Sensitivity Analysis of Radionuclide Transport and Radiation Dose Simulations

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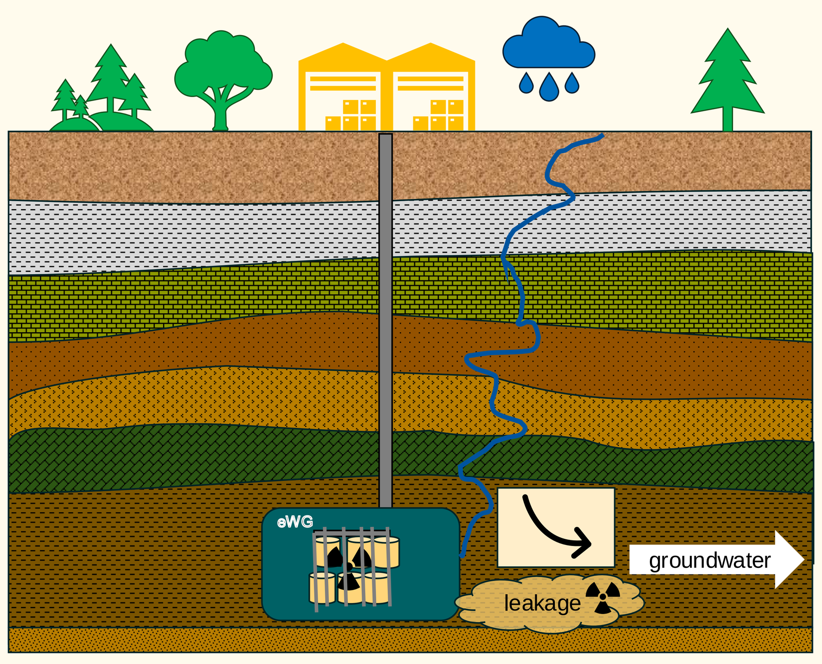
1. Motivation

Physics-based impact models, describing future risks of radioactive contamination in repository sites, are built in the presence of numerous uncertainties. To ensure a high level of predictive accuracy, it is essential to address these uncertainties.



❖ Reliability Management:

1) Process Model

2) Impact Model

3) Sensitivity Analysis

Assess which measurement would be most beneficial to reduce uncertainty.

2. Theory

2.1 Process Model : Reactive Transport Equation:

$$\phi_i R_i \frac{\partial c_i}{\partial t} = -q\nabla c_i + \nabla(D_i \nabla c_i) - \phi_i R_i \lambda_i c_i + \phi_{i-1} R_{i-1} \lambda_{i-1} c_{i-1}$$

(3) (1) (2) (4), (3) (5), (3)

(1) Advection

- mean fluid velocity:

$$v = q/\phi$$

- Darcy flux:

$$q = -\frac{\kappa}{\mu}(\nabla p - \rho g)$$

κ is medium permeability, μ is fluid viscosity

(2) Diffusion

- $D = \phi D_p$

ϕ is porosity, D_p is pore diffusion coefficient.

(3) Adsorption

- retardation factor:

$$R = 1 + \frac{\rho_b K_d}{\phi}$$

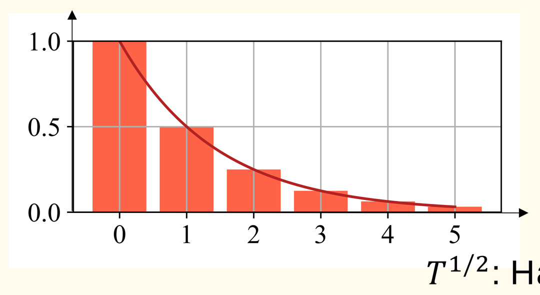
ρ_b is rock density
K_d is adsorption coefficient

(4) Radionuclide Decay

(5) Radionuclide Ingrowth

- Decay rate: $\lambda = \frac{ln2}{T_{1/2}}$, $T_{1/2}$ is Half-life

N: Number of Radionuclides



$T^{1/2}$: Half-life

2.2 Impact Model : Accumulated Dose

➢ Absorbed Dose [Gray]:

$$d = \frac{\Delta E}{\Delta m}$$

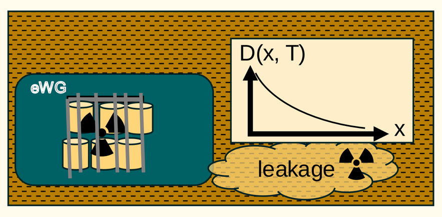
➢ Energy:

$$\Delta E = \sum_{i=1}^{N} \Delta E_i = \sum_{i=1}^{N} a_i \Delta t_j \bar{E}_i$$

