

R-06-112

COMP23 Testbatch

Maria Lindgren, Michael Pettersson
Kemakta Konsult AB

Andrew Cliffe, Martin Kelly
Serco Assurance

December 2008

Svensk Kärnbränslehantering AB

Swedish Nuclear Fuel
and Waste Management Co
Box 250, SE-101 24 Stockholm
Tel +46 8 459 84 00



ISSN 1402-3091

SKB Rapport R-06-112

COMP23 Testbatch

Maria Lindgren, Michael Pettersson
Kemakta Konsult AB

Andrew Cliffe, Martin Kelly
Serco Assurance

December 2008

This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the authors and do not necessarily coincide with those of the client.

A pdf version of this document can be downloaded from www.skb.se

Contents

1	Introduction	5
1.1	Aim of the selected test cases	5
1.2	Summary of test cases	6
2	Test cases	7
	Test case 1 – Solubility limited source term	7
	Test case 2 – Solubility limited source term, increased number of compartments	9
	Test case 3 – Congruent dissolution from source	12
	Test case 4 – Transport into a flowing feature	14
	Test case 5 – Transport through a small hole in canister wall	16
	Test case 6 – Transport through a large hole in canister wall	19
	Test case 7 – Transport through a canister hole with increasing size (ramp)	20
	Test case 8 – Transport through a canister hole with increasing size (step)	22
	Test case 9 – One –dimensional diffusion in a medium bounded by two parallel planes (comparison with analytical solution)	23
	Test case 10 – Calculation case from SR 97, Aberg pessimistic canister related parameters	24
	Test case 11 – Calculation case from SR 97, Aberg special case with immediate fuel dissolution, IRF=1	25
	Test case 12 – Output in Bq instead of mol	25
	Test case 13 – FUELSURFACE	27
	Test case 14 – Dissolution due to alpha radiolysis – decay model	28
	Test case 15 – Dissolution due to alpha radiolysis – explicit model	30
	Test case 16 – Shared solubility	32
	Test case 17 – Probabilistic calculation	33
	Test case 18 – Calculation case from SR 97, Aberg pessimistic canister related parameters, shared solubility	35
	Test case 19 – Consistency Check when Multiple FARF31 Modules are Used	40
	Test case 20 – Time-dependent Variations to K_D	42
	Test case 21 – Time-dependent Variations to Porosity	45
	Test case 22 – Time-dependent Variations to Diffusion Coefficient	48
	Test case 23 – Time-dependent Variations to Solubility Limits	51
	Test case 24 – Material-dependent Solubility Limits	54
3	References	57
Appendix A	Execution of the test cases	59
Appendix B	Parameters used in reference calculations with INHOMOG and RARECAN	61

1 Introduction

This report gives a description of the test batch set up for COMP23 Version 1.2.2. The aim is to ensure that the test batch is valid for future versions of COMP23. The results given in this report are only a component of the overall set of results and the complete test cases are available at SKB's SUN computers (/usr/local/skb/comp23/sun/testex), see Appendix A.

1.1 Aim of the selected test cases

A detailed list with features that needs to be covered in the tests was developed in co-operation with Andy Thompson at Serco Assurance. The list is given in Table 1-1.

Table 1-1. Features to be covered by the test cases.

Processes – transport, decay, solubility limitation, sorption	
1	Each of the three alpha-radiolysis models (CONSTANT, DECAY and EXPLICIT).
2	Advective and diffusive transport.
3	Solubility limitation including shared solubility.
4	Sorption.
5	Nuclides of each of the different SOL_TYPE models (OWNSOL, FUELSURFACE and MATRIX).
6	Use of an Instantaneous Release Fraction (IRF).
7	A range of geometries.
8	A number of nuclides and chains, covering a wide range of half lives.
9	Cu/Fe canister type. Note that testing of lead filled canister types is no longer required.
10	Each of the hole growth models – NONE, RAMP and STEP.
General	
11	Use of the analytical solutions that are embedded in COMP23 (transport into a large compartment, transport into a narrow slit and transport into flowing water).
12	Output in moles and Bq.
13	Simple tests that can be compared against analytical solutions. For example, an analytical expression for 1-D diffusive transport can easily be derived, and used to compare against results from COMP23.
14	Tests that can be compared with other codes.
15	Tests that represent realistic scenarios, e.g. calculations used in SKB performance assessments.
16	A range of parameters values, from best case to worst case, via more realistic example(s).
17	Use of the different solvers that are used in COMP23.
18	Ability to make certain parameters time dependent
Application within the PROPER framework	
19	Single and batch simulations.
20	Probabilistic and deterministic calculations.
21	Networks that contain COMP23 as the first submodel.
22	Networks that contain COMP23 connected to upstream and downstream submodels.
23	Networks that contain COMP23 as the last submodel.
24	Networks that contain COMP23 models connected directly.
25	Networks that contain two or more COMP23 models that are not directly connected.
26	Parameters sampled from a range of probability distributions (e.g. CONST, UNIF, LOGUNIF, PWUNIF, PWLUNIF, TRIANG, LOGTRIANG, NORM, LOGNORM, WEIBULL, GAMMA, BOOTSTRAP and COMPUTED).
27	Regeneration of results using the TIMESERIES command.

1.2 Summary of test cases

The test cases were based primarily on old test examples that are compared with other codes /Gould et al. 1996/ and on calculation cases from SR 97 /Lindgren and Lindström 1999/. In addition a test case that is compared with analytical solutions was set up based on a test reported by /Romero et al. 1995/. The decision to use old test examples was intended to make it possible to compare with old results from NUCTRAN/COMP23, since the developments over the last few years have been performed without updated test cases.

A summary of the test cases is given in Table 1-2. A summary of how the test cases cover the requirements is set out in Table 1-1.

Table 1-2. Summary of the test cases.

Test case	Short description of the case
1	Solubility limited source term
2	Solubility limited source term, increased number of compartments
3	Congruent dissolution from source
4	Transport into a flowing feature
5	Transport through a small hole in canister wall
6	Transport through a large hole in canister wall
7	Transport through a canister hole with increasing size (ramp)
8	Transport through a canister hole with increasing size (step)
9	One-dimensional diffusion in a medium bounded by two parallel planes (comparison with analytical solution)
10	Calculation case from SR 97, Aberg pessimistic canister related parameters
11	Calculation case from SR 97, Aberg special case with immediate fuel dissolution, IRF=1
12	Output in Bq instead of mol
13	FUELSURFACE
14	Dissolution due to alpha radiolysis – decay model
15	Dissolution due to alpha radiolysis – explicit model
16	Shared solubility
17	Probabilistic calculation
18	Calculation case from SR 97, Aberg pessimistic canister related parameters, shared solubility
19	Consistency check when multiple FARF31 modules are used
20	Time-dependent variations to sorption coefficient
21	Time-dependent variations to porosity
22	Time-dependent variations to diffusion coefficient
23	Time-dependent variations to solubility limits
24	Material-dependent solubility limits

2 Test cases

Test case 1 – Solubility limited source term

The first test case is the verification of solubility-limited source term (task 2.1) from /Gould et al. 1996/ with input files updated to the present version of COMP23. The results of the calculation are compared with another code, INHOMOG. The description of the INHOMOG model and the test case are to a large extent directly cited from the report by /Gould et al. 1996/. The code INHOMOG permits a one-dimensional spatial description of the distribution of waste disposal units with potentially different chemical and physical characteristics. It calculates a radionuclide source term arising from the interaction of the waste disposal units, assuming the units are connected by groundwater transport processes. The chemical processes are represented by solubility limitation and linear sorption. The model can represent transport by diffusion, advection and dispersion.

The aim of the test is to verify the solubility-limited release of U-238 from a canister into a bentonite region. Decay and diffusive transport is included. The model comprises two regions, the waste and the bentonite. There is no containment of the waste in the canister.

- The inventory of U-238 used in INHOMOG is very much less than would be usual for a canister. The lower U-238 inventory was used to decrease computation time needed by INHOMOG.
- The inventory of U-238 used in the COMP23 calculations was, however, a realistic inventory of $8.06 \cdot 10^3$ moles, i.e. the one used in SR 97. To obtain comparable results the solubility limit was increased in proportion to the inventory.
- The canister dimensions are as follows: diameter 0.8 m, thickness 0.1 m and length 4.5 m.
- It was assumed that the length and diameter included the thickness of the canister wall. Therefore, the dimensions of the wasteform contained in the canister are; diameter 0.6 m and length 4.3 m.
- The top 0.1 m of the canister (i.e. the corroded canister wall) was assumed to be bentonite.
- The length of bentonite above the corroded canister was taken as 1.5 m.
- To make the effects of the boundary insignificant in INHOMOG a long bentonite region was modelled (25.6 m). The U-238 concentration in only the first 1.6 m of the bentonite (including 0.1 m of corroded canister) is reported.
- The value for the beta factor in the bentonite as used in INHOMOG is $(1-\Phi)$ where Φ is the porosity in the bentonite. This converts the material density (or solid density) required by COMP23 to the bulk density required in INHOMOG.

The input data used in the INHOMOG calculations are given in Appendix B Table B-1.

Results for Test case 1

The concentration of U-238 in bentonite at $1.2 < z < 1.6$ m as a function of time as calculated by COMP23 is shown in Figure 2-1. The concentration profile is in agreement with the profile obtained by /Gould et al. 1996/ in task 2.1.

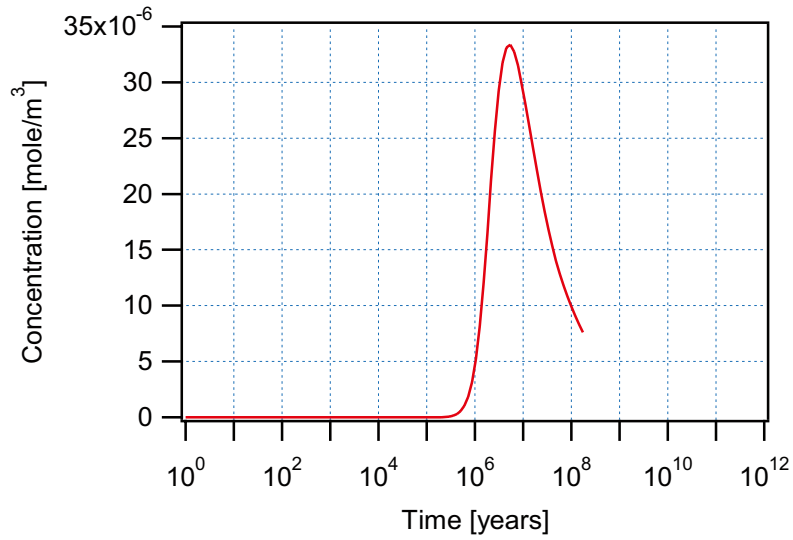


Figure 2-1. Concentration of U-238 in bentonite ($1.2 < z < 1.6$ m) for Test case 1.

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

Test case 2 is equal to Test case 1, except for the number of compartments in the bentonite that was increased from 8 to 16 in the COMP23 calculations. This case is task 2.1b from /Gould et al. 1996/ with input files updated to the present version of COMP23.

Results for Test case 2

The results for Test 2 are shown in the following figures. These figures show the variation of U-238 concentration across the various compartments (23 in total) as a function of time.

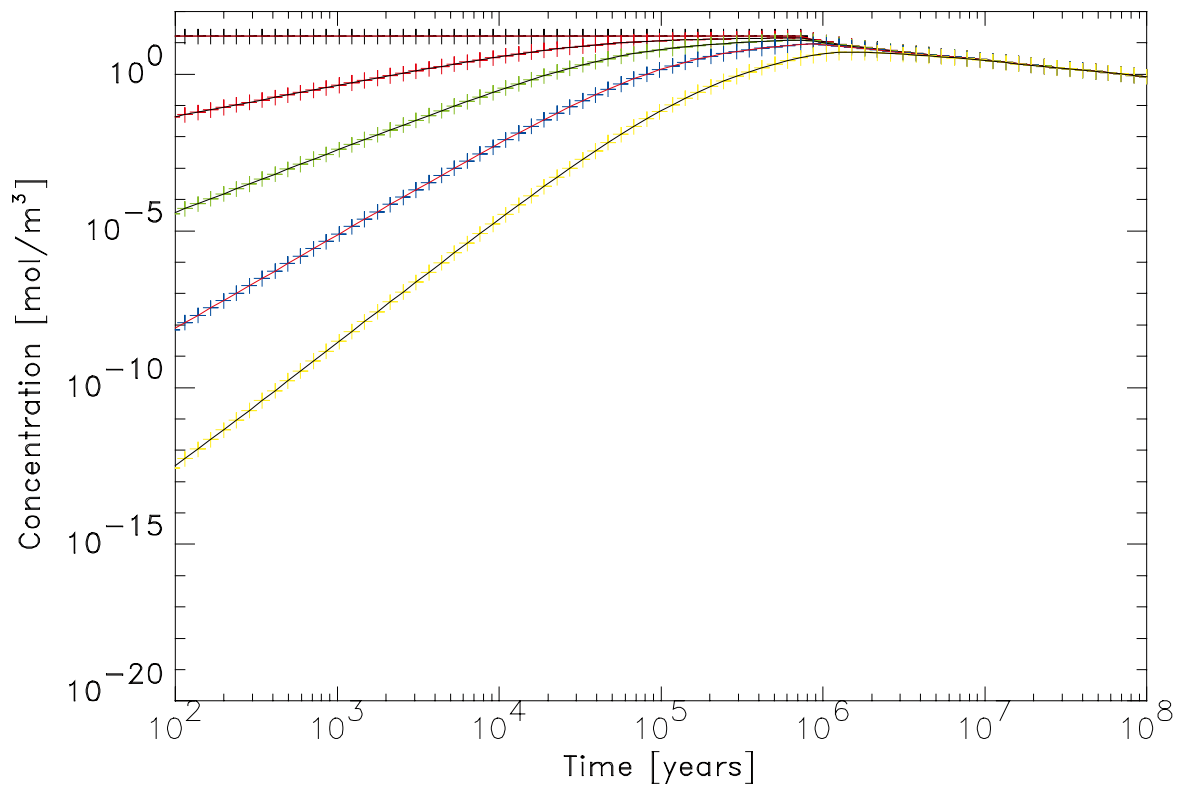


Figure 2-2. Concentration of U-238 in compartments 1 to 5.

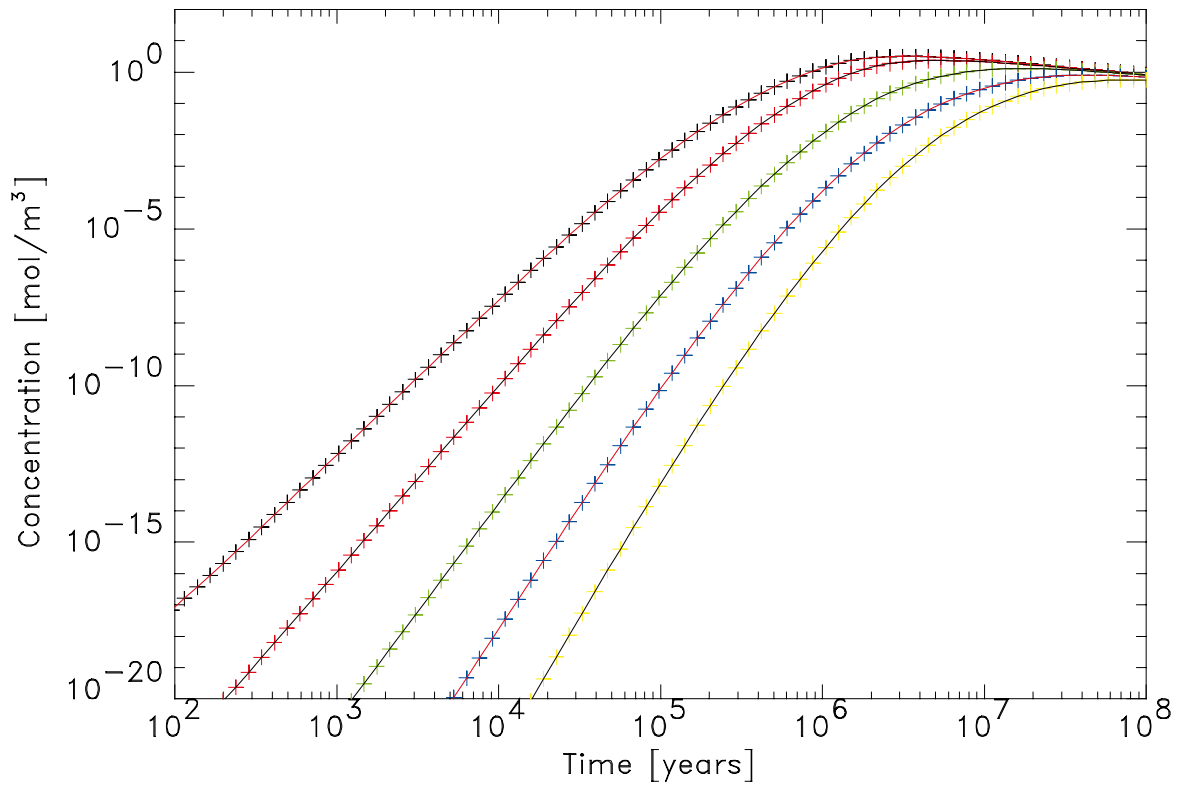


Figure 2-3. Concentration of U-238 in compartments 6 to 10.

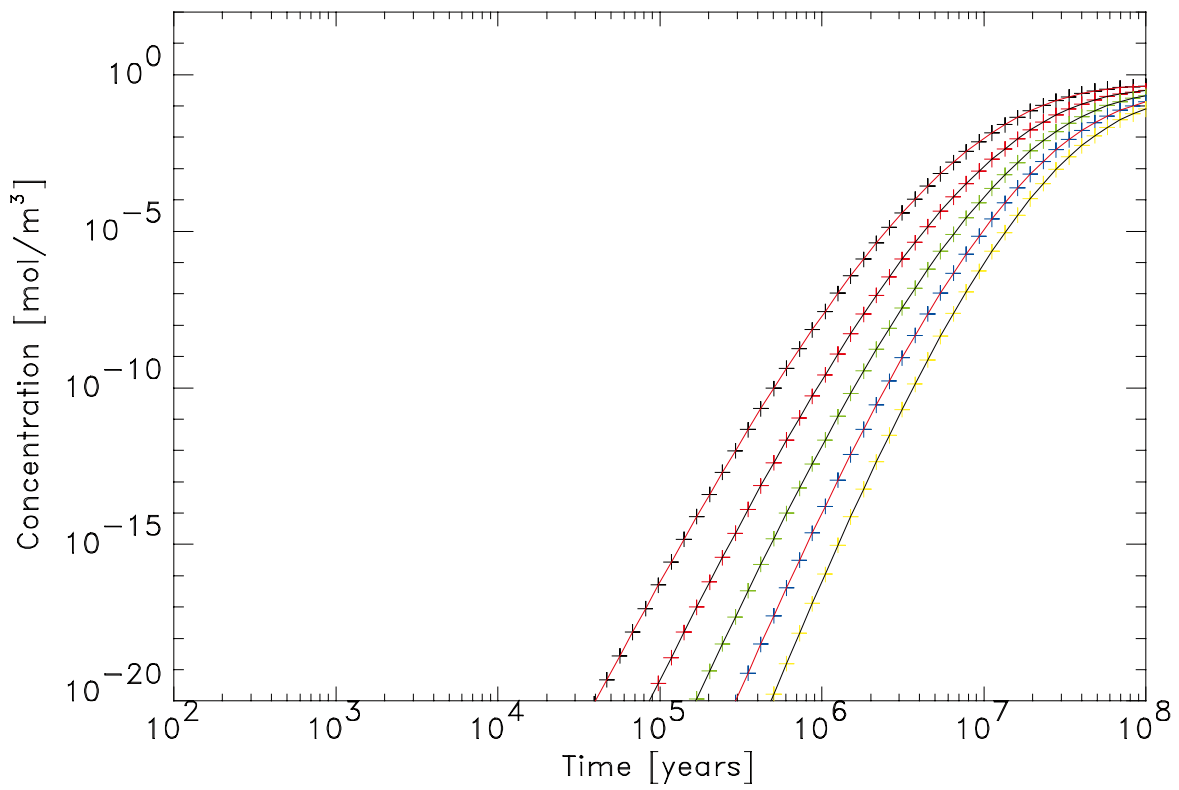


Figure 2-4. Concentration of U-238 in compartments 11 to 15.

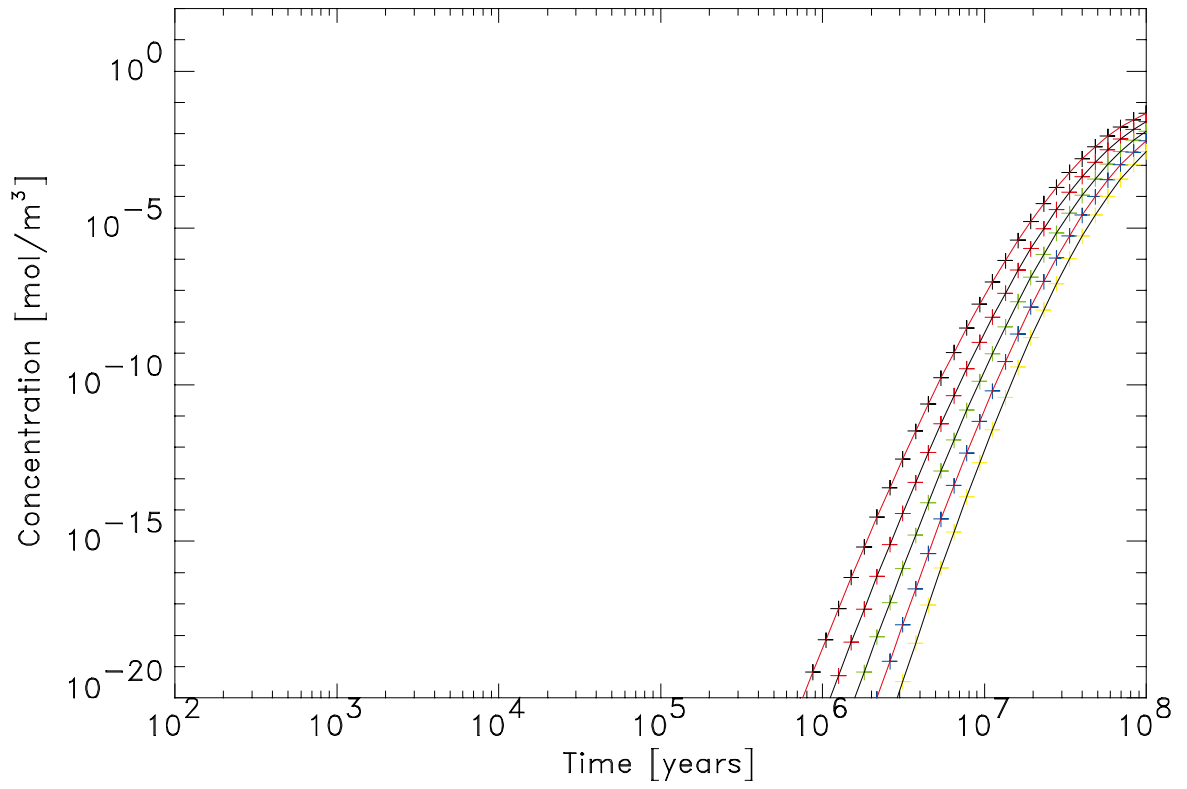


Figure 2-5. Concentration of U-238 in compartments 16 to 20.

