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Final report on benchmark calculation in clay DELIVERABLE (D-N°:4.2.4)

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Foreword

The work presented in this report was developed within the Integrated Project PAMINA: **P**erformance **A**ssessment **M**ethodologies **I**N **A**pplication to Guide the Development of the Safety Case. This project is part of the Sixth Framework Programme of the European Commission. It brings together 25 organisations from ten European countries and one EC Joint Research Centre in order to improve and harmonise methodologies and tools for demonstrating the safety of deep geological disposal of long-lived radioactive waste for different waste types, repository designs and geological environments. The results will be of interest to national waste management organisations, regulators and lay stakeholders.

The work is organised in four Research and Technology Development Components (RTDCs) and one additional component dealing with knowledge management and dissemination of knowledge:

- In RTDC 1 the aim is to evaluate the state of the art of methodologies and approaches needed for assessing the safety of deep geological disposal, on the basis of comprehensive review of international practice. This work includes the identification of any deficiencies in methods and tools.
- In RTDC 2 the aim is to establish a framework and methodology for the treatment of uncertainty during PA and safety case development. Guidance on, and examples of, good practice will be provided on the communication and treatment of different types of uncertainty, spatial variability, the development of probabilistic safety assessment tools, and techniques for sensitivity and uncertainty analysis.
- In RTDC 3 the aim is to develop methodologies and tools for integrated PA for various geological disposal concepts. This work includes the development of PA scenarios, of the PA approach to gas migration processes, of the PA approach to radionuclide source term modelling, and of safety and performance indicators.
- In RTDC 4 the aim is to conduct several benchmark exercises on specific processes, in which quantitative comparisons are made between approaches that rely on simplifying assumptions and models, and those that rely on complex models that take into account a more complete process conceptualization in space and time.

The work presented in this report was performed in the scope of RTDC 4.

All PAMINA reports can be downloaded from <http://www.ip-pamina.eu>.

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1. Introduction

This report describes the work done in Work package WP4.2 of RTDC-4 of the PAMINA integrated project.

This document describes the benchmark test case results obtained by the three partners who have directly contributed to this work, namely CEA IRSN and SCK-CEN. The benchmark was built for the comparison of radionuclide migration calculations in a repository in clay using different levels of geometrical complexity in the repository description. The benchmark results presented hereafter allow studying the impact on radionuclide transport calculations of different modeling/numerical aspects including:

- Dimension of modeling (1D, 2D or 3D).
- Time and space level of refinement (time step and mesh).
- Spatial scheme methods including Finite Elements (FE) [1] (implemented in COMSOL Multiphysics [2] used by SCK•CEN), Mixed Hybrid Finite Element (MHFE) [3] (implemented in Cast3m [4] used by CEA) and Finite Volume (FV) [5] (implemented in PORFLOW [6] used by SCK•CEN, in Cast3m used by CEA and in Melodie [7] used by IRSN).
- Disposal geometry (cylindrical gallery section geometry vs. square section approximation).

The report first recalls the objectives of the benchmark, including the four key point aspects given previously, in Chapter 2. The waste disposal concept chosen is then shortly depicted in Chapter 3 and the benchmark data are depicted in Chapter 4. Chapter 5 includes the presentation of the benchmark results that are discussed in Chapter 6. The conclusions of the work are presented in Chapter 7.

2. Objectives

The benchmark described hereafter is part of the WP4.2 subsection that focuses on clay host rock. The benchmark consists of comparing radionuclide transport calculations performed on a refined 3D complex radioactive waste disposal description on one hand and on the other hand on a coarser description including 1D, 2D and 3D approaches. The benchmark is based on the use of a repository concept and dimensions close to the French vitrified waste one on which public data are available [8].

2.1 Numerical methods

Radionuclide transport calculations performed in the scope of Performance Assessment are today widely based on Finite Element or Finite Volume numerical method approach. The objective of this subsection is to compare the results given using different techniques on real cylindrical geometry representations and simplified “square section” geometry.

2.2 Mesh and time step refinement

The refinement level of meshes used for Performance Assessment calculation purposes is not always derived from a mathematical refinement convergence accuracy study but more usually stems from the modeller's self experience. The objective of this subsection is to study the impact of mesh and calculation time step refinement on transport calculation results. This study will be performed on real cylindrical and simplified “square section” geometries.

2.3 Dimensionality (1D to 3D)

Radionuclide transport calculations are not always performed using 3D approaches but often use simpler and 2D or 1D approach allowing faster computations and sensitivity analysis. Those simplifications are made when the problem presents some symmetry or when the processes involved is mainly 1D or 2D. One objective of the benchmark is to test different dimensional approach to exhibit the level of accuracy of the lowest levels (1D and 2D).

2.4 Geometry (Square / Cylinder)

At present, Performance Assessment approaches often simplify the repository geometry by using disposal connection drifts and cells of square section inside meshes on which radionuclides transport calculations are performed. Meshes are then easier to build (do not require complex meshing tools) but do not represent the real repository geometry made of cylindrical disposal connection drifts and cells assemblage. The objective of this subsection of the benchmark will be to test the added value of using real cylindrical geometry by comparing calculations performed on meshes built according to the “square section” hypothesis and to a real cylindrical geometry.

3. Waste disposal concept

We first define a waste disposal.. As NF-PRO project recently focused on spent fuel waste disposal, a vitrified waste disposal is proposed here. This waste disposal embedded inside a clay host rock formation is only considered surrounded by an aquifer in order to simplify as well as possible geology and hydrogeology of the benchmark. Indeed, in performance assessment calculation methodology, common approaches consist to focus on the host formation in which modelled processes are the slowest as transport processes in aquifers and biosphere appear to be instantaneous and do not need to be included in the model.

3.1 The clayed host rock

The host rock is of argillaceous type with a very low vertical permeability of about 10^{-13} m/s and an anisotropy factor of 10 (horizontal permeability of 10^{-12} m/s). The considered host rock in the model is of parrallelepipedic shape, 100-m-thick and 30×30 km² in lateral extension, surrounded by the aquifer at the top and bottom. The imposed head boundary condition must be chosen to ensure a vertical upward head gradient of about 1 m/m.

3.2 The vitrified waste disposal

The vitrified waste disposal is located in the middle part of the clay host rock (50 meters deep in the clay layer) at the centre of the 30×30 km² square. The waste disposal design as well as dimensions, materials and material properties must be selected according to the “French vitrified waste disposal concept” extensively described in “Dossier 2005 Argile” public report [8]. A representation of the vitrified waste disposal concept is depicted in Figure 1.

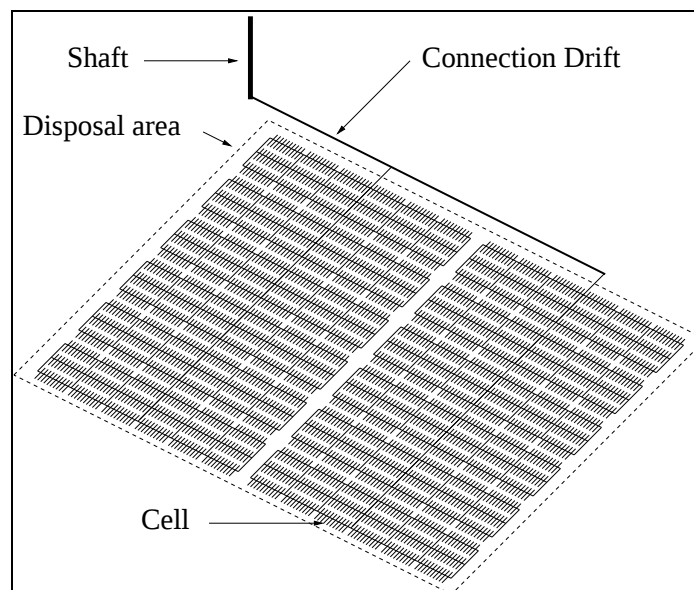


Figure 1: Overview of the vitrified waste disposal concept.

3.3 The radionuclide

Among the full list of radionuclides embedded in vitrified waste, the selected radionuclides of interest are: a sorbed one, a non-sorbed one as well as solubility controlled one. A decay chain is also of interest.

3.4 The outputs

In order to compare the different approaches chosen, time dependent activity fluxes at the interface between host rock disposal top and upper aquifer, over more than one million year period, will be used as main indicator.

4. Benchmark definition

On the basis of the proposed waste disposal system described previously, the benchmark will consist in comparing time dependent radionuclides fluxes at the upper boundary of the clay layer for different calculation approaches including different geometrical complexity description of the waste disposal as defined in the objectives section.

4.1 3D calculation domain geometry

As transport calculations on full 3D description of the repository and geological layer is not feasible with classical computer, the benchmark focuses on an elementary disposal cell. The cell domain extension is chosen taking into consideration the global disposal concept symmetries as depicted on Figure 2.

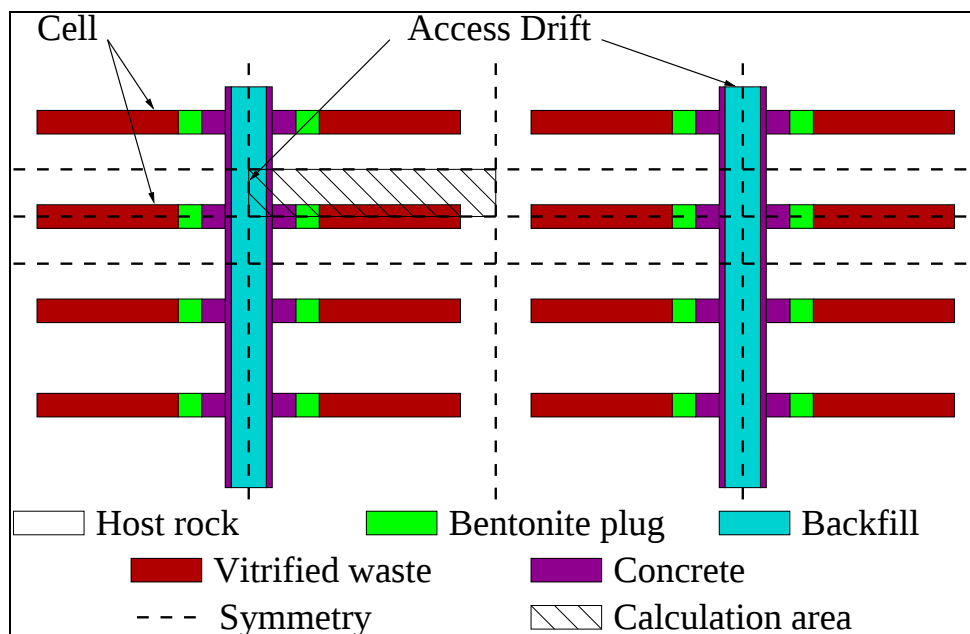


Figure 2: Top view of disposal area part including symmetries and reduced calculation area deduced.

The calculation domain is then restricted to half a cell connected to half a drift embedded in a 100-m-high host rock extension as shown on Figure 3.

The dimensions of the different disposal cell components are listed in Table 1.

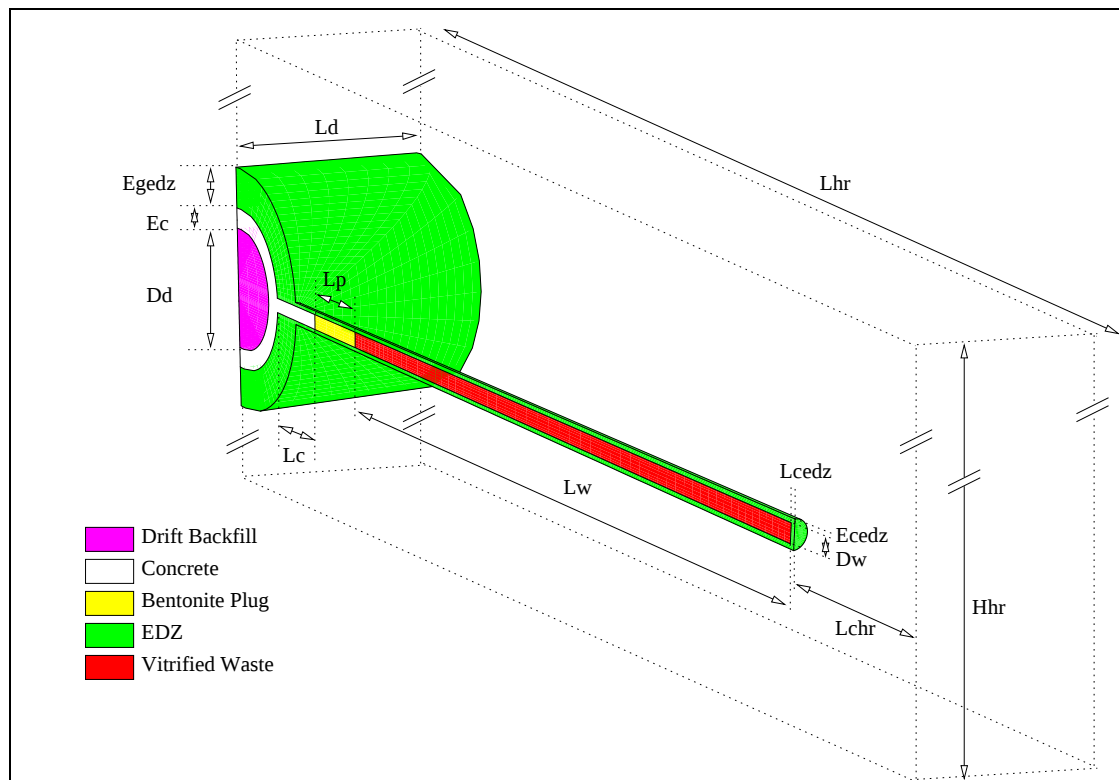


Figure 3: Three-dimensional picture of the calculation domain including dimension notations. The host rock is only represented by the ($L_{hr} \times H_{hr} \times L_d$) dotted box for a better inner view.

