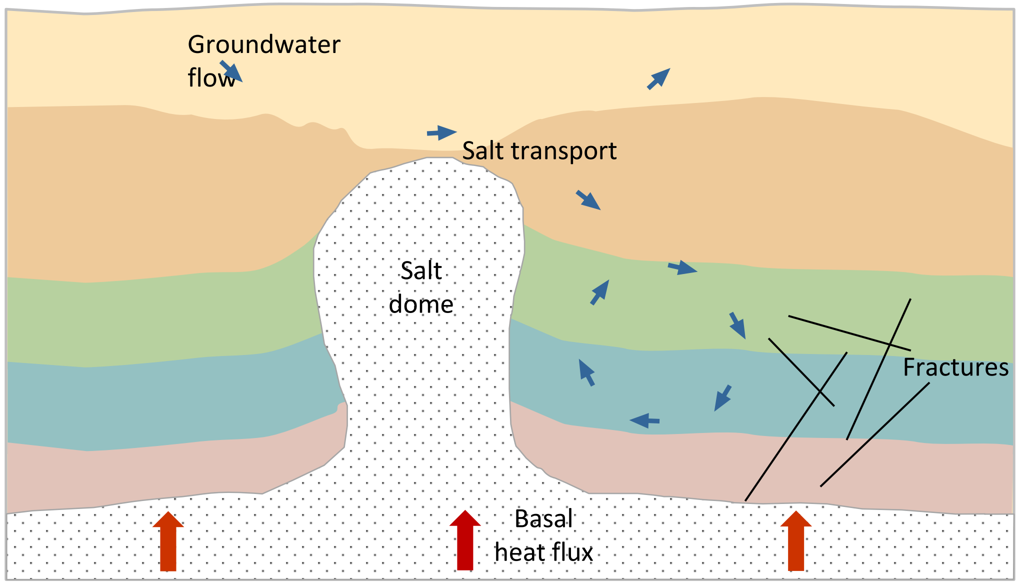
Effect of mixing on groundwater age and life expectancy simulations in density-dependent flow

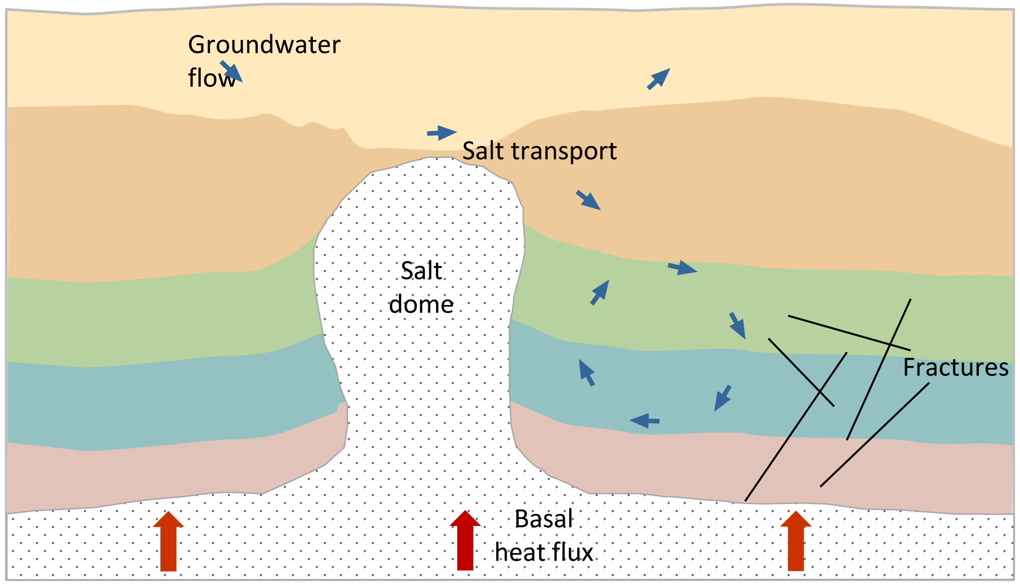


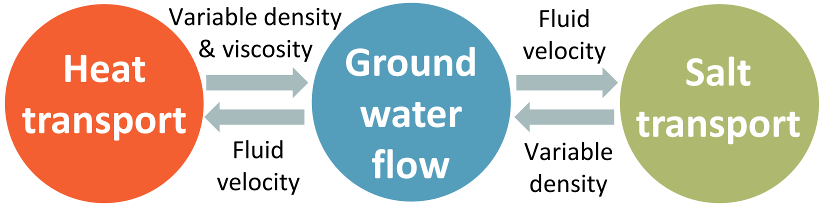
Jonas Suilmann

Motivation

- Salt dome as host rock

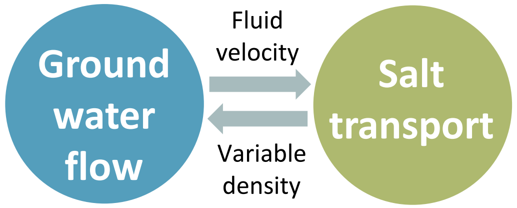
- Relevant methods and processes:
  - Density-dependent flow
  - Heat transport (variable viscosity flow)
  - Groundwater age - as exclusion criterium
  - Potential radionuclide migration
  - Life expectancy - as radionuclide travel time estimate (Cornaton et al. 2008)
  - Uncertain transport parameters

