Modelling, by Scaling Up, the source terms in integrated PA, using homogenization method

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Objectives / Expected Benefits of Homogenization Scaling Up technique

- Improve the modeling approach (**robustness**), for the source term, in integrated performance Assessment, using general Scaling Up methodology working for a wide range of situations (deterministic and stochastic situations, non linear phenomena, ...); even when standard averaging may fail.
- Extend the concept of "conservative value" by providing, magnitude estimates for errors done in the modeling/scaling up process (**estimating accuracy**) .

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Main steps in source term scaling up methodology

- **1 - Define a test case**; for qualifying the Scaling Up process **robustness, sensitivity and efficiency**; IRSN + CEA + UCBL .

  - A vitrified waste disposal embedded inside a clay host rock formation, inspired by WP4.2 test case

  + Two disposal concepts with two different numbers (10 and 20) of connected disposal tunnels for estimating the Scaling up accuracy v.s. the disposal size.

  + Ad hoc and consistent indicators (quantities and localizations).

  + Hydraulic and Transport parameters and boundary conditions, leading to "interesting" radionuclide transport regimes through the facilities (tunnels, drift, gallery).

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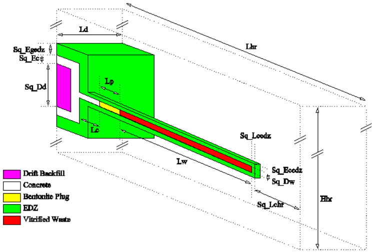
Main steps 1

Fig 1 : Three-dimensional simplified cell geometry.



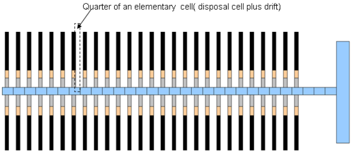
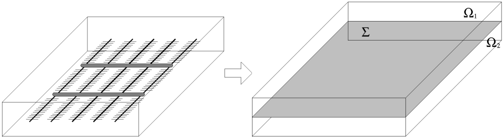


Fig 2 : Disposal concept, to be Scaled up; Double row of 20 Disposal cells connected to an access drift.

Main steps 2

- **2 - Determine the corresponding "Homogenized" Global Problems**: ≈ Only one homogeneous source zone



- **3 -Compare the 3D numerical simulations of radionuclide transport** with different configurations

  + IRSN with MELODIE and CEA with Cast3M ⇒ 3D simulations , using explicit/detailed representation of the source terms (release and geometry)**Local models**,

  + UCBL with Cast3M ⇒ 3D simulations using the Scaled up **Global models**.

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Homogenization main principles

- **Main Principle**:

Provide a Global Model, with parameters defined at the global scale:

1. keeping from the phenomenology, only what is consistent with the global scaling, while neglecting what is appearing only at the smaller scale;

2. **Global model Energy** of the same order as the **Local model Energy**.

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Equations for the Local Model

Radionuclide, ^{129}I; waste disposal embedded inside a clay host rock layer, convection V inside and in the direction of the access drifts, observation during 1 million of years. Data from "Dossier 2005 Argile" French public report

At the local scale:

$$R\theta\frac{\partial u^{\varepsilon}}{\partial t} - \nabla\cdot(\mathbf{A}\nabla u^{\varepsilon}) + (\mathbf{V}\cdot\nabla)u^{\varepsilon} + \lambda R\theta u^{\varepsilon} = f^{\varepsilon},\ \text{in } Q\times(0,\infty);$$

$$u^{\varepsilon}\big|_{t=0} = 0 \text{ in } Q;$$

$$\frac{\partial}{\partial n_A}u^{\varepsilon}\cdot n(x) - \mathbf{V}(\mathbf{x})\cdot n(x)u^{\varepsilon} + \lambda u^{\varepsilon} = 0,\ \text{on } \partial Q\times(0,\infty).$$

$$f^{\varepsilon} = \begin{cases} f(x, x/\varepsilon; t) = \mathbf{\Phi}(t)\psi(x, x/\varepsilon) & \textit{Deterministic} \\ f(x, x/\varepsilon, T_{x/\varepsilon}, \omega; t(\omega)) & \textit{Stochastic} \end{cases}$$

