DECOVALEX 2027 Analog

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Simulation of Radionuclide Transport in Clay

Seminar presentation

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DECOVALEX 2027

Analog

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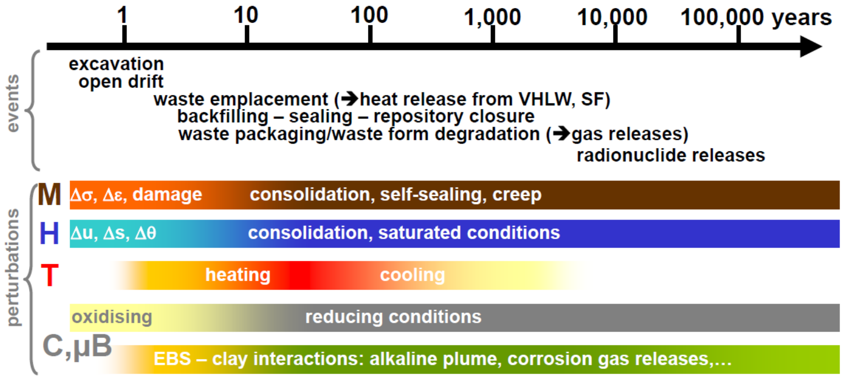
DECOVALEX

DEvelopment of **CO**upled models and their **VAL**idation against **EX**periments

- DECOVALEX was initiated in 1992 as an international cooperative project to address modeling challenges in deep geological repository (DGR) systems, involving nuclear waste organizations, regulators, and research teams.
- DECOVALEX focuses on advancing multiphysics simulations, improving coupled processes (e.g. thermo(T), hydraulic(H), mechanical(M), chemical(C)) models, validating numerical models through laboratory and field experiments, and provide a platform for knowledge exchange and capacity building.

Major T, H, M, and C changes in both engineering and natural barriers during the lifetime of a geologic repository.



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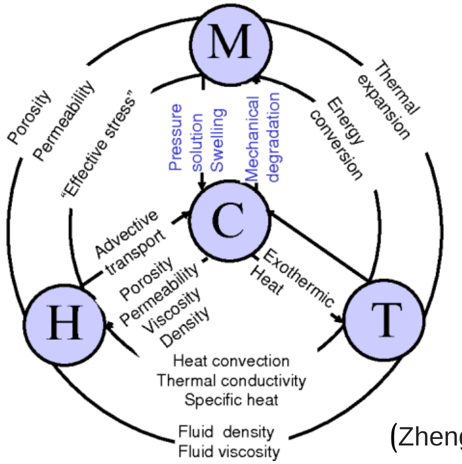


Selected coupling effects between T, H, M, and C processes

(Zheng et al., 2011)

Outline

Introduction

- HLW final disposal
- KBS-3 disposal concept

Modeling Object

- Iodone-129
- Cigar Lake uranium deposit

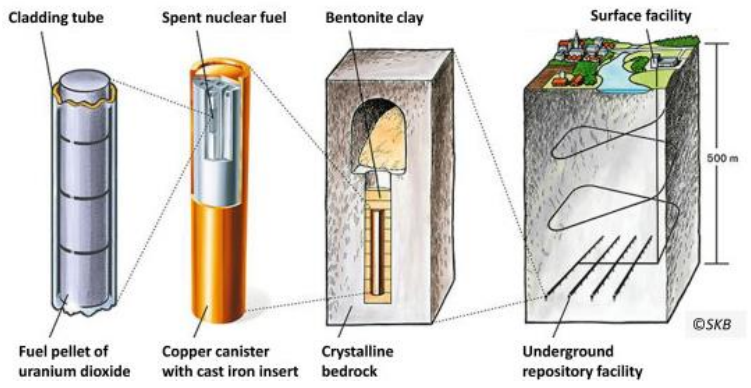
Current Results

Conclusion & Future work

Introduction

- High-level radioactive waste (HLW), comprising spent nuclear fuel (SNF) and reprocessed waste, is highly radioactive, has long half-lives, and poses significant toxicity, necessitating safe disposal and long-term isolation.
- Deep geological disposal with engineering barrier is generally adopted worldwide for final disposal of HLW management.
- KBS-3 disposal concept (SKB, 1983)
  - multi-barrier system = engineering barrier + natural barrier