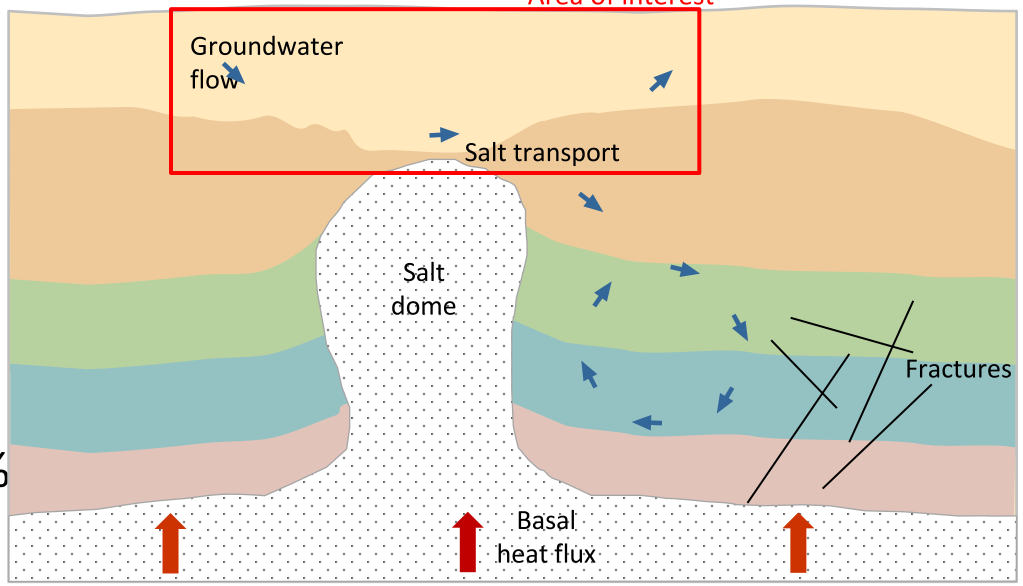


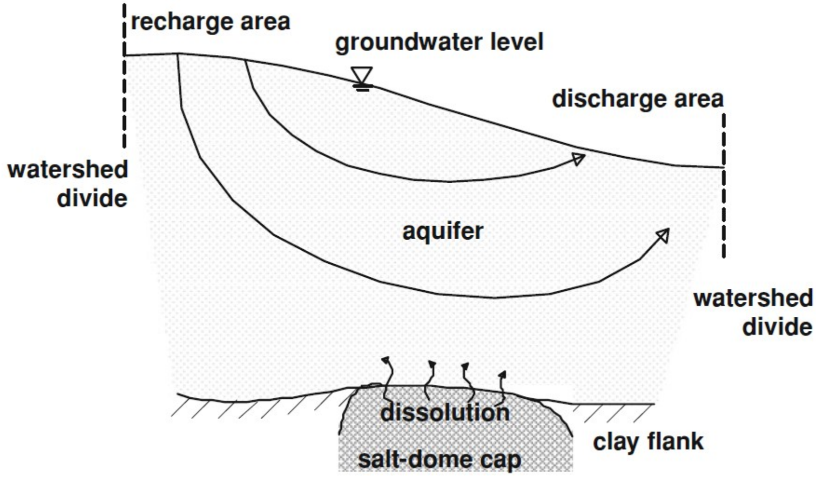


Salt dome Problem

- Simplified hydrogeological situation above saltdome
- **Density-dependent flow** benchmark for numerical codes
- Strongly coupled flow & transport (density variation of 20 %
- Intensively investigated in the 80‘s and 90‘s (Herbert et al. 1988, Oldenburg and Pruess 1995, Kolditz et al. 1998, etc.)
- Different diffusion coefficients and dispersivities used



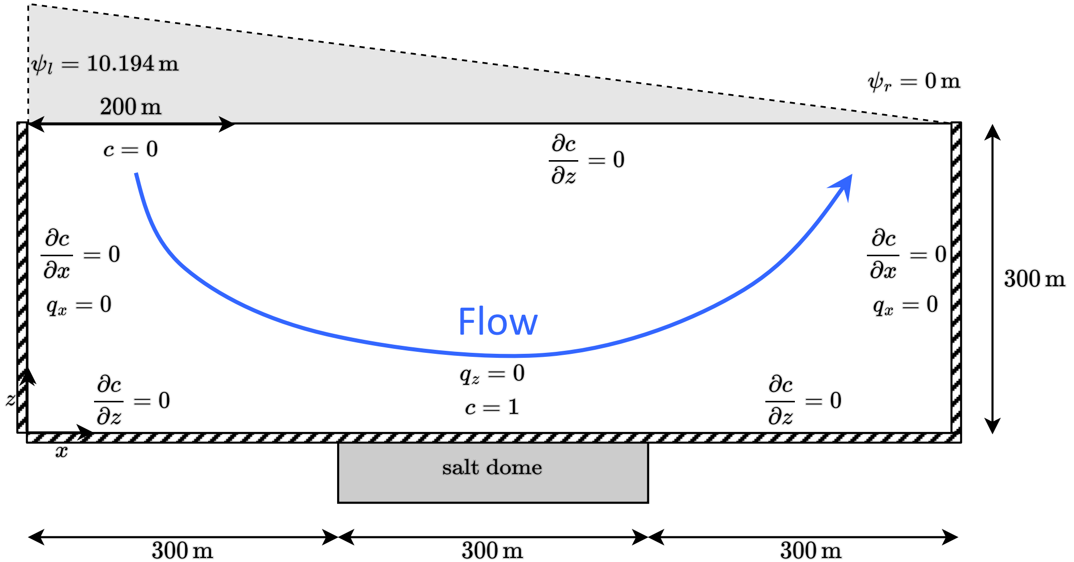




Holzbecher et al. 2010

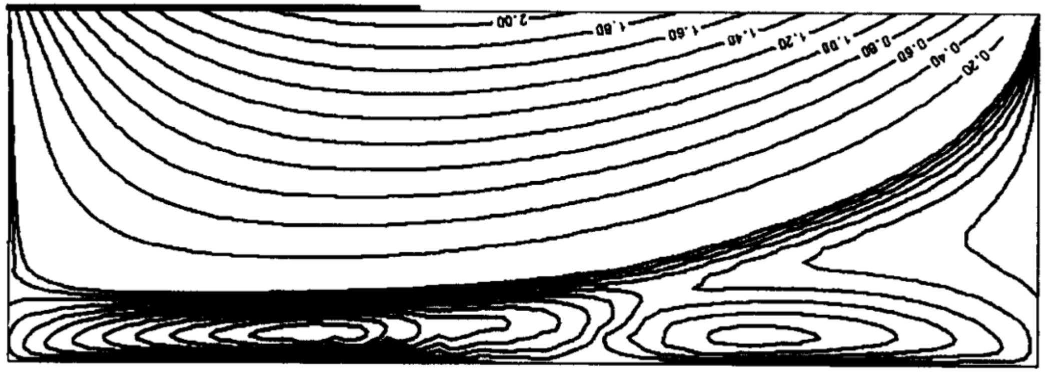
Salt dome Problem

Conceptual model:



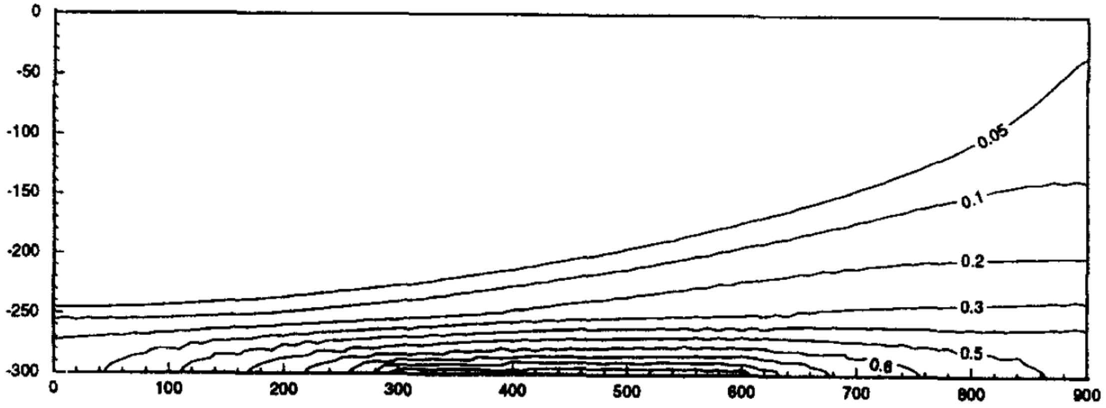
Adapted from Herbert et al. 1988 and Diersch 2013

Flow solution (steady state):