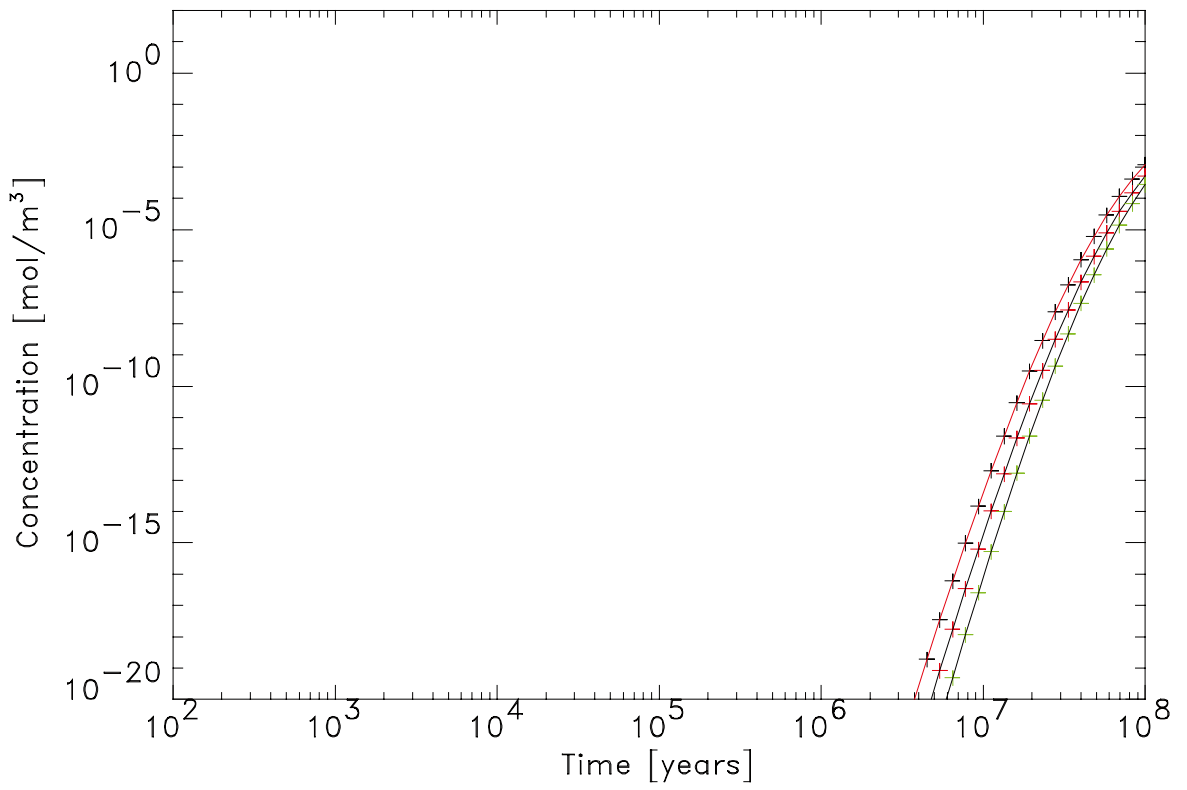


Figure 2-6. Concentration of U-238 in compartments 21 to 23.

Test case 3 – Congruent dissolution from source

Test case 3 is “task 2.2 Verification of congruent source term” from /Gould et al. 1996/ with input files updated to the present version of COMP23. The results from this task are compared with calculations performed with INHOMOG /Gould et al. 1996/. A short description of the INHOMOG code is given in the description of Test case 1. The description given below of the case is to a large extent directly cited from the report by /Gould et al. 1996/.

The aim of the test case is to test the congruent source representation of release from a canister. The release of I-129 from a source in which a small amount of I-129 is embedded in a matrix of predominantly uranium oxide is calculated using COMP23 and INHOMOG. Transport is limited to diffusion into the bentonite region. The decay of U-238 and I-129 is included in the calculation. No canister containment is considered.

The transport parameters, canister/bentonite dimensions and U-238 properties used in this test case is the same as in Test case 1. The additional parameters used in the INHOMOG calculations pertaining to the I-129 embedded in the uranium matrix are given in Appendix B Table B-2.

Results for test case 3

The concentration of I-129 in the bentonite at $1.2 < z < 1.6$ m for Test case 3 is shown in Figure 2-7. The results obtained with COMP23 are in agreement with the results presented for Task 2.2 in /Gould et al. 1996/.

The concentration of I-129 in the hole, corresponding to $0 < z < 0.1$ m in the model, is shown in Figure 2-8 and the concentration in the bentonite ($0.1 < z < 0.2$ m) is shown in Figure 2-9. The concentration profiles obtained by COMP23 in this work are in agreement with the results obtained with NUCSTRAN presented in /Gould et al. 1996/.

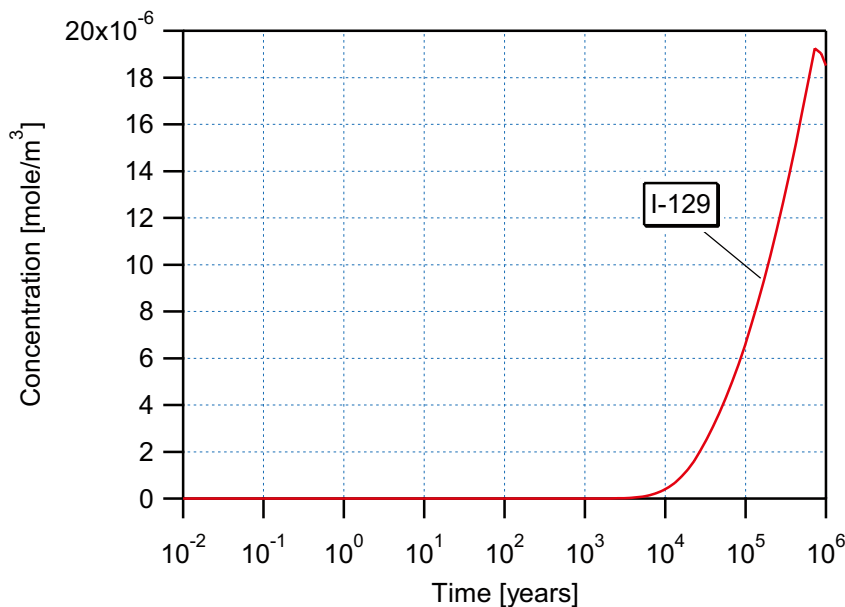


Figure 2-7. Concentration of I-129 in bentonite ($1.2 < z < 1.6$ m) for Test case 3 obtained with COMP23.

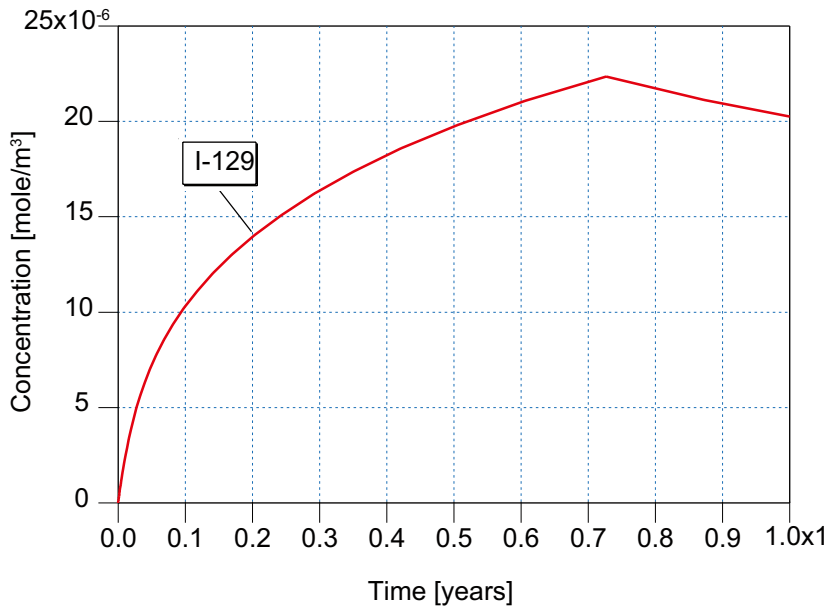


Figure 2-8. Concentration of I-129 in the hole for Test case 3 obtained by COMP23.

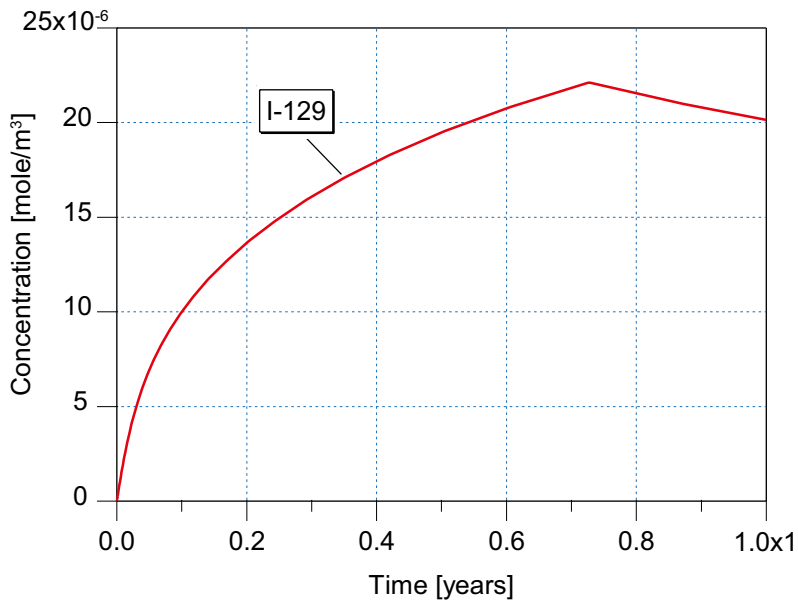


Figure 2-9. Concentration of I-129 in bentonite ($0.1 < z < 0.2$ m) for Test case 3 obtained with COMP23.

Test case 4 – Transport into a flowing feature

Test case 4 is “task 2.3 Verification of transport into a flowing feature” from /Gould et al. 1996/ with input files updated to the present version of COMP23. The results from this test case are compared with calculations performed with INHOMOG /Gould et al. 1996/. A short description of the INHOMOG code is given in the description of Test case 1. The description given below of the case is to a large extent directly cited from the report by /Gould et al. 1996/.

The aim of the test case is to test the capability to predict the rate of transport of radionuclides out of a region of diffusive transport, and into a flowing feature. Release of U-238 from the canister is controlled by solubility-limits. There is no containment in the canister. The decay of U-238 is included. Transport is by diffusion inside the canister and in the bentonite region. In a fracture intersecting the bentonite region, transport by advection is also included.

A 30 m length of rock was used in the INHOMOG and COMP23 calculations. This length was selected to ensure that the boundary did not affect the solution. The concentration in the first 7.5 m was considered. The discretisation of the rock has been modified due to limits in the number of compartments in the current version of COMP23. The rock consists of 12 compartments, 2.5 m long, compared to the NUCTRAN calculation /Gould et al. 1996/ where 30 compartments, each 1 m long, were used.

INHOMOG can only model transport in one dimension. Therefore the direction of advective transport in the flowing fracture in the rock was chosen to be the same as in the bentonite, i.e. in the z-direction. COMP23 is limited so that flow is possible only in one block and only in “one” direction.

The input data used in the INHOMOG calculations are given in Appendix B Table B-3.

Results for Test case 4

The concentrations of U-238 in different parts of the bentonite barrier and in the rock are shown in Figure 2-10 to Figure 2-12. The results obtained with COMP23 are in agreement with the results obtained with NUCTRAN presented for Task 2.3 in /Gould et al. 1996/. The results shown in Figure 2-10 for the rock differ due to the different discretisation used in the COMP23 calculations compared to the NUCTRAN calculations in /Gould et al. 1996/. However, the concentrations are as expected, considering the difference in discretisation.

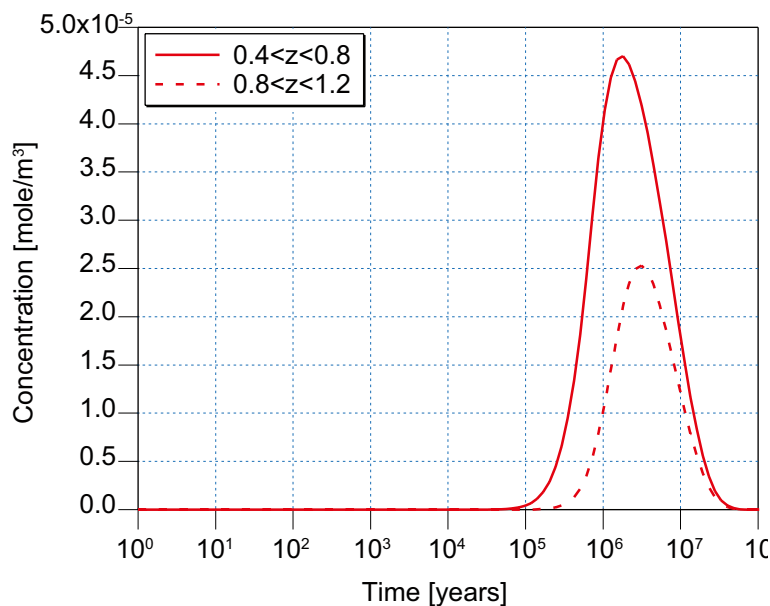


Figure 2-10. Concentration of U-238 in bentonite at two different positions within the bentonite barrier for Test case 4 obtained with COMP23.

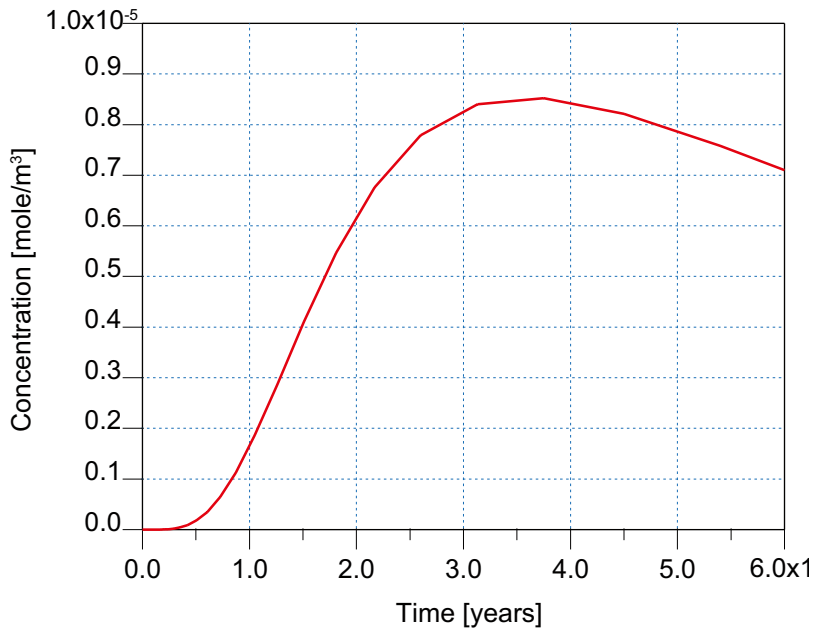


Figure 2-11. Concentration of U-238 at the end of the bentonite barrier for Test case 4 obtained with COMP23.

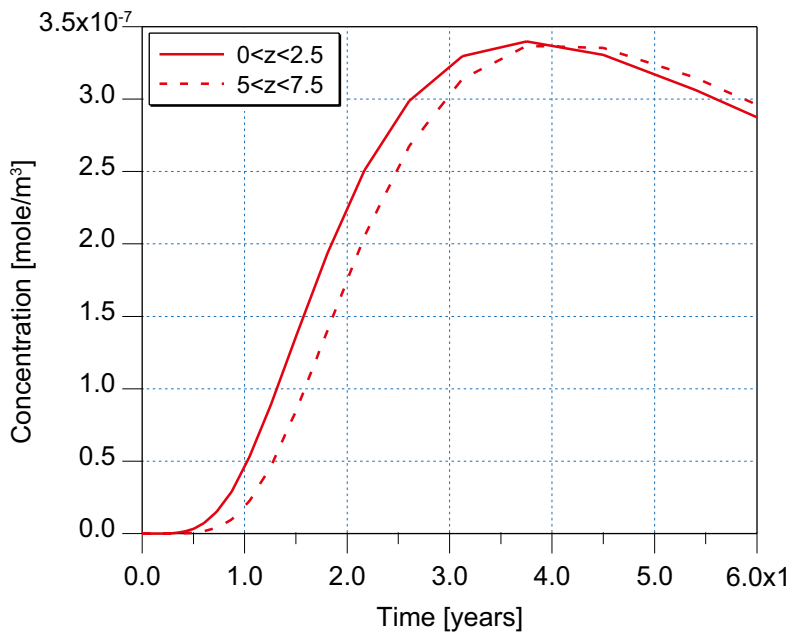


Figure 2-12. Concentration of U-238 at two different positions within the rock for Test case 4 obtained with COMP23.

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

Test case 5 is “task 2.4A Verification of transport through a small hole” from /Gould et al. 1996/ with input files updated to the present version of COMP23. The results from this task are compared with calculations performed with RARECAN /Gould et al. 1996/. The description of RARECAN and the case is to a large extent directly cited from the report by /Gould et al. 1996/. The code RARECAN calculates transfer of radionuclides from within the waste containers to the surrounding backfill, via holes or vents in the containers. RARECAN was developed by AEA Technology within the Nirex Safety Assessment Research Programme to model the effects of corrosion on containment in a metal canister /Porter and Chambers 1995/. The RARECAN model approximates the loss of containment from a stainless steel canister placed in cement, through the formation of increasing number of holes of the same radius (rather than a single hole with increasing radius as used by COMP23).

A model was set up in which there are two regions: one representing the region within the waste canister and one representing the surrounding bentonite. The two regions are connected by a hole, or a number of holes with varying sizes, depending on the case considered. RARECAN treats each of the regions as one block and does not have any spatial discretisation within a region. Transport was restricted to diffusion. The release of the solubility limited radionuclide U-238 was calculated. Decay of U-238 was included.

The following additional points should be noted:

- RARECAN assumes that the wall of the canister is infinitely thin. However, in COMP23, the canister wall must be defined in the input file as block 2. The canister wall must therefore be allocated a non-zero width in a COMP23 calculation. The release rates calculated by COMP23 are dependent on the width of the canister wall when the wall is fairly thick. However, sensitivity studies were carried out /Gould et al. 1996/ to identify a value for the wall width below which the COMP23 results are insensitive to the specified width. These results could then be compared with the RARECAN simulations with an infinitely thin wall. A value of 10^{-10} m was deemed to be acceptable as it gave identical results to simulations with a wall widths of either 10^{-9} or 10^{-12} m /Gould et al. 1996/.
- Since the canister is assumed to have negligible thickness, the outer canister dimensions were used, diameter 0.8 m, length 4.5 m and thickness 10^{-10} m.
- Four calculations were performed with COMP23:
 - a) No “plug”. One bentonite compartment.
 - b) The “plug” facility in COMP23 (analytical solution for transport into a large compartment) was used between the canister hole and the surrounding bentonite. One bentonite compartment.
 - c) No “plug”. Five compartments.
 - d) Plug. Five compartments.

The input data used in the RARECAN calculations are given in Appendix B Table B-4.

Results for Test case 5

The concentration profile obtained with COMP23 using the plug facility and representing the bentonite barrier with one compartment is shown in Figure 2-13. The result is in agreement with that obtained with NUCTRAN as well as RARECAN presented in /Gould et al. 1996/.

For the case where the bentonite barrier is represented by five compartments and the plug facility is not utilised, there is a small deviation between the concentration in the last compartment ($1.2 < z < 1.5$ m) obtained with COMP23 in this work and the corresponding result obtained with NUCTRAN (presented in /Gould et al. 1996/. The results for both codes are shown in Figure 2-14. It can be seen that the concentration profile has the same shape for both codes but there is a small shift in profile with time. Gould and co-workers have not included any input data file for this case in their report. It can not therefore be determined whether the different results are caused by some difference in the codes or in the input data used. In addition the

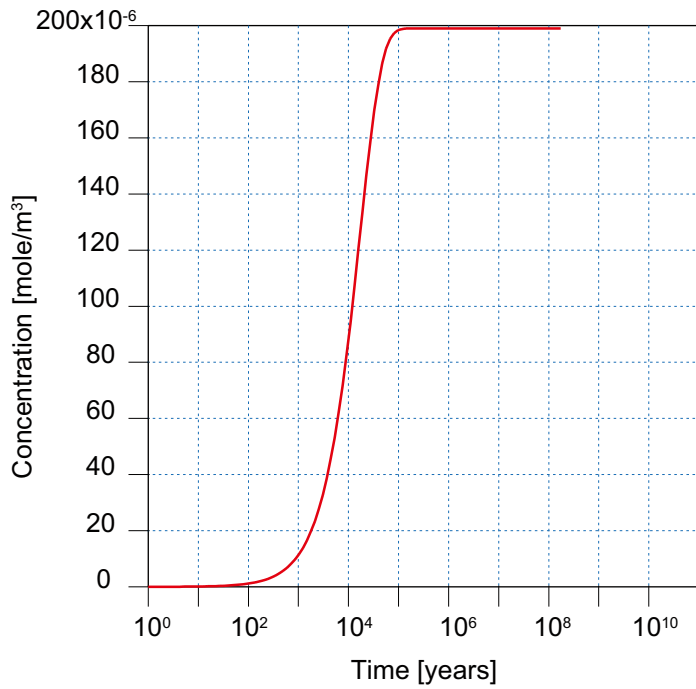


Figure 2-13. Concentration of U-238 using the plug facility and one compartment for the bentonite barrier.

legend in the figure and the figure text are inconsistent in their report. The results might be valid for a “fourth case” with one block and no plug. This has also been tested, but with worse agreement. Nevertheless, it can be concluded that not using the plug facility results in worse agreement with RARECAN than when using the plug facility.

The obtained concentrations in the calculation with five compartment and plug are shown in Figure 2-15. The result is in agreement with that obtained with NUCTRAN presented in /Gould et al. 1996/.

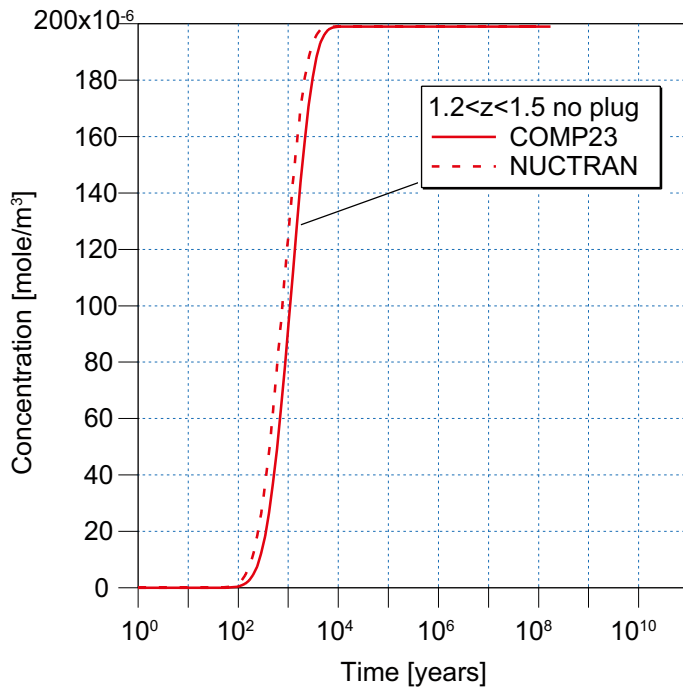


Figure 2-14. Concentration of U-238 without using the plug facility and five compartments for the bentonite barrier. The results obtained with NUCTRAN are from /Gould et al. 1996/.