Engineering barrier system:
Canister
Buffer
Backfill



Natural barrier system:
Host rock

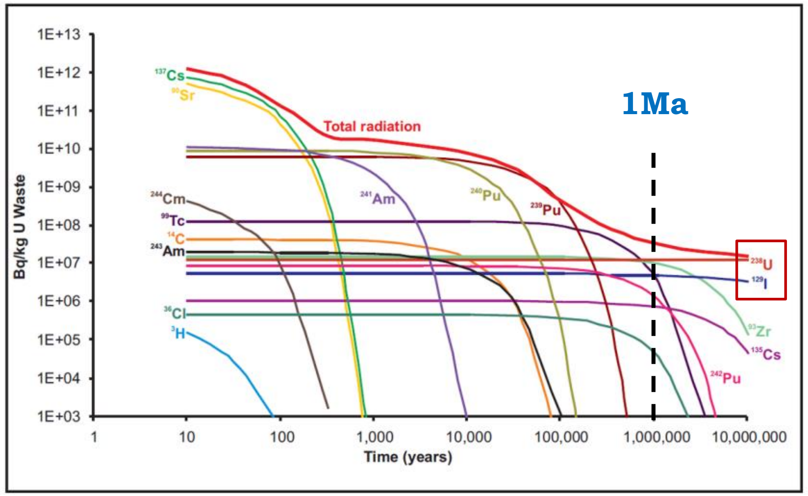
(SKB, 2006)

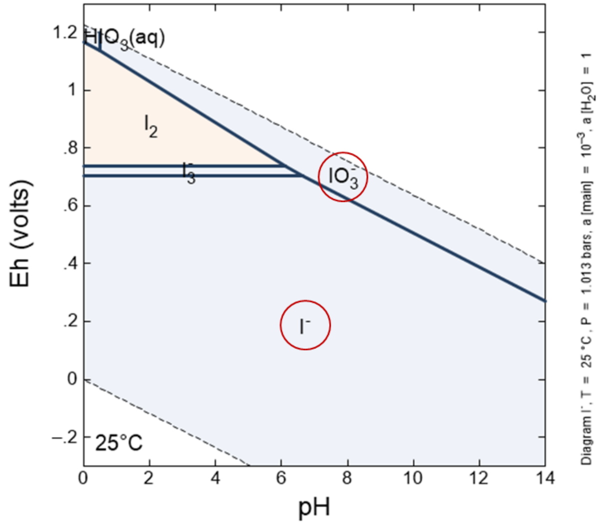
Modeling Object - Iodine-129

- Iodine-129 (I-129) is primarily produced through uranium fission. In the HLW safety assessment, I-129 is a significant radionuclide.
  - Long half-life (15.7Ma): It remains radioactive for an extremely long period.
  - High mobility: In aqueous environments, I-129 primarily exists as iodide (I^-) and iodate (IO_3^-), both of which are highly mobile.
  - Migration modeling and long-term safety analysis are necessary to predict and evaluate its potential effects on the environment and human health.

Dose contribution of major fission products in SNF. The bold red line is the total radiation.

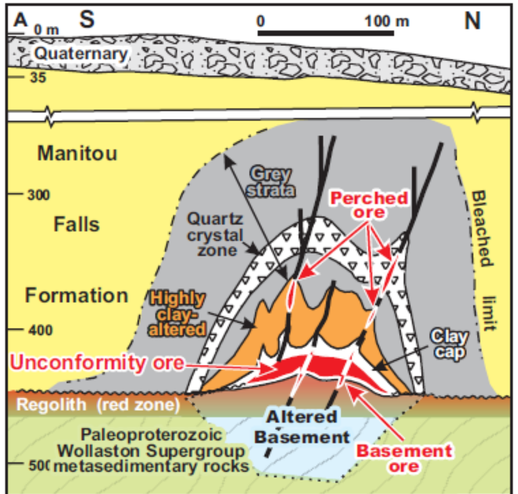
https://commons.wikimedia.org/wiki/File:Radioactivity_of_Fission_Products.png