Name	Description	Value (m)
Dd	Inner drift diameter	6
Ec	Concrete drift extension	1
Egedz	Drift excavated damaged zone extension	2
Ld	Drift length	10
Hhr	Host rock vertical extension	100
Lc	Concrete plug length	4
Lp	Bentonite plug length	4
Lw	Waste disposal cell length	30
Lcedz	Length of the excavated damaged zone at the end of the disposal cell	0.175
Lchr	Extension of host rock at the end of the disposal cell	10
Dw	Waste disposal cell diameter	0.70
Ecedz	Excavation damaged zone extension around waste disposal cell	0.175
Lhr	Total length of the calculation domain	52.175

Table 1: Extensions of the disposal cell components depicted on Figure 3.

4.2 3D simplified domain geometry

The simplified domain geometry was built assuming that drift and waste disposal cell were of square section. On the basis of the geometrical details of Figure 3 and Table 1, equivalent square sections were calculated from cylindrical diameters assuming that the cross-section area must be equal for each description. The square extension Sq (m) was then calculated using relation (1) where D (m) is the diameter for cylindrical description.

$$(Sq)^2 = \pi D^2 / 4 \quad (1)$$

It is to note that this assumption must be considered carefully for the release of solubility controlled radionuclide species.

A three-dimensional representation of the simplified calculation domain including material dimension notations is shown on Figure 4 and values of the calculation domain dimensions are given in Table 2.

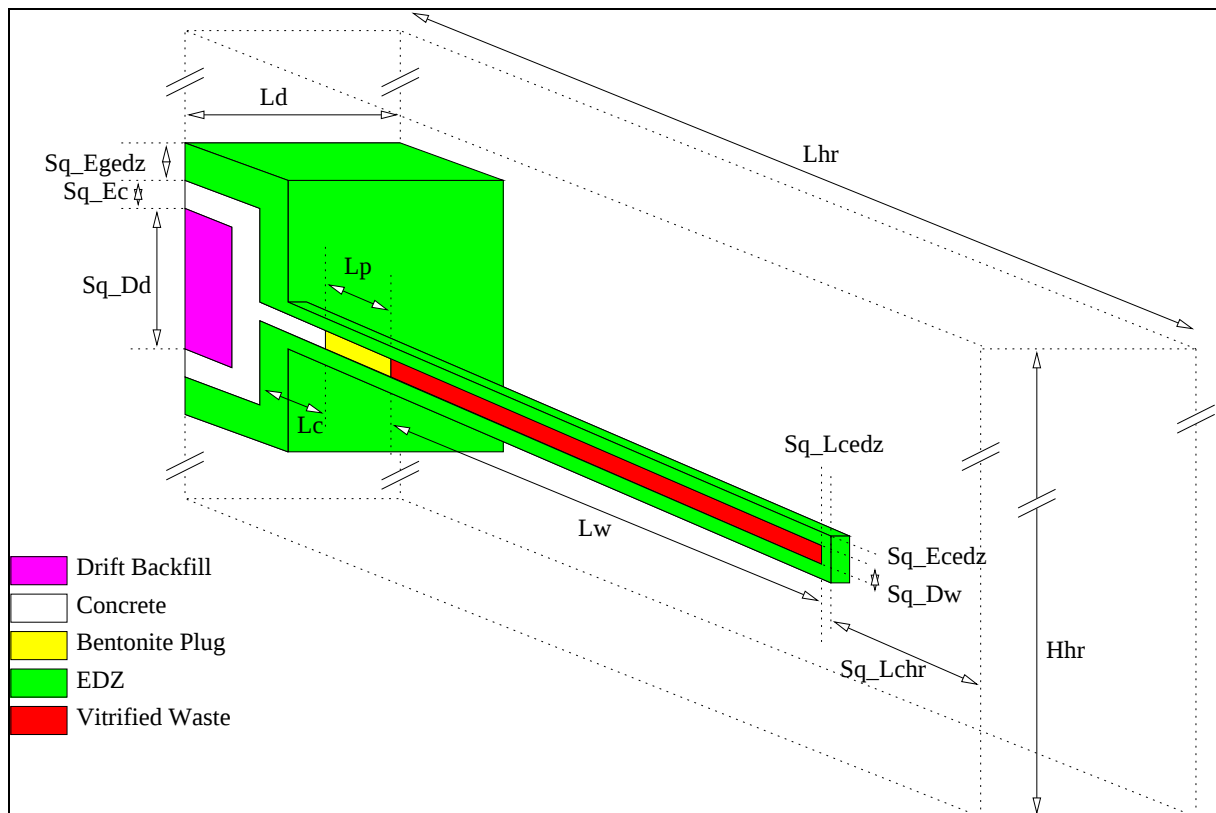


Figure 4: Three-dimensional picture of the simplified calculation domain including dimension notations. The host rock is only represented by the ($L_{hr} \times H_{hr} \times L_d$) dotted box for a better inner view.

Name	Description	Value (m)
Sq_Dd	Inner drift extension	5.32
Sq_Ec	Concrete drift extension	0.885
Sq_Egedz	Drift excavated damaged zone extension	1.77
Ld	Drift length	10
Hhr	Host rock vertical extension	100
Lc	Concrete plug length	4
Lp	Bentonite plug length	4
Lw	Waste disposal cell length	30
Sq_Lcedz	Length of the excavated damaged zone at end of the disposal cell	0.155
Sq_Lchr	Extension of host rock at the end of the disposal cell	10.475
Sq_Dw	Waste disposal cell diameter	0.62
Sq_Ecedz	Excavation damaged zone extension around waste disposal cell	0.155
Lhr	Total length of the calculation domain	52.175

Table 2: Extensions of the disposal cell components depicted on Figure 4.

4.3 2D cylindrical domain geometry

The two-dimensional cylindrical geometry domain is represented in Figure 5. It was obtained from the three-dimensional representation depicted in Figure 3 by using a vertical cut plan crossing the middle of the waste perpendicular to its main direction. The domain then only takes into account the waste, the Excavated Damaged Zone surrounding the wastes and the argillaceous host rock. Useful numerical values are already given in Table 1.

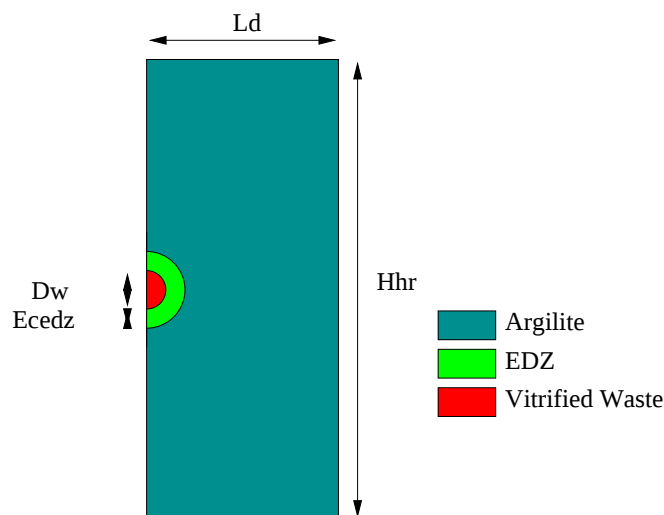


Figure 5: Two-dimensional representation of the cylindrical calculation domain including material dimension notations. The host rock is here represented in blue.

4.4 2D simplified domain geometry

The simplified two-dimensional square domain geometry is built using the equivalent square sections hypothesis from Figure 5 and is represented in Figure 6.

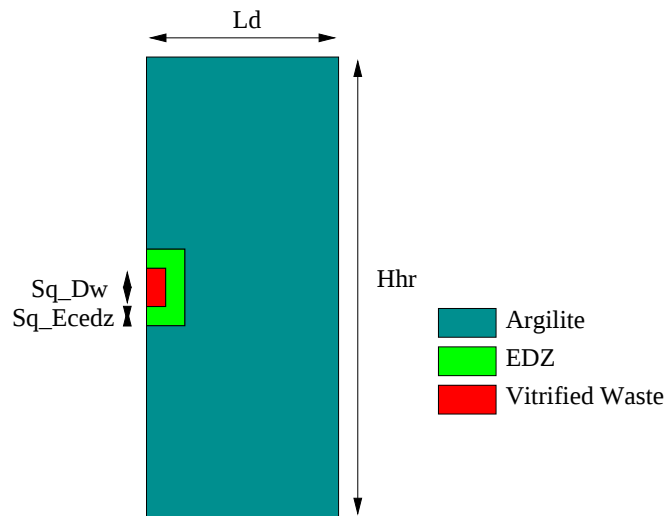


Figure 6: Two-dimensional representation of the simplified calculation domain including material dimension notations. The host rock is here represented in blue.

Useful numerical values are already given in Table 2.

4.5 1D simplified domain geometries

Two simplified Cartesian 1D domain geometries were used. The first one, called 1D cylindrical simplified domain, corresponds to the left vertical boundary of Figure 5 and is built using D_w and E_{cedz} values. The second one, called 1D cubic simplified domain, corresponds to the left vertical boundary of Figure 6 and is built using Sq_Dw and Sq_Ecedz values. The domains then only take into account the waste, the Excavated Damaged Zone surrounding the wastes and the argillaceous host rock and useful numerical values are already given in Table 1 and Table 2.

4.6 Hydro-geological parameters

In order to perform radionuclide transport calculations on the domain calculation geometry described in the previous section, hydro-geological parameters allowing flow calculation are needed.

A steady state flow is assumed considering that the disposal is sealed long (several thousand years) before the transport calculation initial time (which is assumed to start 4000 years after the full saturation of the waste vaults). The flow direction is vertical upward stemming from a vertical head gradient of 1 meter per meter. Upward vertical flow is imposed by means of fixed head conditions at the upper and lower boundaries of the calculation

domain. "No flux" boundary conditions are imposed on the other boundaries of the calculation domain for symmetry reason. Values of the imposed head are given in Table 3.

Boundary	Head value (m)
Upper surface of the host rock	350
Lower surface of the host rock	450

Table 3: Fixed head values at the top and bottom of the calculation domain.

Permeability values, of the different materials constituting the disposal, namely drift backfill, concrete, bentonite, vitrified waste, excavated damaged zone and host rock, are given in Table 4. Note that the argillaceous host rock is considered as anisotropic but is not expected to have a large effect since the lateral extensions of the domain have no flow boundary conditions and only at short distance around the gallery the flow lines are not completely vertical.

Material	Permeability (m/s)
Argillaceous Host rock	10^{-13} (vertical) - 10^{-12} (horizontal)
Excavated Damaged Zone	$5 \cdot 10^{-11}$
Vitrified Wastes	10^{-8}
Concrete	10^{-10}
Bentonite	10^{-11}
Drift Backfill	10^{-6}

Table 4: Permeability values of the engineered barrier materials and the waste.

4.7 Transport parameters

Useful radionuclides transport parameters can be divided in three categories: parameters intrinsic to the nuclide, parameters intrinsic to the material and parameters related to the interaction between the nuclide and the material. Note that from a theoretical point of view, transported solutes always influence transport parameters but we assume that some parameters intrinsic to the material are independent from the considered nuclide.