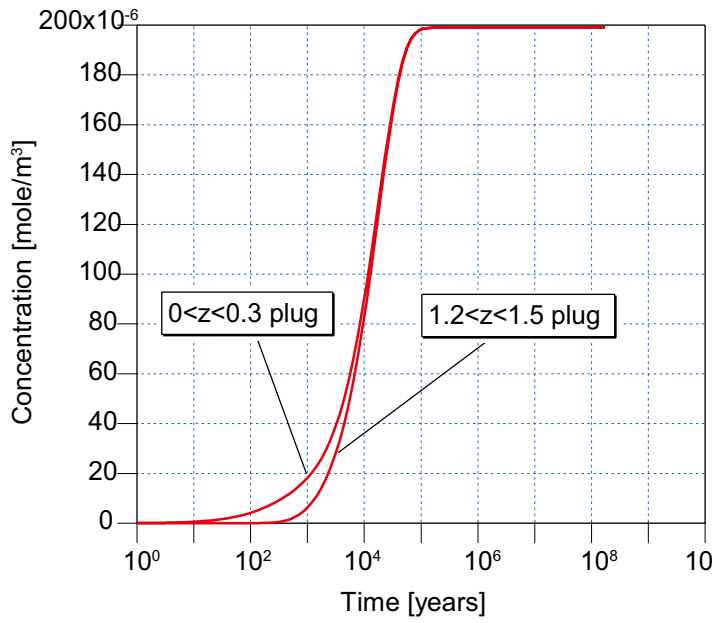


Figure 2-15. Concentration of U-238 using the plug facility and five compartments for the bentonite barrier obtained by COMP23. Results are shown for the first compartment ($0 < z < 0.3$ m) and the last compartment ($1.2 < z < 1.5$ m) representing the bentonite barrier.

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

Test case 6 is “task 2.4B Verification of transport through a large hole” from /Gould et al. 1996/ with input files updated to the present version of COMP23. The results from this task are compared with calculations performed with RARECAN /Gould et al. 1996/. The code RARECAN is briefly described in the description of Test case 5.

Test case 6 is equal to Test case 5, using the plug facility and one compartment in the bentonite, except for a larger hole. The hole has a constant radius ($1.26 \cdot 10^{-1}$ m, which corresponds to an area of $5 \cdot 10^{-2}$ m²). The input data used in the RARECAN calculations are given in Appendix B Table B-4 and B-5.

Results for Test case 6

The concentration of U-238 in the bentonite for Test case 6 is shown in Figure 2-16. The result obtained with COMP23 is in agreement with the result presented for NUCTRAN for Task 2.4b in /Gould et al. 1996/.

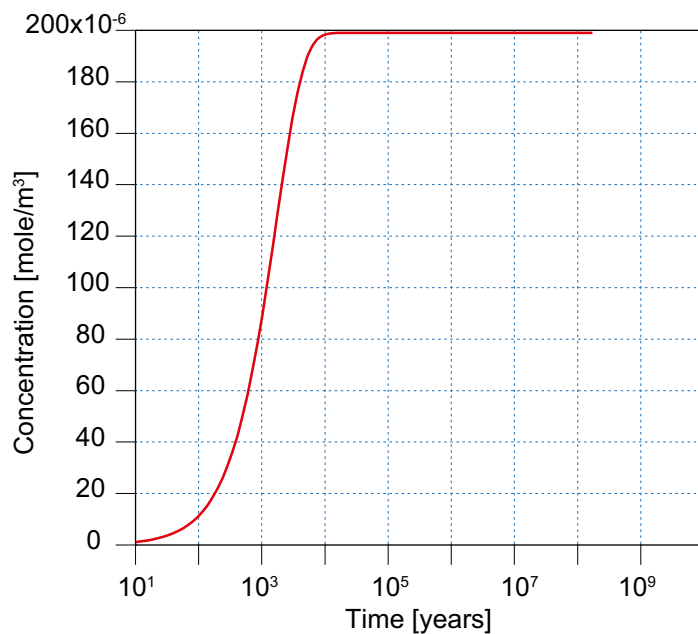


Figure 2-16. Concentration of U-238 in the bentonite barrier for Test case 6 obtained with COMP23.

Test case 7 – Transport through a canister hole with increasing size (ramp)

Test case 7 is “task 2.4D Verification of transport through a canister hole of increasing size” from /Gould et al. 1996/ with input files updated to the present version of COMP23. The results from this task are compared with calculations performed with RARECAN /Gould et al. 1996/. The code RARECAN is briefly described in the description of Test case 5.

Test case 7 is equal to Test case 5, using the plug facility and five compartments, except that the properties of the hole change with time. A gradual loss of containment is represented in RARECAN by an increasing number of holes, and in COMP23 by an increasing cross sectional area of a single hole.

The number of new holes (of radius $1.26 \cdot 10^{-2}$ m) per year, as used by RARECAN was $1 \cdot 10^{-6}$ year⁻¹. In COMP23 the initial area of the hole is $5 \cdot 10^{-4}$ m², which corresponds to a radius of $1.26 \cdot 10^{-2}$ m, increasing linearly (ramp) to $3 \cdot 10^{-3}$ m² at $5 \cdot 10^6$ years.

The input data used in the RARECAN calculations are given in Appendix B Table B-4 and B-5.

Results for Test case 7

The concentration of U-238 in the last bentonite compartment for Test case 7 is shown in Figure 2-17. The result obtained with COMP23 is in agreement with the result presented for NUCTRAN for Task 2.4d in /Gould et al. 1996/, except for a slightly lower concentration during the time period 200 until 2,000 years. The release rate from the canister is shown in Figure 2-18. The result obtained with COMP23 is in agreement with the result presented for NUCTRAN for Task 2.4 d in /Gould et al. 1996/ for longer times (over 10,000 years). For earlier times the difference is up to about 4% at about 1,000 years.

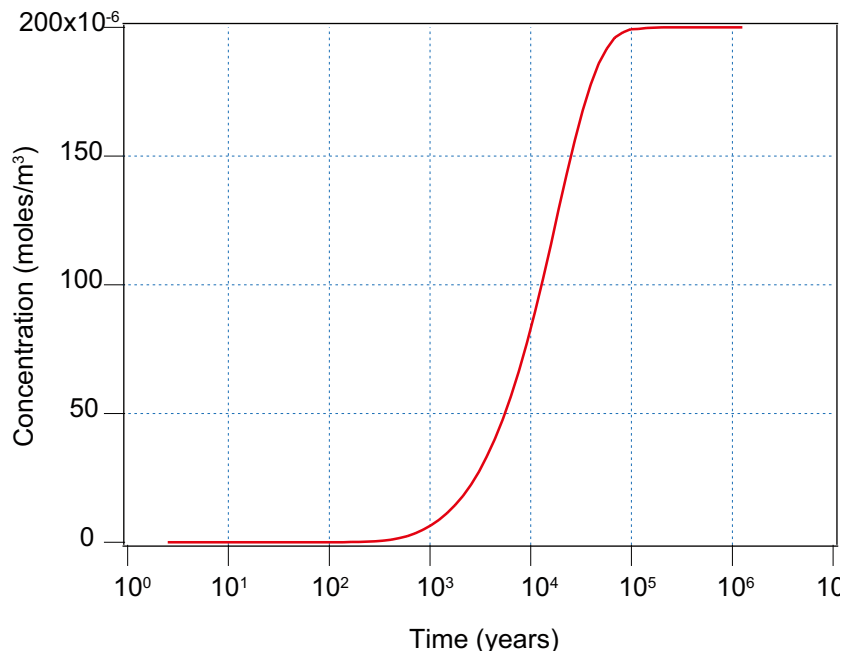


Figure 2-17. Concentration of U-238 in the bentonite barrier for Test case 7 obtained with COMP23.

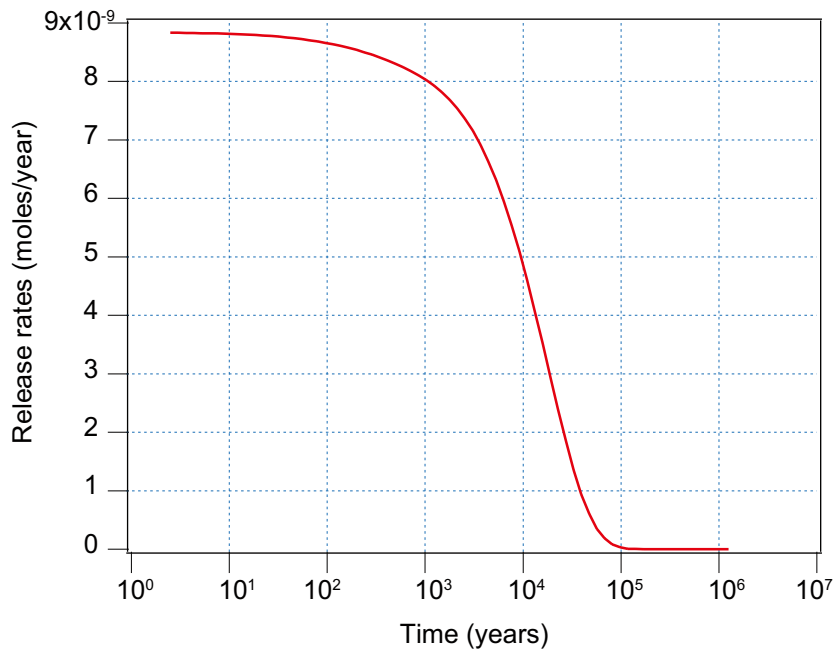


Figure 2-18. Release rate of U-238 from the canister for Test case 7 obtained with COMP23.

Test case 8 – Transport through a canister hole with increasing size (step)

This case is equal to Test case 7 except that the hole is initially small and grows stepwise to a larger hole. This test case is a simple case that includes the hole growth model with stepwise increased size of the hole. This hole growth model is also used in Test case 10, a realistic performance assessment case.

The initial area of the hole is $5 \cdot 10^{-4} \text{ m}^2$, which corresponds to a radius of $1.26 \cdot 10^{-2} \text{ m}$, increasing at 1,000 years to $1 \cdot 10^{-3} \text{ m}^2$.

Results for Test case 8

The concentration of U-238 in the last bentonite compartment for Test case 8 is shown in Figure 2-19. Compared to the corresponding concentration in Test 7 it increases faster in this case due to a larger hole size (during the time period 1,000 to 1,000 000 years) in Test 8. The release rate from the canister is shown in Figure 2-20. In the figure the step in the rate corresponds to the increase in hole size.

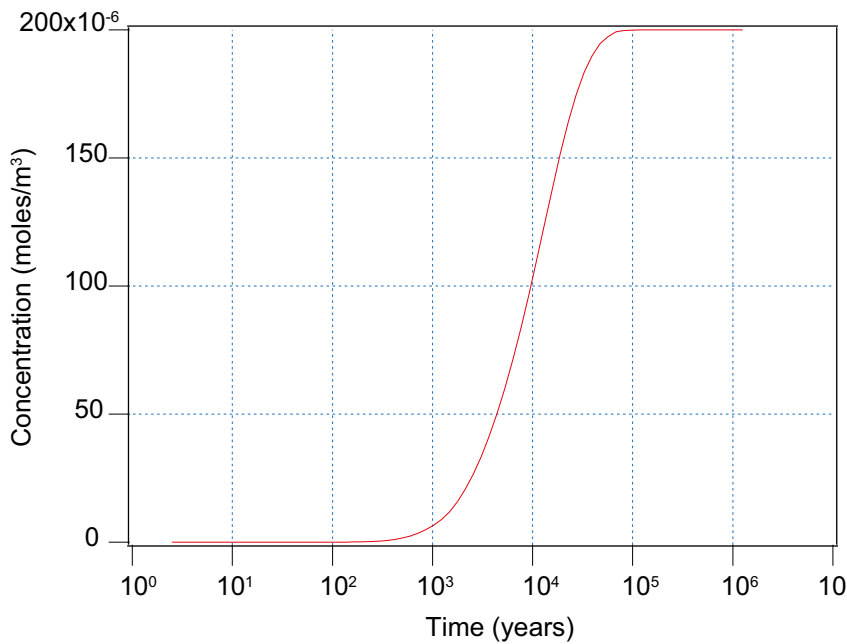


Figure 2-19. Concentration of U-238 in the bentonite barrier for Test case 8 obtained with COMP23.

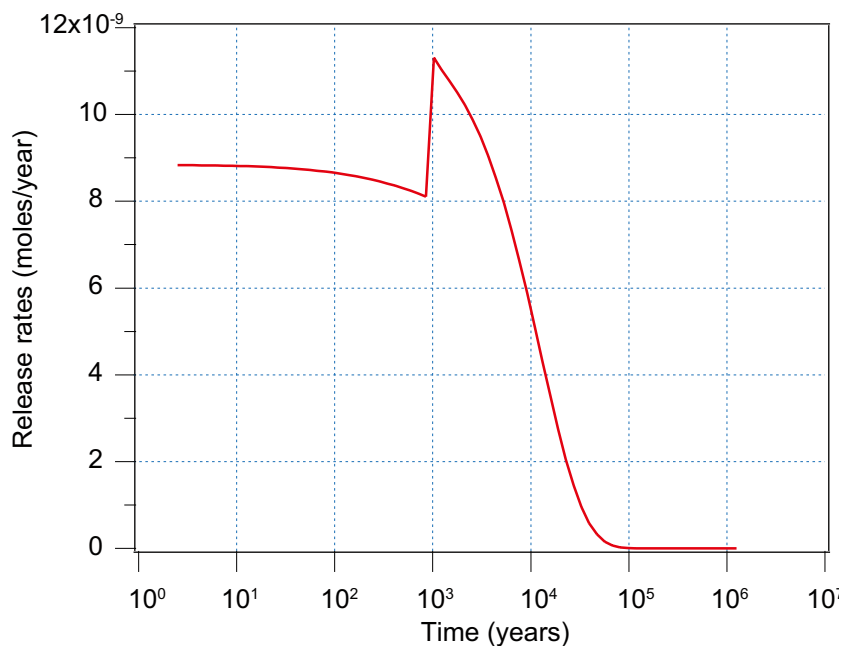


Figure 2-20. Release rate of U-238 from the canister for Test case 8 obtained with COMP23.

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

Verification of the code has also been made by comparing the results given by the model with an analytical solution for the one-dimensional diffusive transport in a medium bounded by two parallel planes. A constant concentration c_0 (mole/m³) at the inlet and zero concentration at the outlet is assumed. The mass transport rate to this problem is /Romero 1995/:

$$N = -\frac{D_e A c_0}{L} \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \exp\left(-\frac{n^2 \pi^2 D_p t}{L^2}\right) \right]$$

where N is the mass transport rate (mol/year), A is the mass transfer area (m²), c_0 is the concentration at the inlet (mol/m³), L is the distance between the two planes, t is the time (year) and D_e and D_p are the effective and the pore diffusivity (m²/year), respectively.

The release rate of U-238 from a bentonite barrier with a cross sectional area of 0.7854 m² (corresponding to a cylinder with a radius of 0.5 m) and 1 m length is used for the comparison. No sorption is assumed. The concentration at the inlet was 1 mol/m³, obtained in COMP23 by assigning a solubility limit of 1 mol/m³ and a sufficient initial amount to maintain the solubility limit during the whole period of the calculations. The effective diffusivity was $3 \cdot 10^{-3}$ m²/year, the pore diffusivity $1.2 \cdot 10^{-2}$ m²/year. The pore diffusivity is not given as input to COMP23, because the effective diffusivity of $3 \cdot 10^{-3}$ m²/year and a porosity 0.25 gives the same input ($D_p = D_e / \varepsilon$). Two COMP23 calculations were performed; one with 8 compartments and one with 16 compartments. They are named Test 9a and Test 9b, respectively.

Results for Test case 9

The normalized release rate for this test case are shown in Figure 2-21 for the two different discretisations. In one calculation the bentonite barrier is divided into eight compartments and in the second calculation into sixteen compartments. Also included in the figure is the normalized release rate obtained from the analytical solution given above. It can be seen that the results obtained with COMP23 deviate from the analytical solution at early times using eight compartments for the bentonite barrier, but the accuracy increases with increasing time. Increasing the number of compartments for the bentonite barrier to sixteen leads to good agreement with the analytical solution at earlier times as well. The result is in agreement with the result presented in /Romero 1995/. In addition to the results in the figure it was concluded that the release rate at steady-state was $2.36 \cdot 10^{-3}$ mol/year ($N_{ss} = D_e c_0 A / L$) for both the analytical and the COMP23 calculation.

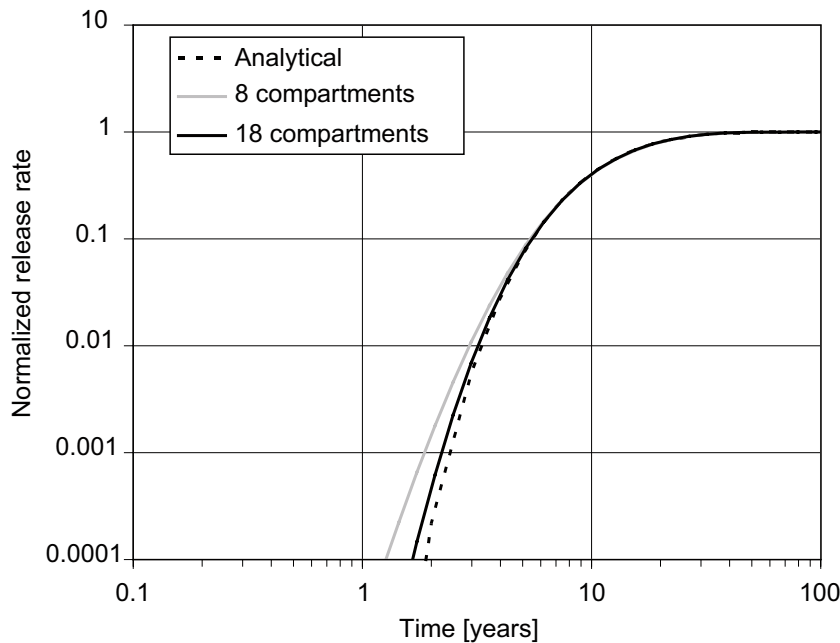


Figure 2-21. Normalized release rate for Test case 9, comparison between analytical solution and COMP23 calculations with 8 and 16 compartments, respectively.

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

For Test case 10, a realistic performance assessment case was chosen from SR 97 /Lindgren and Lindström 1999/. The case is a deterministic case that illustrates the effect of choosing pessimistic canister-related parameters. That is, the number of defective canisters, defect growth and delay time are given pessimistic values, while all other parameters are reasonable. There are five initially damaged canisters. The canister defects are assumed to appear after a time period of 300 years. The defect is initially small, i.e. 1 mm², and the release is therefore limited at early times. The defect increases at 20,000 years and only offers small transport resistance thereafter.

Results for Test case 10

The results for Test case 10 are shown in Figure 2-22 as release from the near field (COMP23) as a function of time. The results have been compared with the results given in /Lindgren and Lindström 1999/ and only negligible differences were found. The results for some nuclides within the chains differ significantly. This is due to the fact that the solubility for isotopes of minor importance must now be assigned a value. None of these is shown in the figure. The new keyword ADDITIONAL_OUTPUT was used to specify some extra output times, around the times when large changes occur. By doing this, changes in the form of the output can be seen more clearly. In this test case four extra outputs have been specified at times (1.99E+4, 2.00E+4, 2.01E+4 and 2.05E+4).

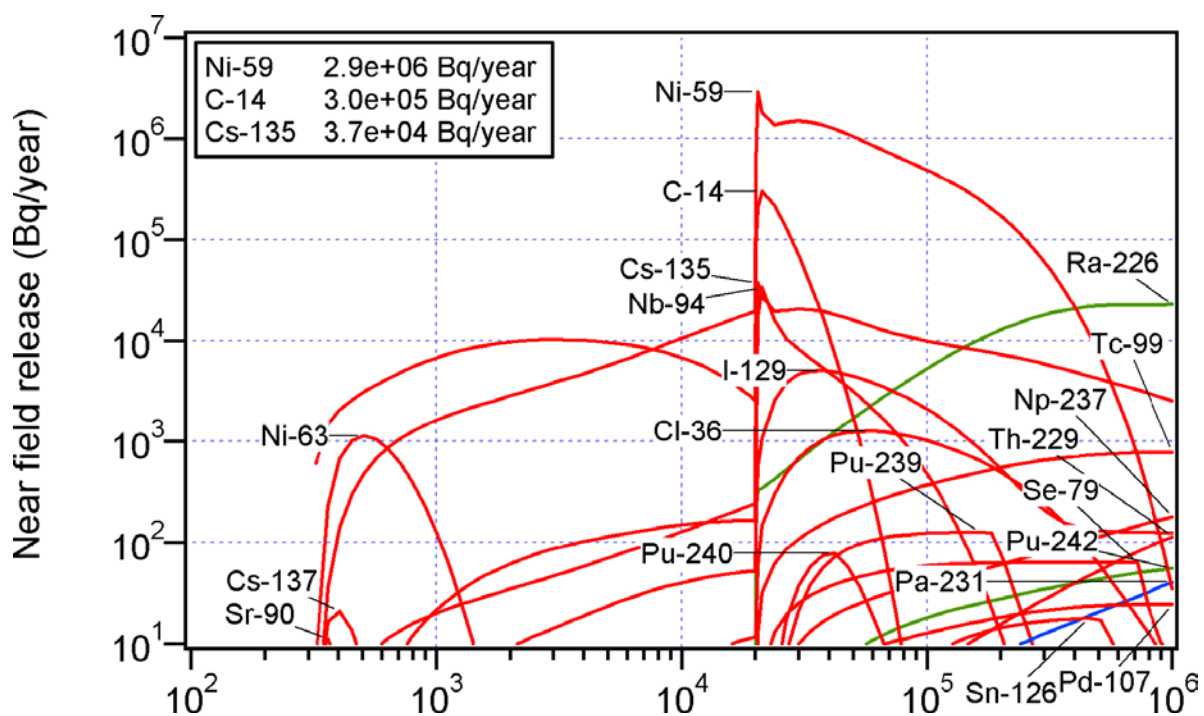


Figure 2-22. Release from the near field as a function of time for Test case 10.

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

This case is a special case from SR 97 /Lindgren and Lindström 1999/ with immediate fuel dissolution, i.e. the whole fraction of all nuclides is free for release immediately for Aberg. This is not a realistic case, but it shows the influence of the fuel dissolution used for the normal cases. The dissolution model used is OWNSOL for all nuclides and IRF=1 for all nuclides.

Results for Test case 11

The results for Test case 11 are shown in Figure 2-23 as release from the near field (COMP23), release from the far field (FARF31) and biosphere dose as a function of time. The results from COMP23 are given in moles/year and have been recalculated before plotting. FARF31 requires input data in mass units (moles). The results have been compared with the results given in /Lindgren and Lindström 1999/ and only negligible differences were found.

It can be concluded that the output of some nuclides, in particular I-129, Cl-36 and Cs-135, vary in proportion to the IRF-value. The number of nuclides that reach their solubility limit increases in this case compared to the reasonable case.

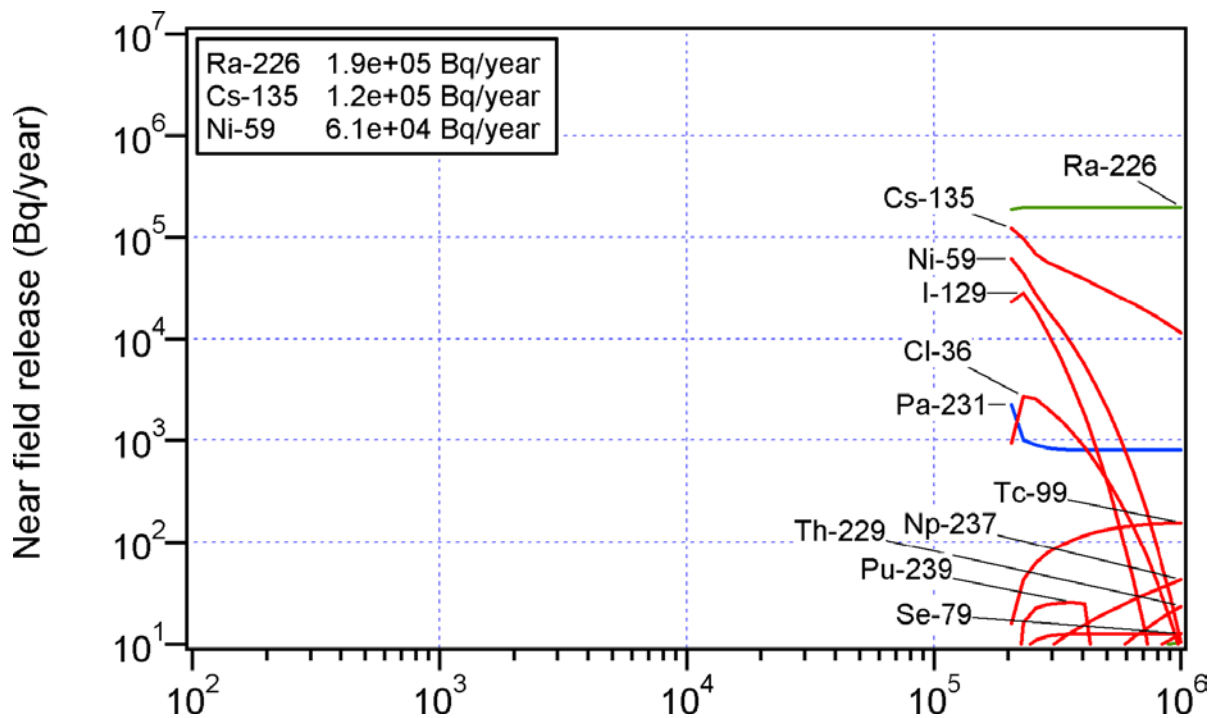


Figure 2-23. Release from the near field as a function of time for Test case 11.

