mathcal{C}}, \quad (2.6)$$

where ϕ is the porosity, and the retardation factor R_s is given by (ρ_{solid} being the density of the solid phase and the distribution coefficient K_{ds} taking adsorption into account in a simplified way):

$$R_s = 1 + \rho_{\text{solid}} \frac{1 - \phi}{\phi} K_{ds}.$$

We have denoted by

- ρ_p : the precipitate concentration (4.2 10⁴ mole/m³);
- ν_p : the precipitation speed (6 10⁻⁹ m/year);
- λ_p : the inverse of specific surface (between 8 10⁻¹⁰ m and 10⁻³ m);
- S_p : the precipitated phase solubility (5.4 10⁻¹ mol/m³).

Precipitation of silica follows a first order kinetic law.

We propose two different models for the dissolution of glass. A detailed model of glass dissolution follows a first order kinetic law. The complete free boundary model associated to the dissolution of the container \mathcal{C} is simplified into a Fourier boundary condition on $\partial\mathcal{C}$, the glass-bentonite interface assuming that this interface remains fixed:

$$-\mathbf{D}_s \frac{\partial C_s}{\partial n} = \rho_m \nu_m \left(1 - \frac{C_s}{S_m}\right), \quad \text{on } \partial\mathcal{C}; \quad (2.7)$$

where we have set:

- ν_m , the initial dissolution velocity (1.5 10⁻⁵ m/year);
- ρ_m , the available concentration that can be dissolved in the matrix (4.2 10³ mol/m³);
- S_m , the maximal silica concentration (or saturated silica concentration), (8.2 10⁻¹ mole/m³).

Alternatively, a simplified model of glass dissolution could be used, reduced to a known constant flux on the glass-bentonite interface:

$$-\mathbf{D}_s \frac{\partial C_s}{\partial n} = \tau, \quad \text{on } \partial \mathcal{C}; \quad (2.8)$$

with the release factor $\tau = 10^{-2} \text{mol/m}^2/\text{year}$. Note that this simplification will in turn make the congruent emission of nuclides simpler in eq. (2.18) in section 2.2.5 below.

The initial concentration in silica is taken equal to its reference value in the geologic medium, $9.9 \cdot 10^{-5} \text{ mole/l}$. The boundary and interface conditions are :

- On the container boundaries, the condition is that given in (2.7) above;
- $C_s = 0$ on the top and bottom boundaries of R^* ;
- Periodic boundary conditions on the 4 outer vertical sides of $R^* \setminus \bar{\mathcal{C}}$.

2.2.5 Nuclide transport

We take into account one isolated nuclide, Cesium 135, and two nuclide chains $^{238}\text{Pu} \rightarrow ^{234}\text{U}$ and $^{242}\text{Pu} \rightarrow ^{238}\text{U}$. This choice lets us study element-wise precipitation. The periods are :

^{135}Cs	^{238}Pu	^{234}U	^{242}Pu	^{238}U
$2.3 \cdot 10^6 \text{ years}$	87.74 years	$2.45 \cdot 10^5 \text{ years}$	$3.76 \cdot 10^5 \text{ years}$	$4.47 \cdot 10^9 \text{ years}$

Table 3: Nuclide periods

To make writing the equations easier, we associate to each nuclide an index k in the following way:

isotope	^{135}Cs	^{238}Pu	^{234}U	^{242}Pu	^{238}U
index k	0	1	-1	2	-2

Table 4: Nuclide-Index association

For instance, for $k = 1$ or $k = 2$, element k is by definition the father of element $-k$. Isotope -1 and -2 correspond to the same chemical element, as do isotopes 1 and 2.

Each nuclide satisfies a convection-diffusion-reaction equation analogous to (2.6), obviously with an added radioactive decay term. It can possibly precipitate.