4.7.1 Radionuclide transport parameters

We selected a limited set of radionuclides, among the full list of ones embedded in vitrified waste, on the basis of their particular chemical behaviour: a sorbed one, a non-sorbed one, a solubility-controlled one and a decay chain. The selection was made considering long lived and highly concentrated radionuclides. For every selected nuclide, the molecular diffusion coefficient, the radionuclide's half life as well as the solubility limit are given in Table 5.

Name	Radionuclide type	Molecular diffusion coefficient (m ² /s)	half-life (years)	Solubility limit (mol/l)
¹²⁹ I	Non-sorbed	1.08 10 ⁻⁹	1.57 10 ⁷	-
¹³⁵ Cs	Sorbed	0.72 10 ⁻⁹	2.3 10 ⁶	-
⁷⁹ Se	Solubility controlled	1.13 10 ⁻⁹	3.56 10 ⁵	5.5 10 ⁻⁸ x 0.085*
²⁴⁵ Cm	Decay chain	1.08 10 ⁻⁹	8500	-
²⁴¹ Pu		1.08 10 ⁻⁹	14.4	5.0 10 ⁻⁷
²⁴¹ Am		1.08 10 ⁻⁹	433	-
²³⁷ Np		1.08 10 ⁻⁹	2.14 10 ⁶	1.0 10 ⁻⁶
²³³ U		1.08 10 ⁻⁹	1.59 10 ⁵	3.2 10 ⁻⁸
²²⁹ Th		1.08 10 ⁻⁹	7340	5.0 10 ⁻⁷

Table 5: Molecular diffusion, half-life and solubility limit for every considered nuclide type. For ⁷⁹Se, the solubility limit used was corrected taking into account the amount of stable Se present in the waste.

In order to simplify the system and reduce the calculation time, only a part of the decay chain will be considered. The chain will be then simplified to the following elements: ²³⁷Np → ²³³U → ²²⁹Th, and the inventory for these actinides will be recalculated taking into account the inventory of the parents. This simplification is often done in PA calculations because the selected radionuclides of the chain (Np, U and Th) are the most important based on half-life and inventory considerations.

4.7.2 Material transport parameters

Properties of materials expected to be independent from the radionuclide considered for transport are porosity ω (-), tortuosity τ (-) and longitudinal and transversal dispersivities α_L and α_T (m). Values are given in Table 6.

Material	Porosity (-) ω	Tortuosity (-) τ	Dispersivity (m) $\alpha_L - \alpha_T$
Argillaceous Host Rock	0.06	0.01	1 (horizontal) – 0.1 (vertical)
Excavated Damaged Zone	0.20	0.1	1 (horizontal) – 0.1 (vertical)
Vitrified Wastes	0.10	0.1	1 (horizontal) – 0.1 (vertical)
Concrete	0.20	0.1	1 (horizontal) – 0.1 (vertical)
Bentonite	0.20	0.01	1 (horizontal) – 0.1 (vertical)
Drift Backfill	0.40	0.3	1 (horizontal) – 0.1 (vertical)

Table 6: Porosity, tortuosity and dispersivity for every disposal material.

Note that for clay host rocks, porosity is often considered as RN dependent. Indeed, considering electrical double layer theory for the pore surface, accessible pore space depends on the electrical charge of the RN species and allows taking into account anion exclusion phenomena. In this case, it is called "diffusion accessible porosity".

Note that at starting radionuclide release time, the waste steel canisters are supposed to be fully corroded and vitrified waste appears as a highly fractured media with given permeability and porosity.

4.7.3 Material/radionuclide transport parameters

Transport parameters linked to radionuclide interaction with materials are retardation factor and effective diffusion.

Retardation factor is expressed as a function of porosity ω (-), material density ρ_s (g/cm³) and distribution coefficient K_d (cm³/g) by relation (2).

$$R = 1 + ((1 - \omega) / \omega) \rho_s K_d \quad (2).$$

Retardation factors for each radionuclide interacting with materials are given in Table 7.

R (-)	¹²⁹ I	¹³⁵ Cs	⁷⁹ Se	²⁴⁵ Cm	²⁴¹ Pu	²⁴¹ Am	²³⁷ Np	²³³ U	²²⁹ Th
Argillaceous Host Rock	1	20*	1	NR	NR	NR	1000	300	500
Excavated Damaged Zone	1	20*	1	NR	NR	NR	1000	300	500
Vitrified Waste	1	1	1	NR	NR	NR	1	1	1
Concrete	1	1	1	NR	NR	NR	1	1	1
Bentonite	1	1	1	NR	NR	NR	1	1	1
Drift Backfill	1	1	1	NR	NR	NR	1	1	1

Table 7: Retardation factor values (NR denotes "not relevant"). *Retardation factor for Cs was initially chosen to be 3600 but arbitrary reduced to 20 in order to capture Cs release pick before 2 million years.

Note that values depicted in Table 7 are not those used for the safety assessments of the "dossier Argile 2005" [8] but only indicative test values selected for these benchmark calculations.

Effective diffusion is expressed as a function of porosity ω (-), tortuosity t (-) and molecular diffusion D_0 (m²/s) by relation (3).

$$D_e = \omega \tau D_0 \quad (3).$$

Effective diffusion values are presented on Table 8 on the basis of relation (3) and values depicted in Table 5 and Table 6.

$D_e \times 10^{-13} (m^2/s)$	^{129}I	^{135}Cs	^{79}Se	^{245}Cm	^{241}Pu	^{241}Am	^{237}Np	^{233}U	^{229}Th
Host Rock	6.48	4.32	6.78	NR	NR	NR	6.48	6.48	6.48
EDZ	216	144	226	NR	NR	NR	216	216	216
Vitrified Waste	108	72	113	NR	NR	NR	108	108	108
Concrete	216	144	226	NR	NR	NR	216	216	216
Bentonite	21.6	14.4	22.6	NR	NR	NR	21.6	21.6	21.6
Drift Backfill	1296	864	1356	NR	NR	NR	1296	1296	1296

Table 8: Effective diffusion coefficient values.

4.8 Radionuclide source term

The disposal cell description depicted in Figure 3 is a simplification of the real case where disposal cells are alternately filled with 8 vitrified waste canisters 1.60-m-long and 7 intercalary canister 2.45-m-long. A more precise mesh description is maybe of interest. In any case the total amount of selected nuclides to be considered in the cell is the one embedded in 8 vitrified canisters.

As a simplification, the release from the source term is defined as a constant degradation rate C ($years^{-1}$) calculated from the total time needed for the glass to dissolve. We will assume a total dissolution time of 100 000 years in this benchmark. The steel canister life time would be about 4000 years according to ANDRA's "Dossier 2005 Argile" [8].

Source term data are depicted in Table 9. Note that data depicted in Table 9 are test data defined for the benchmark. Reader can refer to RTDC 3 for a more realistic source term linking it to real scientific evidence.

Radionuclide	^{129}I	^{135}Cs	^{79}Se	^{245}Cm	^{241}Pu	^{241}Am	^{237}Np	^{233}U	^{229}Th
Initial amount (g/can)	2.3	590	6.16	5.4	0.149	369	682	9.63×10^{-3}	2.15×10^{-6}
Initial concentration C_0 (g/m ³)	1.6	409	4.27	3.74	0.103	256	473	6.68×10^{-3}	1.49×10^{-6}
Initial activity A_0 (Bq/m ³)	1.04×10^7	1.75×10^{10}	2.02×10^9	2.38×10^{10}	3.95×10^{11}	3.25×10^{13}	1.24×10^{10}	2.39×10^6	1.15×10^4

Table 9: initial radionuclide amount embedded in 1 vitrified waste canister (COGEMA universal canister).

Initial concentration C_0 is an averaged concentration calculated assuming that waste vault of volume $V = 11.54 \text{ m}^3$ ($V = 0.25 \times D_w^2 \times L_w$) is filled with 8 waste canisters (and 7 non active intercalary canisters). As C_0 is a waste volumetric concentration, C_0 must be multiplied by waste porosity (0.1) in order to calculate waste pore water concentration.

5. Benchmark results

5.1 Codes description and used meshes

Code and meshes used by CEA

CEA used the Cast3m tool [4] which allows solving flow equation (5) and transport equation (4) using Finite Volume and Mixed Hybrid Finite Element spatial schemes. The Cast3m tool also allows using different type of solvers ranging from direct solver to multi-grid solver and including conjugate gradient solvers.

The CEA contribution includes 1D, 2D and 3D calculations with both rectangular and cylindrical description for all selected radionuclides except for the decay chain. Calculations were performed using different level of mesh refinement. An example of meshes used is presented on Figure 7.

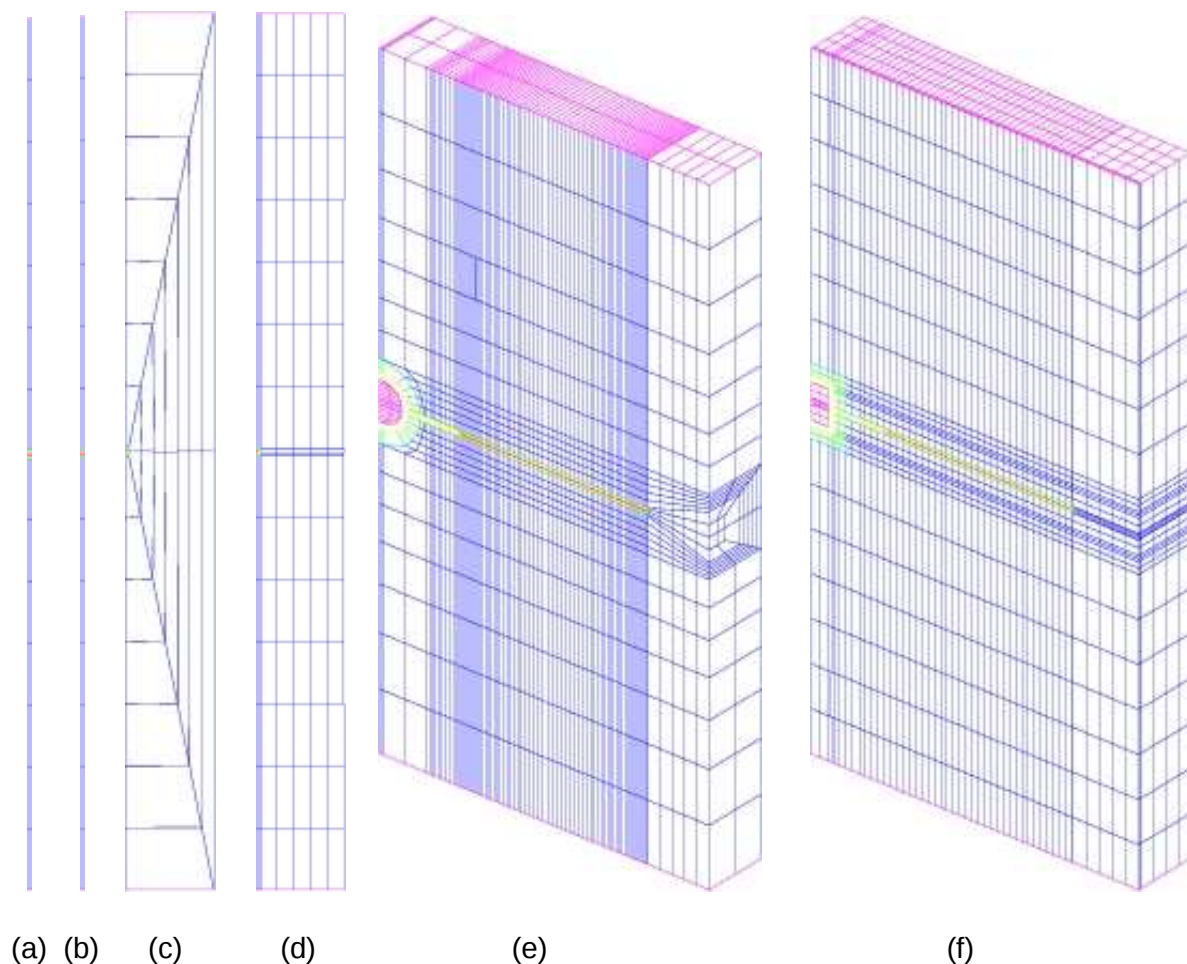


Figure 7: Coarser refined meshes used (the host rock is blue). (a) 1D cylindrical shape (18 cells), (b) 1D cubic shape (18 cells), (c) 2D cylindrical shape (34 cells), (d) 2D cubic shape (126 cells), (e) 3D cylindrical shape (5536 cells), (f) 3D cubic shape (8640 cells).