Kolditz et al. 1998

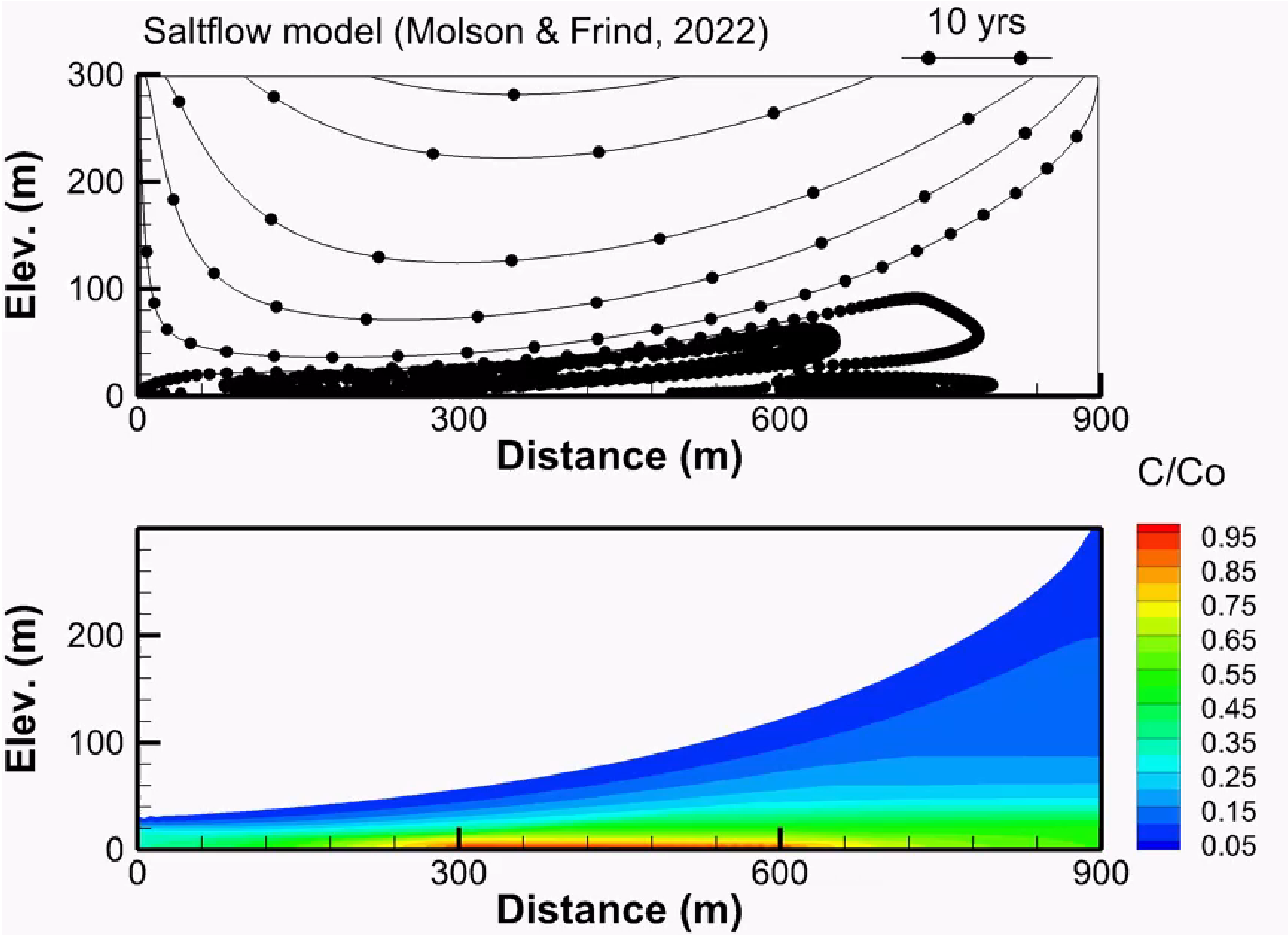
Transport solution (steady state):



Kolditz et al. 1998

Salt dome Problem

- Base case from literature:
  $\alpha_L = 20$ m, $\alpha_T = 2$ m, D = 1.39e-8 m²/s
- 150x75 elements
- Steady-state flow field:
- Steady-state salt concentration:



Governing Equations

Darcy equation: $$\mathbf{q}_i = -\mathbf{K}_{ij}\left[\frac{\partial \psi}{\partial x_j} + \rho_r \mathbf{n}_j\right]$$

Flow equation: $$\frac{\partial}{\partial x_i}\left[\mathbf{K}_{ij}\left(\frac{\partial \psi}{\partial x_j} + \gamma\, c\, \mathbf{n}_j\right)\right] = S_s \frac{\partial \psi}{\partial t}$$

Mass transport equation: $$\frac{\partial}{\partial x_i}\left(\mathbf{D}_{ij}\frac{\partial c}{\partial x_j}\right) - \mathbf{v}_i \frac{\partial c}{\partial x_i} = \frac{\partial c}{\partial t}$$

FEM code **Saltflow** (Molson and Frind 2023)

Density-Dependent Flow and Mass or Age Transport Model in Three Dimensions

Methods: Dispersion

- Hydrodynamic dispersion tensor $\mathbf{D}_{ij}$

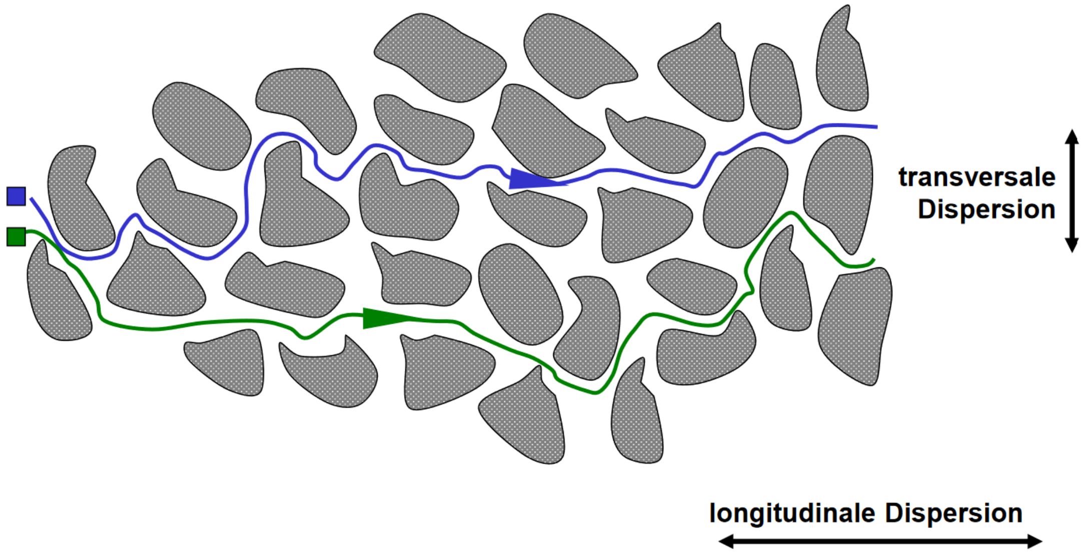
$$\mathbf{D}_{ij} = D_m \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{v}_i \mathbf{v}_i^T}{|\mathbf{v}|} + \alpha_T |\mathbf{v}| \mathbf{I}$$

$$\frac{\partial}{\partial x_i}\left(\mathbf{D}_{ij} \frac{\partial c}{\partial x_j}\right) - \mathbf{v}_i \frac{\partial c}{\partial x_i} = \frac{\partial c}{\partial t}$$

- Molecular Diffusion coefficient D_m

- Macroscopic dispersion
  - Mixing effect due to aquifer heterogeneity
  - Different flow paths
  - Dependent on flow velocity

  - Longitudinal dispersivity α_L in flow direction
  - Transverse dispersivity α_T perpendicular to flow