As far as Cesium (index $k = 0$) is concerned, we shall assume that adsorption follows a Langmuir isotherm, and that the solubility limit is so high that Cesium does not precipitate. Following (2.4), the corresponding transport equation becomes:

$$\phi \frac{\partial}{\partial t} (R_0 C_0) + L_0(C_0) + \phi R_0 \lambda_0 C_0 = 0 \quad \text{in } R^* \setminus \bar{\mathcal{C}} \quad (2.9)$$

where the retardation factor now depends on the concentration

$$R_0 = 1 + \rho_{\text{solid}} \frac{1 - \phi}{\phi} K_{d_0} \quad (2.10)$$

through the (concentration dependent) distribution coefficient

$$K_{d_0} = \frac{\kappa \text{CEC}}{1 + \kappa C_0}. \quad (2.11)$$

In the previous equation, $\kappa = 150 \text{ (mol/l)}^{-1}$ and CEC is the Cationic Exchange Capacity (CEC = 80 mmol/100g).

On the contrary, since Plutonium and Uranium may precipitate, we introduce the concentration of the solid phase, denoted by F_k , $k = -2, -1, 1, 2$. The transport of each isotope is described by the following equations:

- For $k = 1$ and 2 :

$$\rho\phi R_k \frac{\partial C_k}{\partial t} + \rho L_k(C_k) + \rho\phi R_k \lambda_k C_k = \rho\phi S_k \quad \text{in } R^* \setminus \bar{C} \quad (2.12)$$

$$\rho_{\text{solid}}(1 - \phi) \frac{\partial F_k}{\partial t} + \rho_{\text{solid}}(1 - \phi) \lambda_k F_k = -\phi S_k \quad \text{in } R^* \setminus \bar{C} \quad (2.13)$$

- For $k = -1$ and -2 :

$$\rho\phi R_k \frac{\partial C_k}{\partial t} + \rho L_k(C_k) + \rho\phi R_k \lambda_k C_k - \rho\phi R_{-k} \lambda_{-k} C_{-k} = \rho\phi S_k \quad \text{in } R^* \setminus \bar{C} \quad (2.14)$$

$$\rho_{\text{solid}}(1 - \phi) \frac{\partial F_k}{\partial t} + \rho_{\text{solid}}(1 - \phi) \lambda_k F_k - \rho_{\text{solid}}(1 - \phi) \lambda_{-k} F_{-k} = -\phi S_k \quad \text{in } R^* \setminus \bar{C} \quad (2.15)$$

In (2.12)– (2.15), the retardation factor R_k is still given by an isotherm similar to (2.10)

$$R_k = 1 + \rho_{\text{solid}} \frac{1 - \phi}{\phi} K_{d_k}$$

but with a constant coefficient K_{d_k} .

In (2.12)– (2.15), the dissolution-precipitation term S_k takes into account precipitation per species, by assuming that each isotope precipitates in proportion to its mass concentration. The dissolution-precipitation term is given by

$$S_k = \begin{cases} \sigma(C_k - C_k^{\text{sat}}) & \text{if } C_k^{\text{sat}} \leq C_k \\ 0 & \text{if } C_k \leq C_k^{\text{sat}} \text{ and } F_k = 0 \end{cases} \quad (2.16)$$

where

$$C_k^{\text{sat}} = C_{e(k)}^{\text{sat}} \frac{\phi R_k C_k + \rho_{\text{solid}}(1 - \phi) F_k}{\sum_{\substack{|k'|=1,2 \\ k' \text{ has same} \\ \text{sign as } k}} (\phi R_{k'} C_{k'} + \rho_{\text{solid}}(1 - \phi) F_{k'})}, \quad (2.17)$$

with C_e^{sat} , $e \in \{\text{Pu}, \text{U}\}$ being the solubility limit of the considered species, and $e(1) = e(2) = \text{Pu}$, $e(-1) = e(-2) = \text{U}$, and $\sigma = 10^4 \text{ year}^{-1}$.

The dissolution of glass causes a congruent emission of the nuclides still present in the waste. Taking into account the radioactive decay of the nuclides leads to a boundary condition with time dependent coefficients:

$$\mathbf{D}_k \frac{\partial C_k}{\partial n} = \frac{N_k(t)}{N_s^0} \mathbf{D}_s \frac{\partial C_s}{\partial n}, \quad k = -1, 1, 0, 1, 2 \quad (2.18)$$

on the glass–bentonite interface $\partial \bar{\mathcal{C}}$ (supposed fixed as in (2.7)). The constant N_s^0 is the initial number of moles of silica in the container, and is equal to $N_s^0 = 4.56 \cdot 10^4$ (the density of silica in the container is equal to the number ρ_m that appears in eq. (2.7)).

