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► To cite this version:

Alain Genty, Christophe Le Potier, Stephane Gounand. Flow and radionuclide transport modelling in geological radioactive waste repository. MAMERN11: 4th International Conference on Approximation Methods and Numerical Modelling in Environment and Natural Resources, May 2011, Saidia, Morocco. <hal-04108166>

HAL Id: hal-04108166

<https://hal.science/hal-04108166v1>

Submitted on 2 Jun 2023

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Flow and radionuclide transport modelling in geological radioactive waste repository

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Keywords: Radionuclide Transport, Geological Repository, Numerical Error.

Abstract. *In the context of radioactive waste repository simulations, the numerical accuracy of the radionuclide transport calculations performed on repository objects is rarely estimated and considered as the best as possible. In this paper, we present a basic numerical accuracy estimation technique and the value obtained when applying it to the iodine transport simulation in a part of a geological radioactive waste repository.*

1 Introduction

In the context of high-level radioactive waste repository simulations, numerical codes based on sophisticated space en time discretization approaches are used to solve flow and radionuclide transport models. In the practical case, the radionuclide transport simulations performed on the considered geological repository object are carried out on the most refined mesh and the smallest calculation time steps as possible. The space and time refinement level used mainly depends on the available computer resources and on the maximum calculation time that the user agree to wait for. At the end, the numerical accuracy is considered as best as possible but never evaluated. In this paper, we present a basic numerical accuracy estimator that we applied to the radionuclide transport simulation in a part of a geological radioactive waste repository.

2 Radionuclide transport problem

The flow and radionuclide transport equations we consider here are given by relations (1) and (2)

$$\begin{cases} \operatorname{div} \mathbf{U} &= 0 \\ \mathbf{U} &= -\bar{K} \nabla H \end{cases} \quad (1)$$

$$\omega \frac{\partial C}{\partial t} = \nabla \cdot (\bar{D} \nabla C - C \mathbf{U}) - \omega \lambda C \quad (2)$$

where $\mathbf{U} [m \cdot s^{-1}]$ is the Darcy velocity, $H [m]$ is the head, $\bar{K} [m \cdot s^{-1}]$ is the hydraulic conductivity tensor, $\omega [-]$ is the porosity, $\lambda [s^{-1}]$ is the radioactive decay constant, $C [mol \cdot m^{-3}]$ is the concentration, and $\bar{D} = \bar{D}_e + \bar{\alpha} \mathbf{U} [m^2 \cdot s^{-1}]$ is the dispersive tensor (expressed in velocity coordinates) where $\bar{D}_e [m^2 \cdot s^{-1}]$ is the effective diffusion tensor and $\bar{\alpha} [m]$ is the dispersivity tensor.

We solve equations (1) and (2) numerically using a finite volume method for the space discretization scheme and an implicit time discretization scheme for equation (2). We chose a finite volume method using the Multi-Point Flux Approximation (MPFA) which is flux conservative and leads to a resulting discretization global matrix of dimension equal to the mesh cells number. Finally, the discretization matrix was solved using a multi-grid solver.

3 Description of the repository

We focused on the French vitrified waste repository design devoted to the isolation of radioactive waste resulting from spent fuel reprocessing. The design of the repository includes a vertical shaft that permits access to the middle of the host rock layer and a network of horizontal connecting galleries that contain about 3,600 horizontal repository cells in which vitrified waste canisters will be inserted.

The flow and radionuclide transport calculation on the whole repository geometry is beyond the reach of computational resources and we chose to perform computation on elementary parts of the system like the repository unit shown in Figure 1. The chosen repository unit includes a dead end connecting gallery allowing access to a double row of 10 waste disposal cells and is then embedded in an argillaceous box 100 meters long in x direction, 320 meters long in y direction and 100 meters long in z direction.

The repository unit components consist of disposal cells filled with waste canisters, of a connecting gallery filled with backfill material just before disposal closure and of engineered materials like bentonite and concrete plugs used to seal the disposal cells. Finally, gallery and disposal cell excavation are

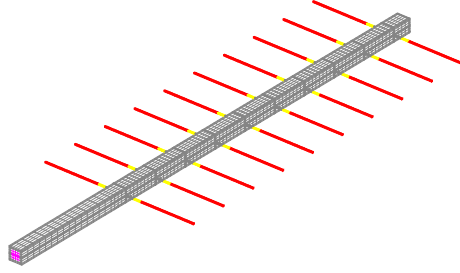


Figure 1: Three dimensional view of the repository unit (without host rock and EDZ).

known to damage the host rock at the repository walls. This area is called the Excavation Damaged Zone (EDZ) and surrounds the repository.