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Global model

A

For parameters values inside the range of values in "Dossier 2005 Argile" French public report, the Global model is of same type as the Local model(standard averaging works):

$$R\theta \frac{\partial u^0}{\partial t} - \mathrm{div}\,(\mathbf{A}\nabla u^0) + (\mathbf{v}\cdot\nabla)u^0 + \lambda R\theta\, u^0 = |V_e|\delta_\Sigma \mathbf{\Phi}(t) \text{ in } \tilde{\Omega}^T$$

$$u^0(x,0) = u_0^0(x) \;\; x \in \tilde{\Omega} = \Omega\backslash\Sigma$$

$$u^0 = 0 \quad \text{on} \;\; S_1$$

$$\mathbf{n}\cdot(\mathbf{A}\nabla u^0 - \mathbf{v}u\, u^0) = 0 \;\; \text{on} \;\; S_2$$

where $|V_e|$ is the elementary volume of a package. **And there is an asymptotic expansion:**

$$u^\varepsilon \simeq u^0 + \varepsilon \left(\underbrace{\chi_\varepsilon^k(\frac{x}{\varepsilon})\frac{\partial u^0}{\partial x_k}}_{shape} + \underbrace{w_\varepsilon(\frac{x}{\varepsilon})\mathbf{\Phi}}_{source} - \underbrace{u^0\rho_\varepsilon^k(\frac{x}{\varepsilon})v_k^1}_{convection} \right)$$

Out of range situations

B

<u>For some extreme values</u>, Out of the range of values in "Dossier 2005 Argile" French public report,

- High Concentration level at the access drift heads (the connecting gallery/access drifts intersections)
- Fast Darcy's Velocity inside the backfilled access drifts

the Global model has a different type than the local model(standard averaging would be wrong): *Transport only in the site horizontal middle plan, in the direction of the drifts .*

Situation not studied here

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Out of range situations II

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C **In some intermediate situations, the Global model connects:**

- strong Transport on the site horizontal middle plan

- to diffusion in the whole 3D domain;

$$R\theta \,\frac{\partial u^0}{\partial t} - \mathrm{div}\,(\mathbf{A}^h\,\nabla u^0) + (\mathbf{v}\cdot\nabla) u^0 + \lambda R\theta\; u^0 = 0 \;\text{ in } \tilde{\Omega}^T;$$

$$u^0(0,x) = u_0^0(x) \text{in } \tilde{\Omega};$$

$$\mathbf{n}\cdot(\mathbf{A}\,\nabla u^0 - \mathbf{v}\,u^0) = \kappa(u^0 - g) \;\text{ on } S^T$$

$$[\mathbf{e}_3\cdot(\mathbf{A}\,\nabla u^0 - \mathbf{v}\;u^0)] = -\mathcal{M}\Phi - \frac{\partial}{\partial x_1}(\langle a\rangle \frac{\partial u^{00}}{\partial x_1}) + \langle v_1^d\rangle \frac{\partial u^{00}}{\partial x_1} \;\text{ on } \Sigma^T$$

$$\langle a\rangle \frac{\partial u^{00}}{\partial x_1}(t, L, x_2, 0) + \langle v_1^d\rangle u^{00}(t, L, x_2, 0) \;= \kappa g^d.$$

Detailed Homogenized Comparison

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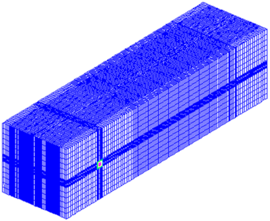
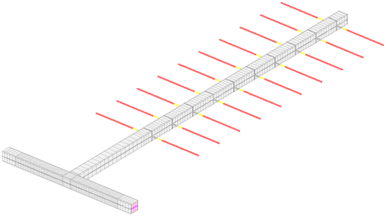
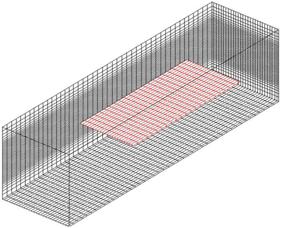
Homogenized detailed Comparison







Meshes:

- Detailed: 486 528 Parallelepipeds;
- Homogenized: 55 440 Parallelepipeds.