- N is number of radionuclides
- a is activity

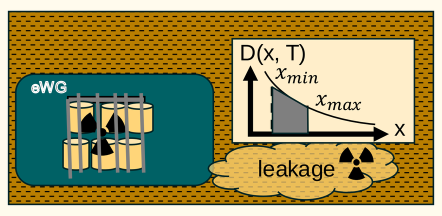
➢ Accumulated Dose:

$$D(x_k, T_{end}) = \frac{N_A}{\rho_k} \sum_{i=1}^{N} \lambda_i \bar{E}_i \int_0^{T_{end}} c_i(x_k, t)\, dt$$



➢ Accumulated Dose in Critical Regions:

$$D^*(T_{end}) = \int_{x_{min}}^{x_{max}} D(x, T_{end})\, dx$$



2.3 Sensitivity Analysis : Sensitivity Indices

- First-order Index:

Measures the contribution to the output variance by a single model input.

$$S_i = \frac{V_{X_i}(E_{X\sim i}(Y|X_i))}{V(Y)}$$

- Second-order Index:

Measures the contribution to the output variance caused by the interaction of two model inputs.

$$S_{ij} = \frac{V_{X_{i,j}}(E_{X\sim i,j}(Y|X_i, X_j))}{V(Y)} - S_i - S_j$$

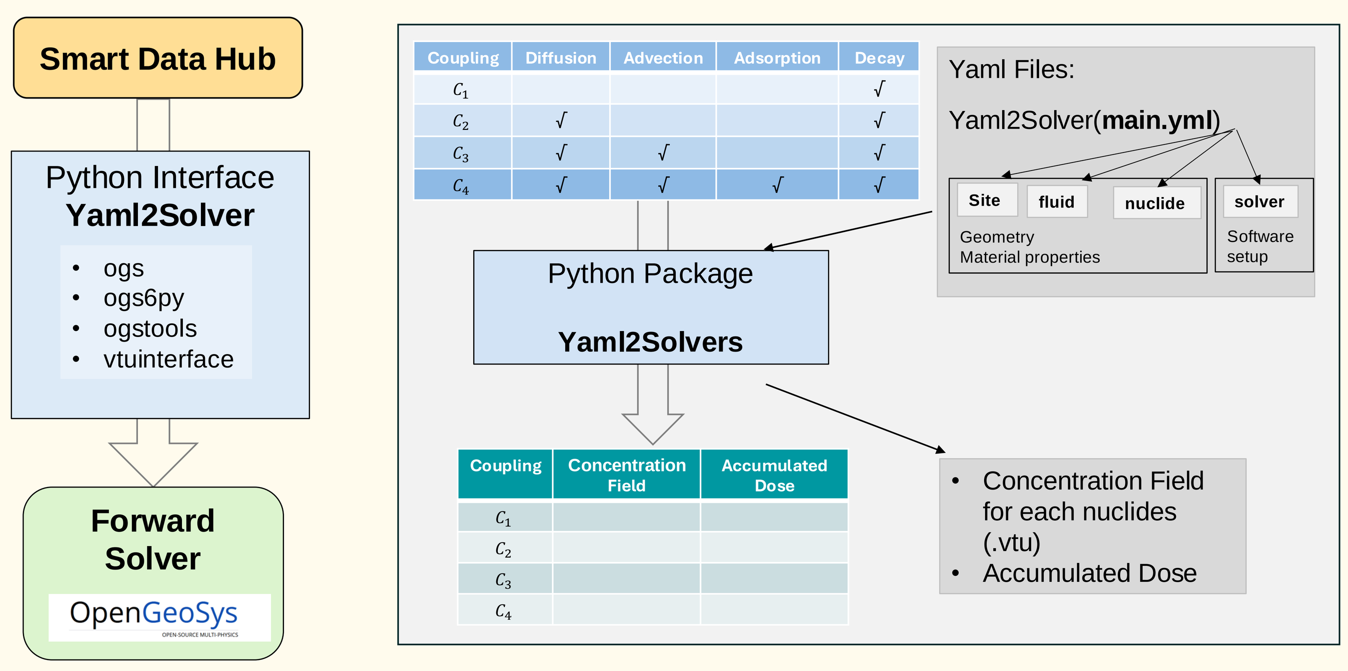
- Total Effect Index:

Measures the contribution to the output variance caused by a model input, accounting for its interactions with all other factors.