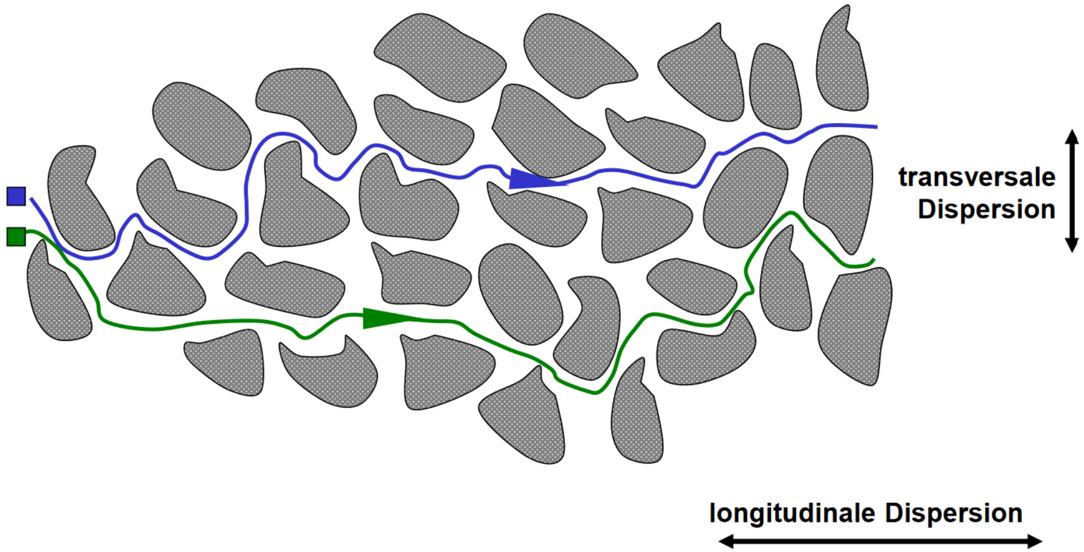
Graf 2022: Lecture on Groundwater modeling

Methods: Dispersion

- Macro dispersion increases with travel distance
- Despite many attempts: No universal scaling law (Zech et al. 2015)

- Dipersivities are largely site-specific
- $\alpha_L \approx 0.1 \ldots 0.01\ \alpha_{TH}$
- $\alpha_{TH} \approx 0.1\ \alpha_{TV}$ (Zech et al. 2019)

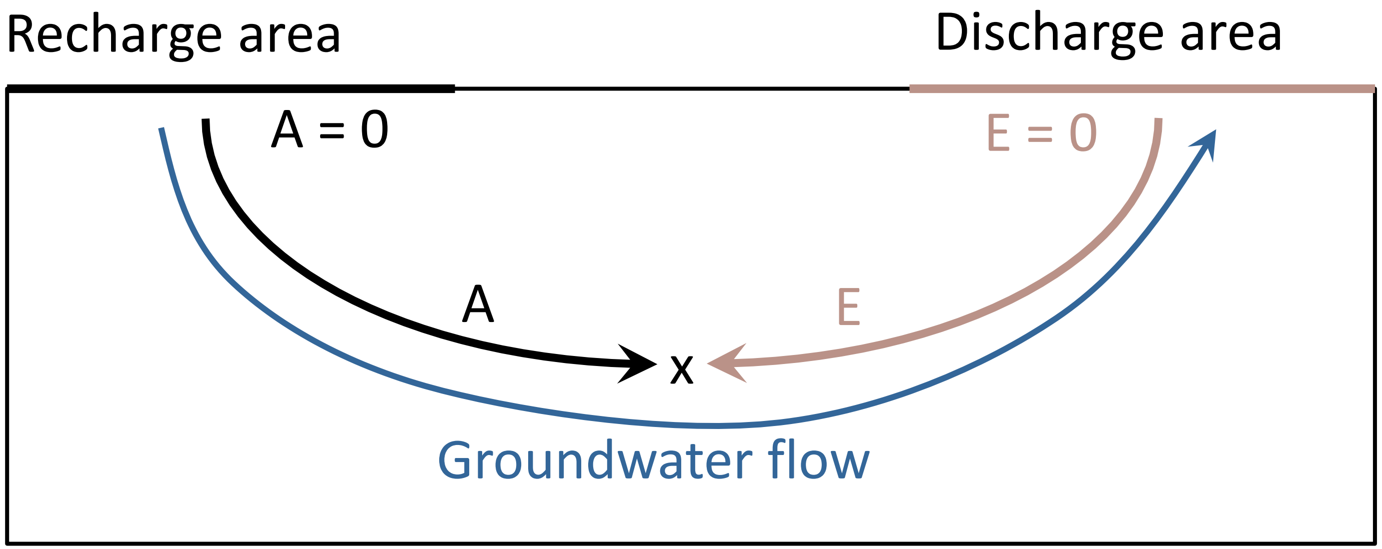
- BUT, fixed ratios are site-specific
- No general law
- Dispersivities are subject of high uncertainty



Graf 2022: Lecture on Groundwater modeling

Methods: Groundwater Life Expectancy

- Concept of groundwater age and life expectancy



T = A + E

T – residence time; A – groundwater age; E – life expectancy

Methods: Groundwater Life Expectancy

- Concept of groundwater age and life expectancy
- Can be simulated directly using a transport equation (Goode 1996)
- Groundwater age

$$\frac{\partial}{\partial x_i}\left(\mathbf{D}_{ij}\frac{\partial A}{\partial x_j}\right) - \mathbf{v}_i\frac{\partial A}{\partial x_i} + 1 = 0$$

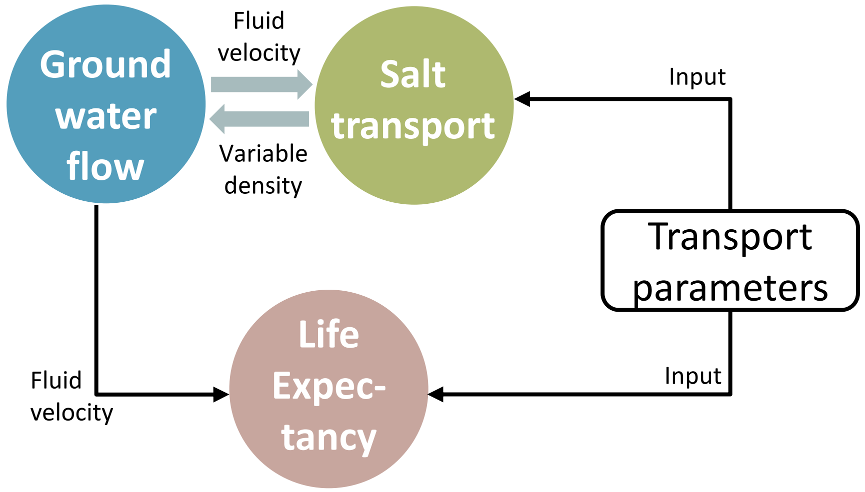
- Groundwater life expectancy

$$\frac{\partial}{\partial x_i}\left(\mathbf{D}_{ij}\frac{\partial E}{\partial x_j}\right) + \mathbf{v}_i\frac{\partial E}{\partial x_i} + 1 = 0$$

Workflow

1. Transient simulations of coupled flow and transport using uncertain transport parameters

2. Using steady-state flow velocities as input for groundwater age and life expectancy simulations using uncertain transport parameters



Research Objective

Principle study using the Salt dome problem as example for:

- Investigating effects of **uncertain transport parameters**
  - on **density-dependent flow** above salt dome (Salt dome problem)
  - on resulting **groundwater age** and **life expectancy** in density-dependent flow