Code and meshes used by IRSN

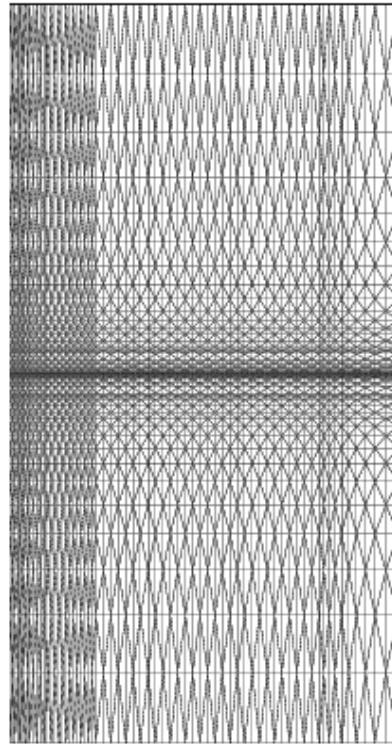
IRSN used a commercial code, GoldSim, and the Melodie software, which is a numerical tool developed by IRSN in collaboration with the Paris School of Mines to model the transport of radionuclides in the context of radioactive waste disposal.

The initial design of the Melodie software was based on Finite Element (FE) method for numerical approximation of flow (1) and transport (2) equations. The FE method, commonly used to solve parabolic and elliptical problems, is not satisfactory for dealing with possible discontinuities in calculation results and with advection terms, especially when the advection is predominant compared to diffusion. To improve the accuracy and the reliability of calculations, a method called Finite Volume Finite Element (FVFE) has been adapted in Melodie. Using 3D models, FVFE method operates on tetrahedral elements and requires constructing a dual mesh. In the modeling case, the dual mesh is based on centres of gravity. A first mesh has thus been built using tetrahedral elements fulfilling the dihedral angle criterion. FE method has been tested on the same tetrahedral mesh, as well as on a hexahedral mesh. The tetrahedral mesh is composed of 80,199 computational nodes and 443,520 elements and a hexahedral mesh is composed of 80,199 nodes and 73,920 elements (Figure 8).

GoldSim code was used to simplify the phenomenological 3D modelling into a compartmental modelling (not presented in that document). GoldSim is a general purpose simulation environment with an integrated graphical user interface for modelling and data output. A contaminant transport module provides the ability to simulate the transport and fate of radionuclides through the environment (e.g. for performance assessment).



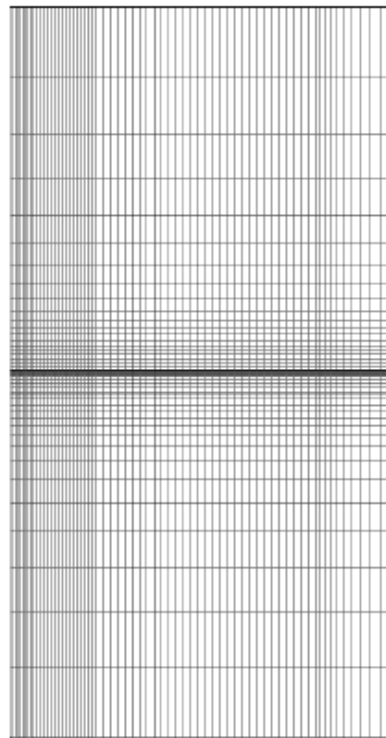
(a)



(b)



(c)



(d)

Figure 8: Tetrahedral ((a) tunnel axis and (b) longitudinal views) and hexahedral ((c) tunnel axis and (d) longitudinal views) meshes.

Code and meshes used by SCK-CEN

SCK•CEN used two commercial codes. The first one based on Finite Volume spatial scheme was PORFLOW 3.07 [6] and the second one based on Finite Element spatial scheme was COMSOL Multiphysics 3.2 (earth science module) [2].

The SCK•CEN contribution so far includes 1D and 2D calculations with a rectangular gallery approximation, using a FE method (COMSOL multiphysics [2]) and a FV code (PORFLOW 3.07 [6]). An example of the grids used in the calculations is shown in Figure 9.

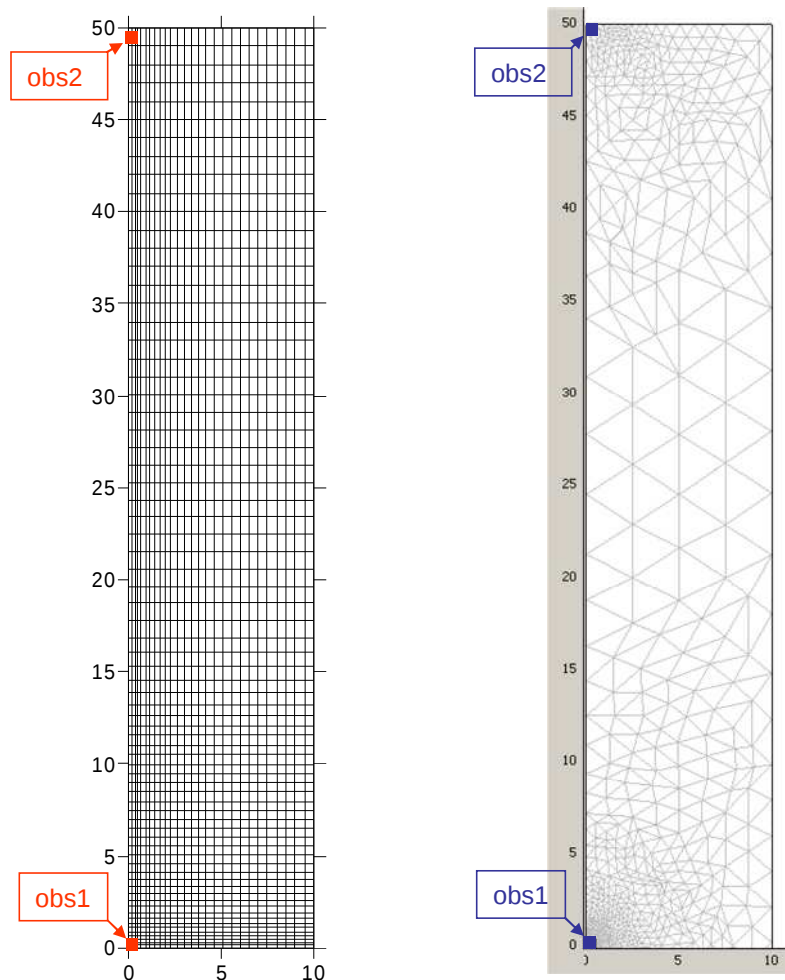


Figure 9: Example of grid spacing used with PORFLOW (left) and FE mesh used with COMSOL multiphysics (right) (zoom on the upper half of the model domain), and position of observation nodes.

As output parameters, SCK•CEN systematically recorded the instantaneous radionuclide flux to the overlying aquifer, the concentration in the source zone (obs1 in Figure 9), and the concentration in the clay in close proximity of the overlying aquifer (obs2 in Figure 9).

5.2 Flow calculation results

Flow calculations were performed by CEA, IRSN and SCK-CEN on each domain dimensionality and geometry described previously.

CEA flow calculation results:

CEA used different meshes of increasing level of refinement as well as Finite Volume and Mixed Hybrid Finite Element spatial scheme. No noticeable impact of refinement neither spatial numerical scheme was found concerning flow calculation results. An example of calculated heads results for cubic shape (Finite volume, 1D, 2D and 3D) are presented on Figure 10.

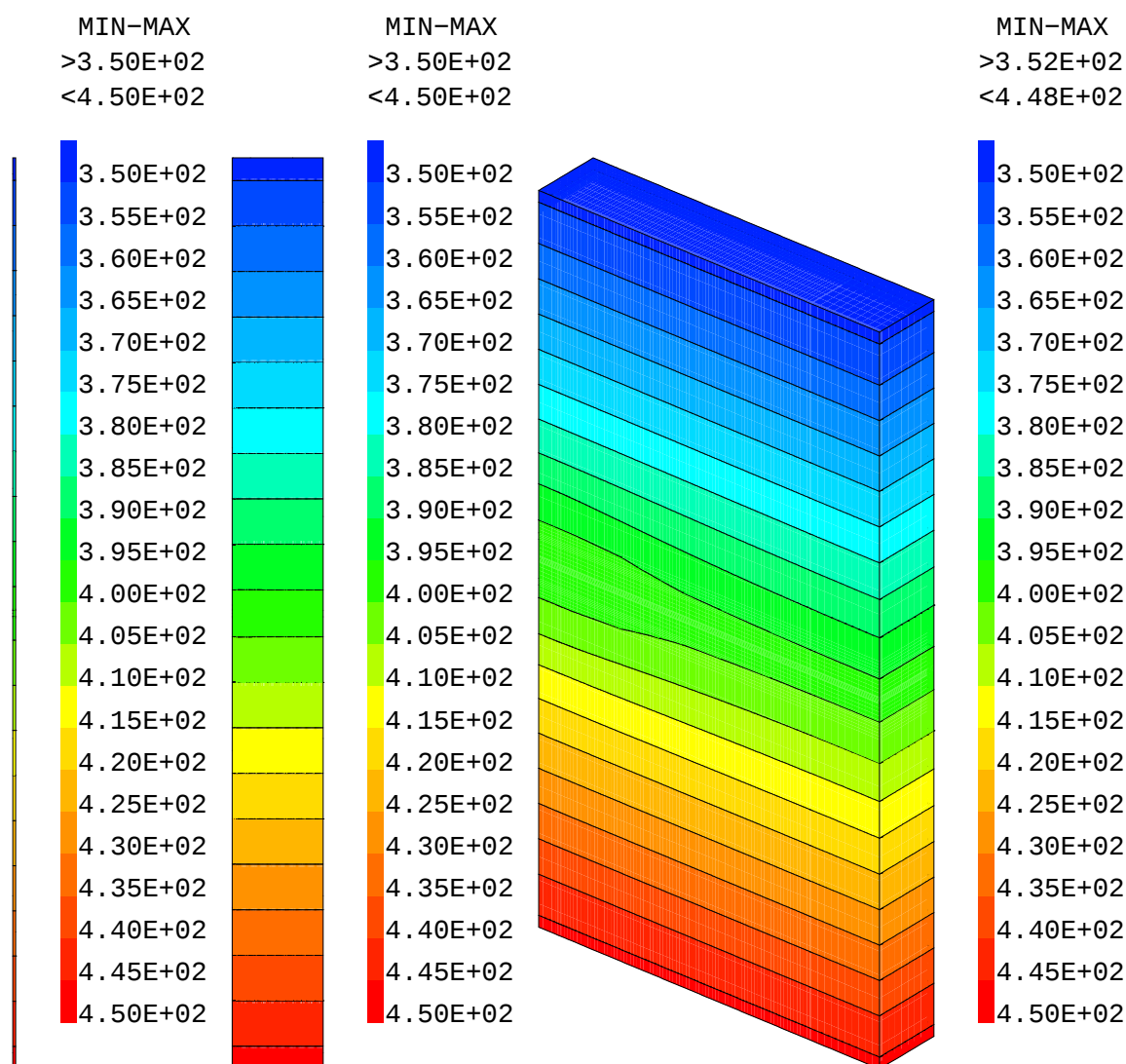


Figure 10: Calculated head for 1D, 2D and 3D cubic shape using finite volume scheme.

IRSN flow calculation results:

Flow calculations have been performed on 3D meshes using FE on tetrahedral and hexahedral meshes and FVFE on a tetrahedral mesh. Figure 11 represents the head results calculated using FVFE methods, but FE method give the same results. The head values are comprised between 350 m and 450 m from the upper part to the lower part of the model corresponding to a vertical upward flow. The colour gradation is only slightly disturbed at the middle of the layer by the presence of the tunnel and the drift.

In accordance with the head results, flow results are similar for all the calculations. It was worth mentioning that there is a little influence of the mesh on the flow calculations. For the hexahedral mesh, the zone surrounding the engineered components has a higher flow value (factor 2) than for tetrahedral mesh. This very located increase of flow do not really influence radionuclide transport throughout the layer, since flow values into the host rock are in the order of magnitude (10^{-6} m/yr). Radionuclide transport remains dominated by diffusion.