Test case 12 – Output in Bq instead of mol

Test case 12 has been set up to test the facility to provide outputs in Bq rather than moles. The test case is equal to Test case 3 except that the output is specified to be given in Bq instead of moles. That is, the keyword RELEASE_TYPE BQ is used instead of RELEASE_TYPE MOL.

Results for Test case 12

The concentrations in the different compartments for all time steps are given in the optional output file “comp32”. Concentrations in activity units (Bq/m³) were converted in EXCEL to mass units (mol/m³) and compared with the corresponding file for Test case 3. The calculation was performed using the following expression:

$$C = \frac{A}{N_A \cdot \lambda} \quad [mol / year]$$

where:

A is the concentration [Bq/m³],

N_A is Avogadro's number [mol⁻¹] ($6.023 \cdot 10^{23}$),

λ is the decay constant [s⁻¹].

The comparison between the two calculations shows only negligible differences.

Test case 13 – FUELSURFACE

Test case 13 has been set up to test the dissolution model FUELSURFACE, for which the dissolution rate is controlled by the solubility of each radionuclide. Only a fraction of the nuclide inventory is available for release (controlled by the IRF value). The test case is the same as Test case 3 except that SOL_TYPE for I-129 is FUELSURFACE and an IRF value of 0.1 is assigned for I-129, which means that only 10% of the inventory is released and that all of it is released instantaneously. The solubility assigned for I-129 is high and will not limit the release in this case.

Results for Test case 13

The concentrations in the different compartments for all time steps are given in the optional output file “comp32”. The concentration of I-129 in the source is given in Figure 2-24 as a function of time. In addition the concentrations obtained for Test 3 and an extra case with IRF = 1 are shown. Compared to Test 3 the concentration is initially higher but after about 10,000 years the concentration is lower. The difference between this case and the extra case with IRF = 1 is that this case has concentrations a factor of 10 smaller, which is as expected.

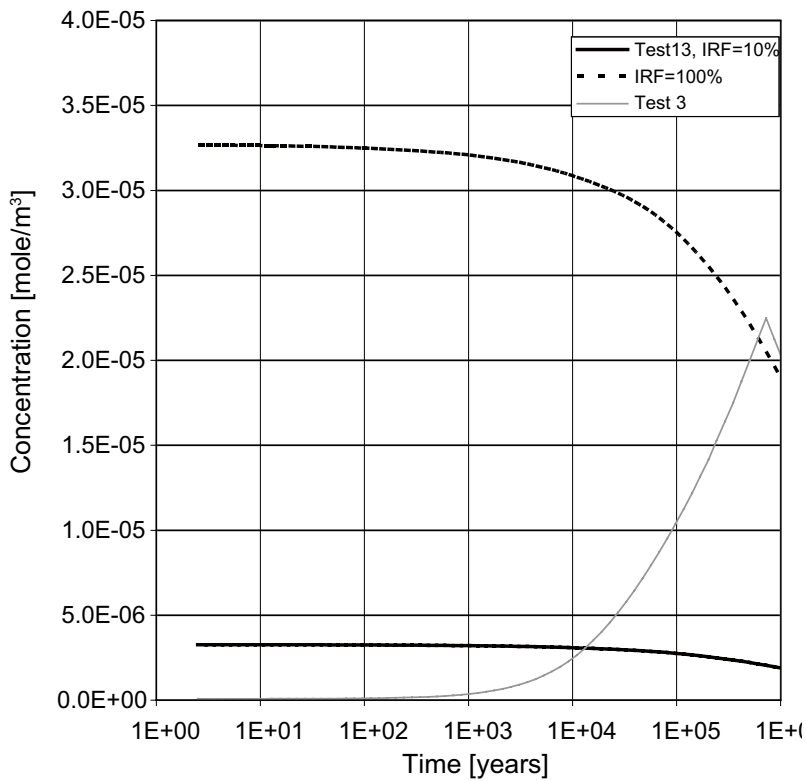


Figure 2-24. Concentration of I-129 in the source (compartment 1) for Test case 13 obtained with COMP23. The concentration from test 3 as well as a case with IRF=1 are also shown.

Test case 14 – Dissolution due to alpha radiolysis – decay model

Test case 14 has been set up to test the fuel dissolution due to alpha radiolysis with the decay model.

The test case is based on the same SR 97 calculation as used in Test case 10, but with a number of simplifications. Only the most important nuclides are included and one canister is assumed to have a defect in all calculations. Only one exit path, Q1, was used. The model then consists of the canister, with a hole and outside 0.35 m bentonite and at the outside a boundary condition, Q1. The nuclides included are Pu-242, U-238, U-234, Th-230, Ra-226, Am-243, Pu-239, Cm-245, Am-241, Np-237, I-129 and Pu-240. The calculation of the biosphere dose is performed with one BIO42-module instead of several SUM41-modules. In addition a PICK51 is used to obtain the output release rates from the near field.

The canister defects are assumed to appear after a time period of 300 years. The defect is initially small, i.e. 1 mm², and the release is therefore limited at early times. The defect increases at 20,000 years and only offers small transport resistance thereafter.

The “decay model” is described in the User’s guide /Romero et al. 1999/. The description below is to a large extent taken from that report. In the decay model it is assumed that four nuclides, Am-241, Pu-239, Pu-240 and Np-237, contribute to the alpha radiolysis. The alpha energy release from the fuel is related to the amount of each of these nuclides present in the fuel matrix and the energy of the alpha emission for each of the nuclide. The alpha radiolysis dose rate as a function of time is:

$$r_{ox} = \sum_{i=1}^4 A_i \exp\left(\frac{t \ln 2}{B_i}\right)$$

where t is the time.

A_i and B_i are fuel specific constants for the nuclides Am-241, Pu-239, Pu-240 and Np-237. In COMP23 these constants are “hard coded” for a BWR 33 MWd/kgU fuel. The fuel chosen as reference fuel in SR 97 is a BWR 38 MWd/kgU. The latter is used for the inventory and hence the input data is not strictly valid for the reference fuel in SR 97. However, it will serve as a test case.

The rate of dissolution of U-238 from the fuel matrix due to alpha radiolysis, r_α , is given by:

$$r_\alpha = K_{DEC} r_{ox}$$

where K_{DEC} is the proportionally constant and has units mol yr⁻¹/(units of A_i).

Thus the governing equation for the loss of U-238 from the fuel matrix is:

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

where:

M is the amount of U-238 in the fuel matrix at time t,

λ is the decay constant for U-238.

In this case a value of K_{DEC} of $1 \cdot 10^{-5}$ was used.

Results for Test case 14

The results for Test case 14 are shown in Figure 2-25 as near field release rates (mol/yr) for some chosen nuclides, U-238, Ra-226, Np-237 and I-129. The figure also shows the release calculated with the two other alpha radiolysis models, namely “constant” and “explicit” (Test case 15).

Compared to the constant model, which is normally used, the release rate for I-129 shows that when the 3% initially free for release (IRF=0.03) has been released the release rate decreases to a lower level using the decay model than for the constant model.

The release of U-238 is equal in the decay case compared to the constant case.

The release rates for Np-237 and Ra-226 are both initially about the same as for the constant case, but after about 20,000 years the releases are lower than in the constant case.

Test case 15 – Dissolution due to alpha radiolysis – explicit model

Test case 15 has been set up to test the fuel dissolution due to alpha radiolysis with the explicit model. The case is equal to Test case 14 except for the fuel dissolution model used.

The model is described in the User's guide /Romero et al. 1999/. The description below is to a large extent taken from that report. The nuclides Am-241, Pu-239, Pu-240 and Np-237 are explicitly included in the calculation and using the time-dependent amount of these nuclides the alpha radiolysis dose rate is calculated. In the explicit model the rate of loss from the matrix is given by the expression:

$$\frac{\partial M}{\partial t} = -K_{EXP} \sum_{i=1}^4 C_i M_i - \lambda M$$

where:

K_{EXP} is the proportionality constant and has units $\text{yr}^{-1}/(\text{units of } C_i)$,

M_i is the amount of alpha emitting nuclide i in the fuel matrix at a time t [mol].

C_i is a fuel specific constant for the nuclides Am-241, Pu-239, Pu-240 and Np-237. In COMP23 these constants are "hard coded" for a BWR 33 MWd/kgU fuel. The fuel chosen as reference fuel in SR 97 is a BWR 38 MWd/kgU. The latter is used for the inventory and hence the input data is not strictly valid for the reference fuel in SR 97. However, it will serve as a test case.

In this case a value of K_{EXP} of $1 \cdot 10^{-4}$ was used.

Results for Test case 15

The results for Test case 15 are shown in Figure 2-25 as near field release rates (mol/yr) for selected nuclides, U-238, Ra-226, Np-237 and I-129. The figure also shows the release calculated with the two other alpha radiolysis models, constant and decay (Test case 14).

Compared to the constant model, normally used, the release rate for I-129 shows that when the 3% initially free for release (IRF=0.03) has been released the release rate decreases to a lower level using the explicit model. The shape of the release curve is almost equal to the one for the decay model.

The release of U-238 is equal in all three cases.

The release rates for Np-237 and Ra-226 are both lower than in the corresponding constant and decay cases.

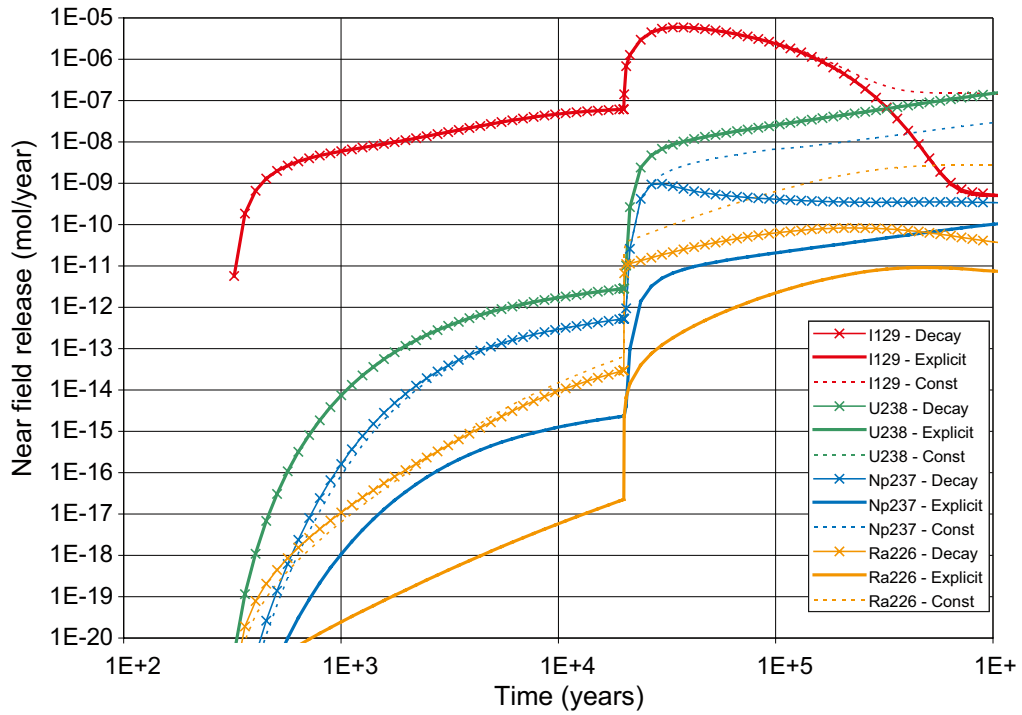


Figure 2-25. Near field release rate (mol/yr) as a function of time for the nuclides I-129, U-238, Np-237 and Ra-226 for the three different alpha radiolysis models.

Test case 16 – Shared solubility

The objective of Test case 16 is to test the shared solubility facility in COMP23. Assuming that the only factor limiting the amount of a certain element to be dissolved is the solubility limit and that the outflow of radionuclides from the canister is negligible the only process changing the canister inventory will be radioactive decay. By using the OWNSOL model for fuel solubility the full inventory will be available for dissolution.

By comparing the terms for outflow with the term for loss through radioactive decay in the transport equation, the maximum allowed half-life for which the nuclide outflow may be neglected can be estimated for a geometry corresponding to the SR 97 case using

$$V_i K_i \lambda \gg \frac{A_{hole} De_{Bentonite}}{L} + De_{Water} \sqrt{2\pi A_{hole}}$$

where L is the diffusion length of the first bentonite block outside the canister and De is the effective diffusivity. If a hole area of 10^{-9} m² is used together with material data for Plutonium, the longest allowed half-life will be of an order of 10^9 years which is much larger than the half-life for both Pu-242 and Pu-240.

An analytic expression that describes the change of the concentration of nuclides in the canister is simple. Since the concentration, c_i , of each nuclide, i , in the water will be proportional to the amount of each nuclide available, the concentration of each nuclide in a solubility group consisting of k nuclides can be expressed as:

$$c_i(t) = c_{shared} \frac{M_{0i} e^{-\lambda_i t}}{\sum_{j=1}^k M_{0j} e^{-\lambda_j t}}$$

where c_{shared} is solubility limit for the group and M_{0i} is the initial amount of nuclide i in the canister.

Results for Test case 16

The canister concentration calculated with COMP23 shown in Figure 2-26 shows good agreement with the concentration calculated with the analytical expression. The initial inventory was 6.0260 mole Pu-242, 11.8900 mole Pu-240 and 8,061 mole U-238.

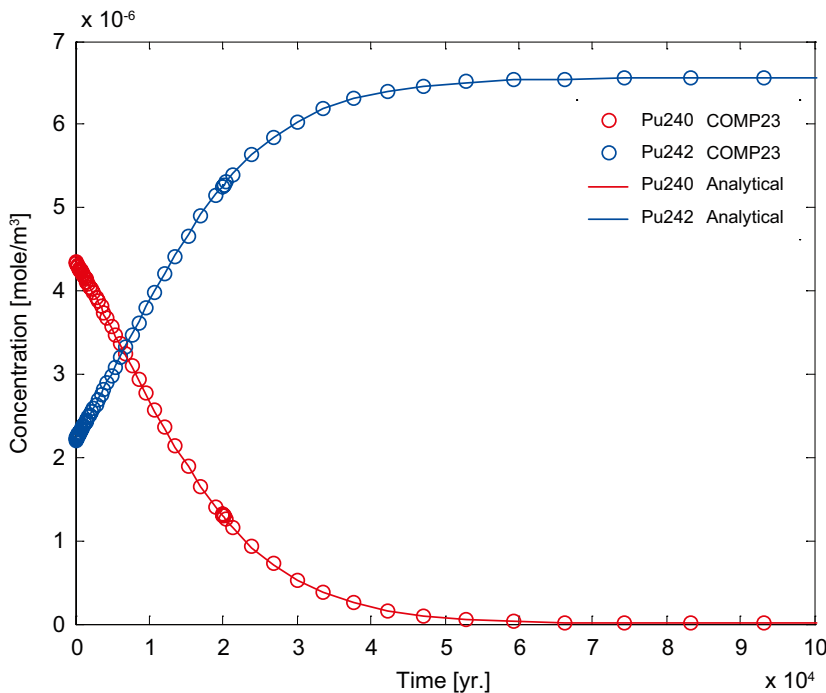


Figure 2-26. Concentration in the canister for Pu240 and Pu-242 for test 16 compared with the analytical solution.

Test case 17 – Probabilistic calculation

Test case 17 is a simplified probabilistic test case that tests the PROPER Monitor rather than COMP23. However, it shows that COMP23 works for a range of parameter values. The test case is based on the same SR 97 calculation as used in Test case 10, but with a number of simplifications. 20 batches with 15 simulations in each were performed. Only the most important nuclides are included and one canister is assumed to have a defect in all calculations. Only one exit path, Q1, was used. The model then consists of the canister, with a hole and outside 0.35 m bentonite. At the outside a boundary condition, Q1, that is dependent on the near-field water flux is applied. The near-field water fluxes calculated for Aberg in SR 97 are used (the first 15 simulations only). The nuclides included are Pu-242, U-238, U-234, Th-230, Ra-226, I-129 and Sn-126. In addition to these simplifications the distribution functions have been changed to test all possible distribution functions in PROPER. The calculation of the biosphere dose is performed with one BIO42-module instead of several SUM41-modules. In addition there are three PICK51-modules that obtain the release rates from the near field, far field and biosphere, respectively.

The different parameter distribution types available with the PROPER Monitor are:

CONST (value)

single-valued distribution

value = the constant value

UNIF (min max)

uniform distribution

min = minimum value

max = maximum value

LOGUNIF (min max)

log-uniform distribution

min = minimum value

max = maximum value

PWUNIF (n x(1) .. x(n+1) p(1) .. p(n) eps)

piecewise uniform distribution

n = number of bins

x(i) = knot point values, in general $x(i) < x(i+1)$, but by setting $x(i) = x(i+1)$ it is possible to enable a discrete distribution

p(i) = probability of value being in bin i

eps = tolerance, if left out = 0.01, $1.0 - \text{eps} < \text{sum}(p(i)) < 1.0 + \text{eps}$

PWLUNIF (n x(1) .. x(n+1) p(1) .. p(n) eps)

piecewise log-uniform distribution

n = number of bins

x(i) = knot point values, $x(i) < x(i+1)$

p(i) = probability of value being in bin i

eps = tolerance, if left out = 0.01, $1.0 - \text{eps} < \text{sum}(p(i)) < 1.0 + \text{eps}$

TRIANG (min mode max)

triangular distribution

min = minimum value

mode = mode (peak) value

max = maximum value

LOGTRIANG (min mode max)

log-triangular distribution

min = minimum value

mode = mode (peak) value

max = maximum value

NORM (mean sigma lprob uprob)
normal (gaussian) distribution
mean = mean value of non-truncated distribution
sigma = standard deviation of non-truncated distribution
lprob = lower cutoff probability (0.->1.)
uprob = upper cutoff probability (0.->1.)

LOGNORM (mu sigma loc lprob uprob)
log-normal distribution
mu = mean value of lg (base 10) of variable of non-truncated distribution
sigma = standard deviation of lg of variable of non-truncated distribution
loc = location parameter
lprob = lower cutoff probability (0.->1.)
uprob = upper cutoff probability (0.->1.)

WEIBULL (scale shape loc lprob uprob)
Weibull distribution
scale = scale parameter
shape = shape parameter
loc = location parameter
lprob = lower cutoff probability (0.->1.)
uprob = upper cutoff probability (0.->1.)

GAMMA (scale shape loc lprob uprob)
gamma distribution
scale = scale parameter
shape = shape parameter
loc = location parameter
lprob = lower cutoff probability (0.->1.)
uprob = upper cutoff probability (0.->1.)

BOOTSTRAP (file)
Parameters sampled from values in a Bootstrap Data File.
The file must have one value on each line and must be sorted in ascending order.
file = Bootstrap Data File name containing the sorted values.

PTABLE (file)
Parameters are taken from a file containing values in a table (see Appendix D).
In each realisation the parameters are single-value distributed.
file = name of the file containing parameter values in a table format.
i = number (integer) of the column storing the parameter.

COMPUTED
Parameters that are calculated inside a module shall be marked "computed".
They are not entered into the sampling scheme.

Results for Test case 17

One of the important outputs to check for this test case is the "proper.sta"-file, which includes all input values chosen from the distributions assigned to the parameters. This file has been studied in EXCEL.

It is noted that there are a few problems associated with the presentation of results arising from the GAMMA distribution. However, it is not anticipated that the GAMMA distribution will be used in subsequent studies, and consequently these issues have not been addressed to date.

Test case 18 – Calculation case from SR 97, Aberg pessimistic canister related parameters, shared solubility

Test case 18 is identical to Test case 10, except that shared solubility is used throughout.

Results for Test case 18

The results for Test case 18 are shown in the following figures. They show the concentration of I-129 and Ra-226 as a function of time, across the various compartments.

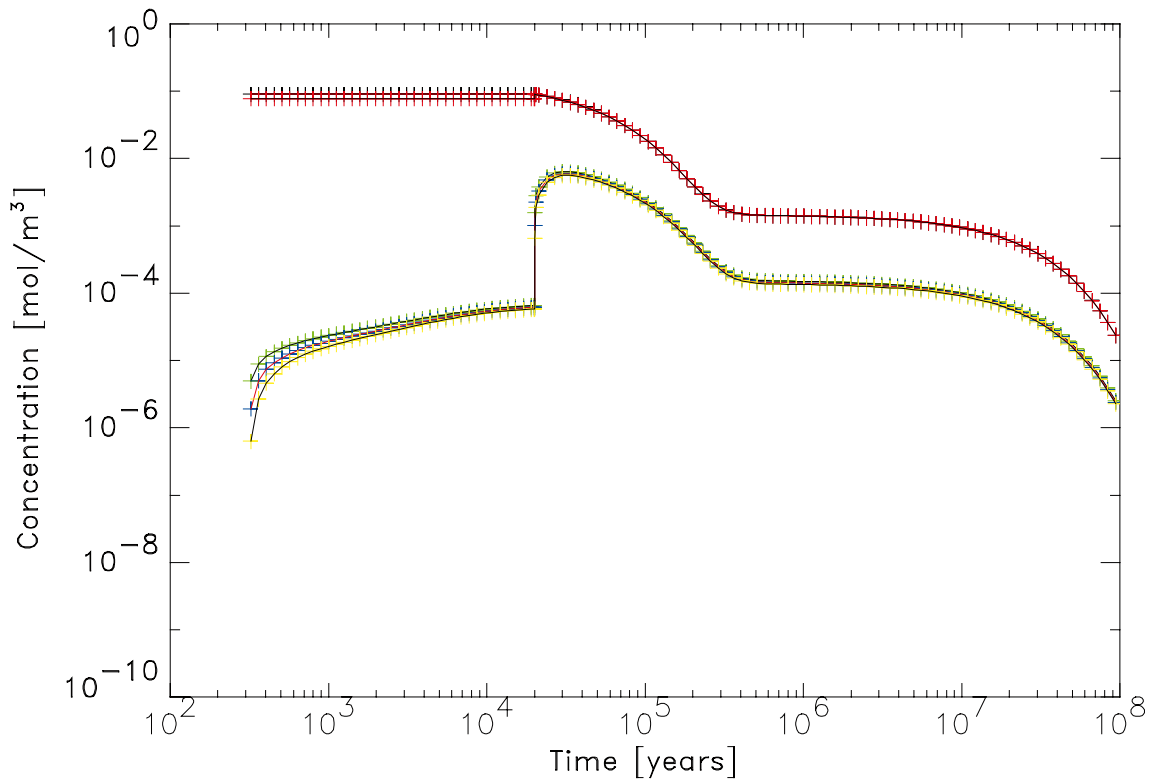


Figure 2-27. I-129 concentrations in compartments 1 to 5.