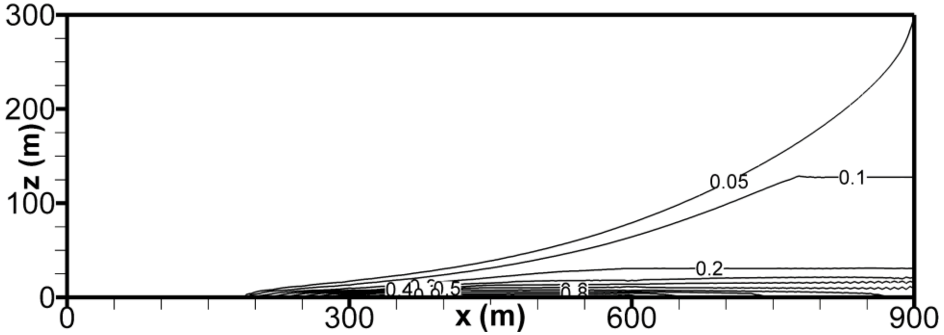
- Understand how mixing processes affect life expectancy in DDF in **the safety assessment of nuclear waste disposal**

Uncertain Transport Parameters

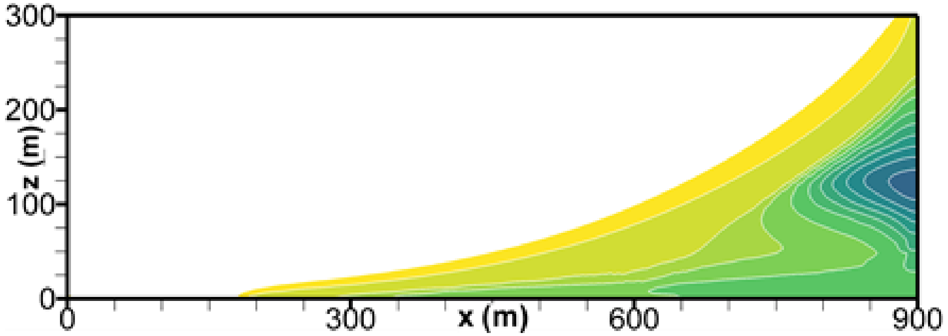
- Longitudinal Dispersivity α_L = [5, 10, 20] m
- Transverse Dispersivity α_T = [0.1 - 2] m
- Diffusion coefficient D_m = [5e-9, 1e-9, 5e-10] m^2/s
- Base case: α_L = 10 m, α_T = 0.4 m, D_m = 1e-9 m^2/s

Results - Base Case

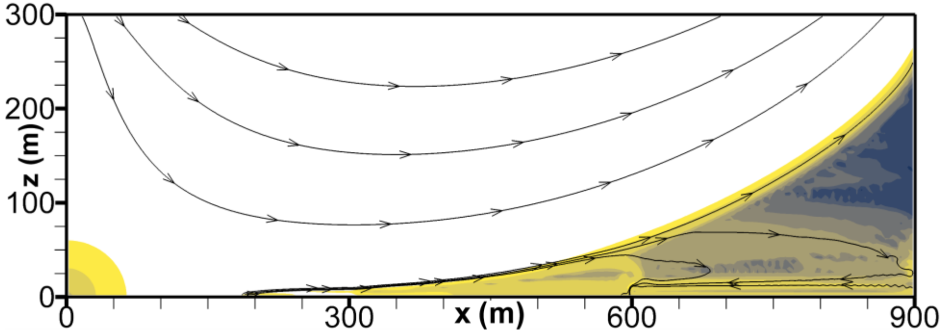
Salt concentration



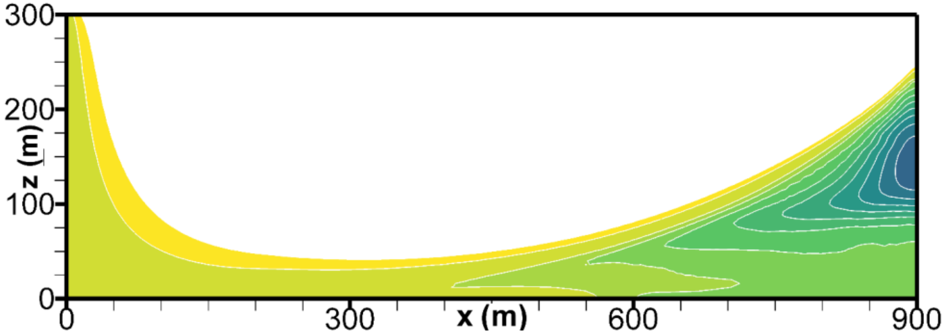
Groundwater age



Streamlines and flow velocity



Life expectancy



α_L = 20 m, α_T = 0.4 m, D_m = 1e-9 m²/s

Results

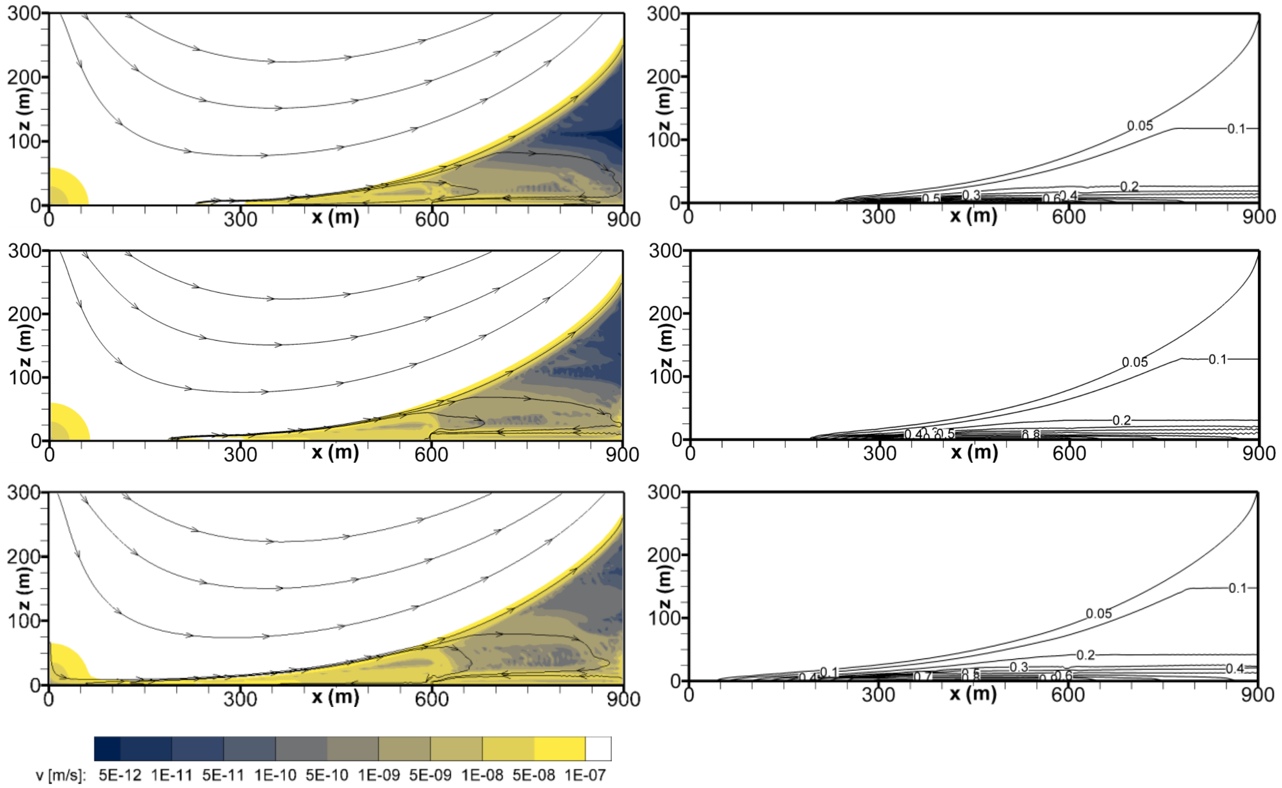
- Effect of longitudinal dispersivity on DDF