Note that in case the simplified model of glass dissolution given in eq. (2.8) is used, eq. (2.18) simplifies to:

$$\mathbf{D}_k \frac{\partial C_k}{\partial n} = \tau \frac{N_k(t)}{N_s^0}, \quad k = -1, 1, 0, 1, 2 \quad (2.19)$$

with $\tau = 10^{-2} \text{ mol/m}^2/\text{year}$.

The functions $N_k(t)$ are the number of moles of the corresponding element at time t . They are solution of a coupled set of differential equations expressing the decay of the element under consideration. A simple computation gives the expression for $N_k(t)$:

$$\begin{cases} N_k(t) = N_k^0 e^{-\lambda_k t}, & k = 0, 1, 2 \\ N_k(t) = N_{-k}^0 \frac{\lambda_{-k}}{\lambda_k - \lambda_{-k}} e^{-\lambda_{-k} t} + \left(N_k^0 + N_{-k}^0 \frac{\lambda_{-k}}{\lambda_{-k} - \lambda_k} \right) e^{-\lambda_k t}, & k = -1, -2 \end{cases} \quad (2.20)$$

The constants N_k^0 (initial values of the number of mole for each nuclide) are given in table 5 below. They were computed from the (known) activities for each nuclide, as detailed in Appendix B. These numbers are valid for one alveolus.

Isotope	^{135}Cs	^{238}Pu	^{234}U	^{242}Pu	^{238}U
Number of moles	41.6	$2.01 \cdot 10^{-2}$	$1.40 \cdot 10^{-2}$	$2.03 \cdot 10^{-2}$	21.1

Table 5: *Initial number of moles for the 5 nuclides in one alveolus*

2.2.6 Remarks

The simulation should cover a period of 10^6 years.

Boundary conditions for the nuclides are as follows:

- As given in (2.18) above on the container boundary $\partial \mathcal{C}$;
- $C_k = 0$, $k = -2, -1, 1, 2$ on the top and bottom sides of the elementary cell R^* ;
- Periodic boundary conditions on the 4 outer vertical sides of R^* .

2.3 Output requirements

The following output quantities are expected from the simulations (both tables and graphical representations):

- Total fluxes for all nuclides on the top and bottom horizontal boundaries of R^* , as a function of time;
- Total fluxes through the seal – backfill interfaces, as a function of time;
- Total fluxes through the buffer – seal interfaces, as a function of time;
- Total fluxes through the backfill – geological medium interfaces, as a function of time;
- Concentration profiles for all nuclides along the 2 symmetry planes, at times $10^2, 10^3, 5 \times 10^2, 10^4, 10^5, 10^6$ years;
- Total cumulative concentration of dissolved silica as a function of time;
- Exact time at which the total initial amount of silica has been dissolved;
- Total cumulative precipitation for each element, each isotope, as a function of time.

2.4 Physical coefficients

Note the the buffer and the seal are actually the same material.

	buffer	backfill	geological medium
permeability K (m/s)	10^{-13}	10^{-9}	10^{-13}
porosity ϕ (%)	25	40	15
solid density ρ_{solid}	1.8	2.1	2.1

Table 6: *General physical properties*

silica ($k = s$)	buffer	backfill	geological medium
effective diffusion coeff. d_s (m^2/s)	$5 \cdot 10^{-11}$	$2 \cdot 10^{-10}$	$5 \cdot 10^{-11}$
longitudinal dispersion coeff. α_{l_s} (m)	0	0	0
transverse. dispersion coeff. α_{t_s} (m)	0	0	0
distribution coeff. K_{d_s} (m^3/kg)	10^{-4}	10^{-4}	10^{-4}

Table 7: *Physical properties for the silica*

Cesium ($k = 0$)	buffer	backfill	geological medium
effective diffusion coeff. d_0 (m ² /s)	$5 \cdot 10^{-11}$	$2 \cdot 10^{-10}$	$5 \cdot 10^{-11}$
longitudinal dispersion coeff. α_{l0} (m)	0	5	5
transverse. dispersion coeff. α_{t0} (m)	0	1	1
Distribution coeff. K_{d0} (m ³ /kg)	cf. eq. (2.11)	10^{-3}	10^{-3}