Ratio 9

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Indicators

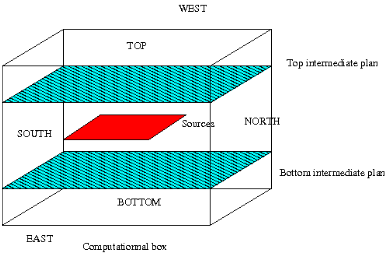

Figure: Flux Indicators

- Outward fluxes through two horizontal plans.
- Outward fluxes on South and Top faces.

Numerical Comparison

Numerical Comparison

One compares:

- Concentration and fluxes solutions coming from detailed model
- Concentration and fluxes solutions coming from homogenized model

One onsideres two homogenized models:

1. Model with only one source on Σ for low convection velocity.
2. Model coupling 2D- transport model and 3D convection-diffusion model for high convection velocities in the drift.

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Low convection in the drifts

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Detailed Homogenized Solutions Comparison

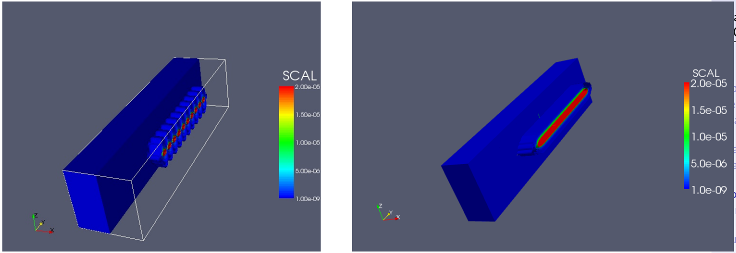


Figure: t = 1000 years

Low convection in the drifts

Detailed Homogenized Solutions Comparison

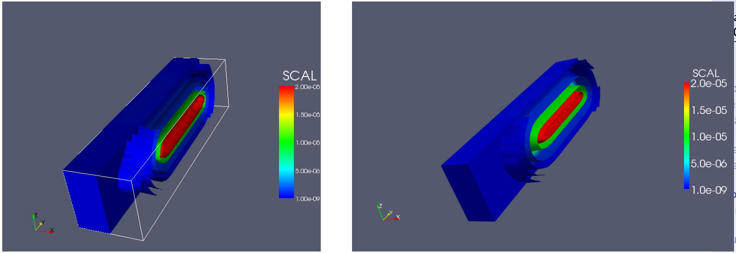
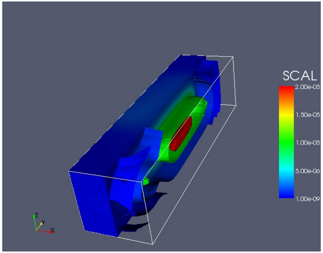


Figure: t = 25000 years

Detailed Homogenized Solutions Comparison



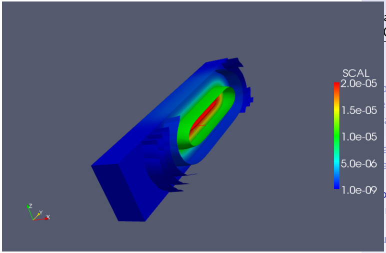
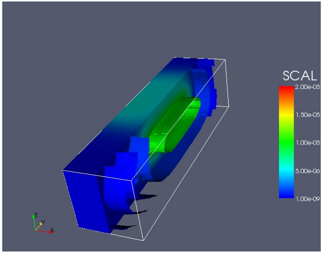


Figure: t = 50000 years

Detailed Homogenized Solutions Comparison



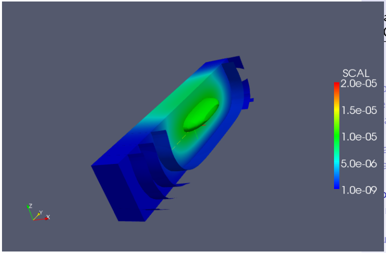


Figure: t = 100000 years

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Detailed Homogenized Solutions Comparison

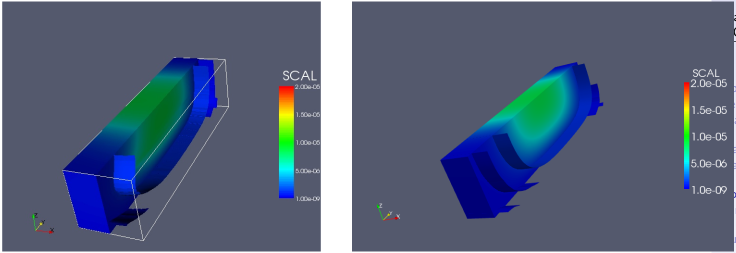

Figure: t = 100000 years

Low convection in the drifts

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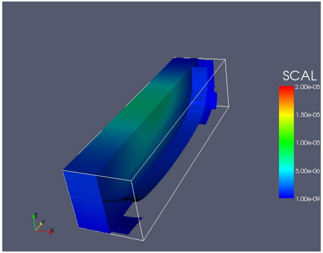
Detailed Homogenized Solutions Comparison