Modeling Object – Cigar Lake

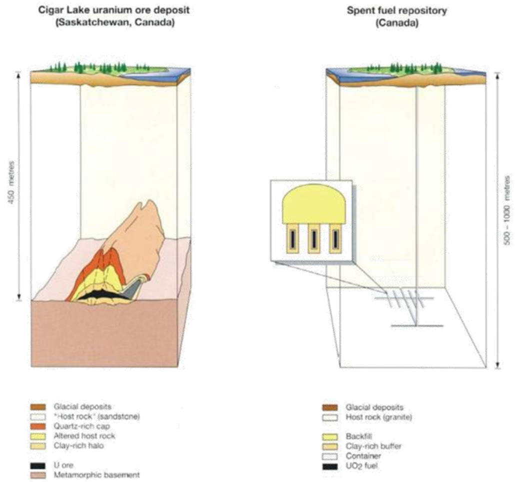
- Cigar Lake uranium deposit located in Canada, at a depth of approximately 450 m, formed by hydrothermal processes.
- Hydrothermal alteration of the host sandstone leads to the formation of an illite-rich clay layer, ranging in thickness from 5 to 30 m. These geological features prevent radionuclides from migrating to the surface.
- Due to its geological structure being similar to the concept of HLW final disposal, it is regarded as an important natural analogue for study.



(Jefferson et al., 2007)

sandstone host rocks

basement

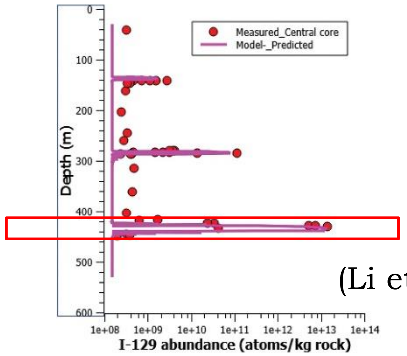


(Miller et al., 2006)

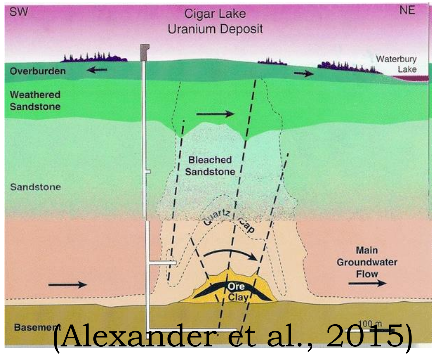
Objectives

- To verify the feasibility of the model by comparing simulation results with field data.
- To understand the long-term transport behavior of I-129 in fractured and porous media.
- To calibrate long-term simulation predictions and contribute to the HLW final disposal.

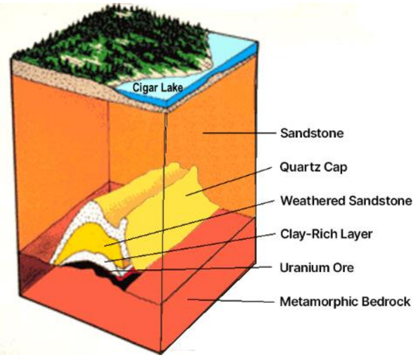
1 dimension → 2 dimension → 3 dimension



(Li et al., 2024)



(Alexander et al., 2015)

