Modelling radionuclide transport using different representations of sorption

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Introduction:

Radionuclide migration assessments are an important part of any radioactive waste storage and disposal facility safety assessment. Sorption is one of the key factors that strongly affects contaminants retention and transport. This parameter encompasses a number of reactions of dissolved contaminants with solid surfaces, this includes surface complexation and ion exchange reactions, among others. There is a multitude of methods of describing sorption. One of the more common approaches is to describe the interactions of contaminants with the solid using sorption coefficients or Kd values. These Kd values represent the ratio of the concentration of the sorbed contaminant to its concentration in the solution. A less common approach is modelling reactive transport of the contaminants with surface complexation and ion exchange reactions. This allows for a more detailed representation of the processes occurring in the engineered or natural barrier and their effect on radionuclide transportation. This approach however, requires significantly more computational resources and specific input data, that is not available for all cases.

The aim of this study is to investigate the difference in contaminant distribution in soil obtained with different contaminant sorption implementation. To achieve this, an evaluation of contaminant migration in clayey soils using two different approaches is performed. In the first case, a simple solute transport model is created, where sorption is described with a Kd value. In the second case, Kd values are introduced in a reactive transport model.

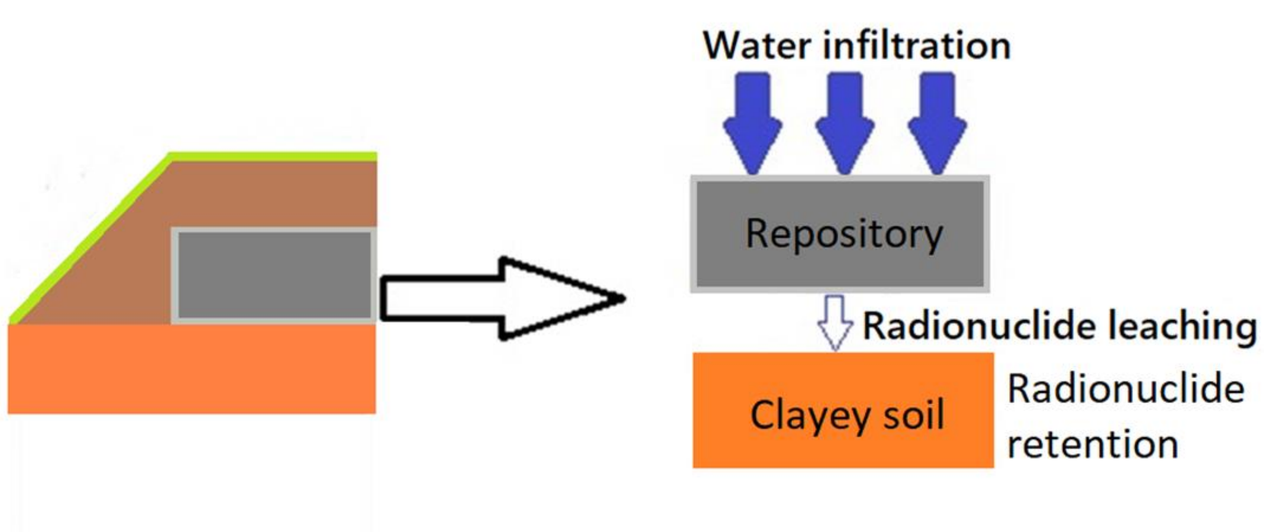

Fig. 1 Analyzed system

Modelling scenario:

A contaminant/radionuclide is assumed to be leached from the repository into the clayey soil, where undergo sorption and radioactive decay.

Cases considered:

- Non-decaying well sorbed contaminant;
- Non-decaying poor sorbed contaminant;
- Well sorbed long-lived radionuclide;
- Poor-sorbed short-lived radionuclide.