4 Numerical accuracy estimation

The numerical solution of the transport problem S_n^m , where n and m refer to the space and time refinement level used respectively, can reach the real solution S^* as close as needed by increasing n and m . The L^2 error $E_n^m = \sqrt{\int |S_n^m - S^*|^2 / \int S^{*2}}$ can then be decreased as low as wanted. The error E_n^m is known to be of the form $E_n^m = Cn^{-\alpha} + Dm^{-\beta}$ where C and D are constants and α and β refer to the convergence order of the space and time schemes respectively. We chose $m = n^{\alpha/\beta}$ to obtain $E_n = An^{-\alpha}$.

The problem in estimating E is that S^* is not known. We can only calculate S_n for different value of n . Let then consider two levels of refinement calculation n and p with $p > n$. Dividing E_n by E_p leads to the relation $E_n/E_p = (p/n)^\alpha = K = \sqrt{\int |S^* - S_n|^2 / \int |S^* - S_p|^2}$ which allow to write $K^2 \int |S^* - S_p|^2 = \int |S^* - S_n|^2 = \int |S^* - S_p + S_p - S_n|^2 < \int |S^* - S_p|^2 + \int |S_p - S_n|^2$ where the left part is maximised using the triangular inequality relation. Rearranging the previous relation allow to exhibit a new error ξ_p giving access to the accuracy of the performed calculation S_p which is maximized by a value depending on S_p and S_n .

$$\xi_p = \sqrt{\int |S^* - S_p|^2 / \int S_p^2} < 1/\sqrt{K^2 - 1} \cdot \sqrt{\int |S_p - S_n|^2 / \int S_p^2} \quad (3)$$

In order to evaluate the accuracy of our computations, we focus on the radionuclide activity flux across the upper boundary of the calculation domain by the mean of the error ξ . Note that for dominant diffusive transport problems, Finite Volume scheme is second order ($\alpha = 2$) and we chose $p = 2n$ ($K = 4$).

5 Computation Results

We performed flow and iodine transport computation on the system presented in Figure 1 using a coarse space and time steps discretization (361,800 cells, 16 time steps) and a refined space and time steps discretization (2,894,400 cells, 64 time steps). The time evolution of the calculated iodine plume inside the system indicates that the transport is mainly diffusive (see Figure 2).

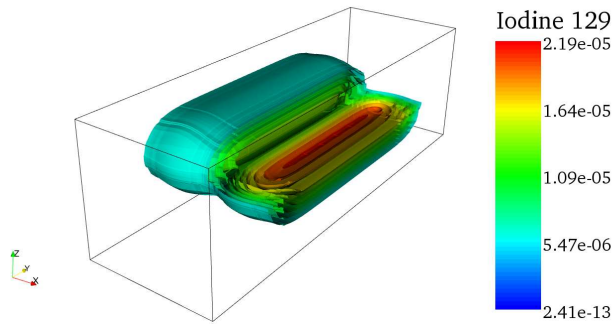


Figure 2: Iodine concentration plume in the repository at time $t = 50,000$ years.

The output flux calculated for the two refinement level is presented as a function of time in Figure 3. The calculation of the numerical accuracy of the

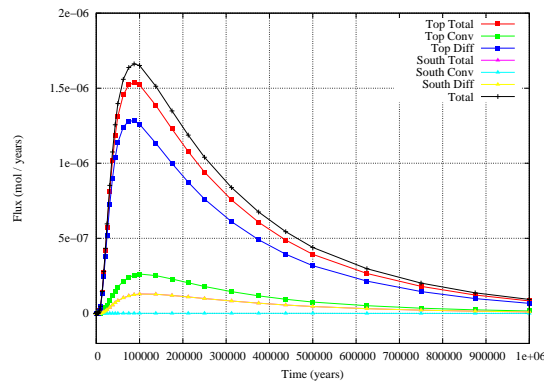


Figure 3: Iodine output flux evolution.

obtained output flux curve with the finest level lead to $\xi < 0.0X$.