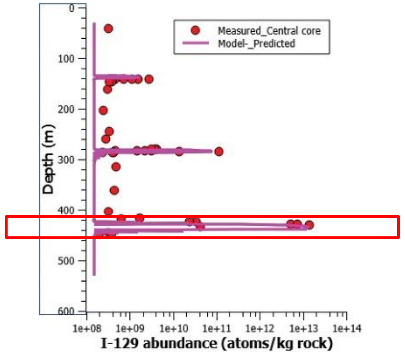


https://en.wikipedia.org/wiki/Cigar_Lake_mine

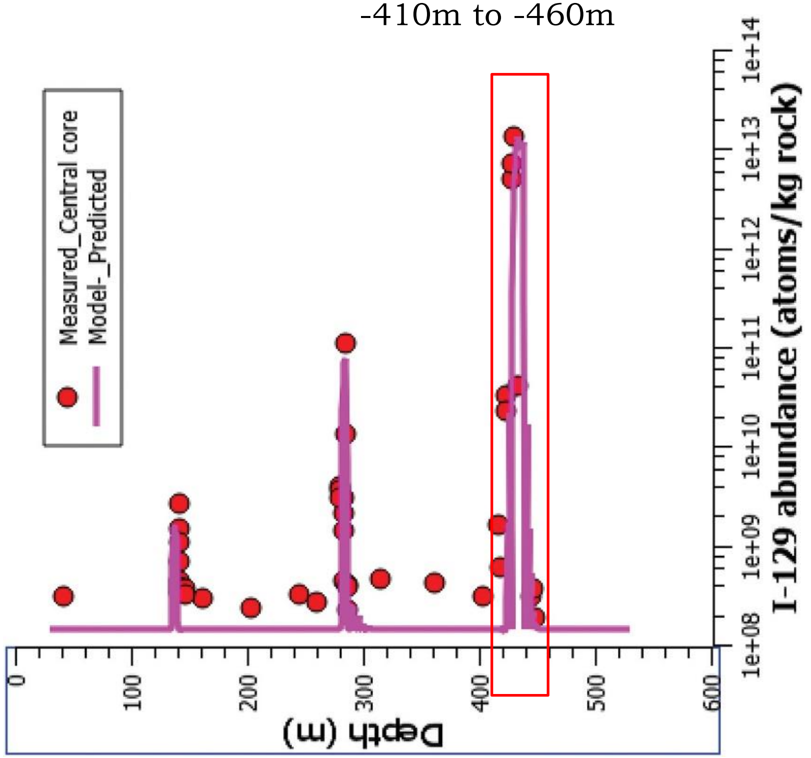
8 Current Result

Model Setting

- Simulation focuses on a depth range from -410 meters to -460 meters.
- The model is in the range from -25m to 25m, with center of uranium orebody located at 0.
- The material is homogeneous.
- Diffusion-only study case.



-410m to -460m



(Li et al., 2024)

Model Setting

- I-129 is primarily produced through uranium fission.
- Initial concentration of
  - I-129 is set as 0.
  - U-238 follows a normal gaussian distribution.
- Dirichlet boundary condition
  - Concentration of I-129 on right and left ends are set as 0.
- Simulation time
  - The model can be run for up to 1.4 billion years, which is the age of the uranium formation.

Governing Equation

- Diffusion equation (1D)

$$\varepsilon \frac{\partial c}{\partial t} + k_d \rho \frac{\partial c}{\partial t} = \mathrm{D}_e \frac{\partial^2 c}{\partial x^2}$$

$$R = 1 + \frac{k_d \rho}{\varepsilon}$$

retardation factor

$$\frac{\partial c}{\partial t} = \frac{\mathrm{D}_e}{R} \frac{\partial^2 c}{\partial x^2}$$

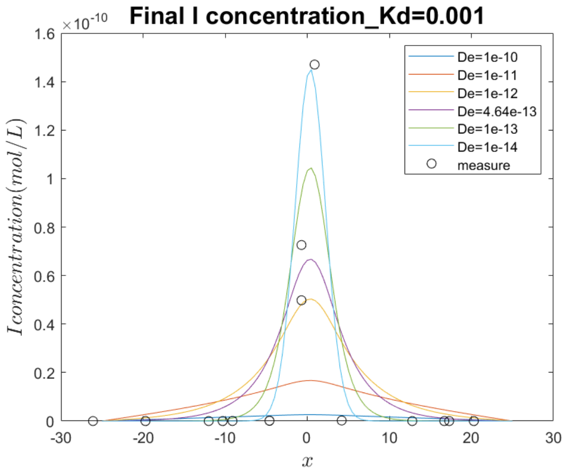
Model Parameters		
concentration	c	mol/L
location	x	m
porosity	ε	-
Diffusion coefficient	D_e	m^2/s
Distribution coefficient of I	K_d	m^3/kg
Density	ρ	kg/m^3