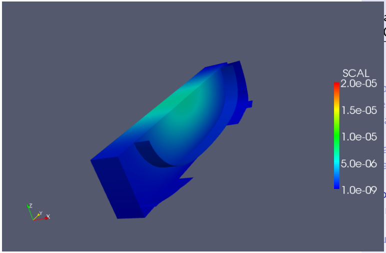


Figure: t = 250000 years

Low convection in the drifts

Detailed Homogenized Solutions Comparison

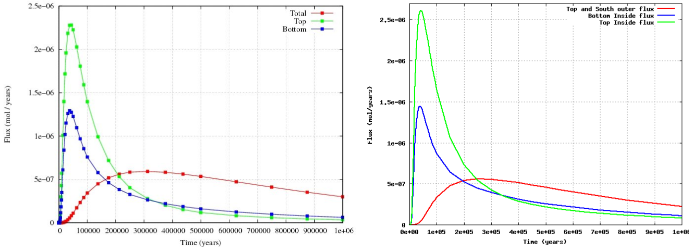


Figure: Time evolution of the outward fluxes for DH/Lyt = .1m/m

High Convection in the drifts

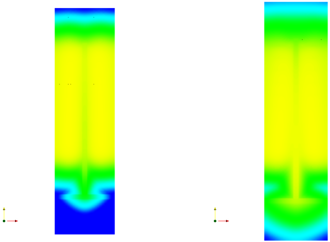


Figure: Concentration in the middle plan at t= 25 000 years: low convection in the drift (Left) and high convection in the drift (Right)

Out of range situations II (Flashback)

C In some intermediate situations, the Global model connects:

- strong Transport on the site horizontal middle plan

- to diffusion in the whole 3D domain;

$$R\theta \frac{\partial u^0}{\partial t} - \mathrm{div}\,(\mathbf{A}^h \nabla u^0) + (\mathbf{v} \cdot \nabla) u^0 + \lambda R\theta\, u^0 = 0 \text{ in } \tilde{\Omega}^T;$$

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High Convection in the drifts

Numerical Dificulties

- In a such approach, one need to solve time and spatially coupling between 3D and 2D partial differential problems.
- $\Rightarrow$ Iterativ Domain decomposition Algorithms.

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High Convection in the drifts

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Detailed Homogenized Comparison

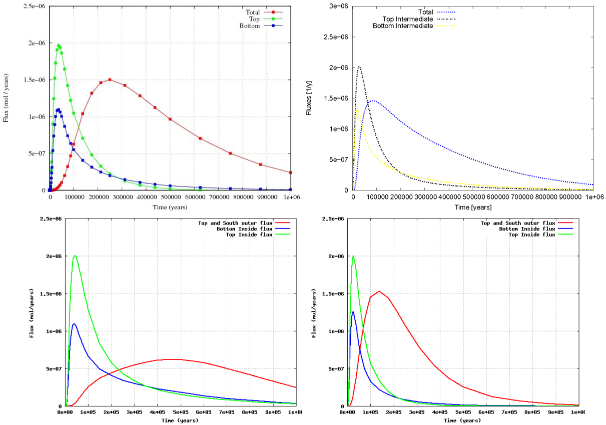

Figure: Time evolution of the outward fluxes for DH/Lyt = .5m/m (Top left CEA COmputations) (Top right IRSN Computations) (Bottom left UCBL Computations with non coupled model) (Bottom right UCBL Computations with 3D-2D coupled model)

Conclusion

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Conclusions

- Homogenization approach gives solutions:
  1. In Deterministic cases (linear or non linear)
  2. In stochastic cases (PAMINA Workshop in PRAHA (2007))
  3. Even when standart averaging fails (Convection dominant in drifts).
- Homogenization gives "cheap" models to PA in Far Field studies.