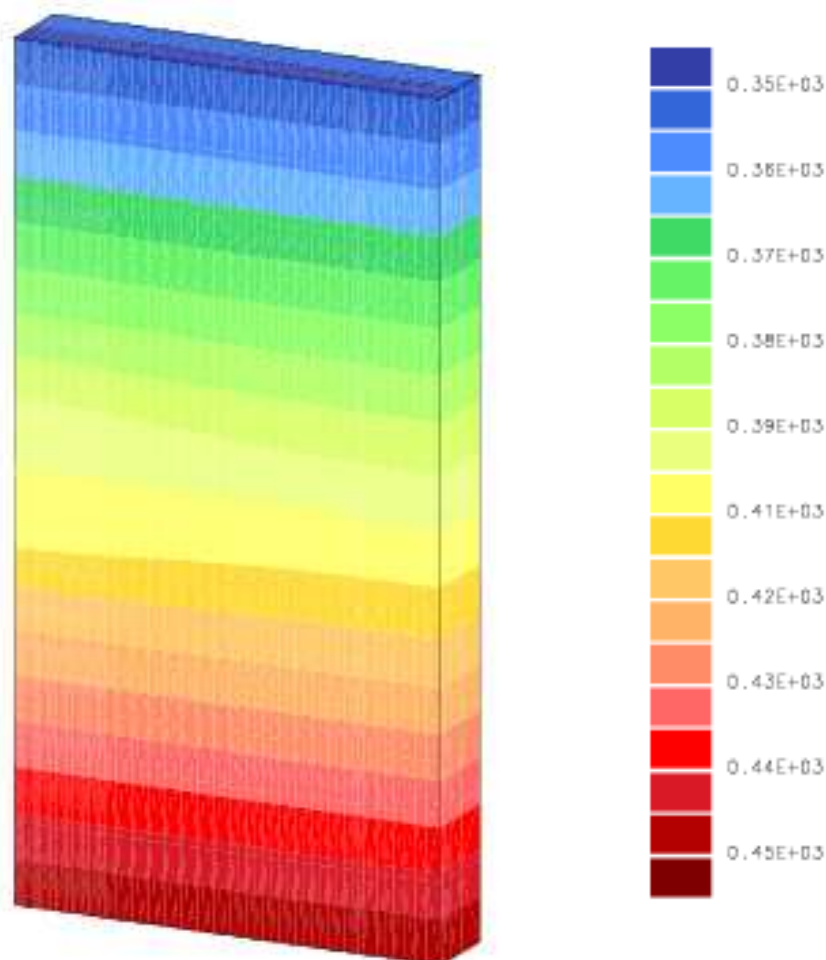


Figure 11: Hydraulic head results (m) using FE and FVFE scheme.

SCK-CEN flow calculation results:

Since the hydraulic gradient (1m/m in upward direction) over the clay formation is quite high, advection can not be neglected, even though the hydraulic conductivity is very small ($K_z=10^{-13}$ m/s). As such, radionuclide transport is both governed by diffusion and advection. When adsorption of solutes to clay is assumed to be linear with concentration and reversible, it can be represented by a retardation factor R and the transport equation can be written as follows:

$$\frac{\partial C}{\partial t} + \frac{1}{R} \nabla \cdot (\mathbf{v}_p C) = \frac{1}{R} \nabla \cdot ((\mathbf{D} + D_p \mathbf{I}) \cdot \nabla C) - \lambda C + S \quad (4)$$

With C (Bq/m³) the RN concentration, R (-) the retardation factor, $\mathbf{v}_p$ the pore velocity vector (m/s), $\mathbf{D}$ (m²/s) the dispersion tensor, D_p (m²/s) the pore diffusion coefficient, $-\lambda C$ is the radioactive decay and S the local source term.

To obtain the local $\mathbf{v}_p$, we must solve the flow equation, which is in this case assumed to be steady state:

$$\nabla(K \nabla h) = 0 \quad (5)$$

with h (m) the hydraulic head and K (m/s) the hydraulic conductivity. Solving this equation will result in the hydraulic head field $h(x,y,z)$ from which, through application of Darcy's law, the field of pore velocities can be obtained. A zoom of the steady state flow field in the vicinity of a gallery (at (0,0)) of the repository under consideration is shown in Figure 12.

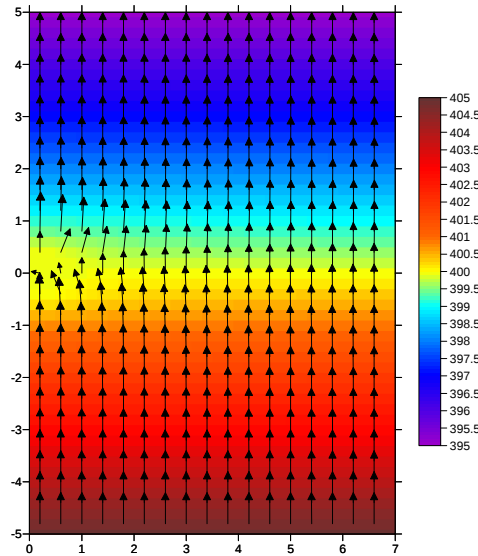


Figure 12: Hydraulic heads and orientation of Darcy velocities in the vicinity of a disposal gallery.

We can also opt (since flow is considered to be steady state) to calculate solute transport with a fixed and uniform Darcy velocity (ignoring the effects close to the gallery), calculated as follows:

$$v_D = \frac{v_p}{\eta} = K \frac{\Delta h}{\Delta z} \quad (6)$$

The Darcy velocity v_D becomes then 3.16×10^{-6} m/y.

Flow calculation conclusion:

Results obtained by the benchmark partners show that the flow is mainly vertical upward and very slightly modified by the repository. The upward vertical Darcy velocity inside the clay host rock is of the order of 10^{-13} , very close from the Darcy velocity of 10^{-13} m/s (3.15×10^{-6} m/y) induced by a vertical head gradient of 1 m/m inside host rock of vertical permeability of 10^{-13} m/s.

5.3 Iodine (^{129}I) transport results

Comparison of iodine output fluxes calculated by each partners on cubic geometry is presented in Figure 13.

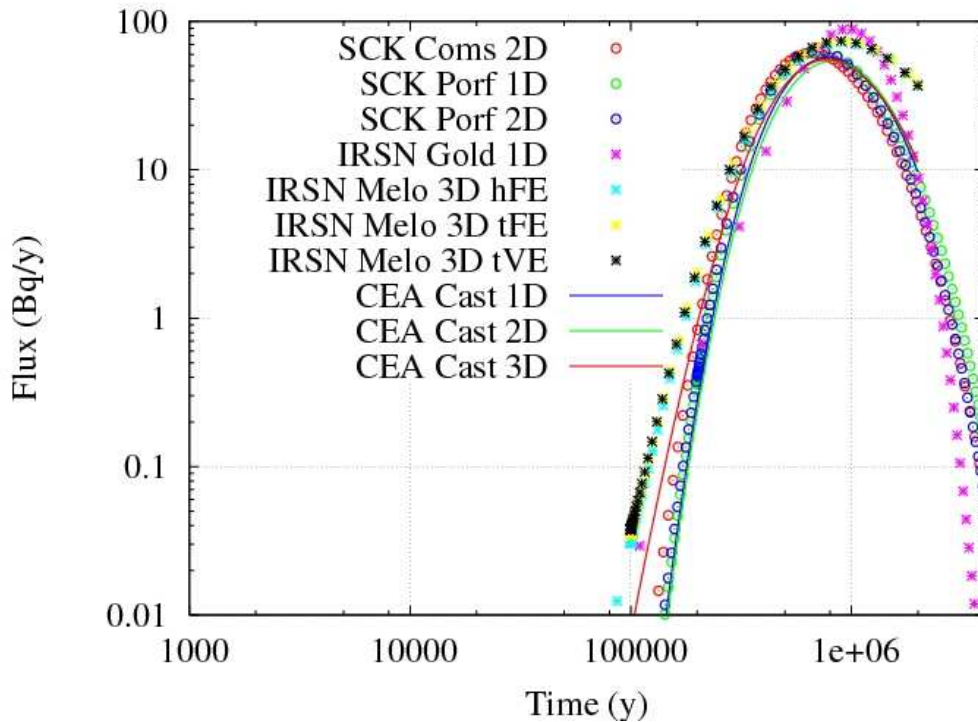


Figure 13: Calculated Iodine output fluxes.

Results obtained by SCK•CEN (SCK) using Comsol (Coms) and Porflow (Porf) codes on 1D and 2D models and by CEA using Castem code (Cast) on 1D, 2D and 3D models are very close. IRSN results, using Goldsim codes (Gold) in 1D and Melodie code (Melo) in 3D with different mesh cell types (h = hexahedrons, t = tetrahedrons) and different spatial schemes (FE = Finite Elements, VE = Finite Volume), have a more diffusive trend.

5.4 Caesium (^{135}Cs) transport results

Comparison of caesium output fluxes calculated by partners on cubic geometry is presented in Figure 14.

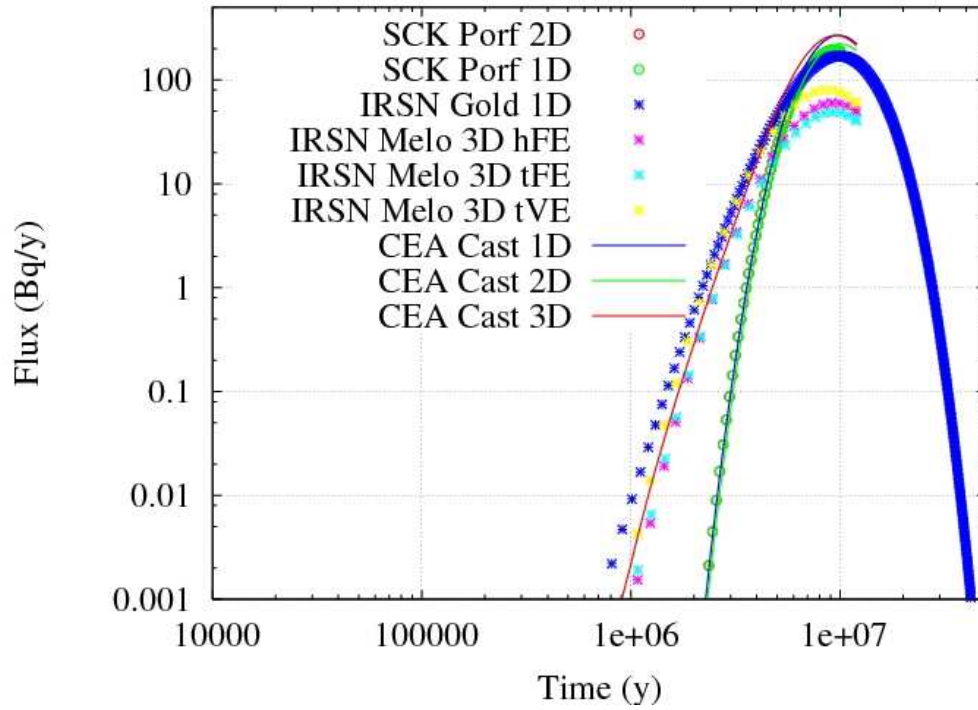


Figure 14: Calculated Caesium output fluxes.

Results obtained by SCK•CEN (SCK), CEA and IRSN are similar except for 3D computations performed by IRSN. A slight difference on source term imposition is maybe of concern.

5.5 Selenium (^{79}Se) transport results

Comparison of selenium output fluxes calculated by partners on cubic geometry is presented in Figure 15.

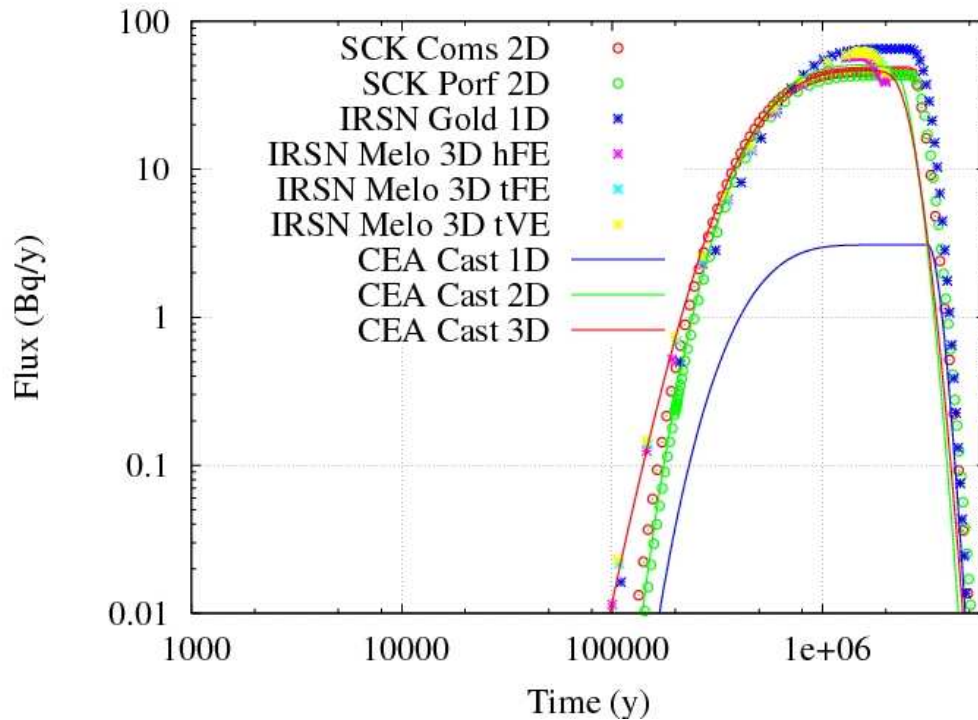


Figure 15: Calculated Selenium output fluxes.