Table 8: *Physical properties for Cesium*

plutonium ($k = 1$ or 2)	buffer	backfill	geological medium
effective diffusion coeff. d_k (m ² /s)	$5 \cdot 10^{-11}$	$2 \cdot 10^{-10}$	$5 \cdot 10^{-11}$
longitudinal dispersion coeff. α_{lk} (m)	0	5	5
transverse dispersion coeff. α_{tk} (m)	0	1	1
distribution coeff. K_{dk} (m ³ /kg)	3	$8.5 \cdot 10^{-3}$	$8.5 \cdot 10^{-3}$
solubility limit C_k^{sat} (mol/l)	$4 \cdot 10^{-9}$	$4 \cdot 10^{-9}$	$4 \cdot 10^{-9}$

Table 9: *Physical properties for Plutonium*

uranium ($k = -1$ or -2)	buffer	backfill	geological medium
effective diffusion coeff. d_k (m ² /s)	$5 \cdot 10^{-11}$	$2 \cdot 10^{-10}$	$5 \cdot 10^{-11}$
longitudinal dispersion coeff. α_{lk} (m)	0	5	5
transverse. dispersion coeff. α_{tk} (m)	0	1	1
distribution coeff K_{dk} (m ³ /kg)	3	$1.7 \cdot 10^{-2}$	$1.7 \cdot 10^{-2}$
solubility limit C_k^{sat} (mol/l)	$2 \cdot 10^{-9}$	$2 \cdot 10^{-9}$	$2 \cdot 10^{-9}$

Table 10: *Physical properties for Uranium*

3 COUPLEX3: Coupling Near and Far Fields

3.1 Introduction

The aim of that final test case is to use the results of the Near Field computation (COUPLEX2) to describe the behavior of the nuclide source term f_i in the Far Field computation (COUPLEX1, eq. (1.3)). In this way, we could include as much as possible of the repository behavior, coming from a Near Field computation, inside the nuclide source term f_i necessary for a Far Field simulation.

The coupling in between the two simulations should then allow possible Near Field / Far Field retroactions.

This test case is more open than the previous two, and the way the coupling should be effected is not a priori specified, and is left up the participants.

The results of the COUPLEX2 Test case on a cell R^* (dimension $27\text{ m} \times 100\text{ m} \times 49.6\text{ m}$) have to be used to define the source behavior of the 2D repository R (dimension $3240\text{ m} \times 6\text{ m}$), as in figure 1 in COUPLEX1 section 1.2, and equation (1.3). The simulation period is $T = 10^7$ years, as in COUPLEX1.

The cell R^* in COUPLEX2 was actually part of a larger repository and we assume for simplicity that the whole repository is made up of 10 parallel lines of containers. Each line of containers is made by repeating 120 times the backfill and alveoles system described in figure 4 in COUPLEX2. The length of a line is then 3240 m . All the lines belong to the same horizontal plane. The distance between two lines is 50 m . The geometry is shown on figure 6.