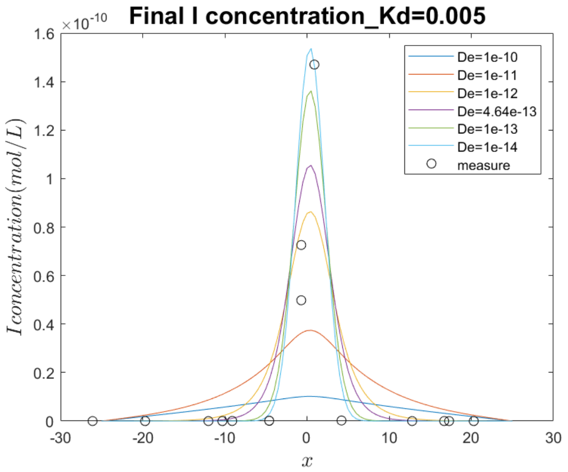
- Source term
- I-129 Production and Decay

$$S = \alpha [U] Y_f \lambda_{sf} - \lambda_d * c$$

Model Parameters	
empirical adjustment factor for I-129	α
fission yield at mass I-129 from the spontaneous fission (half life 16.1 Ma)	Y_f
decay constant for spontaneous fission of U-238 (half life 8.4e15 a)	λ_{sf}
rate of loss of I-129	λ_d
concentration	c