In each case the Kd values and radioactive decay are implemented in two ways:

- Variant 1 – a simple solute transport with a defined Kd value and decay rate.
- Variant 2 – the Kd value is introduced as surface reaction based on a model proposed in [1], radionuclide decay is modelled as a kinetic reaction.

Modelling assumptions:

- A 1D domain of 1 m length clayey soil.
- Contaminant/radionuclide flow pulse duration – 1000 years.
- Contaminant/radionuclide concentration in the infiltrating water – 1e-8 mol/l.
- Kd values: 300 ml/g and 30 ml/g.
- Half life: 75000 years (Ni-59) and 29 years (Sr-90).
- Modelling time frame:
  - Short-lived radionuclide – 1500 years,
  - Other cases – 10000 years.
- The clayey soil domain has homogenous physical and chemical properties.
- Computer tool – HP1 [2].

Modelling results

Non-decaying contaminants

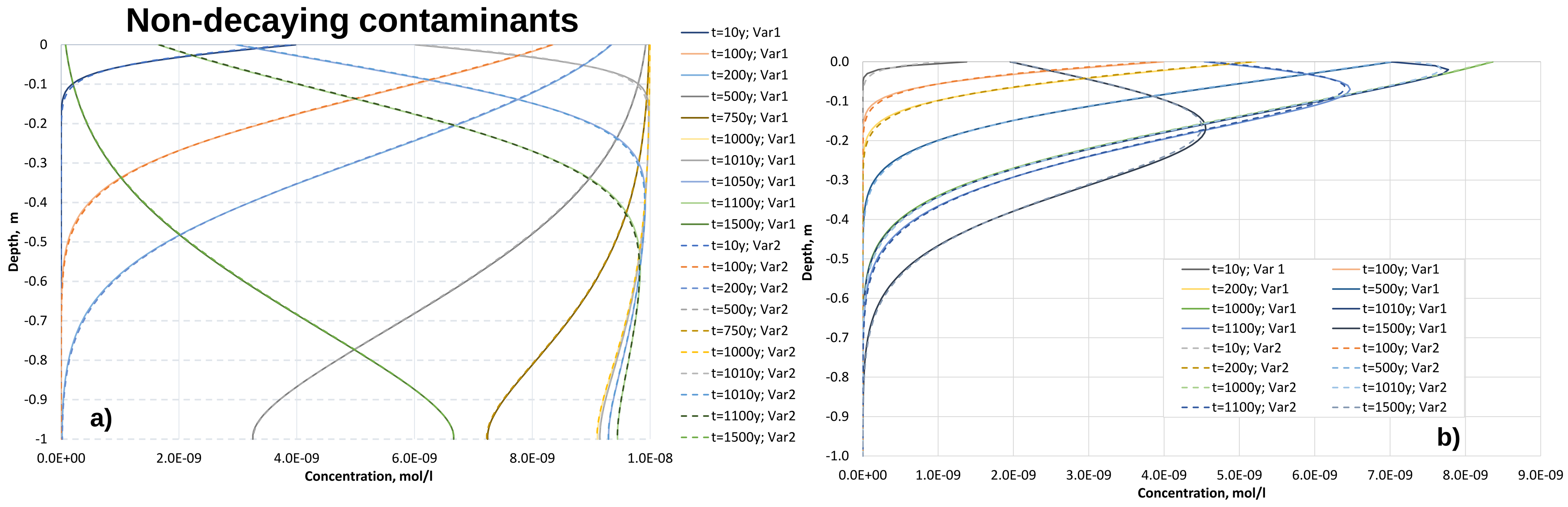

Fig. 2 Contaminant distribution profiles at different time steps a) low sorbing contaminant, b) well sorbing contaminant

Decaying contaminants (radionuclides)