$D_m = 10^{-9}$ m² s^{-1}

α_L = 5 m
α_T = 0.4 m

α_L = 10 m
α_T = 0.4 m

α_L = 20 m
α_T = 0.4 m



Results

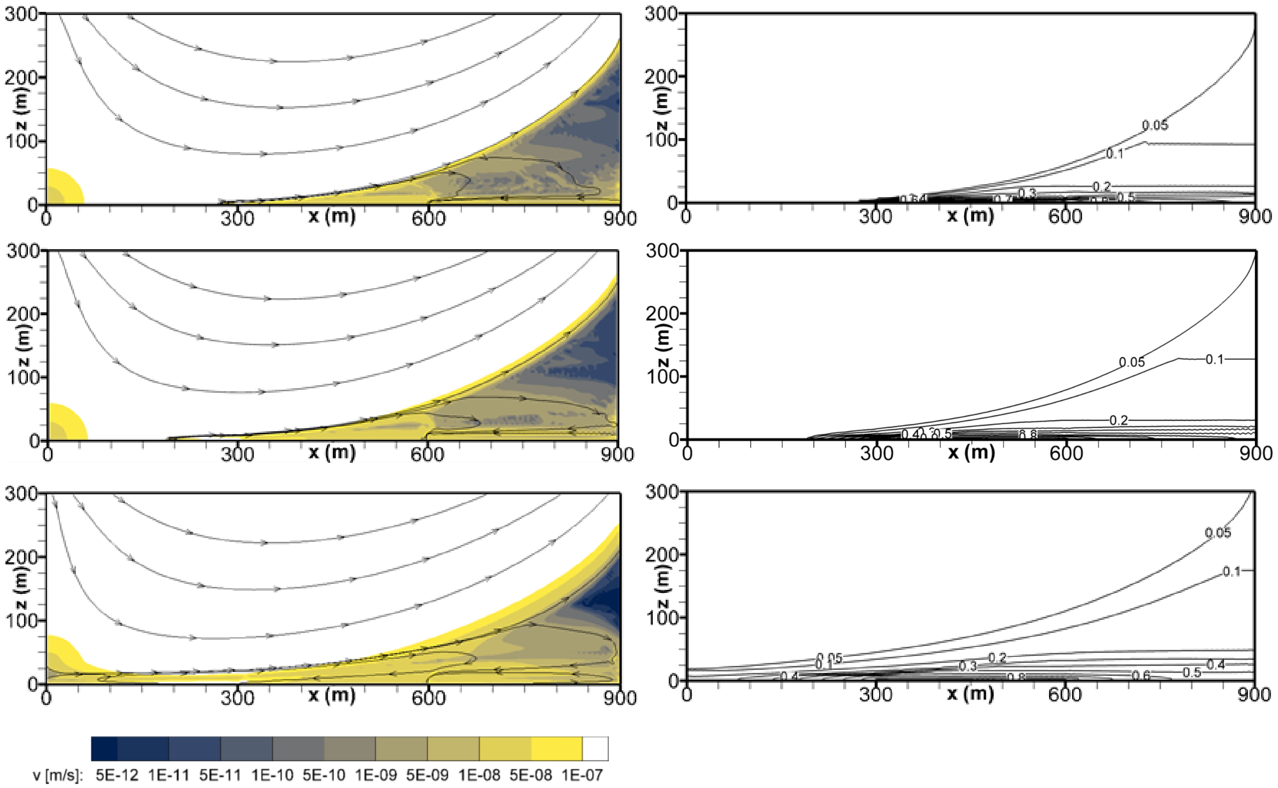
- Effect of transverse dispersivity on DDF