Results


Final I concentration_Kd=0.001
×10^-10
I concentration(mol/L)
x
De=1e-10
De=1e-11
De=1e-12
De=4.64e-13
De=1e-13
De=1e-14
measure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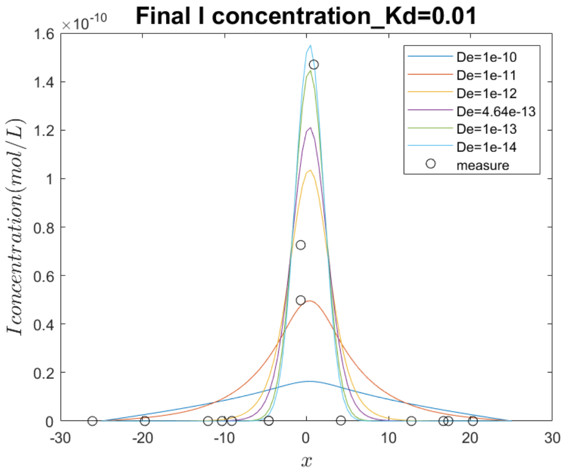
De=1e-14
measure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I concentration(mol/L)
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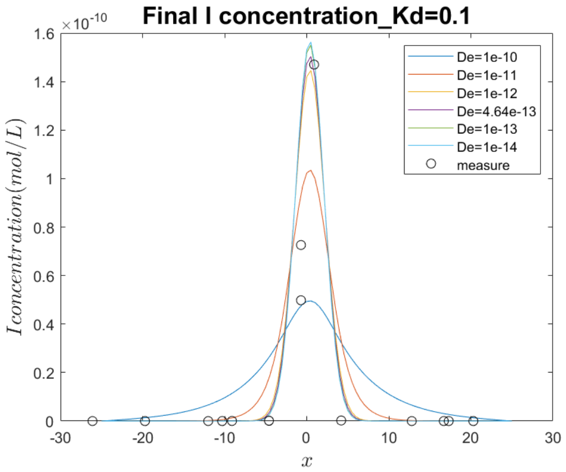
De=1e-14
measure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I concentration(mol/L)
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De=1e-11
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De=4.64e-13
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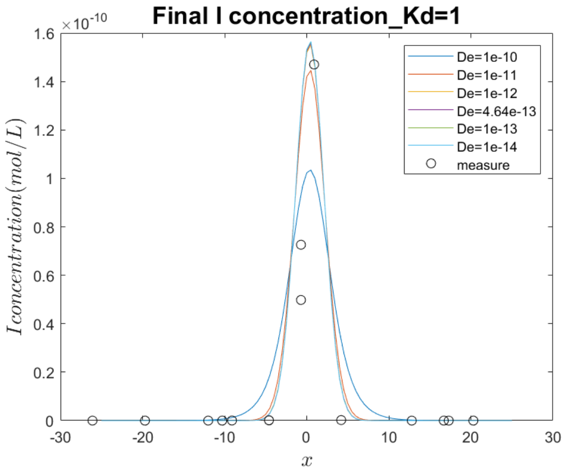
De=1e-14
measure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De=4.64e-13
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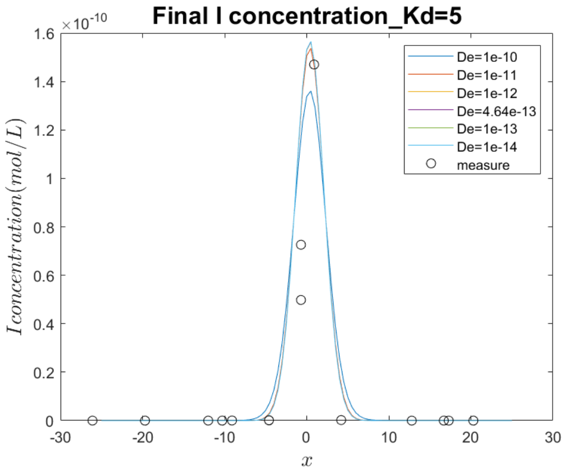
De=1e-14
measure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×10^-10
I concentration(mol/L)
x
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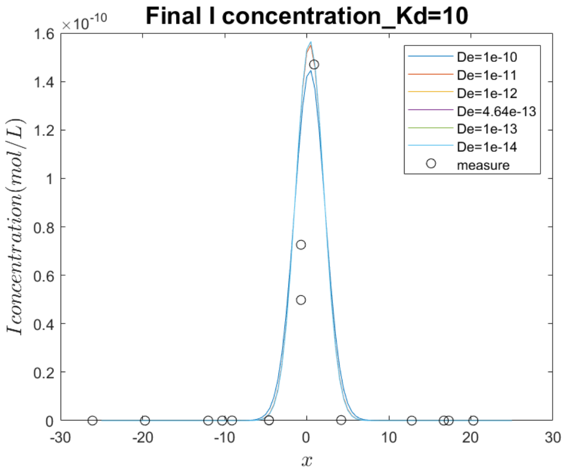
De=1e-14
measure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×10^-10
I concentration(mol/L)
x
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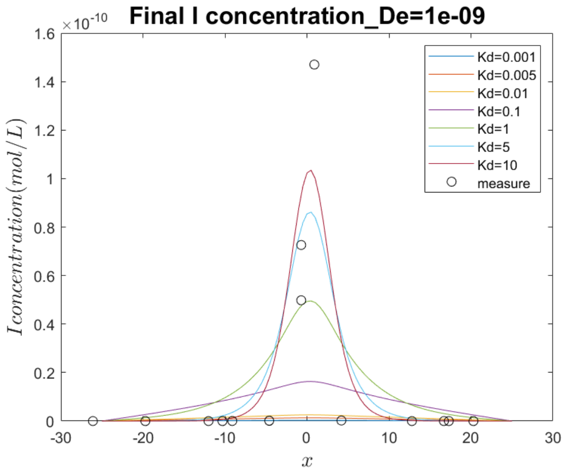
De=1e-11
De=1e-12
De=4.64e-13
De=1e-13
De=1e-14
measure