Results obtained by SCK•CEN (SCK), CEA and IRSN are similar except for 1D computation performed by CEA: In order to compare 1D to 3D computation results, CEA imposed an initial activity as source term in 1D that is larger than solubility limit. This result point out that, depending on source term imposition choice, solubility limits cannot be modelled accurately enough for the 1D model.

5.6 Curium (^{245}Cm) chain (^{237}Np , ^{229}Th , ^{233}U) transport results

Comparison of Neptunium output fluxes calculated by partners on cubic geometry is presented in Figure 16.

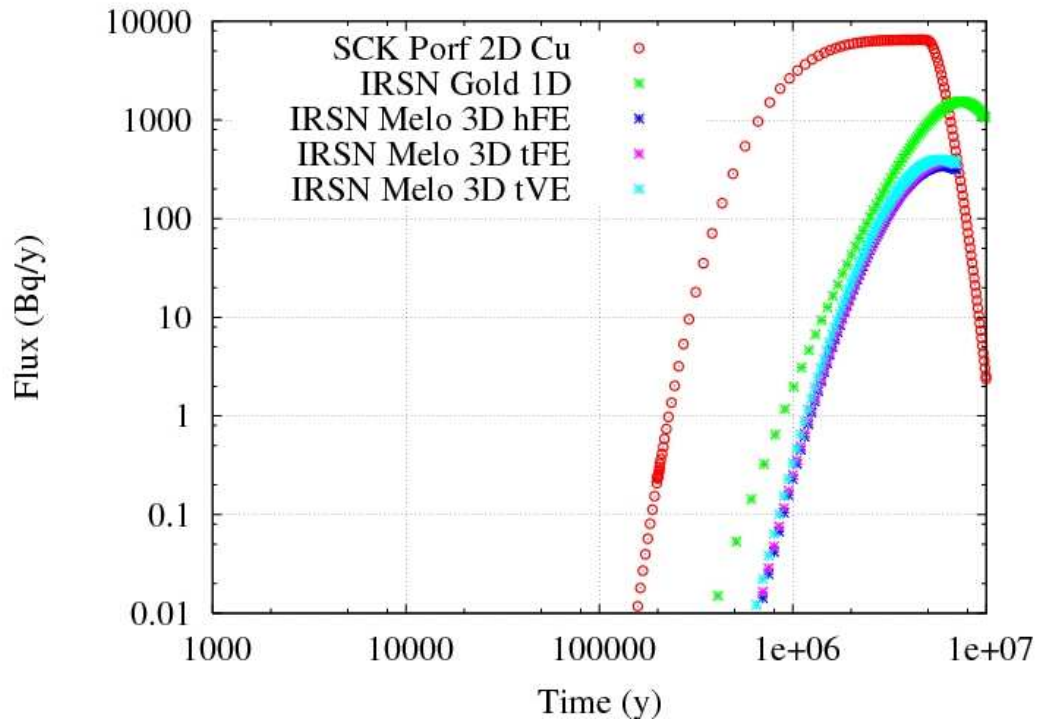


Figure 16: Calculated Neptunium output fluxes.

Comparison of Thorium output fluxes calculated by partners on cubic geometry is presented in Figure 17.

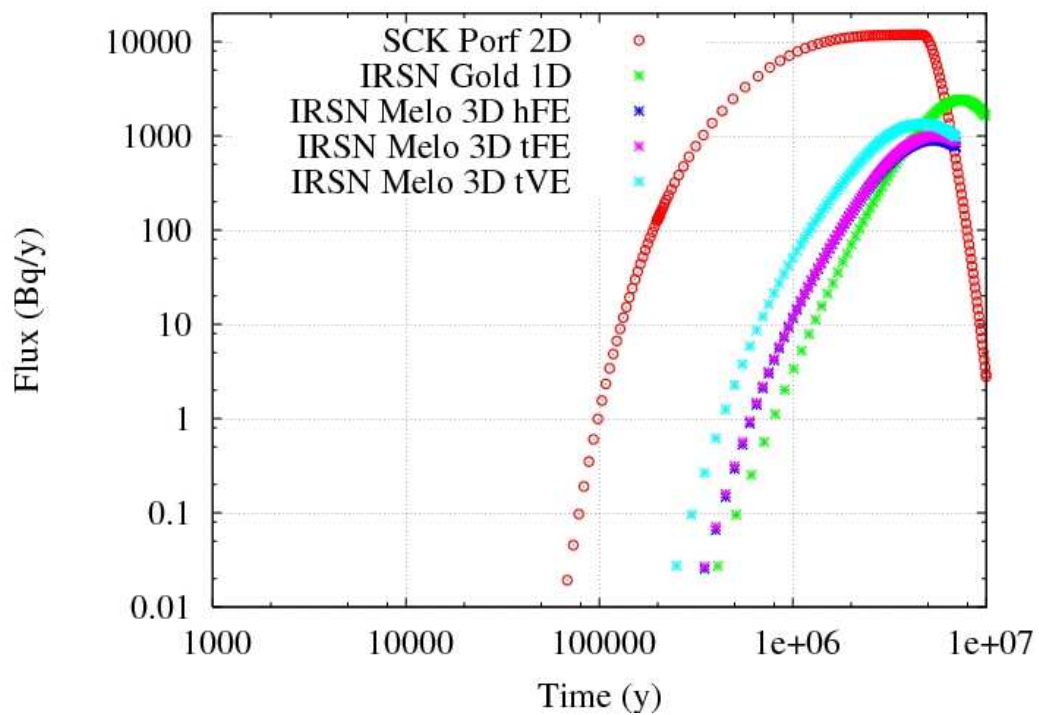


Figure 17: Calculated Thorium output fluxes.

Comparison of Uranium output fluxes calculated by partners on cubic geometry is presented in Figure 18.

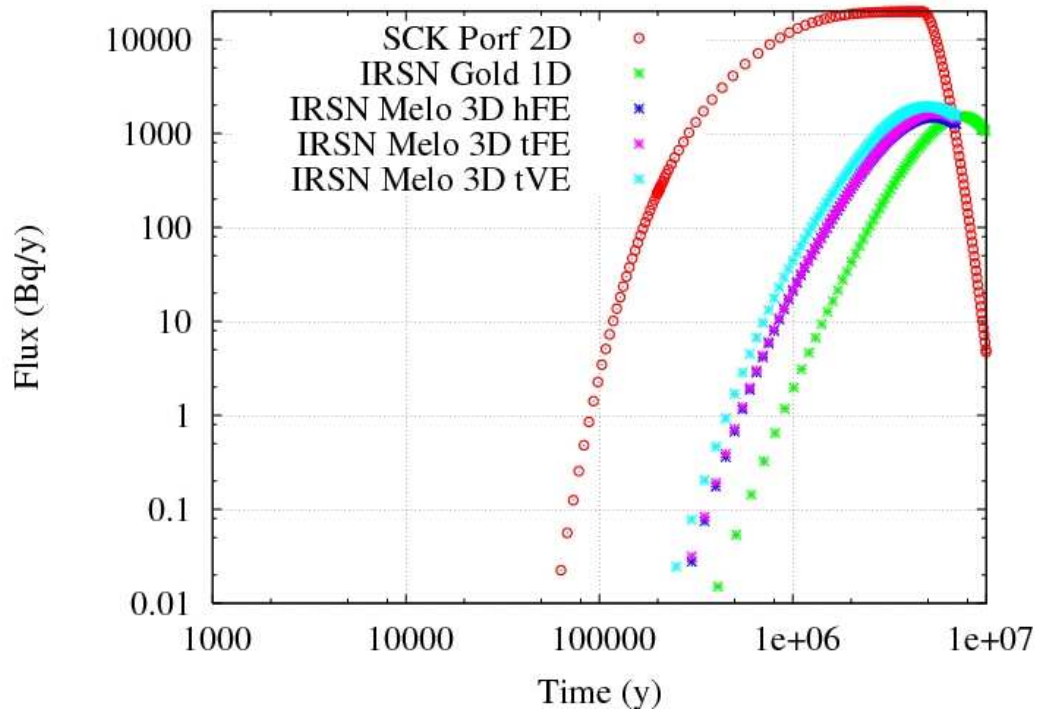


Figure 18: Calculated Uranium output fluxes.

Results obtained by SCK•CEN (SCK) and IRSN are in this case difficult to compare because results obtained by SCK•CEN deal with a reduced clay thickness (to 40 meters). Nevertheless, IRSN results point out that if the use of different spatial scheme has little influence, a larger one is shown between 1D and 3D approach.

6. Results discussion

6.1 Impact of numerical methods

CEA conclusions:

Results obtained by CEA indicated that, as expected, the use of different spatial scheme methods, like Mixed Hybrid Finite Elements or Finite Volume, have a very small impact on the calculation results (see Figure 19).

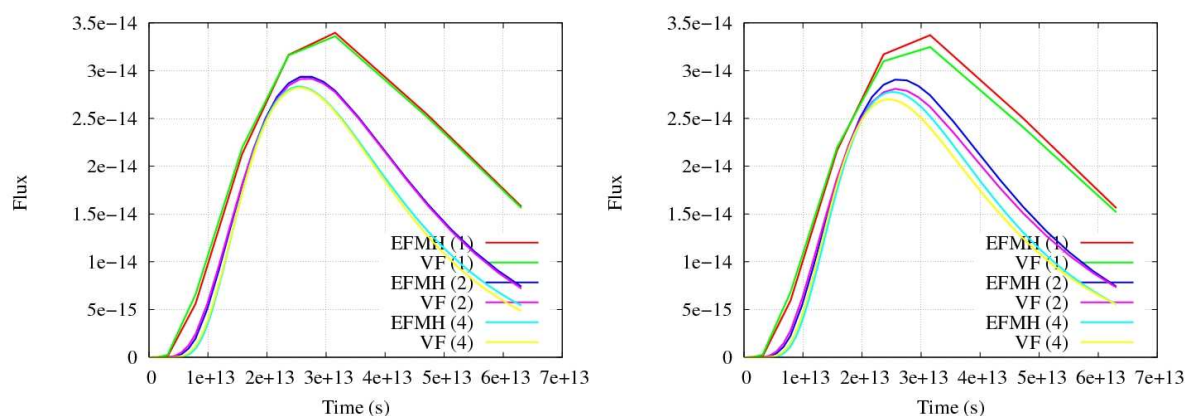


Figure 19: Comparison of calculated normalized Iodine output time evolution fluxes using Finite Volume and Mixed Hybrid Finite Element scheme for different increasing level of refinement for three-dimensional cylindrical approach (left) and cubic approach (right).

In comparison to the impact of time and space refinement level used (see levels (1) to (4) on Figure 19) impact of spatial scheme numerical methods could be considered as negligible for the studied case.

IRSN conclusions:

Concerning calculations carried out using Melodie, results have shown a little influence of the spatial discretization methods due to the mesh refinement when radionuclides are sorbed (e.g. Cs and chains). In fact, FVFE method, as implemented in Melodie, needs mesh elements fulfilling dihedral angle criterion and Péclet number constraint ($Pe < 0.01$). The meshes used in that benchmark have been adapted to Iodine migration (non sorbed anion). For Cs and chains, an adapted mesh refinement should reduce the influence of the mesh.

In addition, FVFE methods have been implemented in order to improve the resolution of the transport equation for advective transport (i.e. through disposal drifts, through fractured components). The low difference between results is due to the dominant diffusive transport. FE methods are thus sufficient to solve diffusion models. A second radionuclide pathway considering an advective transport would have been useful to complicate resolution of the FE methods and highlight advantages of FVFE methods.