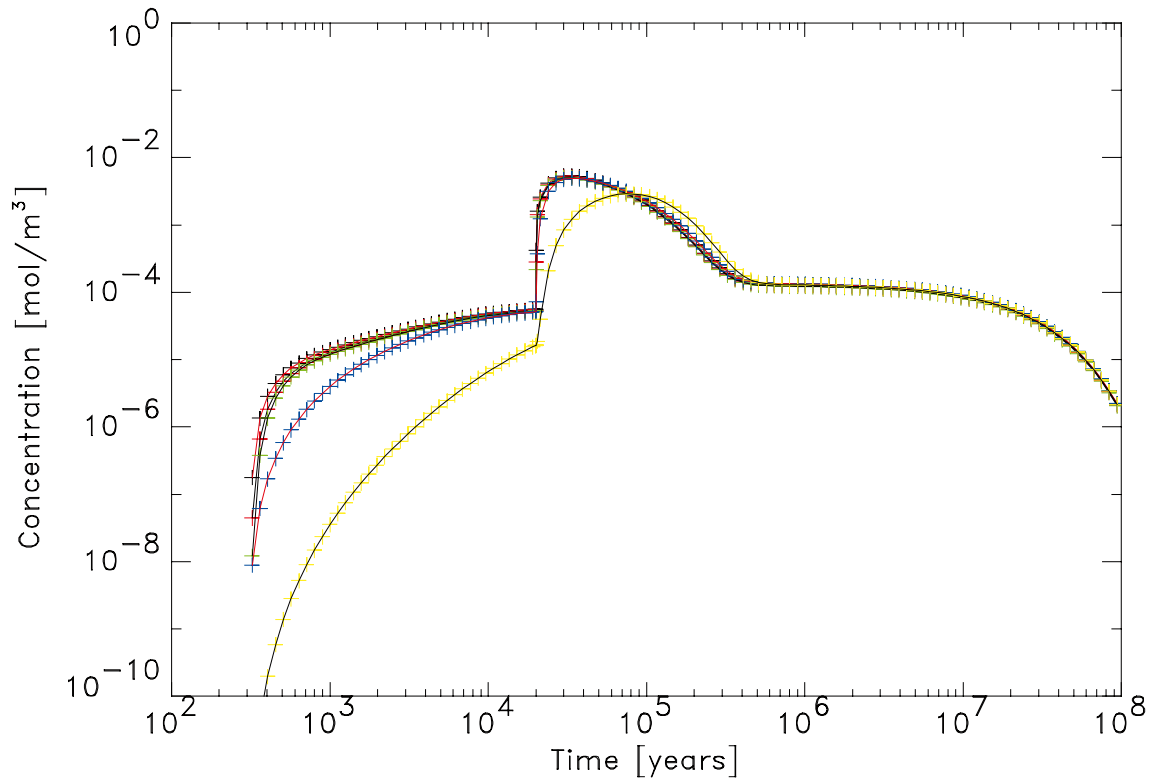


Figure 2-28. I-129 concentrations in compartments 6 to 10.

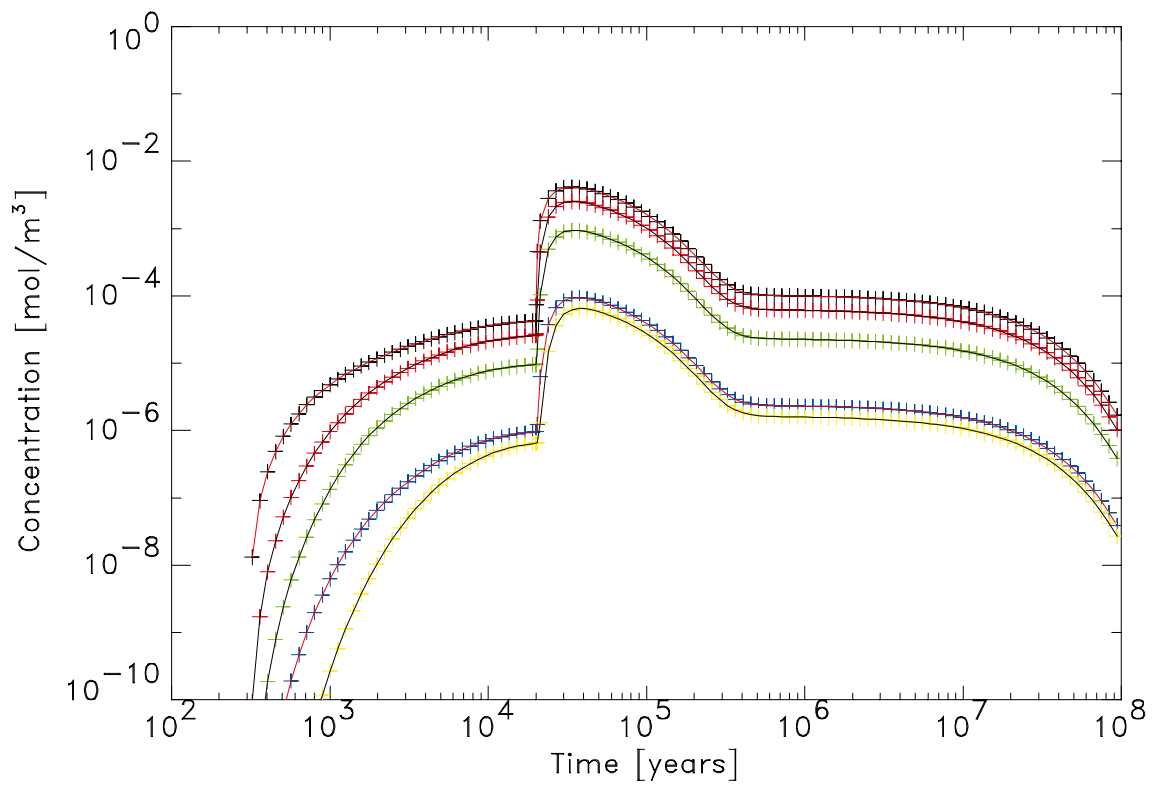


Figure 2-29. I-129 concentrations in compartments 11 to 15.

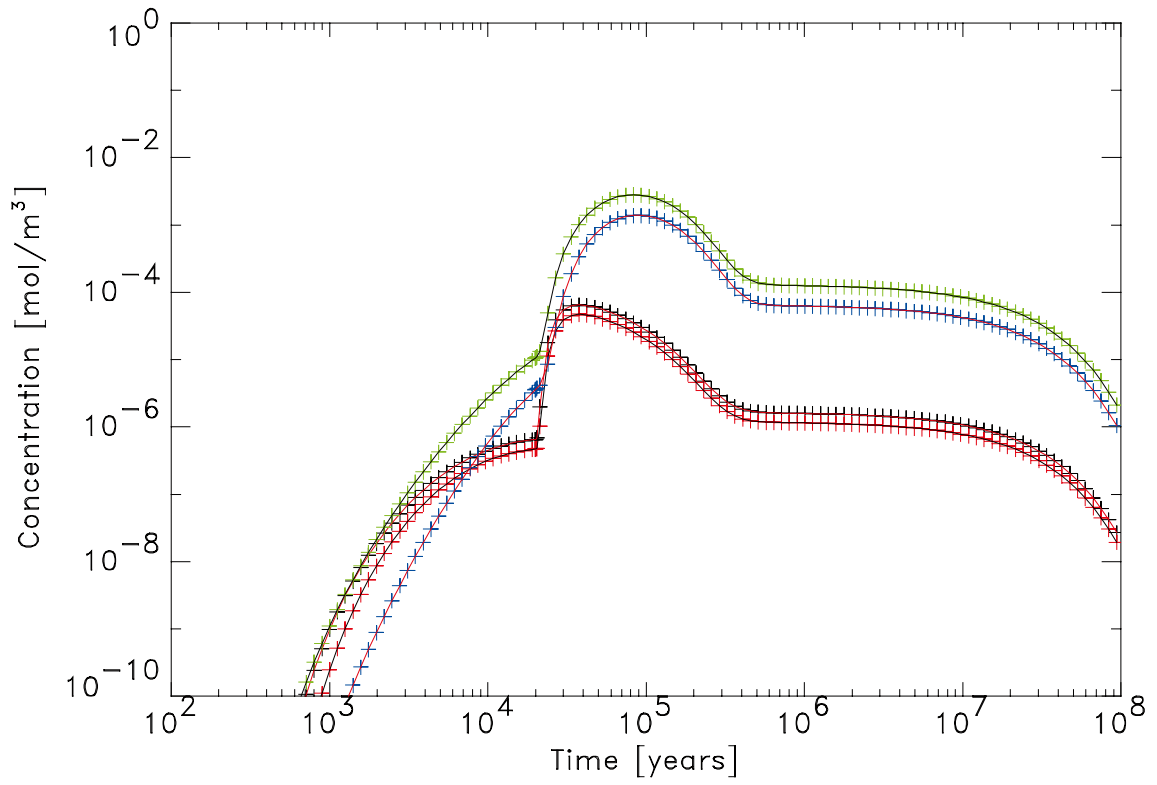


Figure 2-30. *I-129 concentrations in compartments 16 to 19.*

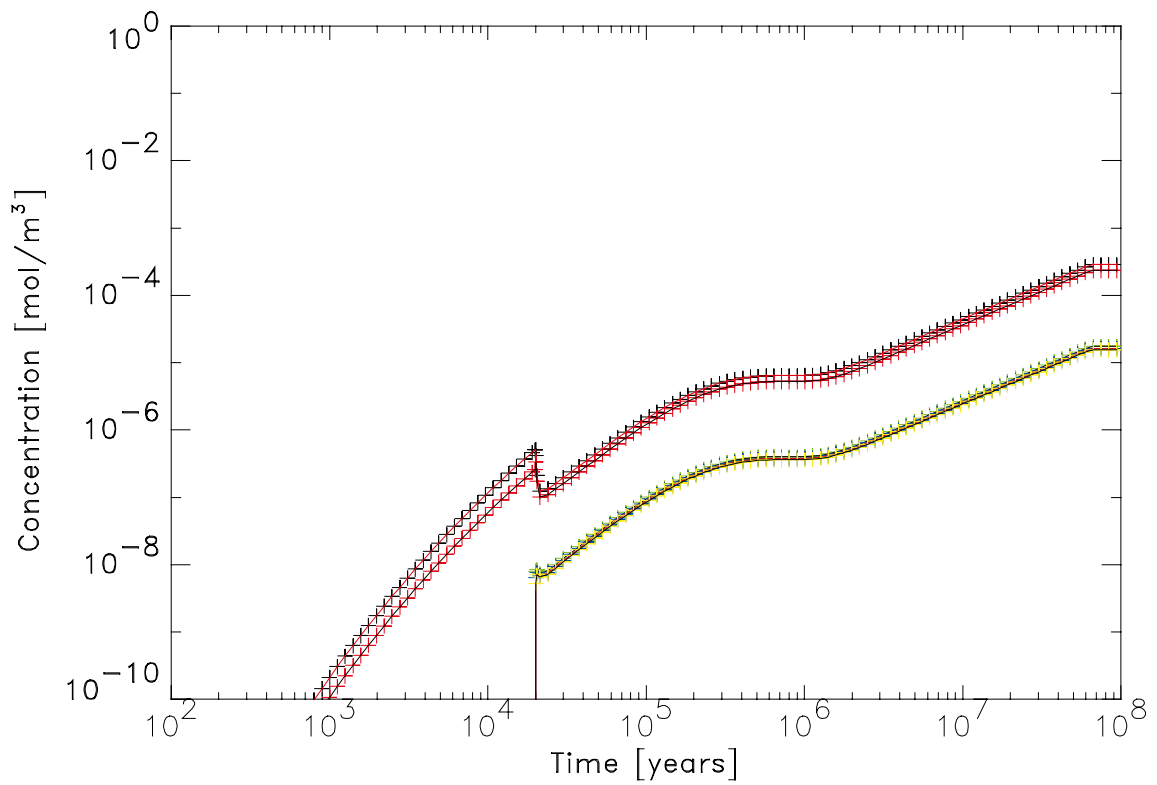


Figure 2-31. *Ra-226 concentrations in compartments 1 to 5.*

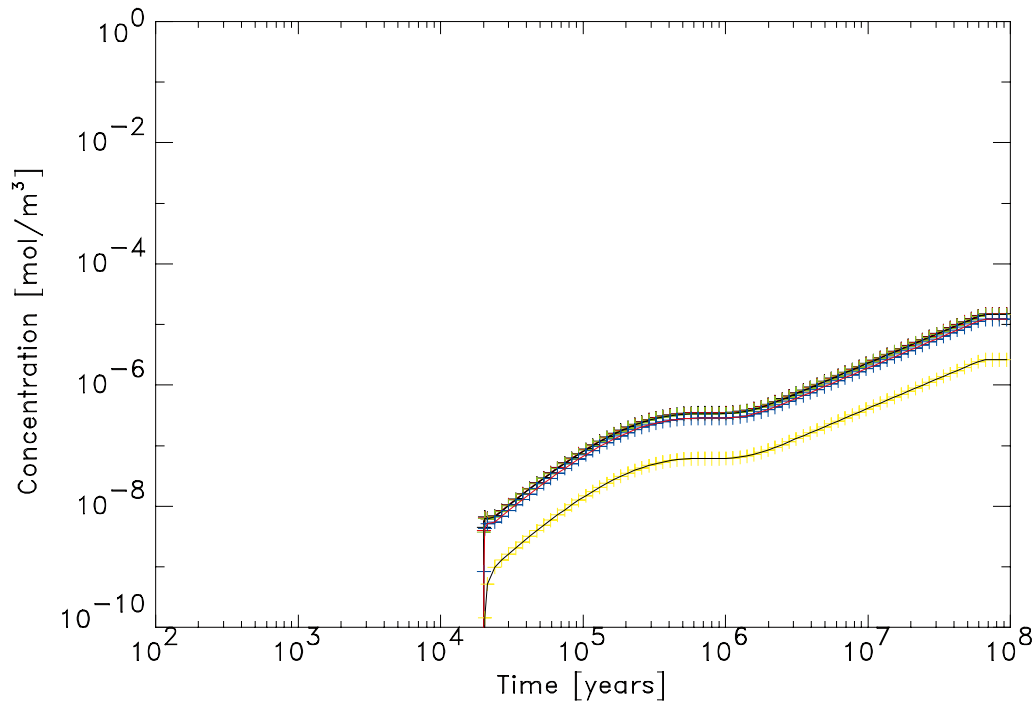


Figure 2-32. Ra-226 concentrations in compartments 6 to 10.

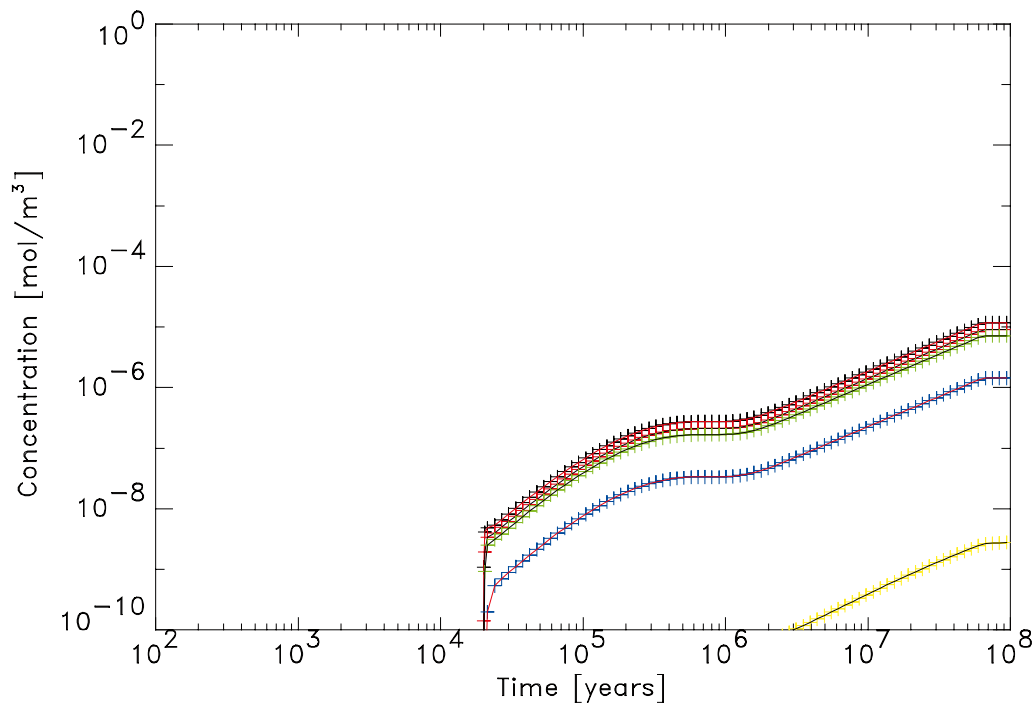


Figure 2-33. Ra-226 concentrations in compartments 11 to 15.

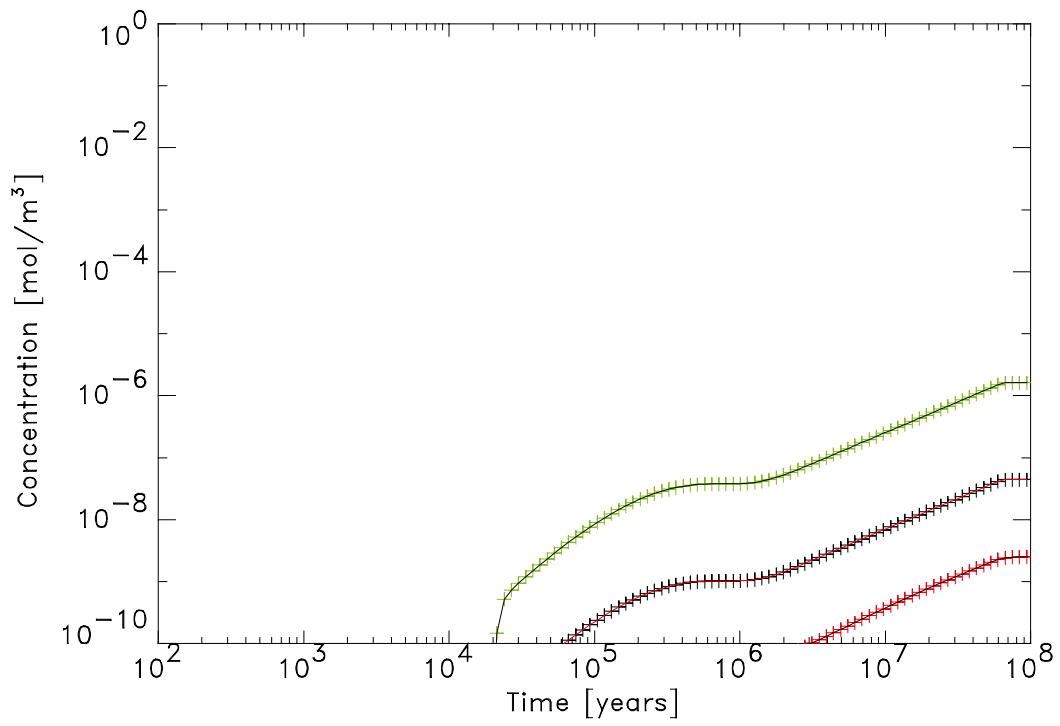


Figure 2-34. Ra-226 concentrations in compartments 16 to 19.

Test case 19 – Consistency Check when Multiple FARF31 Modules are Used

The objective of Test 19 is to ensure that PROPER provides consistent output when multiple sinks are defined in COMP23, and those sinks are used to provide input to separate FARF31 geosphere modules. The test is shown schematically in Figure 2-35.

Each of the FARF modules in this layout have identical properties. If COMP23 is treating multiple sinks in a consistent manner, then $F_1 = F_2 + F_3$.

There are two components to Test 19, namely Test 19a and Test 19b. Test 19a considers the system in the left of the above figure, in which both outputs are fed through a single FARF31 module. Test 19b considers the system on the right of the above figure, in which each output is fed through separate (but identical) FARF31 modules.

Results for Test case 19

Test case 19a provides output fluxes from a single FARF31 module, and Test case 19b provides output fluxes from separate FARF31 modules. The test is passed if the sum of the two fluxes in Test 19b equal the flux obtained in 19a, for all times. Once equilibrium has been obtained, the following fluxes emerge from the FARF31 modules:

Test 19a: $F_1 = 2.04589\text{E-}08 \text{ mol y}^{-1}$

Test 19b: $F_2 = 1.35053\text{E-}08 \text{ mol y}^{-1}$ $F_3 = 6.95362\text{E-}08 \text{ mol y}^{-1}$

Simple summation indicates that $F_1 = F_2 + F_3$ for these fluxes, and similarly the equality also holds for other time points. The following figures illustrate this further.

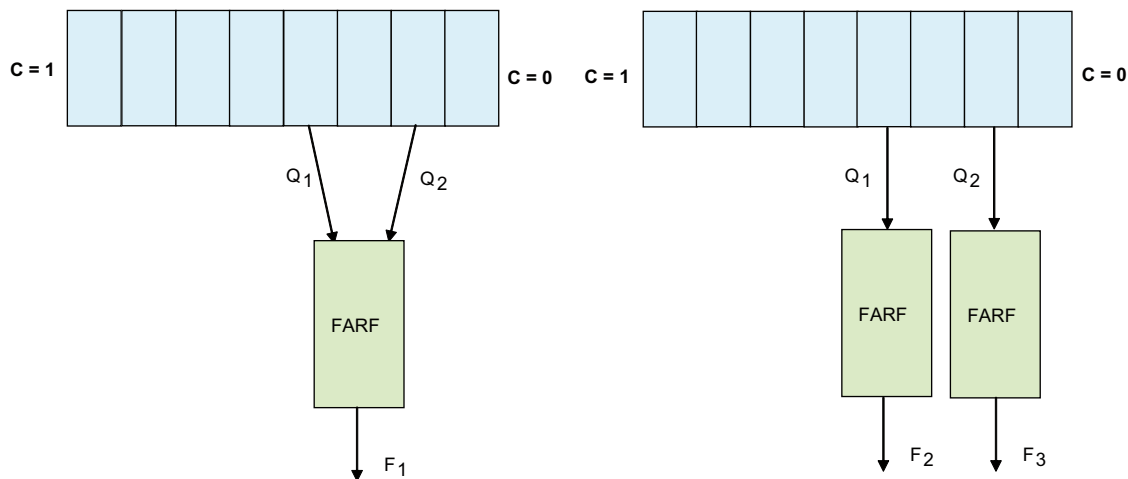


Figure 2-35. Schematic illustration of Test 19.

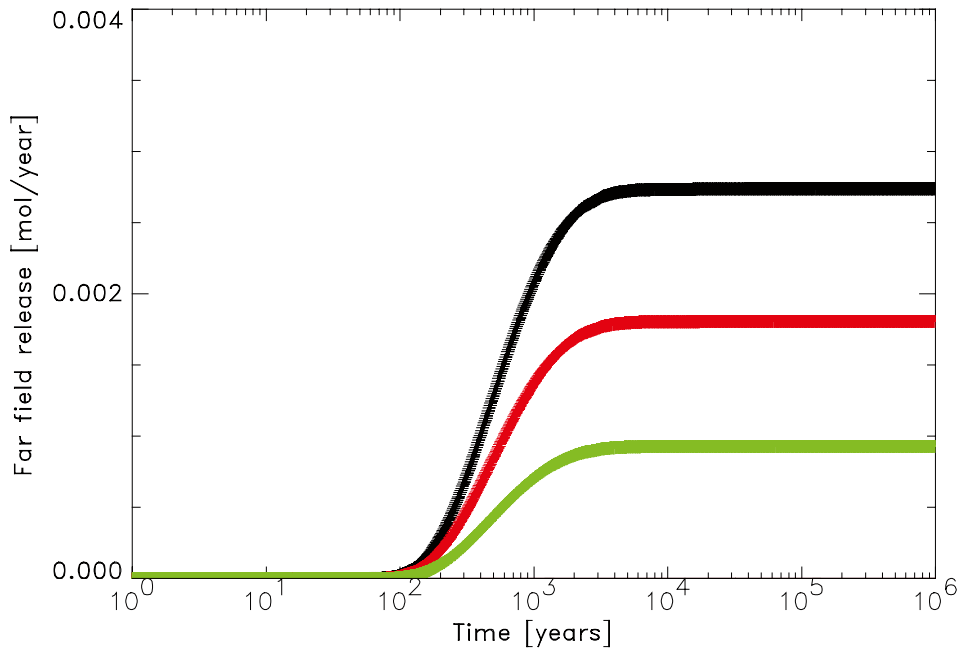


Figure 2-36. Radionuclide release from the far field as a function of time. Black = total, red = near sink, green = far sink.