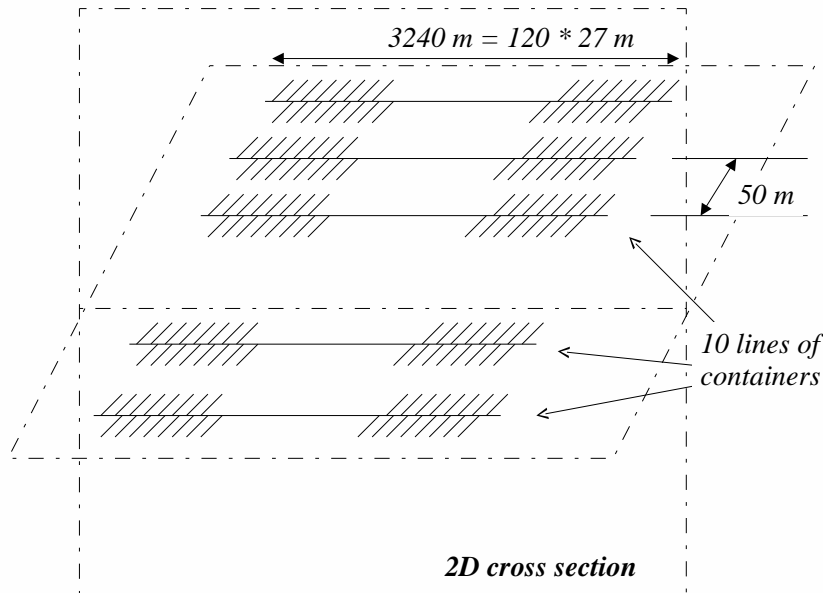


Figure 6: Geometry of the disposal site

The radioactive elements to be considered in the repository for the far field computation are now those used in COUPLEX2, that is an isolated ^{135}Cs and two nuclides filiation chains on ^{238}Pu and ^{242}Pu , as described in section 2.2.5 COUPLEX2, following the transport equation (2.6) and (2.12)–(2.15) (sections 2.2.4 and 2.2.5 in COUPLEX2).

We are interested by the Far Field simulation of a 2D vertical cross-section of the disposal site, similar to the one in the simulation of COUPLEX1. This cross section is parallel to the lines of containers.

Data in Table 2 in COUPLEX1 have to be completed by the ones in Tables 3–10 in COUPLEX2.

The host geological medium is then the clay strata defined in COUPLEX1, but with the same porosity of 15% for all nuclides. Other characteristics of the clay are now the ones of the geological medium defined in Tables 8–10 in COUPLEX2 section 2.4.

3.2 Output requirements

- At least, a simulation using the same kind of sequential coupling as the one used in COUPLEX1 (the repository behavior is a simple input to the Far Field simulation) should be carried out, and the results should be presented following the requirements of section 1.6.
- If an other way of coupling has been chosen, then the results should still be presented following the requirements of section 1.6.

For convenience, we reproduce the contents of section 1.6 below.

The following output quantities are expected from the simulations(both tables and graphical representations):

- Contour levels of C_i at times 200, 10110, 50110, 10^6 , 10^7 years (the following level values should be used: 10^{-12} , 10^{-10} , 10^{-8} , 10^{-6} , 10^{-4});
- Pressure field (10 values uniformly distributed between 180 and 340);
- Darcy velocity field, along the 3 vertical lines given by $x = 50$, $x = 12500$, $x = 20000$, using 100 points along each line;
- Places where the Darcy velocity is zero;
- Cumulative total flux through the top and the bottom clay layer boundaries, as a function of time;
- Cumulative total fluxes through the left boundaries of the dogger and limestone layers;
- The discretization grid of the domains and the time stepping used in the simulations should also be given.

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A Description of the data file for COUPLEX 1

The file `source.dat` contains data needed to compute the source term f_i in eq. (1.3). These data come from a Near Field computation. The file has 212 lines, and each line contains three numbers $t^p, \tilde{f}_1^p, \tilde{f}_2^p$, $p = 1, \dots, 212$, where t^p is the time, and the source term $f_i(t^p)$ is related to \tilde{f}_i^p by: $f_i(t^p) = \tilde{f}_i^p / S$, where S is the surface of the repository.

The times t^p are in years, and the numbers \tilde{f}_i^p are in units of mole /year.

B Conversion between activities and number of moles

The activity (in Becquerel) of a nuclide is the number of disintegration per seconds. The rule for converting the activity to a number of moles is simply:

$$N = T / (\ln(2)\mathcal{N}) A$$

T being the half-life of the element (in seconds), and \mathcal{N} is Avogadro’s number ($\mathcal{N} = 6.02 \cdot 10^{23} \text{ mol}^{-1}$).

The initial activities for the various nuclides are as follows (numbers in table 11 are for 1 package, and there are 8 packages in one alveolus).

Isotope	^{135}Cs	^{238}Pu	^{234}U	^{242}Pu	^{238}U
Activity	$2.99 \cdot 10^{10}$	$3.79 \cdot 10^{11}$	$9.47 \cdot 10^{07}$	$8.94 \cdot 10^{07}$	$7.81 \cdot 10^{06}$

Table 11: *Nuclide inventory for one package*