SCK•CEN conclusions:

In the experience of SCK•CEN, there is no impact on results (which is expected), apart from somewhat larger numerical dispersion for the FV results at later times, which is related to the applied mesh. However, the most substantial difference in both techniques is the calculation time, which is in general much shorter for the FE technique. Of course: this is dependent on a number of settings such as meshes and time stepping, tolerances and convergence criteria. SCK•CEN did not perform a dedicated optimisation in function of computation time. Nevertheless, the following Table 10 is indicative for the order of magnitude of the computation time.

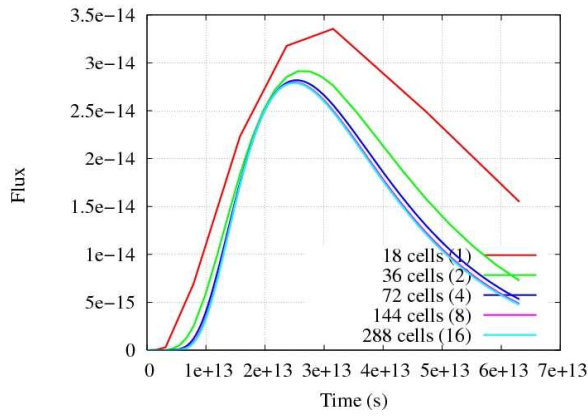
Computation time (min.)	PORFLOW 3.07	COMSOL Multiphysics 3.2
¹²⁹ I	194	3
⁷⁹ Se	195	3
¹³⁷ Cs	198	2
4N+1 actinide chain	215	12

Table 10: Indicative computation times.

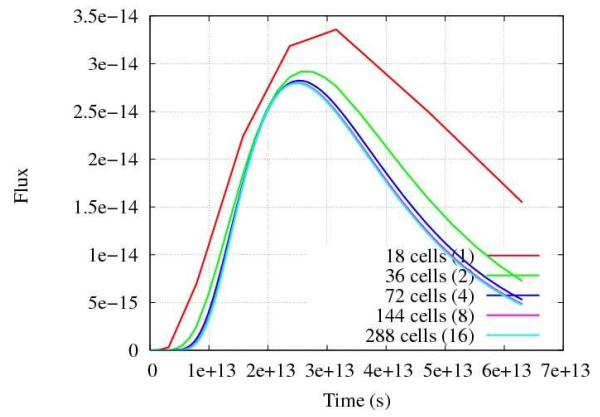
6.2 Impact of refinement level (mesh and time step)

CEA conclusions:

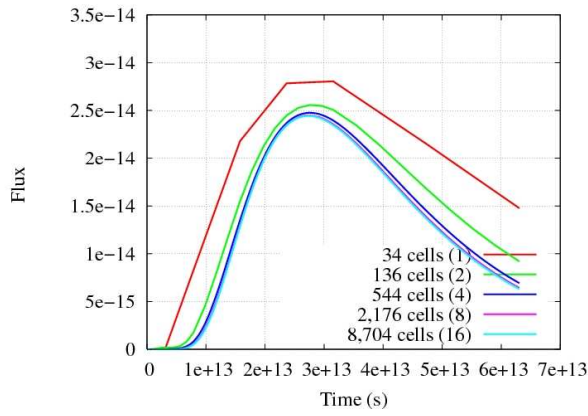
As presented in Figure 20 for Iodine transport calculations and in Figure 21 and Figure 22 for Caesium and Selenium transport calculations respectively, the choice of the refinement of the calculation time step and of the mesh cell size (refinement level) is of importance.



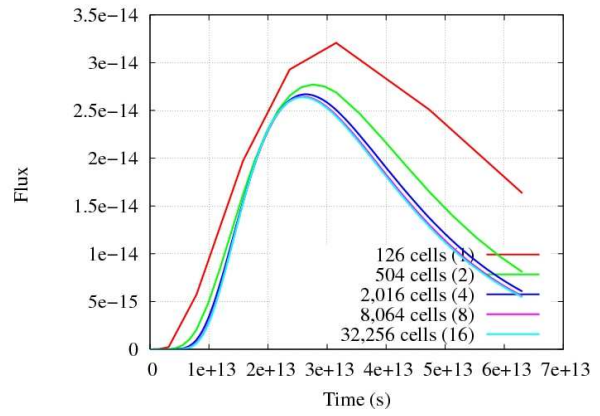
(a) 1D cylindrical



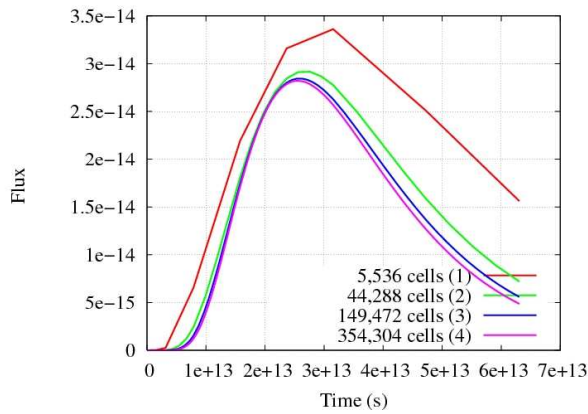
(b) 1D cubic



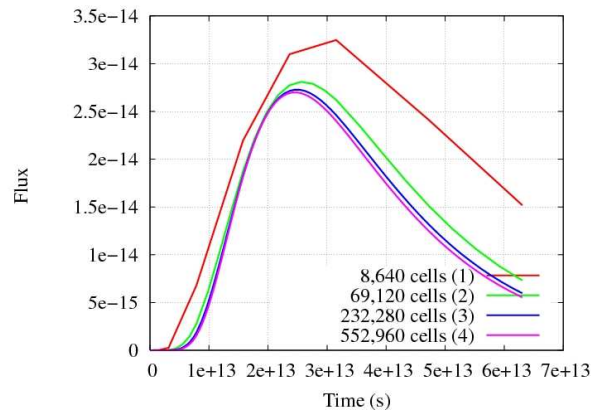
(c) 2D cylindrical



(d) 2D cubic

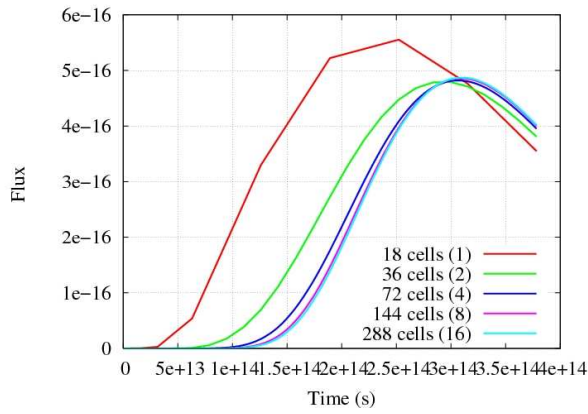


(e) 3D cylindrical

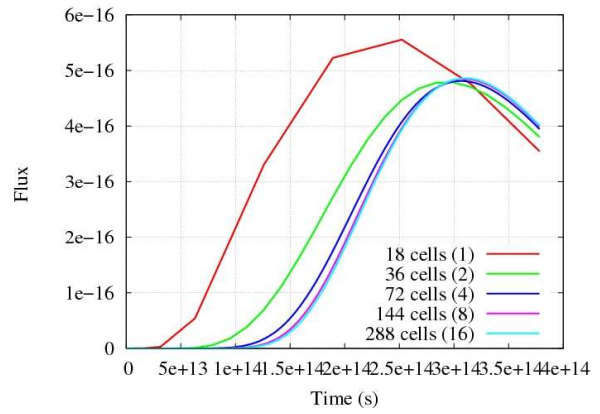


(f) 3D cubic

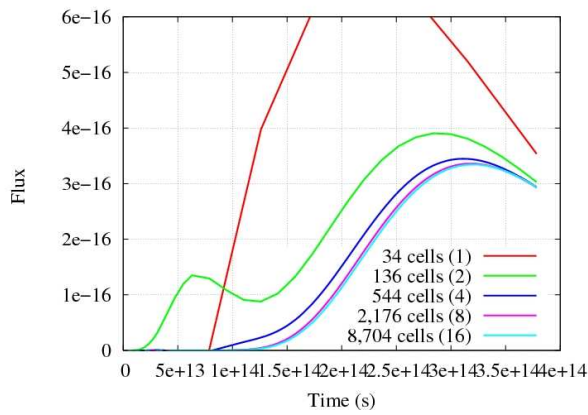
Figure 20: Calculated normalized Iodine output time evolution fluxes using Finite Volume scheme.



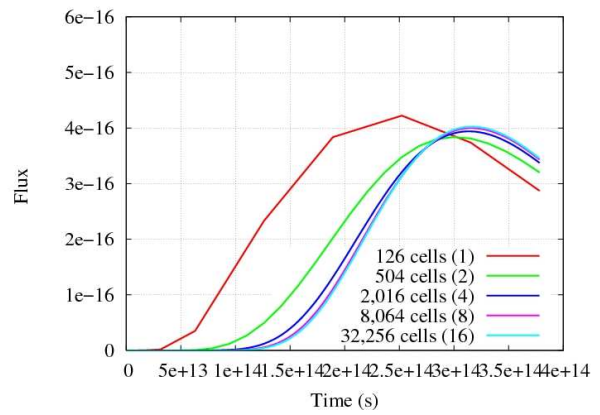
(a) 1D cylindrical



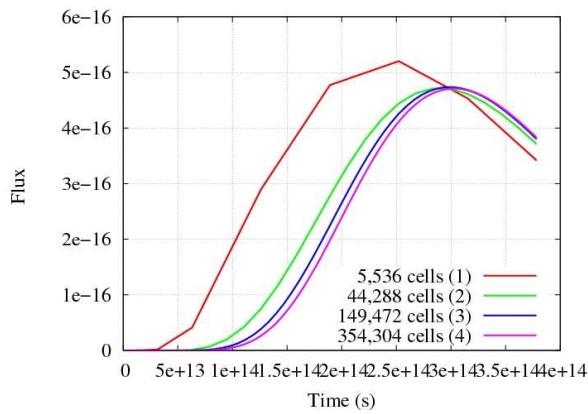
(b) 1D cubic



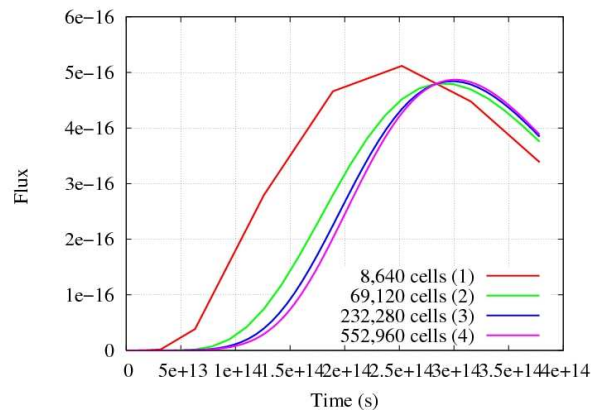
(c) 2D cylindrical



(d) 2D cubic

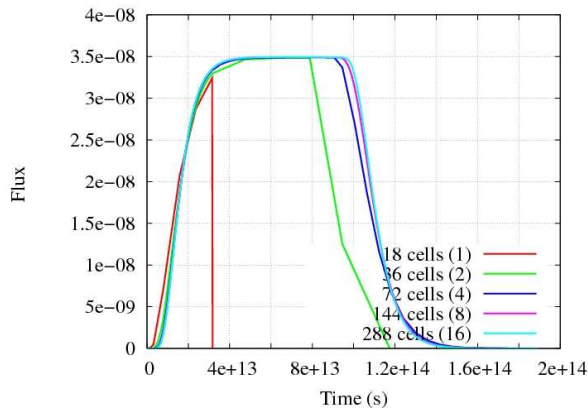


(e) 3D cylindrical

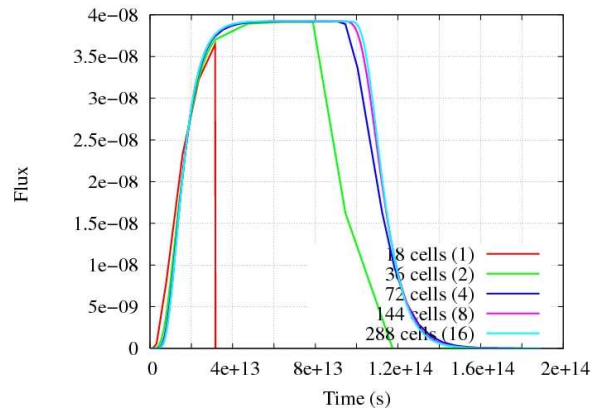


(f) 3D cubic

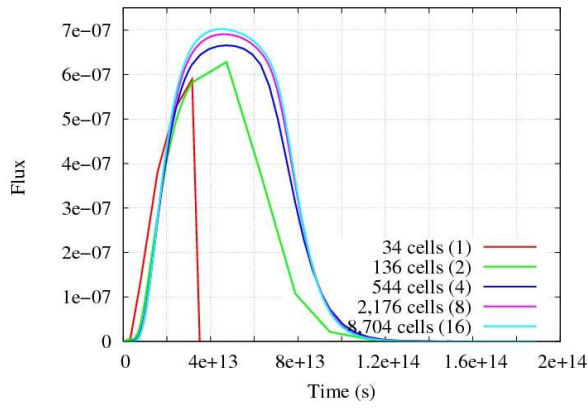
Figure 21: Calculated Caesium output time evolution fluxes using Finite Volume scheme.