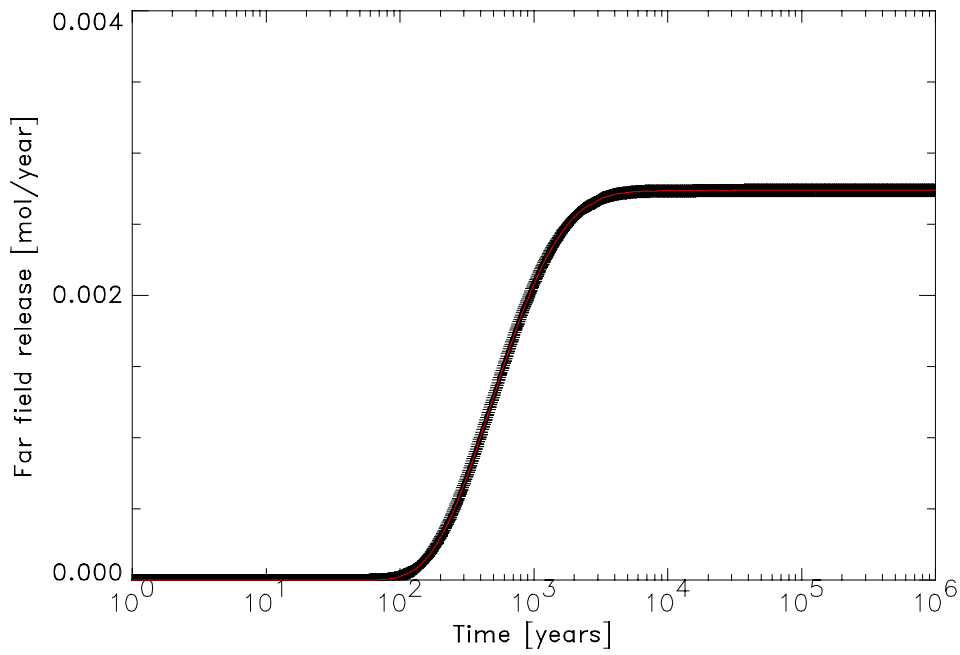


Figure 2-37. Total radionuclide release from far field as a function of time (mol/yr). Solid line corresponds to a single FARF taking the sum of the outputs from COMP23.

Test case 20 – Time-dependent Variations to K_D

The objective of Test 20 is to test the ability of COMP23 to handle time-dependent changes in the sorption coefficient for near-field materials. The basic system is similar to that for Test 9, and is shown in Figure 2-38.

The system is modelled in PROPER with either 8 or 16 compartments. The $C = 1$ boundary condition is enforced in PROPER by choosing a large inventory of U-238 in a canister and setting the solubility limit of U-238 to unity. Test 20 consists of four subtests:

- Test 20a Piecewise linear variations with 8 compartments;
- Test 20b Piecewise linear variations with 16 compartments;
- Test 20c Piecewise constant variations with 8 compartments;
- Test 20d Piecewise constant variations with 16 compartments.

Comparisons were made between the concentrations predicted by COMP23 and analytic solutions (all subtests), and with the output from a simulation of the system undertaken using the ModelMaker code (for subtests 20a and 20c).

The analytic solution is derived from the following form of the diffusion equation:

$$\frac{\partial}{\partial t}(K(t)C) - D \frac{\partial^2 C}{\partial x^2} = 0 \quad K(t) = K_0(1 + at)$$

By defining a new dependent variable as a function of time, it is possible to transform this equation into a standard form for which an analytic solution is known. The derivation and evaluation of the analytic solution was undertaken using Mathematica.

Results for Test cases 20

The following figures illustrate that agreement between the output from PROPER and the analytic solutions described above are in general very good, apart from for the first compartment at early times. The figures shown here are for Test cases 20a and 20c. Agreement is similar, and just as good, for Tests 20b and 20d.

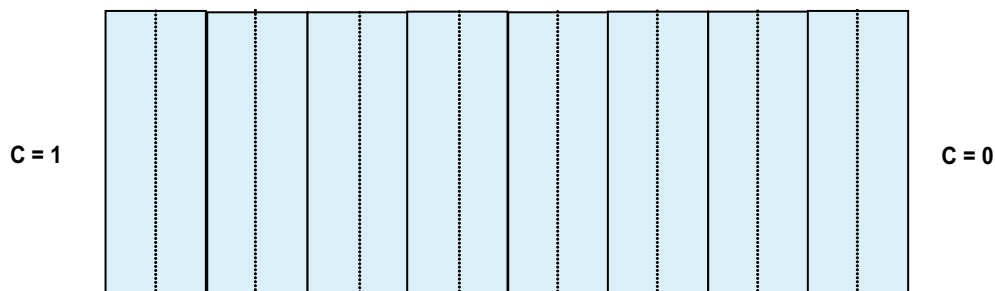


Figure 2-38. Schematic illustration of Test 20.

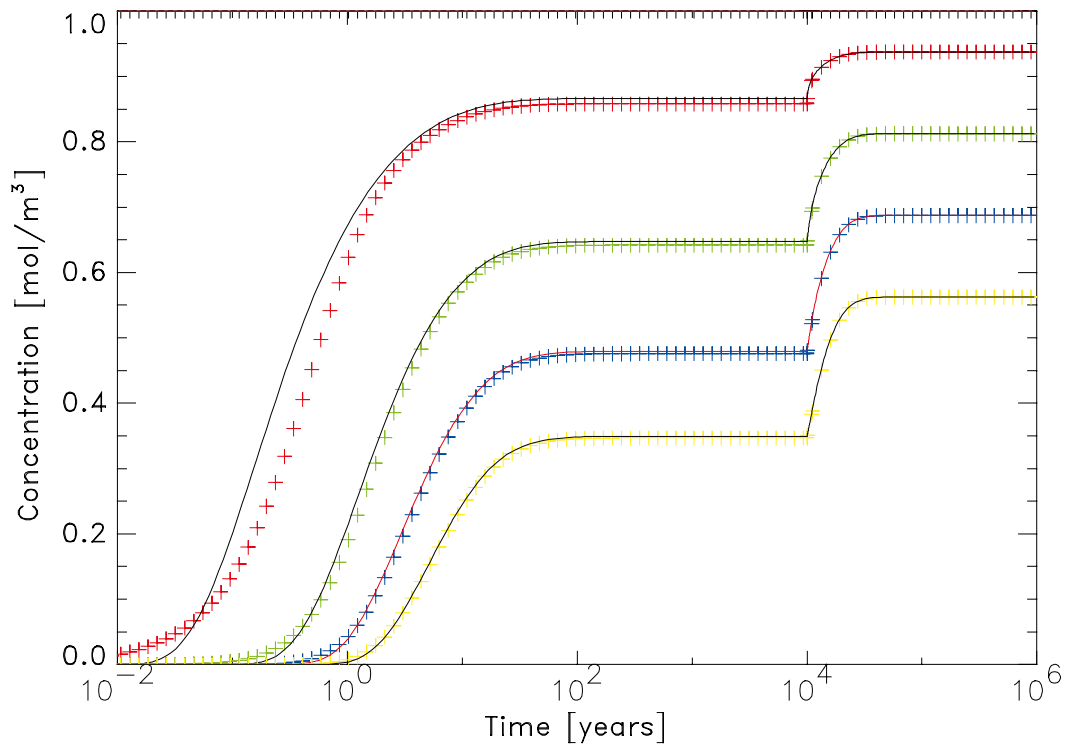


Figure 2-39. Concentrations in compartments 1 to 4 for test case 20a.

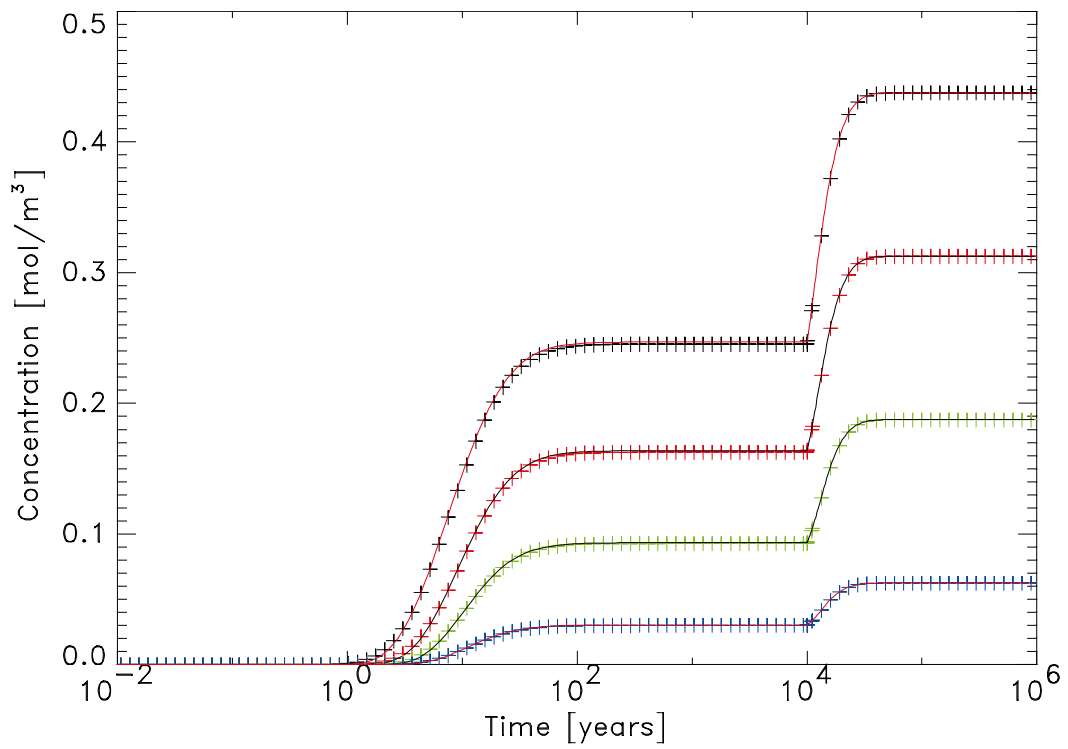


Figure 2-40. Concentrations in compartments 5 to 8 for test case 20a.

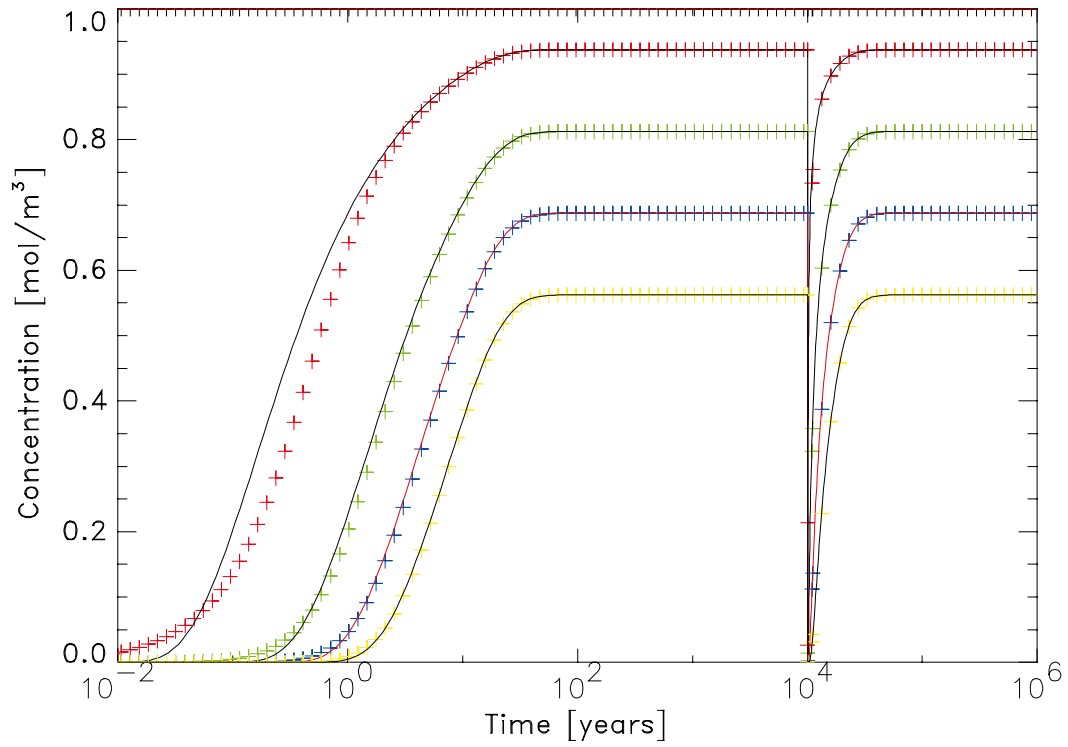


Figure 2-41. Concentrations in compartments 1 to 4 for test case 20c.

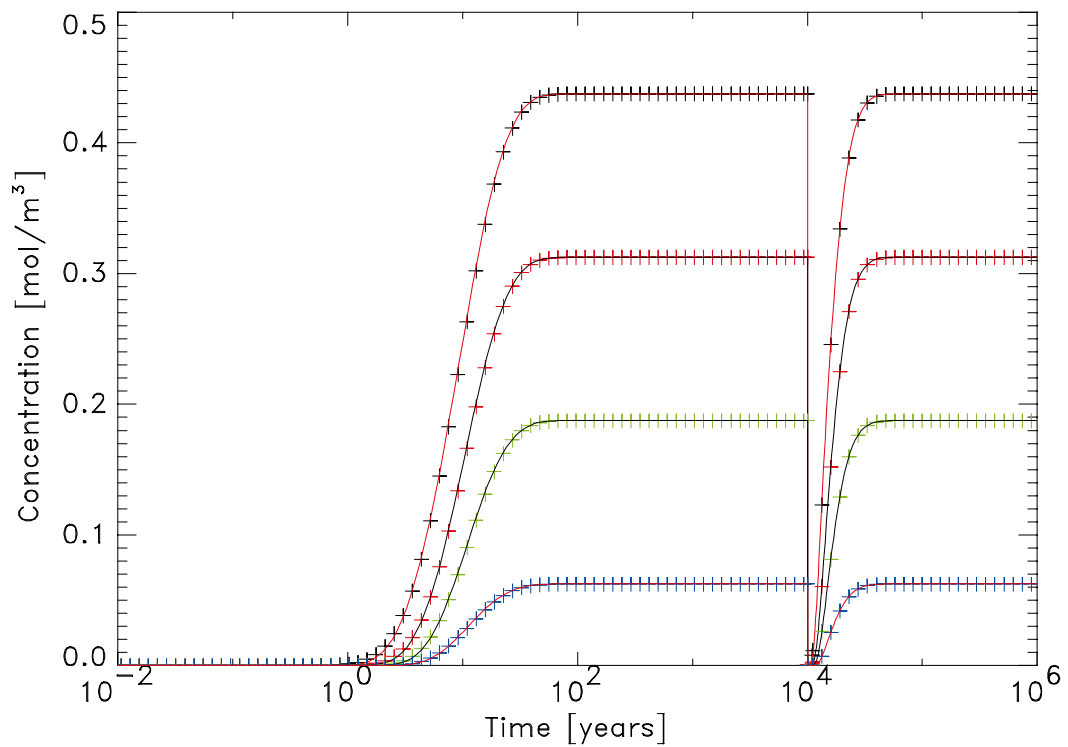


Figure 2-42. Concentrations in compartments 5 to 8 for test case 20c.

Test case 21 – Time-dependent Variations to Porosity

The objective of Test 21 is to test the ability of COMP23 to handle time-dependent changes in the porosities of near-field materials. The basic system is similar to that for Test 9, and is shown in Figure 2-43.

The system is modelled in PROPER with either 8 or 16 compartments. The $C = 1$ boundary condition is enforced in PROPER by choosing a large inventory of U-238 in a canister and setting the solubility limit of U-238 to unity. Test 21 consists of four subtests:

- Test 21a Piecewise linear variations with 8 compartments;
- Test 21b Piecewise linear variations with 16 compartments;
- Test 21c Piecewise constant variations with 8 compartments;
- Test 21d Piecewise constant variations with 16 compartments.

Comparisons were made between the concentrations predicted by COMP23 and analytic solutions (all subtests), and with the output from a simulation of the system undertaken using the ModelMaker code (subtests 21a and 21c).

The analytic solution is derived from the following form of the diffusion equation:

$$\frac{\partial}{\partial t}(K(t)C) - D \frac{\partial^2 C}{\partial x^2} = 0 \quad K(t) = K_0(1 + \alpha t)$$

By defining a new dependent variable as a function of time, it is possible to transform this equation into a standard form for which an analytic solution is known. The derivation and evaluation of the analytic solution was undertaken using Mathematica.

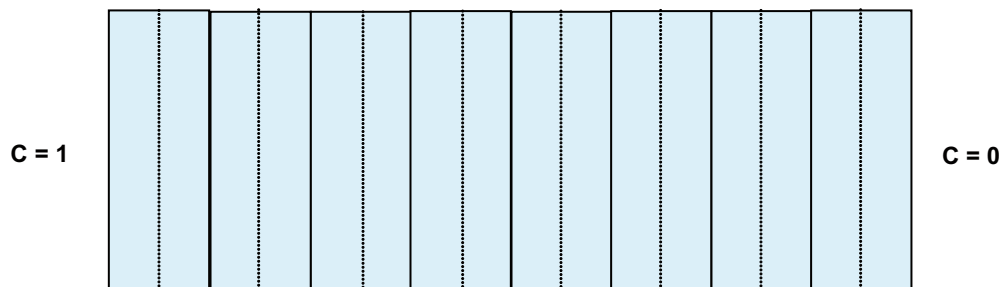


Figure 2-43. Schematic illustration of Test 21.

Results for Test cases 21

The following figures illustrate that agreement between the output from PROPER and the analytic solutions described above are in general very good, apart from for the first compartment at early times. The figures shown here are for Test cases 21a and 21c. Agreement is similar, and just as good, for Tests 21b and 21d.

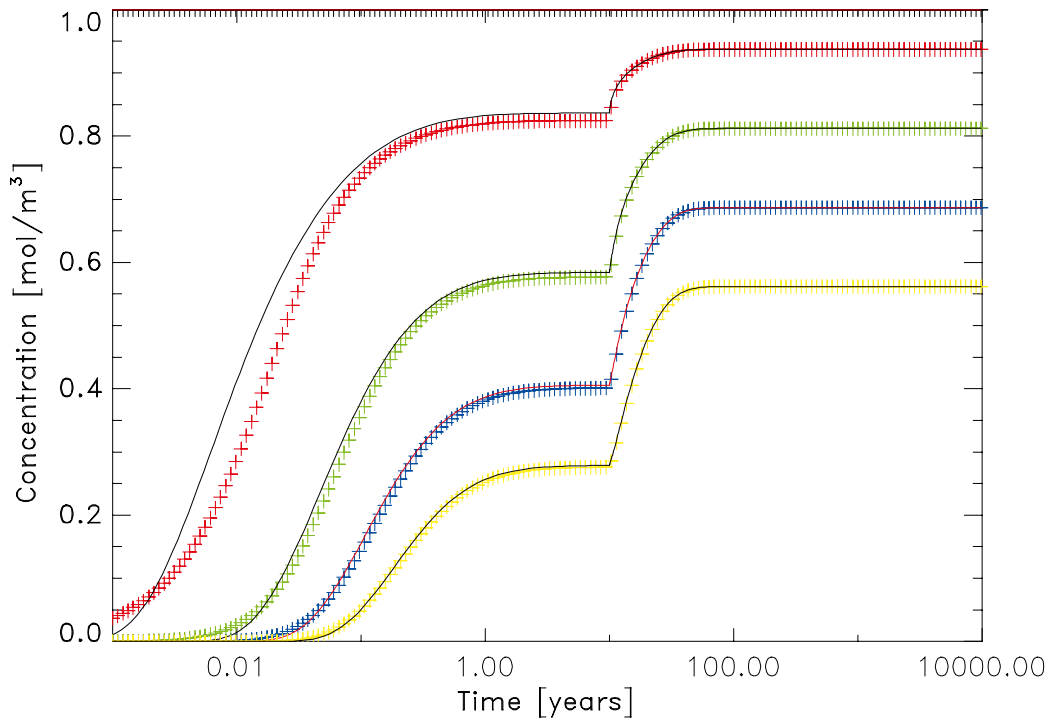


Figure 2-44. Concentrations in compartments 1 to 4 for test case 21a.

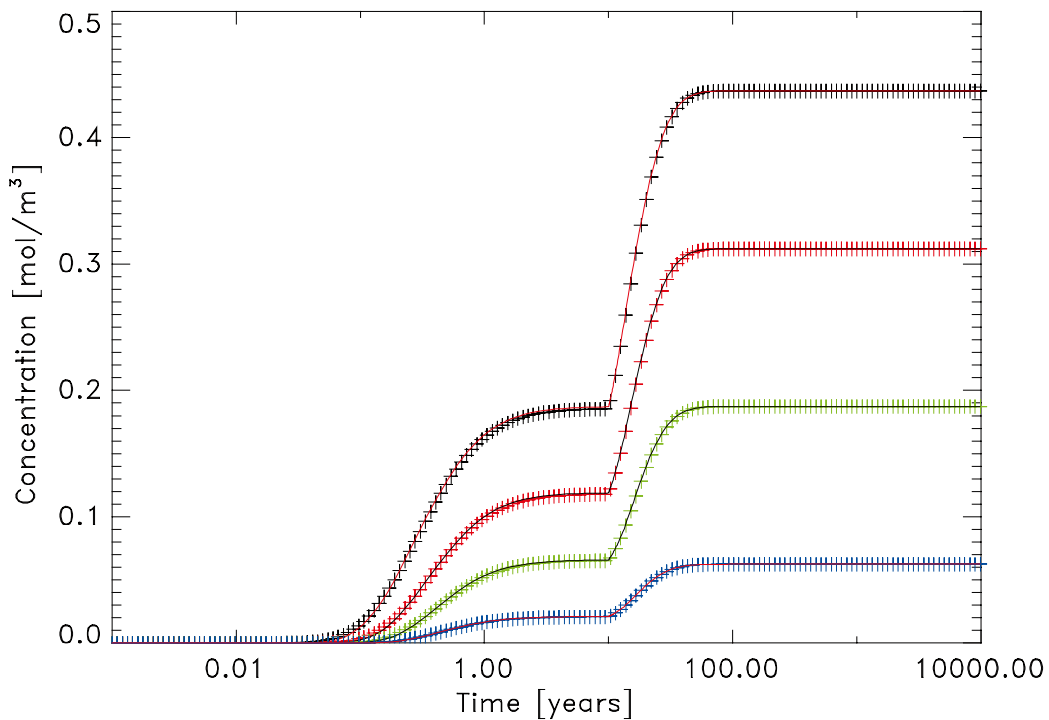


Figure 2-45. Concentrations in compartments 5 to 8 for test case 21a.