Results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Iconcentration(mol/L)
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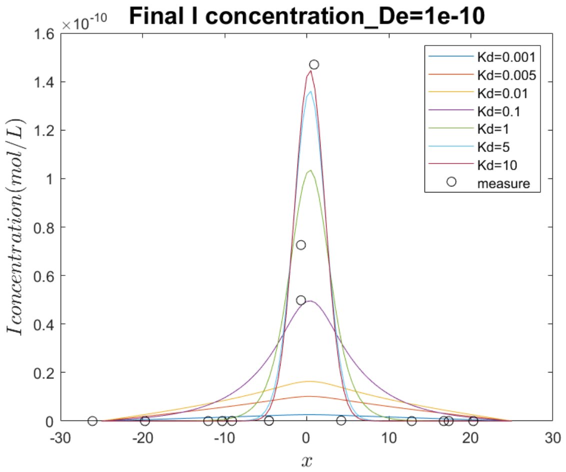
Kd=1
Kd=5
Kd=10
measure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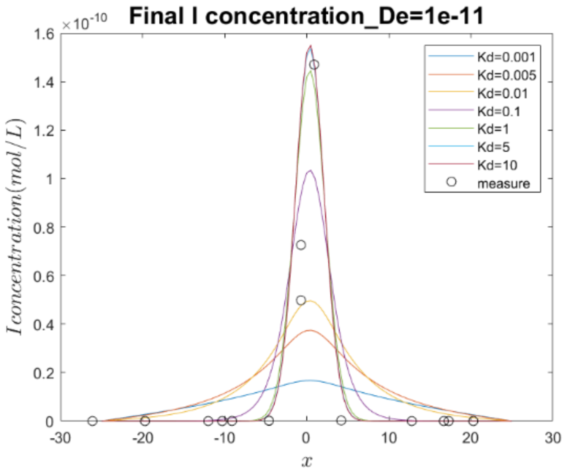
Kd=5
Kd=10
measure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×10^-10
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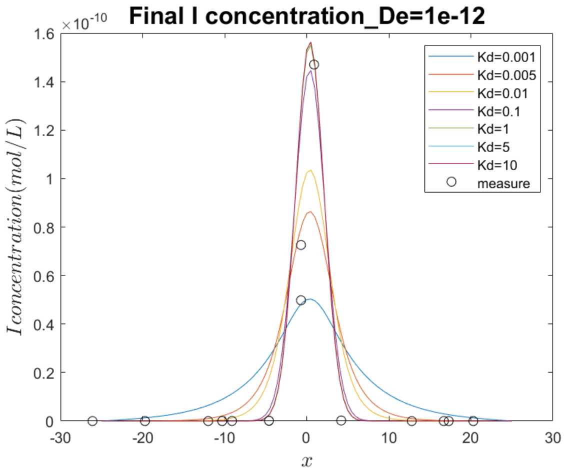
Kd=0.001
Kd=0.005
Kd=0.01
Kd=0.1
Kd=1
Kd=5
Kd=10
measure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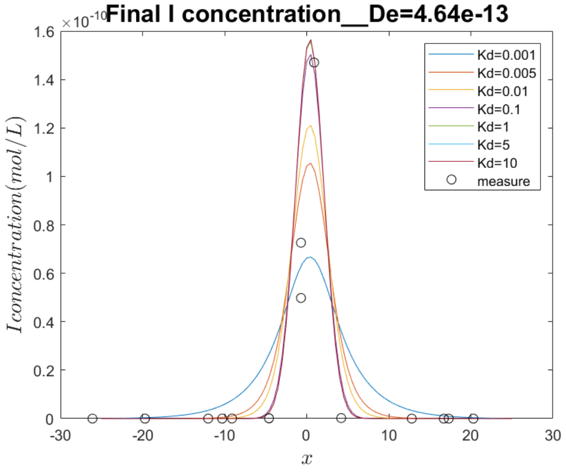
Kd=0.005
Kd=0.01
Kd=0.1
Kd=1
Kd=5
Kd=10
measure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×10^-10
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x
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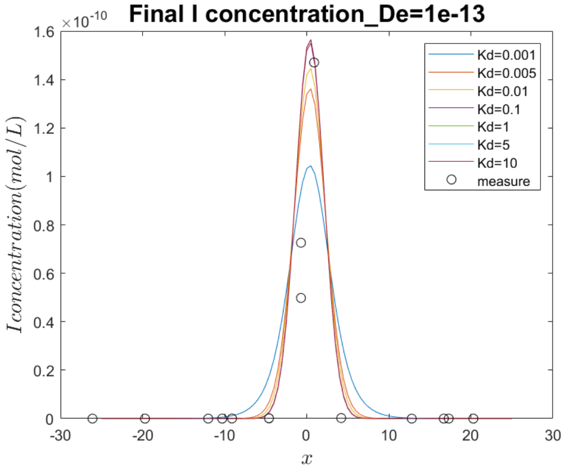
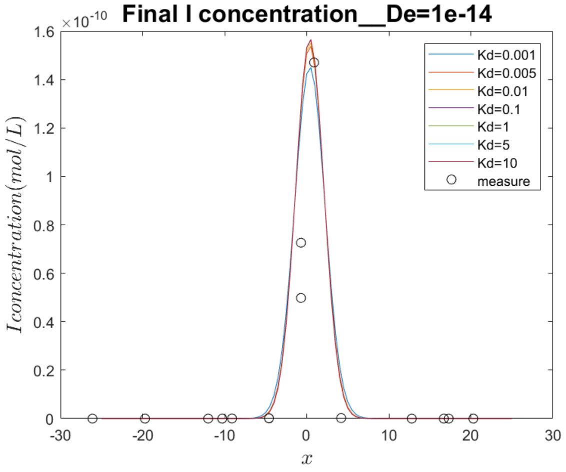
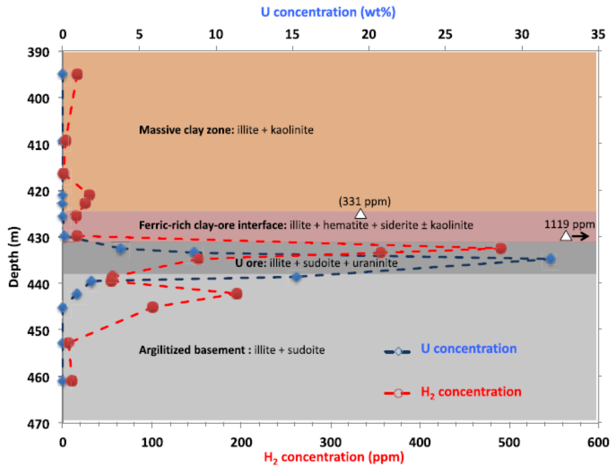
Kd=0.005
Kd=0.01
Kd=0.1
Kd=1
Kd=5
Kd=10
measure


Final I concentration_De=1e-13
×10^-10
Iconcentration(mol/L)
x
Kd=0.001
Kd=0.005
Kd=0.01
Kd=0.1
Kd=1
Kd=5
Kd=10
measure


Final I concentration__De=1e-14
×10^-10
Iconcentration(mol/L)
x
Kd=0.001
Kd=0.005
Kd=0.01
Kd=0.1
Kd=1
Kd=5
Kd=10
measure

Conclusion and Future Work



(Truche et al., 2018)

- The simulation results do not fit well with the measured data. One possible explanation for this might be the assumption of homogeneity in the model. In real case, the geological medium likely exhibits heterogeneity, including variations in mineral composition and porosity.
- The constant De and Kd values used in the model may oversimplify the system. Factors such as chemical reaction, scale effects and localized fractures could alter effective diffusion coefficients and adsorption behavior, influencing radionuclide transport.
- Future work should include heterogeneous conditions, through assigning distinct properties to different regions. Additionally, transitioning to two-dimensional and three-dimensional simulations could provide a more accurate representation of complex transport dynamics in natural systems.

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Thank you for your attention!

Seminar presentation

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