D_m = 10^{-9} m² s^{-1}

α_L = 10 m
α_T = 0.1 m

α_L = 10 m
α_T = 0.4 m

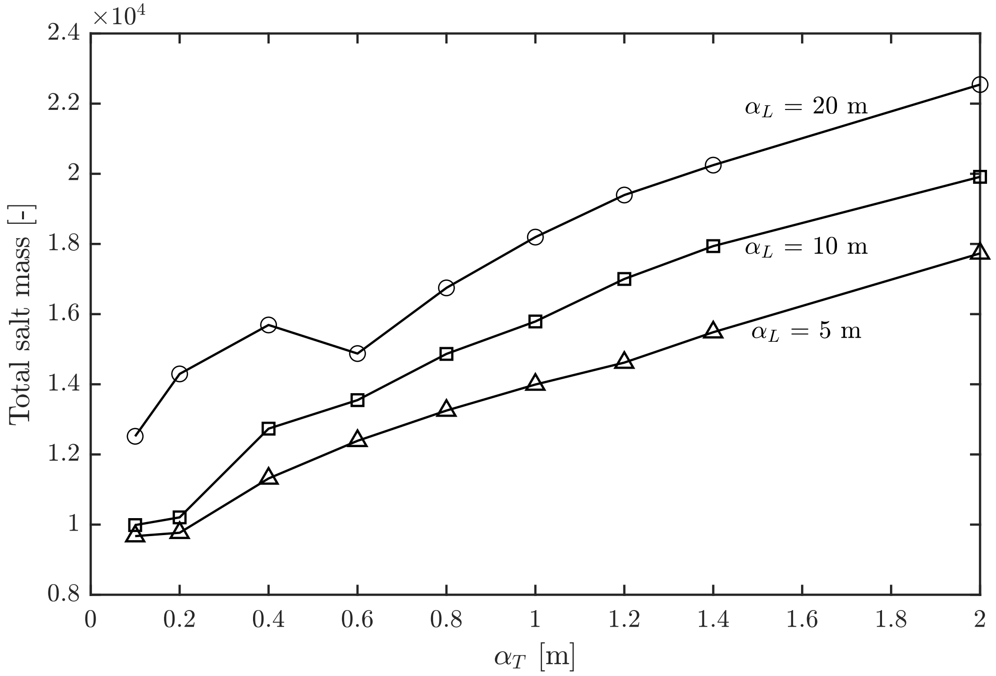
α_L = 10 m
α_T = 2 m



Results

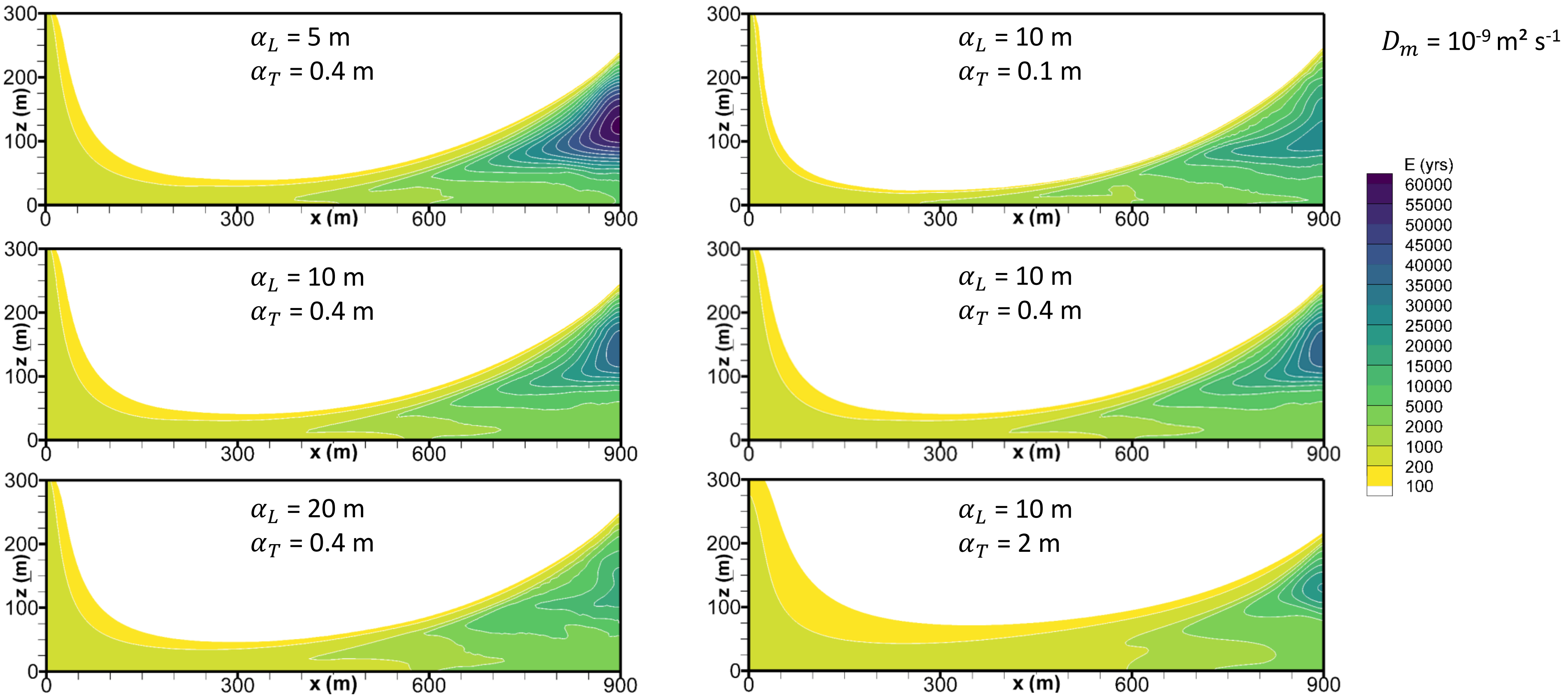
- Effect of longitudinal and transverse dispersivity on total steady-state salt mass

D_m = 10^{-9} m^2 s^{-1}



Results

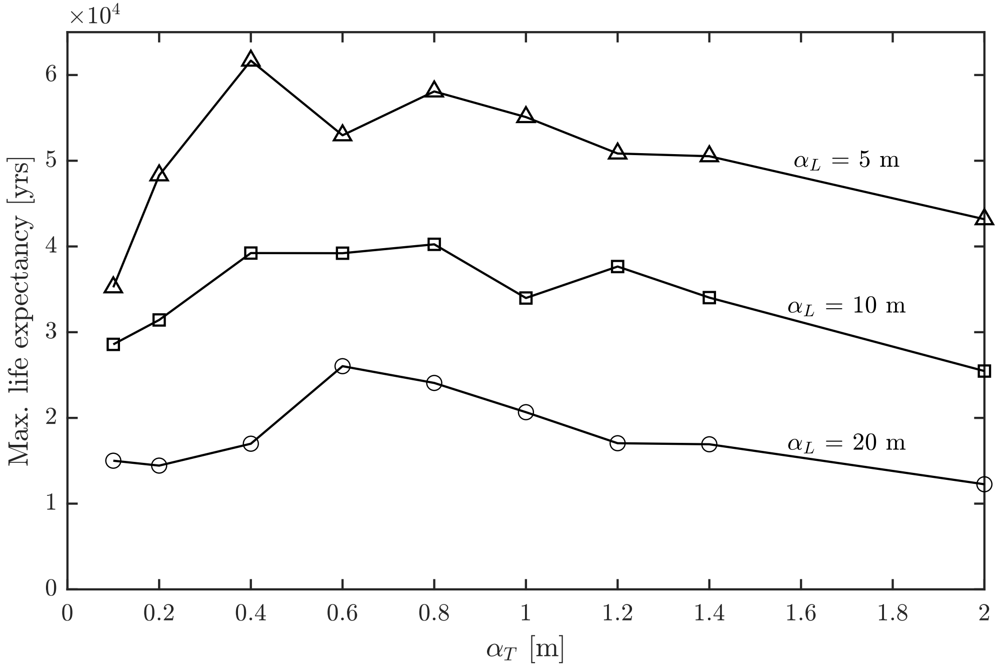
- Effect of longitudinal and transverse dispersivity on life expectancy



Results

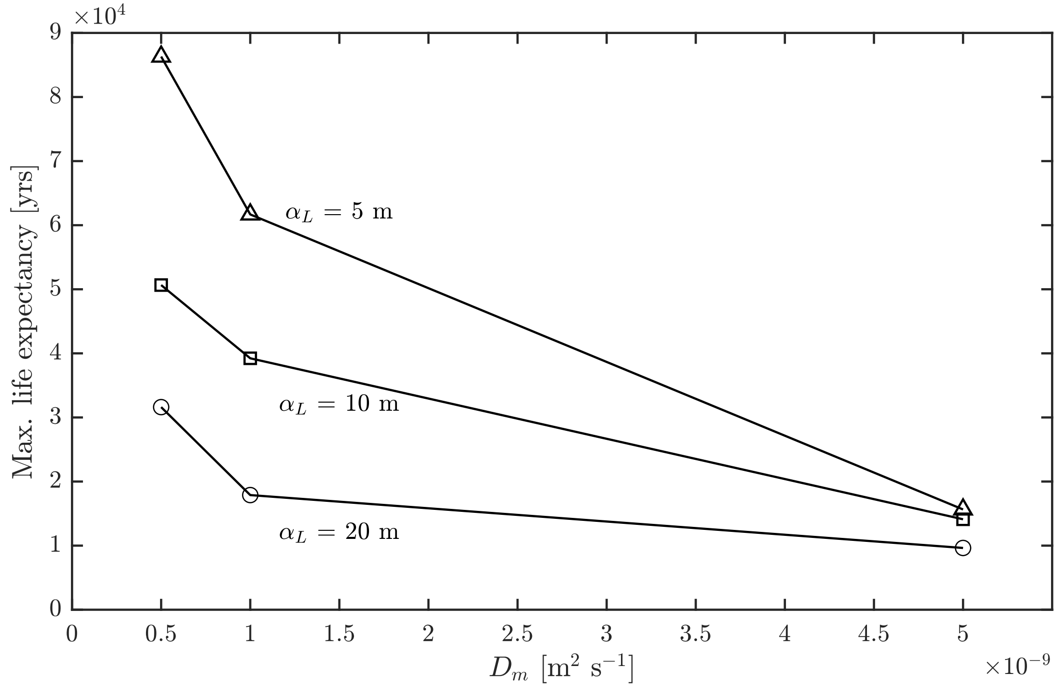
- Effect of longitudinal and transverse dispersivity on maximum life expectancy