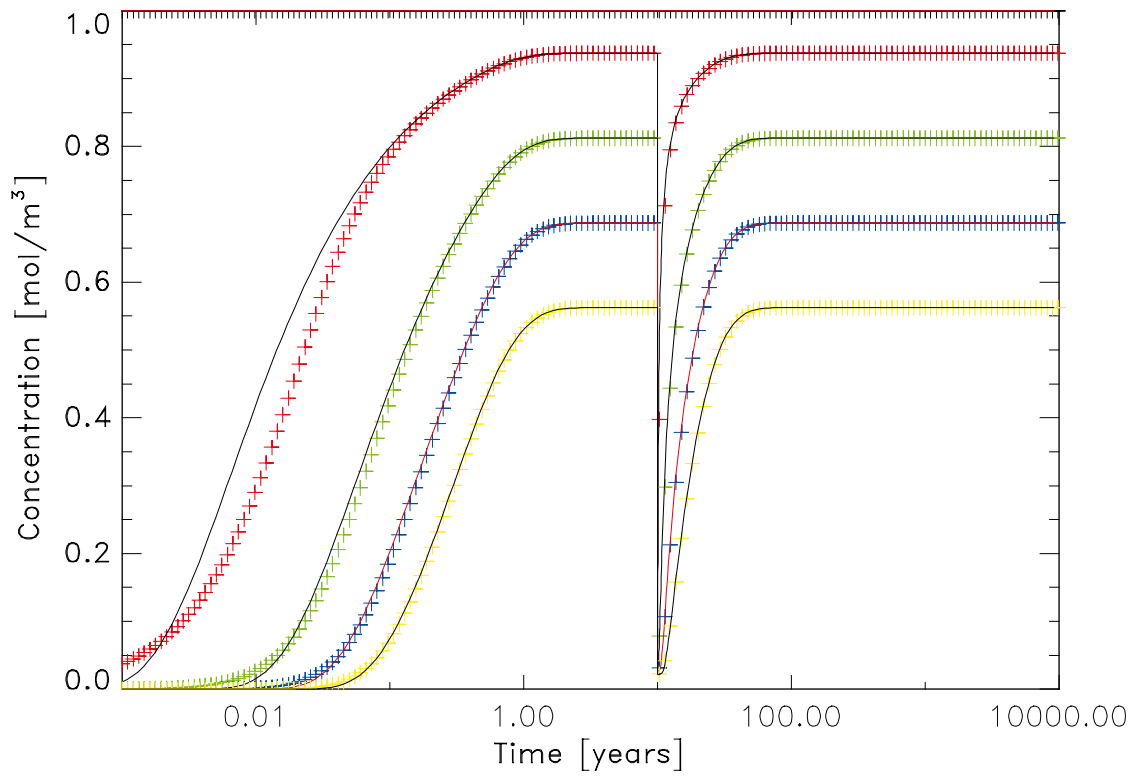


Figure 2-46. Concentrations in compartments 1 to 4 for test case 21c.

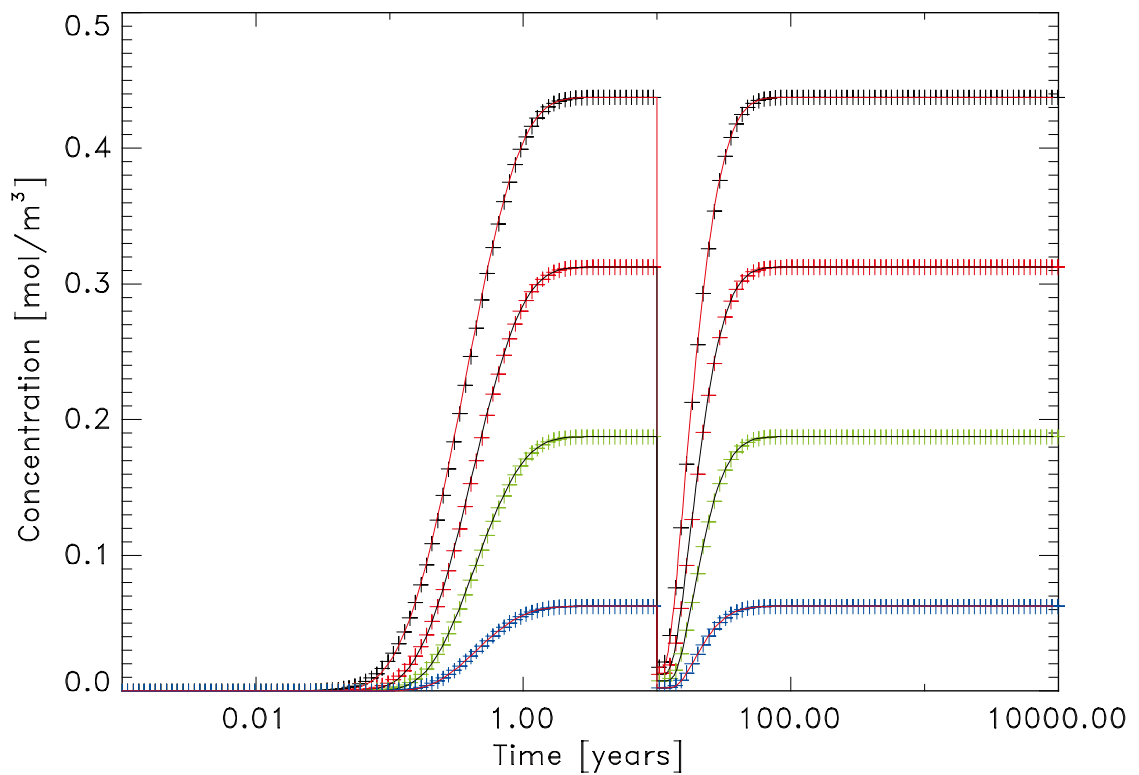


Figure 2-47. Concentrations in compartments 5 to 8 for test case 21c.

Test case 22 – Time-dependent Variations to Diffusion Coefficient

The objective of Test 22 is to test the ability of COMP23 to handle time-dependent changes in the diffusion coefficient of near-field materials. The basic system is similar to that for Test 9, and is shown in the Figure 2-48.

The system is modelled in PROPER with either 8 or 16 compartments. The $C = 1$ boundary condition is enforced in PROPER by choosing a large inventory of U-238 in a canister and setting the solubility limit of U-238 to unity. Test 22 consists of four subtests:

- Test 22a Piecewise linear variations with 8 compartments;
- Test 22b Piecewise linear variations with 16 compartments;
- Test 22c Piecewise constant variations with 8 compartments;
- Test 22d Piecewise constant variations with 16 compartments.

Comparisons were made between the concentrations predicted by COMP23 and analytic solutions (all subtests), and with the output from a simulation of the system undertaken using the ModelMaker code (subtests 22a and 22c).

The analytic solution is derived from the following form of the diffusion equation:

$$\frac{\partial}{\partial t}(K(t)C) - D \frac{\partial^2 C}{\partial x^2} = 0 \quad K(t) = K_0(1 + \alpha t)$$

By defining a new dependent variable as a function of time, it is possible to transform this equation into a standard form for which an analytic solution is known. The derivation and evaluation of the analytic solution was undertaken using Mathematica.

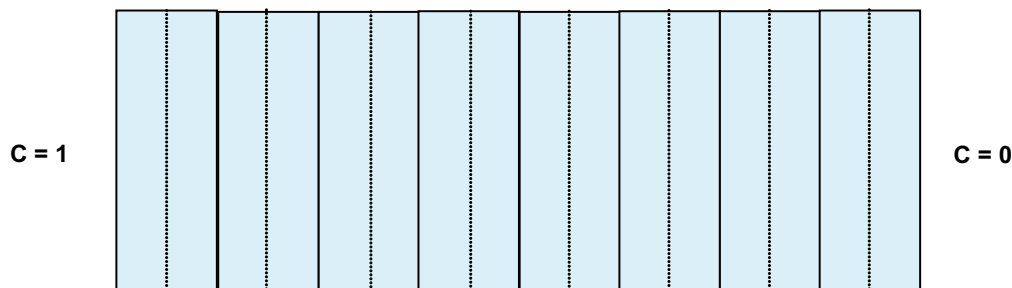


Figure 2-48. Schematic illustration of Test 22.

Results for Test cases 22

The following figures illustrate that agreement between the output from PROPER and the analytic solutions described above are in general very good, apart from for the first compartment at early times. The figures shown here are for Test cases 22a and 22c. Agreement is similar, and just as good, for Tests 22b and 22d.

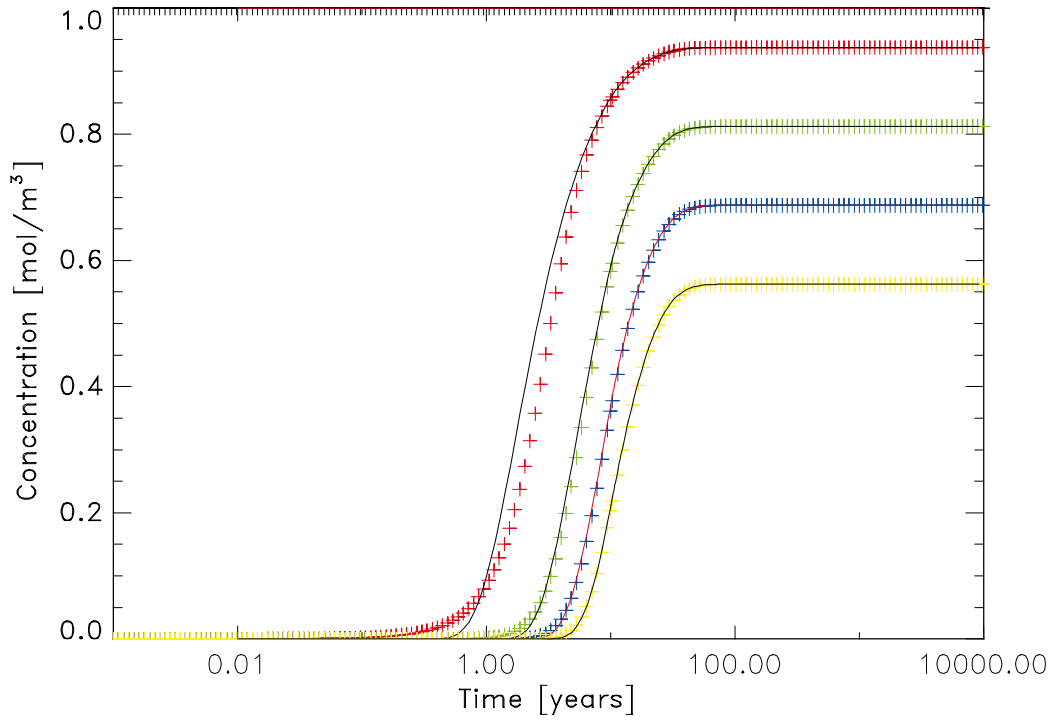


Figure 2-49. Concentrations in compartments 1 to 4 for test case 22a.

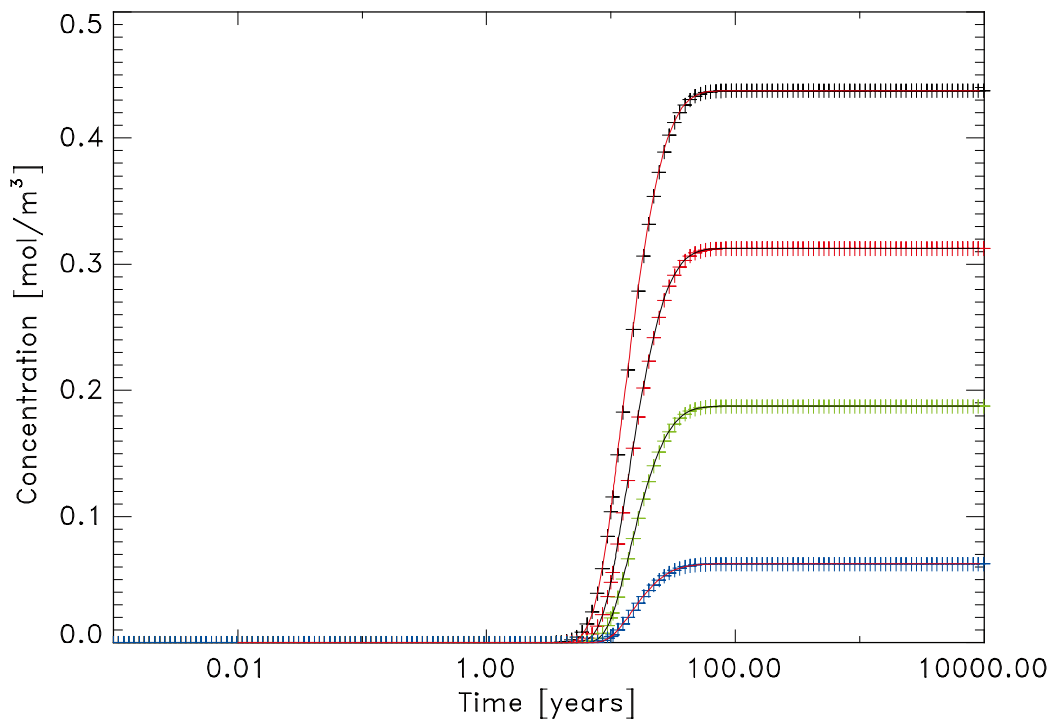


Figure 2-50. Concentrations in compartments 5 to 8 for test case 22a.

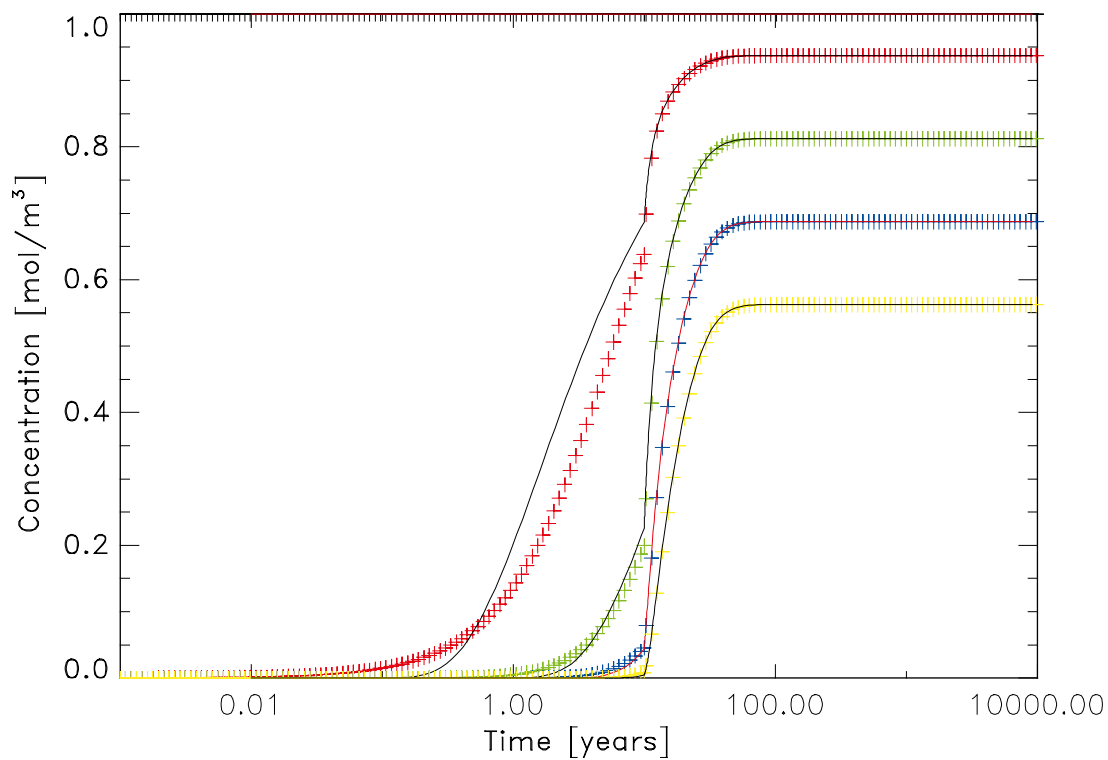


Figure 2-51. Concentrations in compartments 1 to 4 for test case 22c.

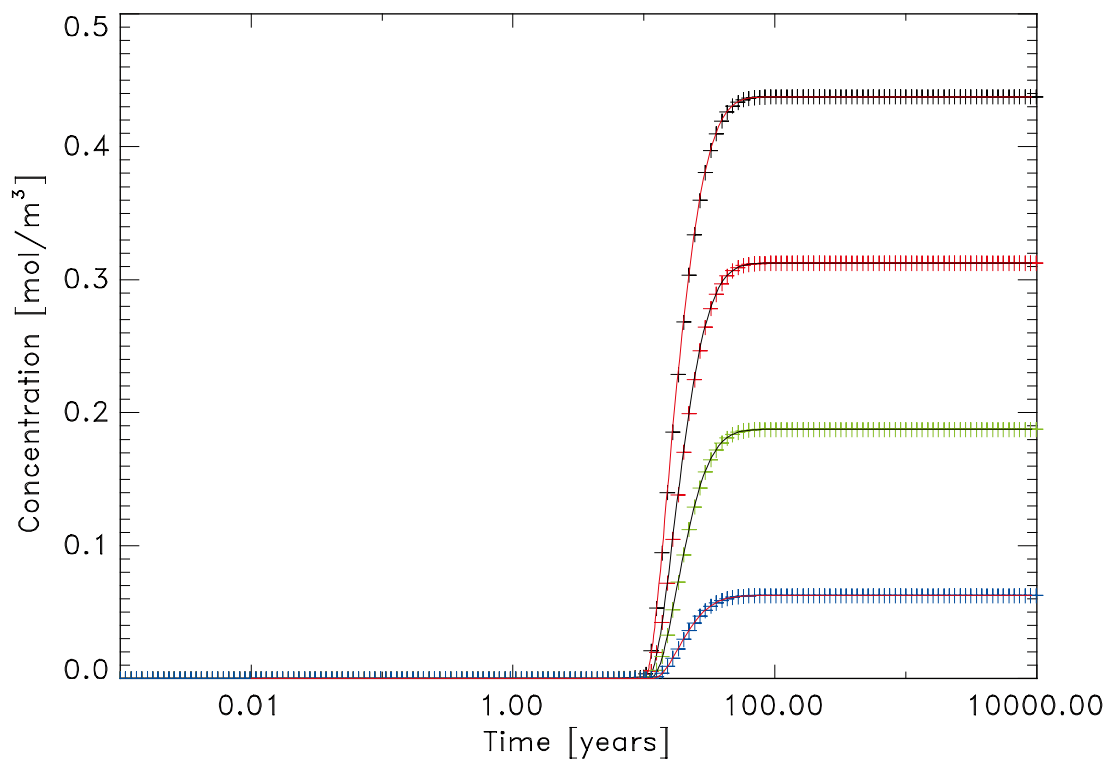


Figure 2-52. Concentrations in compartments 5 to 8 for test case 22c.

Test case 23 – Time-dependent Variations to Solubility Limits

The objective of Test 23 is to test the ability of COMP23 to handle time-dependent changes in the solubility limits of near-field materials. The basic system is similar to that for Test 9, and is shown in Figure 2-53.

The system is modelled in PROPER with 8 compartments. The $C = 1$ boundary condition is enforced in PROPER by choosing a large inventory of U-238 in a canister and setting the solubility limit of U-238 in the canister to unity. Test 23 consists of four subtests:

Test 23a Piecewise linear variations with 8 compartments;

Test 23b Piecewise constant variations with 8 compartments.

Comparisons were made between the concentrations predicted by COMP23 and the output from a simulation of the system undertaken using the ModelMaker code.

ModelMaker is a generalised compartment model solver that is ideally suited for setting up simulations of the simple systems considered in these test cases. ModelMaker models consist of a number of compartments, connections between compartments and functional relationships that define transfers between compartments. ModelMaker is used for comparison purposes in this test as the presence of solubility limitation introduces non-linearity into the governing equation, which precludes obtaining an analytic solution.

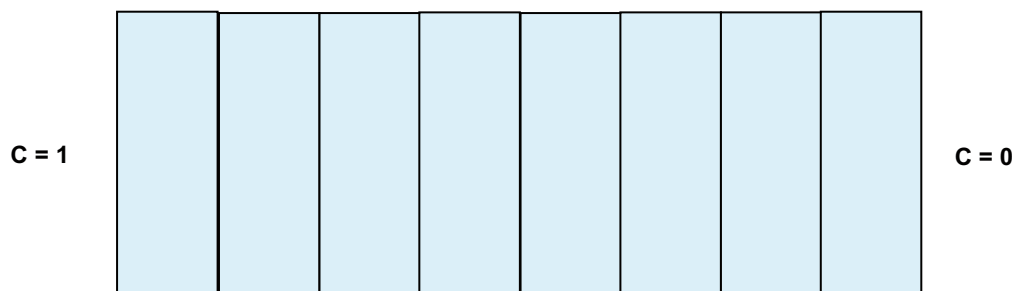


Figure 2-53. Schematic illustration of Test 23.

Results for Test cases 23

The following figures illustrate that agreement between the output from PROPER and the simulation carried out with ModelMaker are in general very good, with no areas where there are discrepancies between the two solutions.

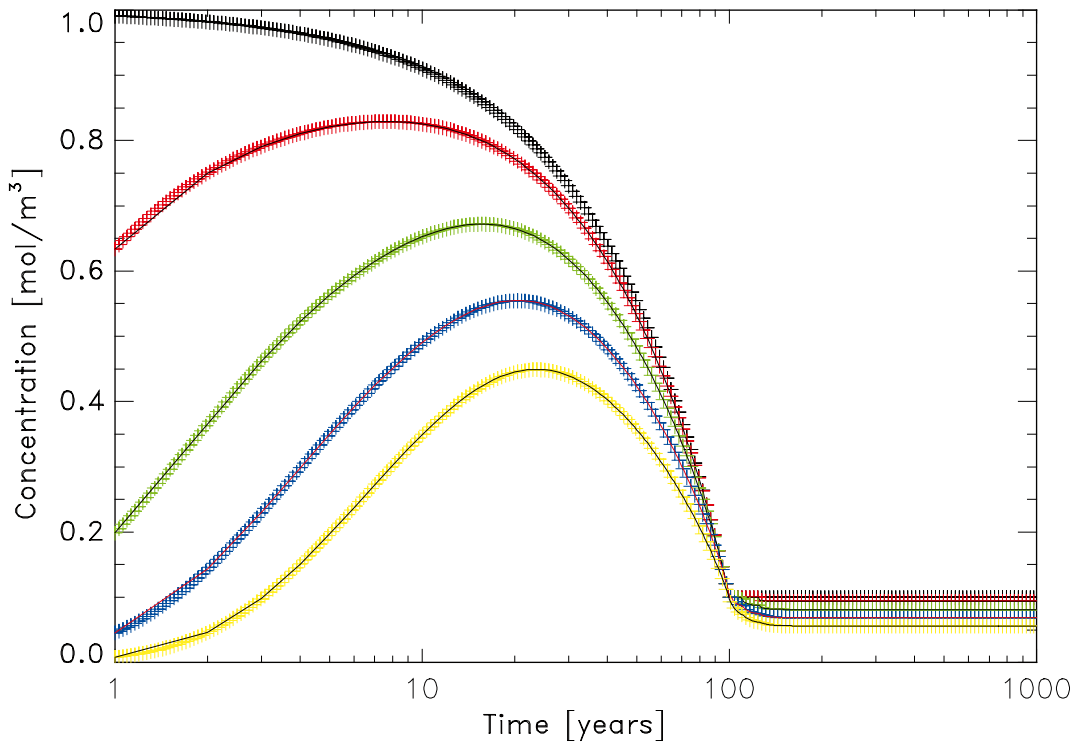


Figure 2-54. Concentrations in compartments 1 to 4 for test case 23a.