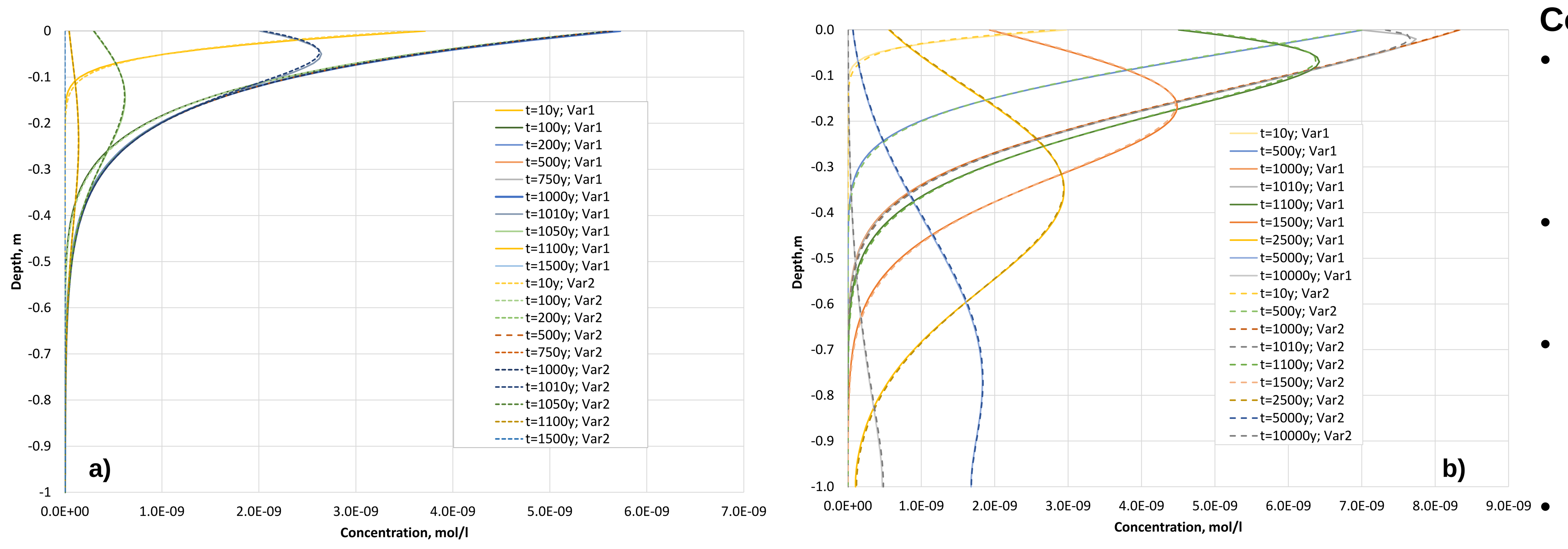

Fig. 3 Radionuclide distribution profiles at different time steps a) Poor sorbing radionuclide, b) well sorbing radionuclide

Non-decaying contaminants

The modelling results between cases when Kd values are used (Variant 1) and when Kd values are introduced in a reactive transport model (Variant 2) in general show very good agreement (around 1% difference for most data points). Somewhat larger differences in the results can be observed only at the very edge of the contaminant propagation front and at the contaminant inflow point (26-38% for individual points).

Decaying contaminants

Again, the results between the different methods have shown good agreement with mostly 1% difference in concentration values. Larger differences were observed only at the edge of the contaminant propagation front and in the top soil layer (radionuclide inflow zone). The differences between concentration values here were about 28-47%.

Conclusions:

- The results using two different approaches to radionuclide sorption evaluation in general yielded very good agreement (the difference in the contaminant concentration values was mostly less than 1%).
- Both methods can be equally used in the modelling of the radionuclide migration (e.g. in performance assessments).
- The main advantage of using reactive transport modelling is the ability to take into account chemical reactions (equilibrium and/or kinetic). This would allow to model the chemical evolution of the modelled system.
- However, introducing these chemical reactions come at a cost to computational time: in a relatively simple case as shown here, the computational time increased around 50 to 65 times in comparison with the case when a simple solute transport model with the defined Kd value and decay rate was used.

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