$$S_{T_i} = 1 - \frac{V_{X\sim i}(E_{X_i}(Y|X_{\sim i}))}{V(Y)}$$

3. Yaml2Solver Python Interface: A Python Interface for Seamless Simulations

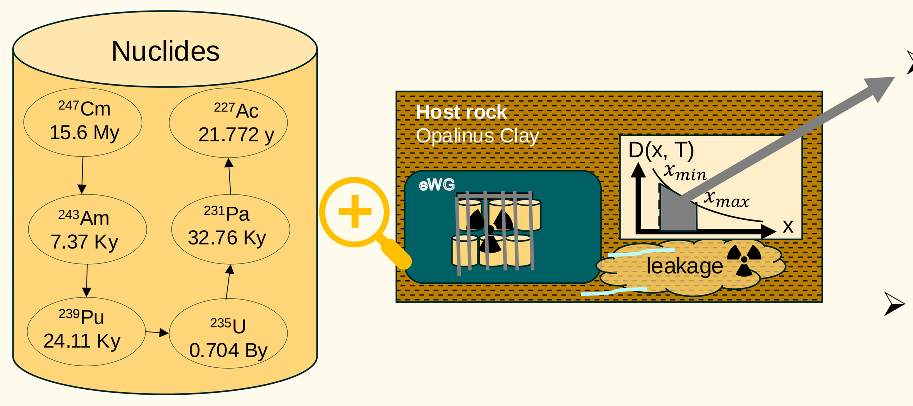
Yaml2Solver employs YAML files to define input parameters, enabling efficient adjustment of values and consideration of various coupled processes.



▲ Functionality of Yaml2Solver

4. Model Setup

4.1 Leakage scenario:



➢ Accumulated Dose in Critical Regions:

$$D^*(T_{end}) = \int_{x_{min}}^{x_{max}} D(x, T_{end})\, dx$$

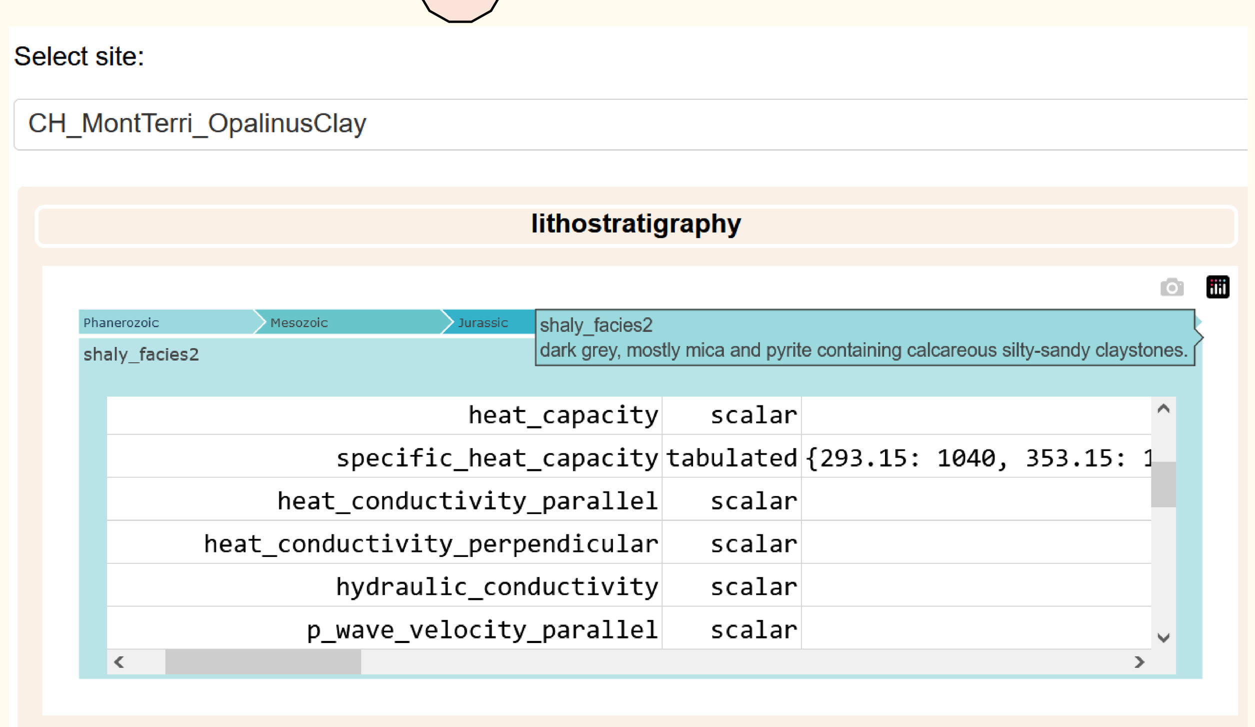
$$D^*(T_{end}) = g(c_i(x,t)) = f(\phi_i, q, D_i, R_i, \dots)$$

➢ Uncertain Parameters:

$$D^*(T_{end}) = f(\phi_i, q, D_i) \quad \text{with } \phi_1 = \phi_2 = \dots = \phi_N,\ D_1 = D_2 = \dots = D_N$$