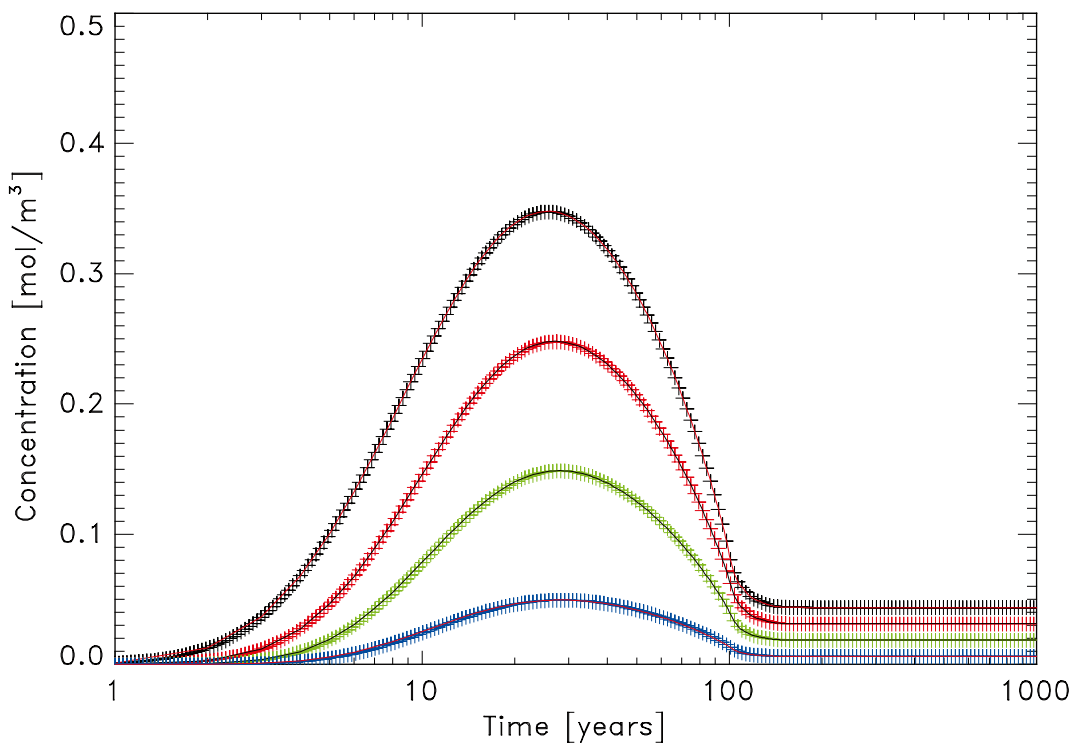


Figure 2-55. Concentrations in compartments 5 to 8 for test case 23a.

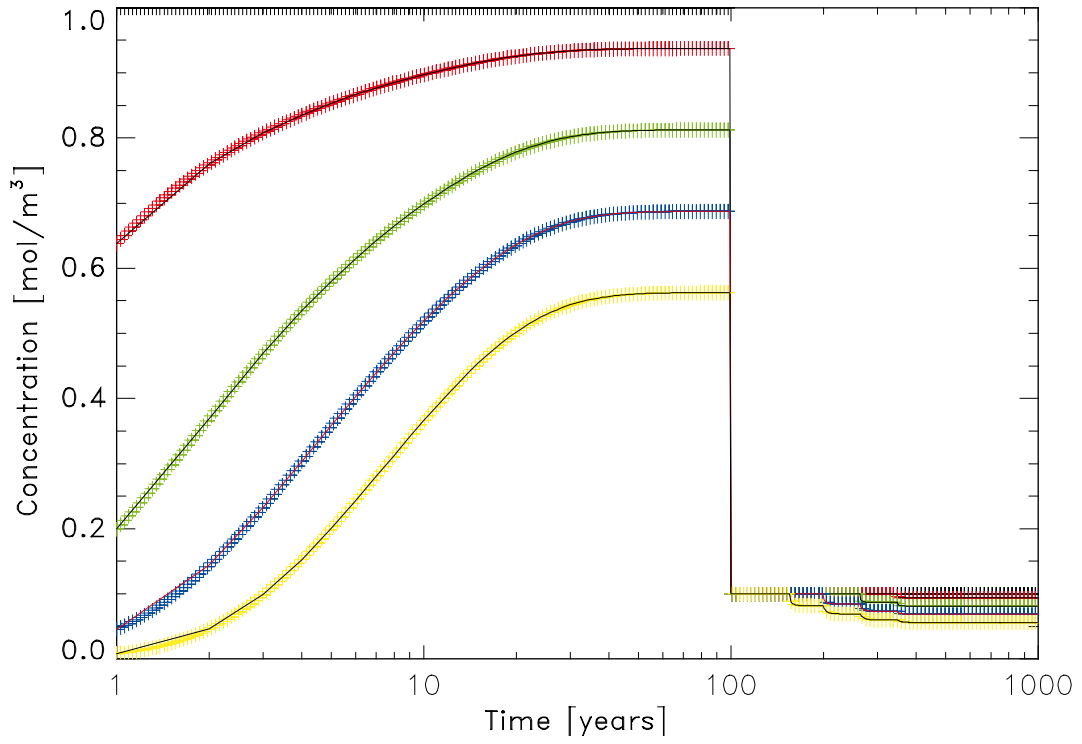


Figure 2-56. Concentrations in compartments 1 to 4 for test case 23b.

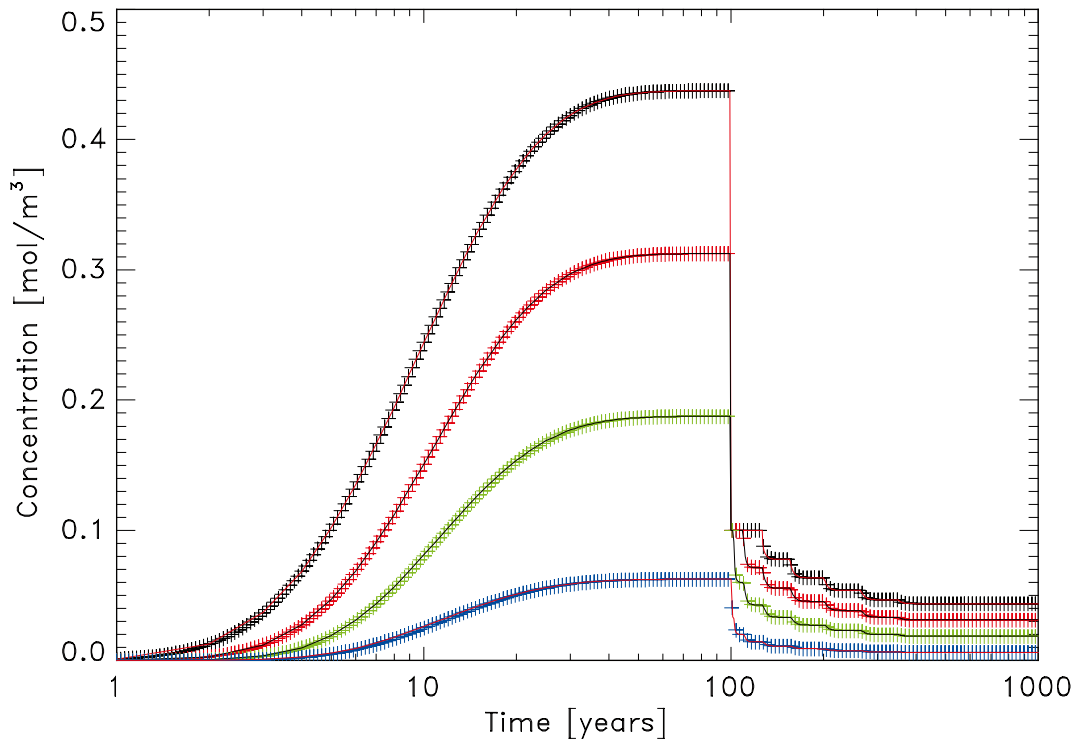


Figure 2-57. Concentrations in compartments 5 to 8 for test case 23b.

Test case 24 – Material-dependent Solubility Limits

The objective of Test 24 is to test the ability of COMP23 to handle systems in which different block materials have different solubility limits. The basic system is similar to that for Test 9, and is shown in Figure 2-58. The first four compartments are assigned a different solubility limit from the final four compartments.

The system is modelled in PROPER with 8 compartments. The $C = 1$ boundary condition is enforced in PROPER by choosing a large inventory of U-238 in a canister and setting the solubility limit of U-238 in the canister to unity.

Comparisons were made between the concentrations predicted by COMP23 and the output from a simulation of the system undertaken using the ModelMaker code.

ModelMaker is a generalised compartment model solver that is ideally suited for setting up simulations of the simple systems considered in these test cases. ModelMaker models consist of a number of compartments, connections between compartments and functional relationships that define transfers between compartments. ModelMaker is used for comparison purposes in this test as the presence of solubility limitation introduces non-linearity into the governing equation, which precludes obtaining an analytic solution.

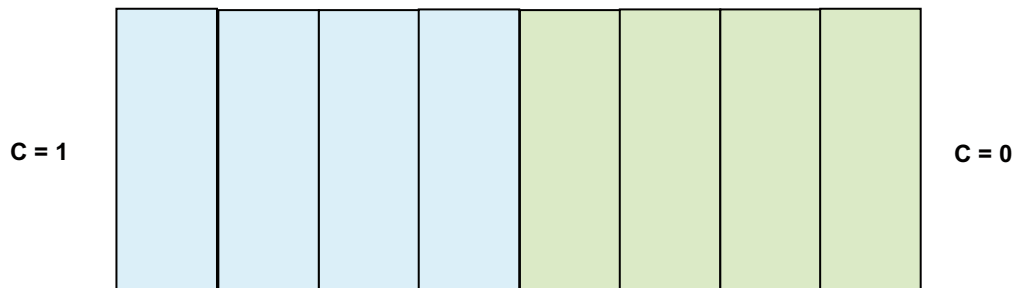


Figure 2-58. Schematic illustration of Test 24.

Results for Test case 24

The following figures illustrate that agreement between the output from PROPER and the simulation carried out with ModelMaker are in general very good, with no areas where there are discrepancies between the two solutions.

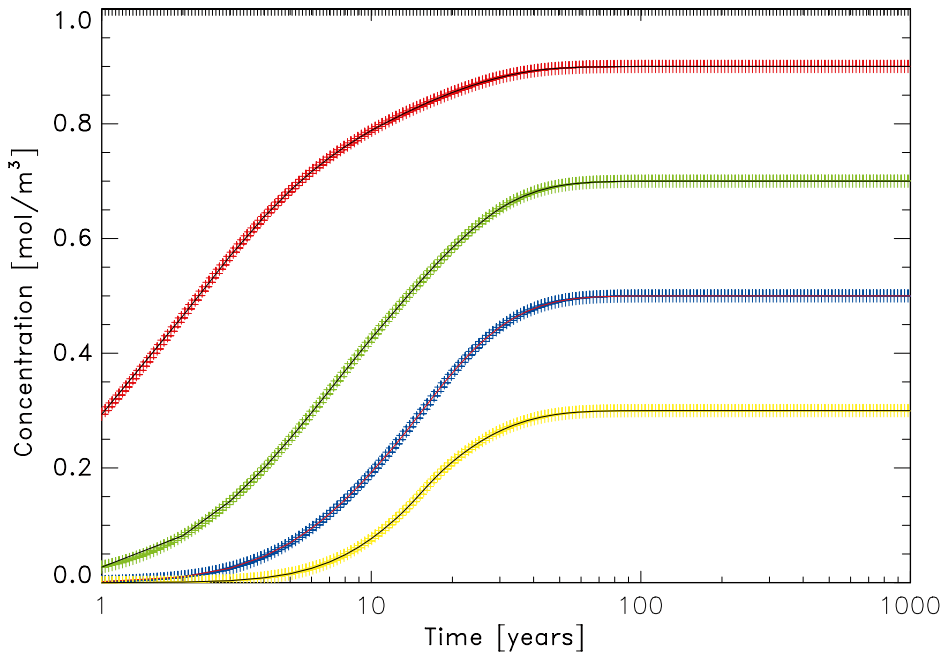


Figure 2-59. Concentrations in compartments 1 to 4 for test case 24.

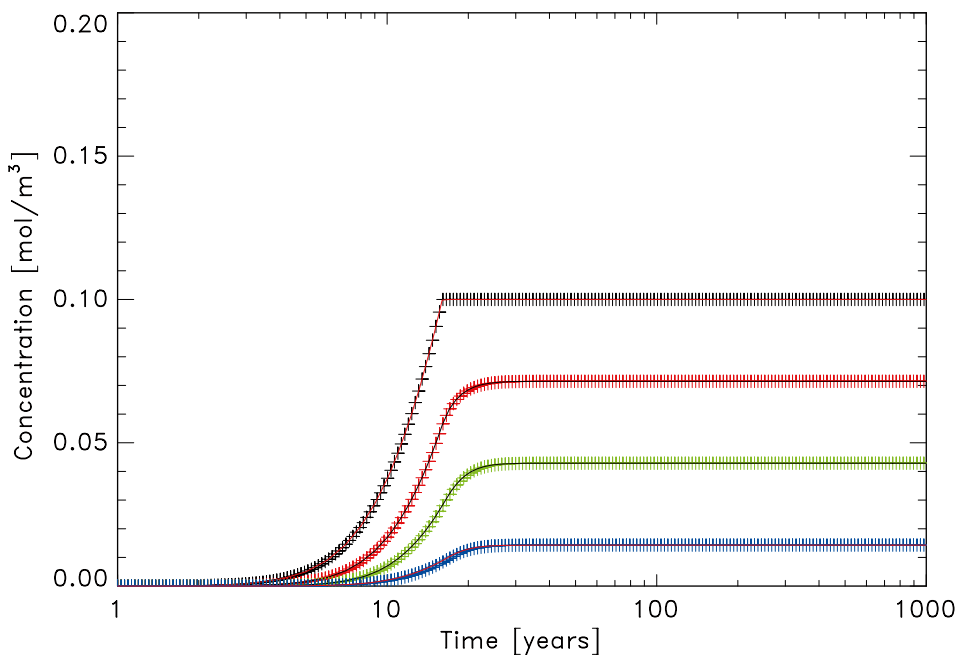


Figure 2-60. Concentrations in compartments 5 to 8 for test case 24.

3 References

Gould L J, Haworth A, Sullivan N, D J Worth, 1996. Verification and optimisation of NUCTRAN. SKB report U-96-22, Svensk Kärnbränslehantering AB.

Lindgren M, F Lindström, 1999. SR 97 – Radionuclide transport calculations. SKB TR-99-23, Svensk Kärnbränslehantering AB.

Porter F M, A V Chambers, 1995. The development and application of RARECAN, Nirex Safety Studies Report NSS/R396.

Romero L, Moreno L, I Neretnieks, 1995. Fast multiple path model to calculate radionuclide release from the near field of a repository, Nuclear Technology, 112 (1), 89–98, 1995.

Romero L, Thompson A, Moreno L, Neretnieks I, Widén H, A Boghammar, 1999. COMP23/NUCTRAN User's guide, PROPER Version 1.1.6. SKB R-99-64, Svensk Kärnbränslehantering AB.

Execution of the test cases

Location of test cases

The main path to the test cases is: /usr/local/skb/comp23/sun/testex/. The test case directories include input files and scripts to run the test case and compare results with reference files. The procedure of using the available scripts is optional. In addition, the directories contain a sub-directory for the Reference files. Packages of the files for the tests are stored in the SCCS-directory /usr/local/skb/comp23/sun/SCCS. The general file structure for the test cases is:

```

/usr/local/skb/comp23/sun/testex/testi/
  input files
  Optional scripts to run the test
  Readme.txt
  Reference/      input files
                  output files
  testrun/       results from the latest run (for tests 2 and
                  18-24))
  Analytic/      Analytic solutions (for tests 20 to 24)
  ModelMaker/    ModelMaker solutions (for tests 20 to 24)

/usr/local/skb/comp23/sun/SCCS/
  Package of input files and reference files

```

Executables

The latest official version of the PROPER-version of COMP23 is executed with the script /usr/local/skb/release/bin/**coprop** (or /usr/local/skb/release/bin/**hycoprop**). If '-h' is passed as argument, the script will list available releases. If a recognised release-name is passed, that particular release will be started. If no argument is passed, the latest release will be started. The Tests 1 and 3–7 were performed with the official PROPER-version **rel 040211** thereafter a new official PROPER-version **rel 080820** were computed with COMP23 version 1.2.2. Tests 2 and 18–24 were performed with the COMP23 version 1.2.2.

The latest official standalone version of COMP23 is executed with the script /usr/local/skb/release/bin/**comp23**. This script works in the same way as the script for the PROPER version, i.e. if '-h' is passed as argument, the script will list available releases. If a recognised release-name is passed, that particular release will be started. If no argument is passed, the latest release will be started. The standalone version has not been tested within this study.

How to run test cases

Test 1 is given as example of how to run the test examples. At the official directory for Test 1 input files, optional scripts and two directories may be found. One of the directories, **Reference**, holds files from a previously executed run (using the release **rel 040211** (Tests 1 and 3–17) or COMP23 version 1.2.2). These files are aimed to be used as a reference case. A source package of the whole set of files for the test including the reference files are stored in /usr/local/skb/comp23/sun/SCCS. The main file structure of Test 1 is:

Readme.txt	General information and advice on how to run the test
RunCoprop.sh*	Script that starts coprop and then runs diff with the reference files
system.dsc_org	Source file to system.dsc
Reference/	Directory with results for reference from a previously executed run using rel 040211 (Tests 1, 3–17) or COMP23 version 1.2.2 (Tests 2, 18–24)

One way to run Test 1 is to check out the file **test1.tar**, un-pack it and then run the test using **RunCoprop.sh**. For example, the sequence of suggested commands is then as follows:

```
% mkdir my_test_directory      (a directory for all tests, a sub-directory named
                                Test1 will be obtained when the Test1.tar file
                                is un-packed)
```

```
% cd my_test_directory
```

```
% ln -s /usr/local/skb/comp23/sun/SCCS SCCS
```

```
% sccs get test1.tar1
```

```
% tar -xf test1.tar
```

- If the official release is not to be used – edit the file RunCoprop.sh by setting the variable Prog to the program that is to be tested.

```
% RunCoprop.sh
```

- The results are stored in a new directory named testrun. (This directory is already present for Tests 2, 18–24).

¹ Some test cases are compressed with gzip, the tar-file is then named testi.tar.gz. This file is checked out and unpacked as follows:

```
% sccs get testi.tar.gz
```

```
% gzip -d testi.tar.gz
```

```
% tar -xf testi.tar
```

Parameters used in reference calculations with INHOMOG and RARECAN

Table B-1. Parameters used in INHOMOG calculations used for comparison with Test case 1, 2 and 3.

Parameter	Value
Nuclide	U-238
Darcy velocity	0
D_i uranium in canister	$3.898 \cdot 10^{-9}$ m ² /s (0.123 m ² /y)
D_i uranium in bentonite	$2.5 \cdot 10^{-11}$ m ² /s ($7.885 \cdot 10^{-4}$ m ² /y)
Porosity canister	1.0
Porosity bentonite	0.25
Bulk density canister	1,000 kg/m ³
Bulk density bentonite	2,000 kg/m ³
Beta factor canister	1.0
Beta factor bentonite	0.75
Uranium sorption coefficient canister	0.0 m ³ /kg
Uranium sorption coefficient bentonite	3.0 m ³ /kg
Uranium solubility limit	$2.0 \cdot 10^{-4}$ moles/m ³
U-238 inventory	0.1 moles
U-238 decay constant	$4.9248 \cdot 10^{-18}$ s ⁻¹
Canister radius	0.3 m
Canister length	4.3 m
Length of bentonite	25.6 m
Number of cells in canister region	1
Number of cells in bentonite region	128

Table B-2. Parameters used in INHOMOG calculations used for comparison with Test case 3.

Parameter	Value
Nuclide	I-129
Darcy velocity	0
D_i iodine in canister	$3.9 \cdot 10^{-9}$ m ² /s (0.123 m ² /y)
D_i iodine in bentonite	$6.25 \cdot 10^{-13}$ m ² /s ($1.972 \cdot 10^{-5}$ m ² /y)
Iodine sorption coefficient canister	0.0 m ³ /kg
Iodine sorption coefficient bentonite	0.0 m ³ /kg
Iodine solubility limit	infinite
I-129 inventory	$3.976 \cdot 10^{-5}$ moles
I-129 decay constant	$1.399 \cdot 10^{-15}$ s ⁻¹

Table B-3. Parameters used in INHOMOG calculations used for comparison with Test case 4.

Parameter	Value
Nuclide	U-238
Darcy velocity in canister	0
Darcy velocity in bentonite	0
Darcy velocity in rock	$3.01 \cdot 10^{-9}$ m/s
D_i uranium in canister	$3.90 \cdot 10^{-9}$ m ² /s (0.123 m ² /y)
D_i uranium in bentonite	$2.50 \cdot 10^{-11}$ m ² /s ($7.885 \cdot 10^{-4}$ m ² /y)
D_i uranium in rock	$5 \cdot 10^{-13}$ m ² /s ($3.2 \cdot 10^{-3}$ m ² /y)
Porosity canister	1.0
Porosity bentonite	0.25
Porosity rock	$5 \cdot 10^{-3}$
Bulk density canister	1,000 kg/m ³
Bulk density bentonite	2,000 kg/m ³
Bulk density rock	2,700 kg/m ³
Beta factor canister	1.0
Beta factor bentonite	1.0
Beta factor rock	1.0
Uranium sorption coefficient canister	0.0 m ³ /kg
Uranium sorption coefficient bentonite	3.0 m ³ /kg
Uranium sorption coefficient rock	2.0 m ³ /kg
Uranium solubility limit	$2.0 \cdot 10^{-4}$ moles/m ³
U-238 inventory	0.1 moles
U-238 decay constant	$4.9248 \cdot 10^{-18}$ s ⁻¹
Canister radius	0.3 m
Canister length	4.3 m
Length of bentonite	1.6 m
Length of rock	30 m
Number of cells in canister region	1
Number of cells in bentonite region	230
Number of cells in rock region	1,860

Table B-4. Parameters used in RARECAN calculations used for comparison with Test case 5, 6 and 7.

Parameter	Value
D _i uranium in canister	3.898·10 ⁻⁹ m ² /s (0.123 m ² /y)
D _i uranium in bentonite	2.5·10 ⁻¹¹ m ² /s (7.885·10 ⁻⁴ m ² /y)
Darcy velocity	0
Bulk density canister	1,000 kg/m ³
Bulk density bentonite ¹⁾	1,000 kg/m ³
Porosity canister	1.0
Porosity bentonite ²⁾	1.0
Canister radius	0.4 m
Canister length	4.5 m
Uranium solubility limit	2.0·10 ⁻⁴ moles/m ³
Uranium sorption coefficient canister	0.0 m ³ /kg
Uranium sorption coefficient bentonite ³⁾	0.0 m ³ /kg
U-238 inventory	8.405·10 ³ moles
U-238 decay constant	4.9248·10 ⁻¹⁸ s ⁻¹
Hole radius	See Table B-5
Number of holes	See Table B-5

¹⁾ RARECAN assumes that the canister and backfill region have the same density. COMP23 defines the canister region (block 1) as water. Therefore, for the purpose of a test case, the density of bentonite is given the value 1,000 kg/m³.

²⁾ As in footnote 1 above, RARECAN assumes that the porosity of the bentonite region equals that of the canister region, which is defined as water in COMP23.

³⁾ RARECAN uses the same sorption coefficient in the bentonite region as in the canister region. Therefore, the sorption coefficient in both regions is taken as that of uranium in pure water with no sorption sites

Table B-5. Parameters used in RARECAN calculations used for comparison with Test case 5, 6, and 7, particular to each test case.

Test case	Vent radius (m)	Number of new holes per year	Hole radius (m)	Number of vents/holes	Total vent/hole area (m ²)
5	1.26·10 ⁻²			1	5·10 ⁻⁴
6	1.26·10 ⁻¹			1	5·10 ⁻²
6b	3.98·10 ⁻²			10	5·10 ⁻²
6c	1.26·10 ⁻²			100	5·10 ⁻²
7	1.26·10 ⁻²	1·10 ⁻⁶	1.26·10 ⁻²	Initially 1	5·10 ⁻⁴ incr. to 3·10 ⁻³ at 5·10 ⁶ yr