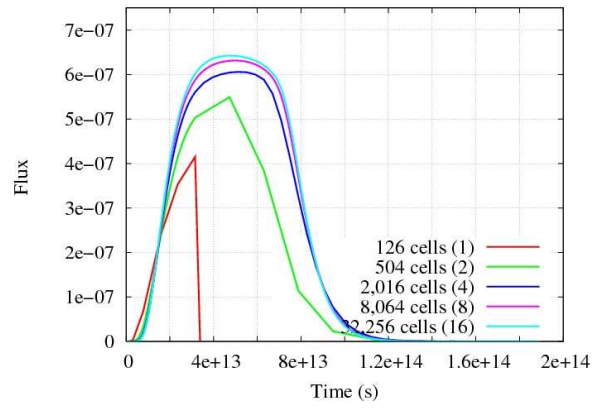
(a) 1D cylindrical



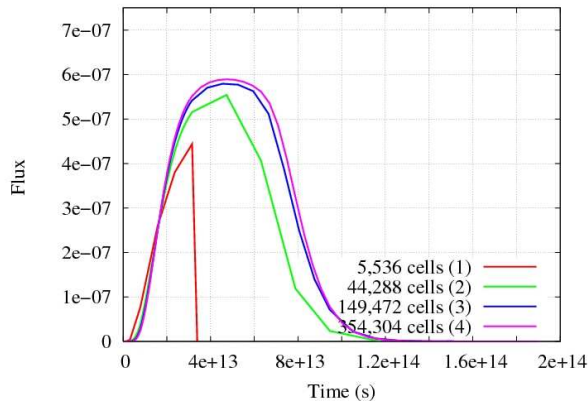
(b) 1D cubic



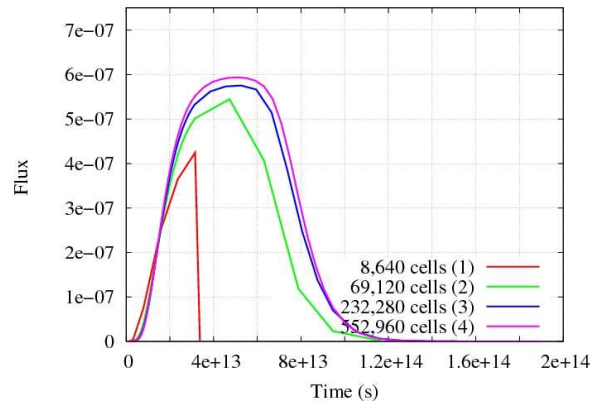
(c) 2D cylindrical



(d) 2D cubic



(e) 3D cylindrical



(f) 3D cubic

Figure 22: Calculated Selenium output time evolution fluxes using Finite Volume scheme.

It is well known that the finer the calculation time step and the mesh size cell are, the more accurate the computed transport calculation is. When comparing the results obtained for the finest meshes to the ones obtained for the coarser ones, the error made due to spatial and time discretisation is at maximum of the order of 6 % for three-dimensional calculations and at maximum of the order of 0.5 % for one and two-dimensional calculations

IRSN conclusions:

IRSN did not perform any sensitivity analysis on grid performance. However, as depicted in the previous chapter, adapted mesh refinement is needed for FVFE methods.

SCK•CEN conclusions

SCK•CEN assumed that the grid spacing was sufficiently fine to obtain an accurate solution (which is actually shown by the calculation results as presented further), and there has been no attempt at using coarser grids to assess accuracy degradation.

6.3 Impact of spatial representation (dimensionality / geometry)

CEA conclusions:

In order to analyze the impact of spatial representation (dimensionality and square or cylindrical representation) on the radionuclide transport calculation results, finest refinement level results are compared for iodine, caesium and selenium on Figure 23, Figure 24 and Figure 25 respectively.

Note that presented fluxes are normalized (in fact the total amount of radionuclide at initial time in the waste is chosen to be equal to 1) and only shape of output fluxes curves add to be compared. Note also that for a better view of the curve peaks discrepancies linear scale were used instead of logarithmic scale commonly used in PA with time in years.

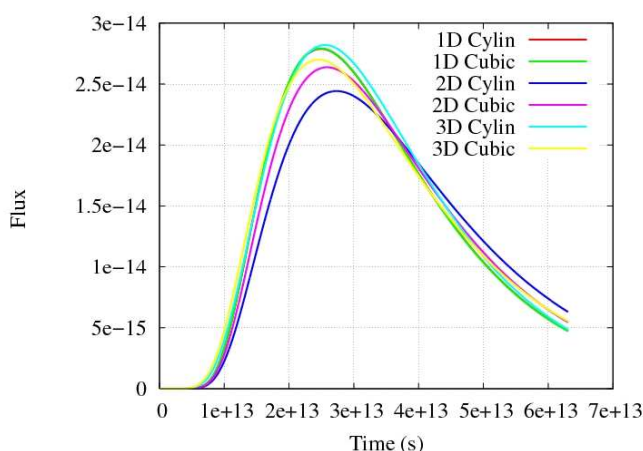


Figure 23: Comparison of calculated iodine output normalized flux using different spatial representations.

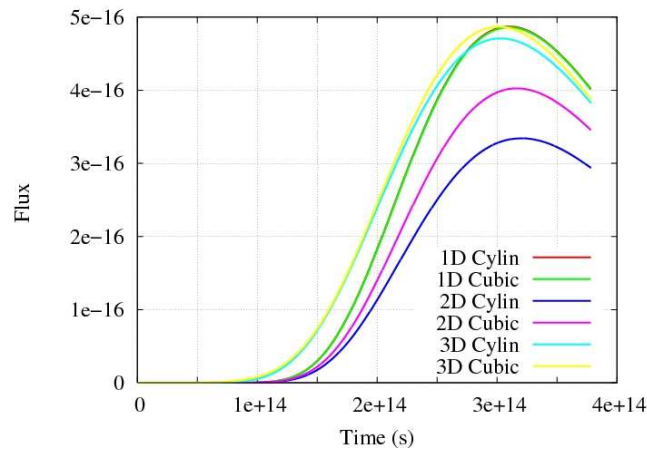


Figure 24: Comparison of calculated caesium output normalized flux using different spatial representations.

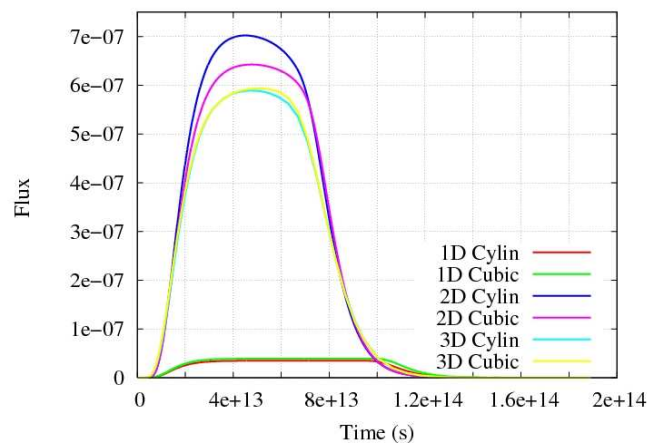


Figure 25: Comparison of calculated selenium output normalized flux using different spatial representations.

Results presented in Figure 23 to Figure 25 indicate that the largest results discrepancy stems from the dimensionality used and that the geometrical shape used is of less importance. This result is probably due to the large distance between the source (of different shape) and the output flux calculation surface (see SCK•CEN results pointing out that the source shape is of importance when indicators close to the gallery are evaluated or in case of solubility limited release). Figure 23 to Figure 25 indicate that there is no global trend linked neither to geometrical shape nor to dimensionality.

For the iodine and caesium cases, the output fluxes are close from each other but less dimensionality underestimate the peak flux value, the worse being the 2D approach.

For the selenium case, the 2D approach overestimate the peak flux value and the 1D approach present a dramatic behaviour with one order of magnitude of underestimating the peak flux value. According to additional calculation results, the 1D approach failure is linked to the solubility limit action that literally stops the radionuclide plume transport in one

dimension as the plume spreading in 2D and in 3D allows the transport of a lower concentration plume but with a wider extension. When the solubility limit is increased, similar results were obtained for all the dimensional approaches. Those results point out that 1D Cartesian is not appropriate when solubility limits are involved.

IRSN conclusions:

Concerning peak magnitudes, IRSN has identified low differences between GoldSim and Melodie results (up to a factor 2 for Cs). For each radionuclide, GoldSim results are always higher than 3D models, since the radionuclide plume in 3D is spread in the whole volume constituting the mesh. When the radionuclide is solubility limited, the fluxes for all the models reach the same plateau value. However, for the 3D models, the decay following that steady state is quicker than for the GoldSim model, since less activity is reaching that exit because of spreading.

In a computational viewpoint, the GoldSim model development and calculation times are of an incommensurable interest, since calculations have been performed in one day, whereas Melodie calculations have been checked in two weeks.

SCK•CEN conclusions:

SCK•CEN did not find significant differences between 1D and 2D calculations. However, a 1D Cartesian geometry is not appropriate when solubility limits are involved.

When indicators close to the source zone are monitored (such as source concentrations monitored by SCK•CEN as additional output), sometimes small differences appear. However, when the flux to the aquifer is evaluated (which is far from the source) differences are negligible because the clay formation buffers/damps the signal. This demonstrates the robustness (insensitivity) of the results to the spatial representation of the near field.

7. Conclusions

Numerical methods and time and space discretization:

In the framework of the defined benchmark, the conducted radionuclide transport calculations allow to point out that if the calculation results are lightly dependent on the numerical methods used and on time stepping and space meshing, it can be reduced as low as wanted by increasing time and space refinement. In fact, for a highly refined problem in space and time, numerical method should not have impact on the results, as long as the conceptual model and solved equations are equal. However, some methods or software can have advantages above others in view of computation time, accuracy for a given time and space refinement or flexibility in defining auxiliary equations. It is for example well known that spatial schemes based on fluxes conservation technique such as Finite Volume or Mixed Hybrid Finite Element are more accurate than classical Finite Element. It is also known that for problems including highly anisotropic dispersive tensors, classical spatial schemes fail and that other schemes must be used. Finally, it is the choice of the modeller to use one or another numerical method as well as space and time refinement based on the pros and cons of each one. It just requires caution from the modeller to verify the accuracy of the results based, for example, on mass balances.

Geometry:

It was found from the radionuclide transport calculation performed that the effect of geometry (square or cylindrical gallery and waste cell cross section) on fluxes to aquifers is very small (few percents for the peak value). Indeed, from a distance of 50 meters, the detailed geometry resembles a line source only. However, caution is required with modelling solubility limited release (both surface area for diffusion and waste concentrations should be realistic). It will off course also have influence when accurate estimations of safety/performance indicators from the Engineered Barrier Systems (EBS) are asked.

Dimensionality:

The conducted radionuclide transport calculations exhibited that dimensionality (1D, 2D or 3D computation) can have an influence. But it depends on the problem to be solved.

- For 1D geometry, boundary conditions and solubility limits cannot be modelled accurately enough leading in some case to large discrepancy with 2D and 3D geometry results. This approach should be used with caution. However, 1D model can be used for probabilistic purposes after being checked with complex models.
- For the present benchmark models, 2D is a good compromise between computation time and accuracy. The radionuclide transport computations performed in the framework of the PAMINA project allow to exhibit that this accuracy (for the defined problems) is of about few percents in comparison to 3D computation results.

- A 3D model has a limited interest for that type of modelling, since the conceptual model is more or less designed as a 2D model. However, 3D modelling remains a valuable tool when considering more complex transfers.

User-sensitivity:

In addition, an element of difference in the results which is not due to differences in the methods or models is the modelling philosophy. This benchmark deals with several ranges of data (e.g. source term) which can be interpreted from different manners (due to numerical tool or modeller). Therefore, the interpretation of those data and the assumptions made by the modellers may strongly influence the results.

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