4.2 Sensitivity Analysis Through Smart Data Hub and Yaml2Solver:

I **Smart Data Hub:**



Host Rock: Opalinus Clay Shaly Facies

Extract Uncertain Parameters

Model Parameters: III

Main.yml:

❑ **site:**
➢ **site_name:** ../../yaml-db/sites/Mont_Terri/Mont_Terri.yml
➢ **modelling_areas:** ['Jurassic-Middle_Aalenian_OpalinusClay_shaly-facies1']

❑ **fluid:**
➢ **type:** ['water']
➢ **fluid_properties:** ['../../yaml-db/fluid/default/water.yml']

❑ **nuclide:**
➢ **nuclides_properties:** ../../yaml-db/nuclide/Cm247_decay_chain_OpalinusClay.yml
➢ **first_nuclide:** Cm-247
➢ **include_nuclides:** ['Cm-247', 'Am-243', 'Pu-239', 'U-235', 'Pa-231', 'Ac-227']

❑ **solver:**
➢ **ogs_solver:**
❖ **simulation_setup:** ../../yaml-db/sim_setup/ogs_sol_setup.yml
➢ **analytical_solution:**
❖ **simulation_setup:** ../../yaml-db/sim_setup/analytical_sol_setup.yml

Uncertain Parameter	Range	Unit
Accessible porosity ϕ_i	[0.2, 0.4]	-
Darcy flow q	[0.1,1]	mm/a
Effective diffusion coefficient D_i	[1e-11, 1e-10]	m^2/s

Generate Samples

Generate Model Evaluations

II SALIB Sensitivity Analysis Library (SALib)

Provide model parameters

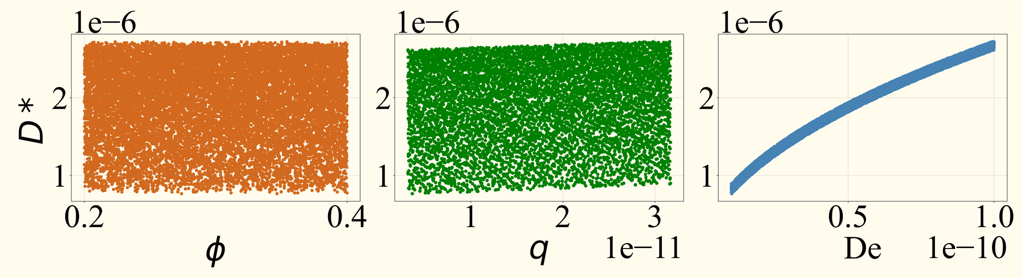
IV **Yaml2Solver**

Solve process and impact models

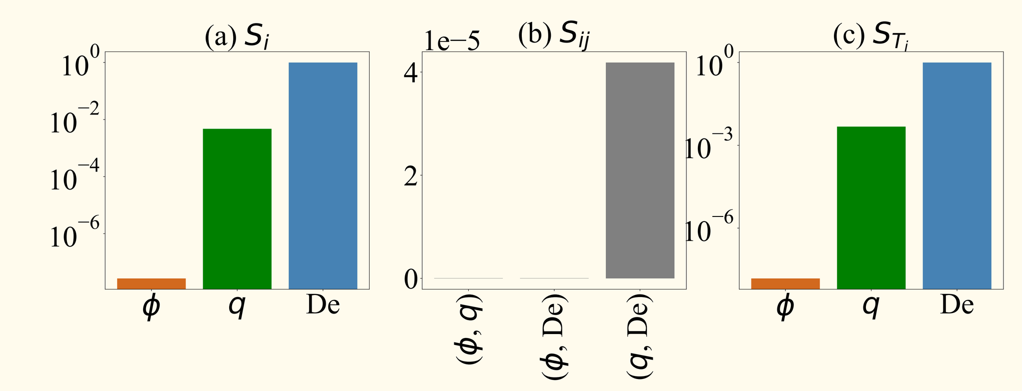
Result: Accumulated Dose in Critical Regions

5. Results and Conclusions

The sensitivity analysis was conducted utilizing three uncertain parameters. The base sample size was set to 2048, resulting in a total of 16384 simulation runs.



◀ Scatterplots of accumulated dose within a critial region D^* versus the porosity ϕ, darcy flow q and effective diffusion coefficient De.



◀ First-, total- and second-order effects for porosity ϕ, darcy flow q and effective diffusion coefficient De.

The results indicate that the effective diffusion coefficient is the most influential factor affecting accumulated dose, while porosity has a minimal impact. Consequently, for future field experiments, it is advisable to focus on setting up experiments that accurately estimate the diffusion coefficient to reduce uncertainty.

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