D_m = 10^{-9} m^2 s^{-1}



Results

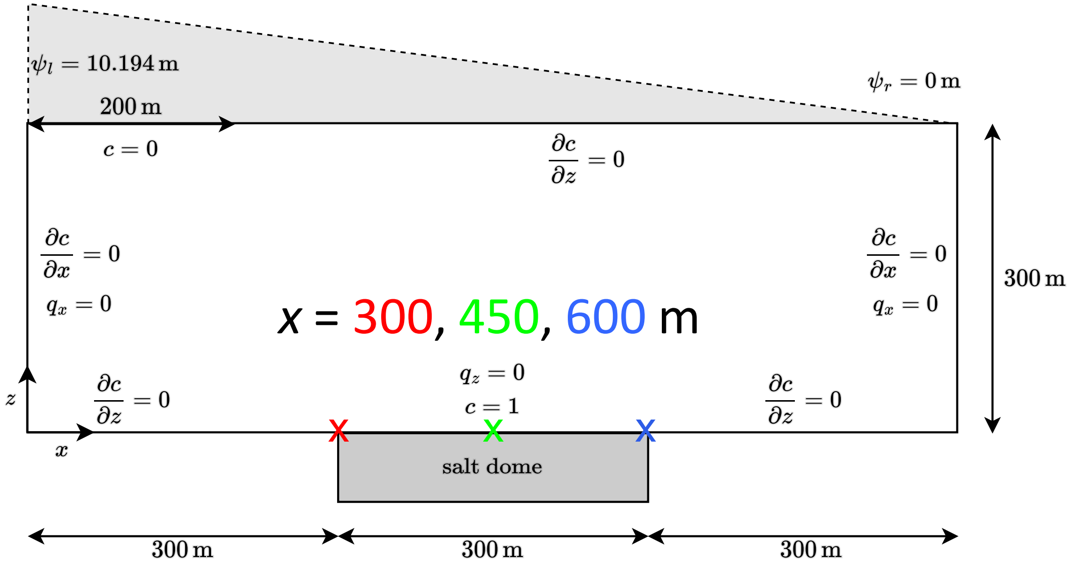
- Effect of diffusion on maximum life expectancy



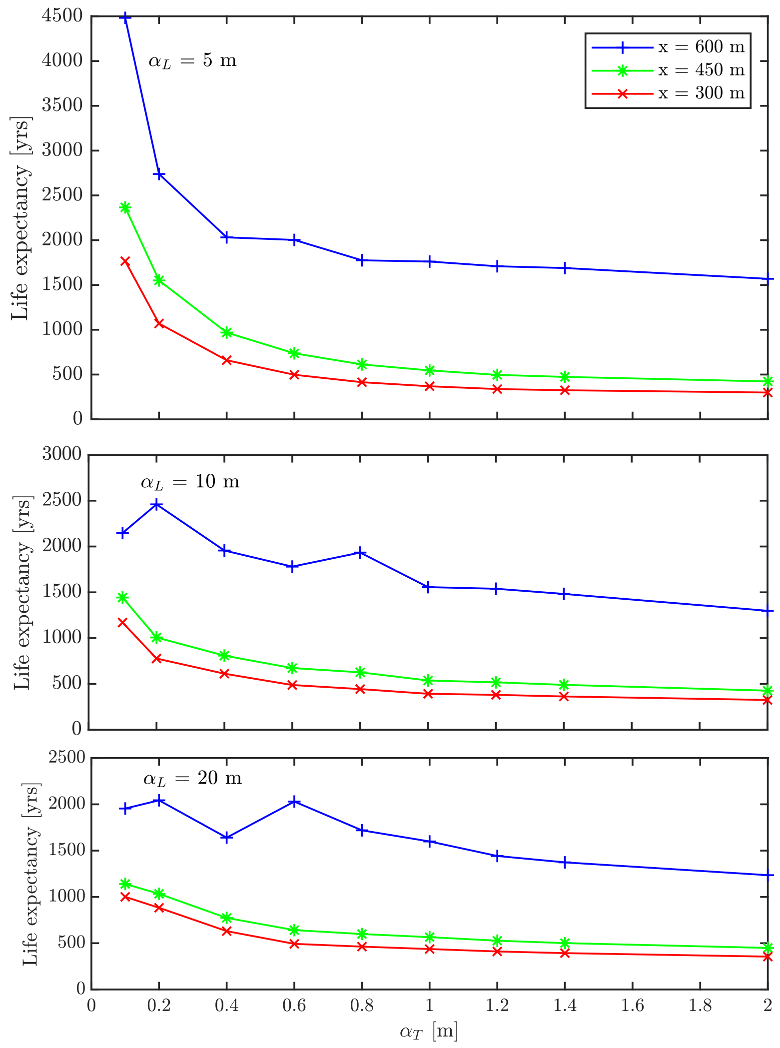
α_T = 0.4 m

Results

- Effect of diffusion on life expectancy along lower boundary



Adapted from Herbert et al. 1988 and Diersch 2013



$D_m = 10^{-9}\ \text{m}^2\ \text{s}^{-1}$

Summary & Conclusion

- DDF system in the salt dome problem is highly sensitive to uncertain dispersivities
- Maximum life expectancy is highly sensitive to the dispersivity-dependent DDF velocities
- Diffusion has a significant direct effect on maximum life expectancies
- Longitudinal and transverse dispersion highly affect life expectancies as used in the safety assessment of repositories

- Underestimating longitudinal and/or transverse dispersivity leads to overestimating life expectancy close to a salt dome and, thus, to **overestimating safety** of nuclear waste disposal sites.

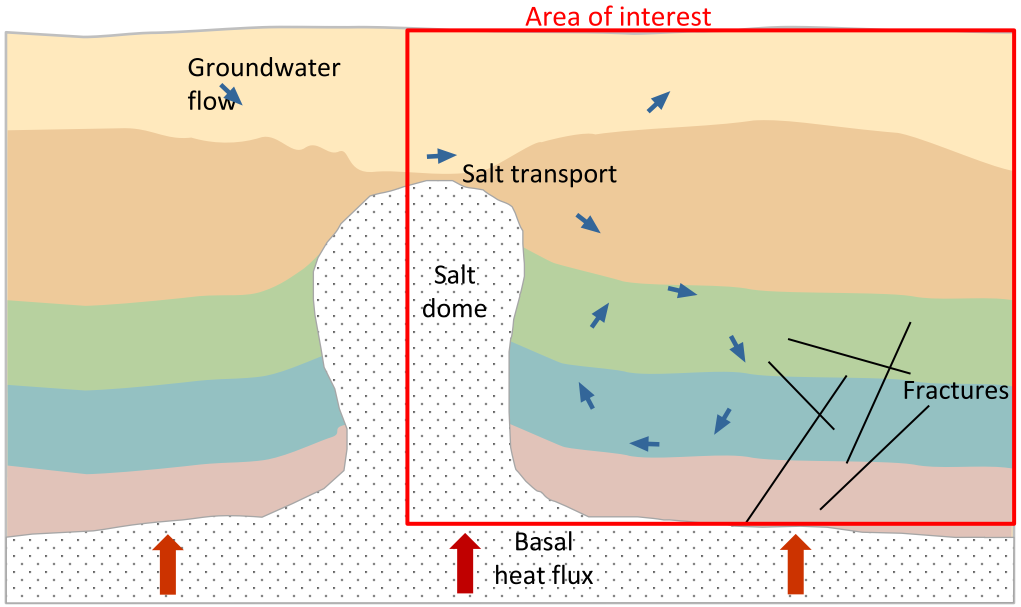
Importance of considering uncertain transport parameters in evaluating life expectancy in the safety assessment in nuclear waste disposal

Outlook

- Results will soon be submitted

Next step:

- Including heat transport
- Investigating **thermohaline flow in fractured-porous media** in a larger model domain of salt dome including adjacent strata
- Investigating **Salt chimney effect** (Canova et al. 2018)
  Convection due to higher thermal conductivity of salt



Thanks for your attention!

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