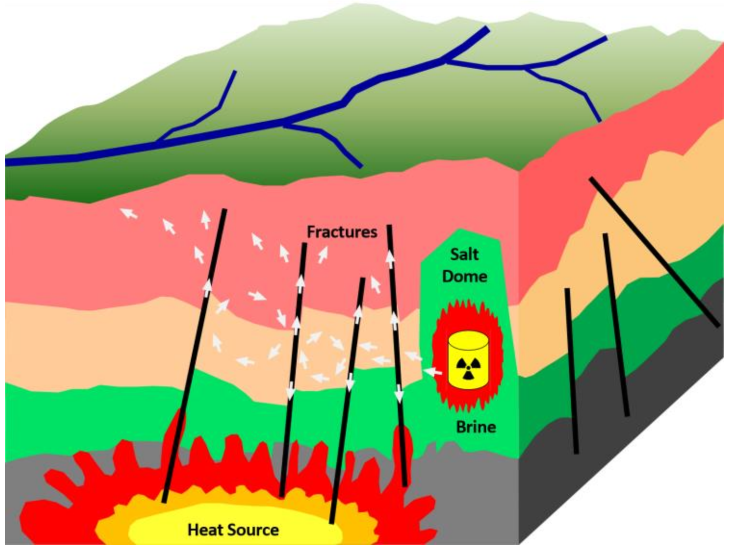
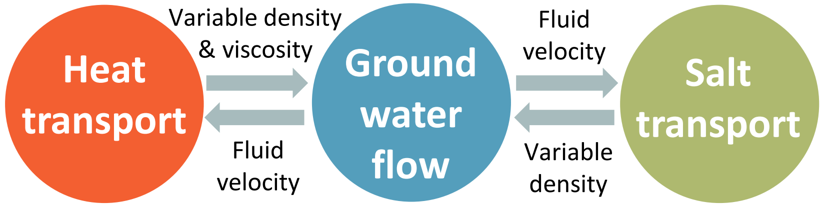
Sensitivity of Salt Concentration and Groundwater Age to Dispersivity in the Salt Dome Problem

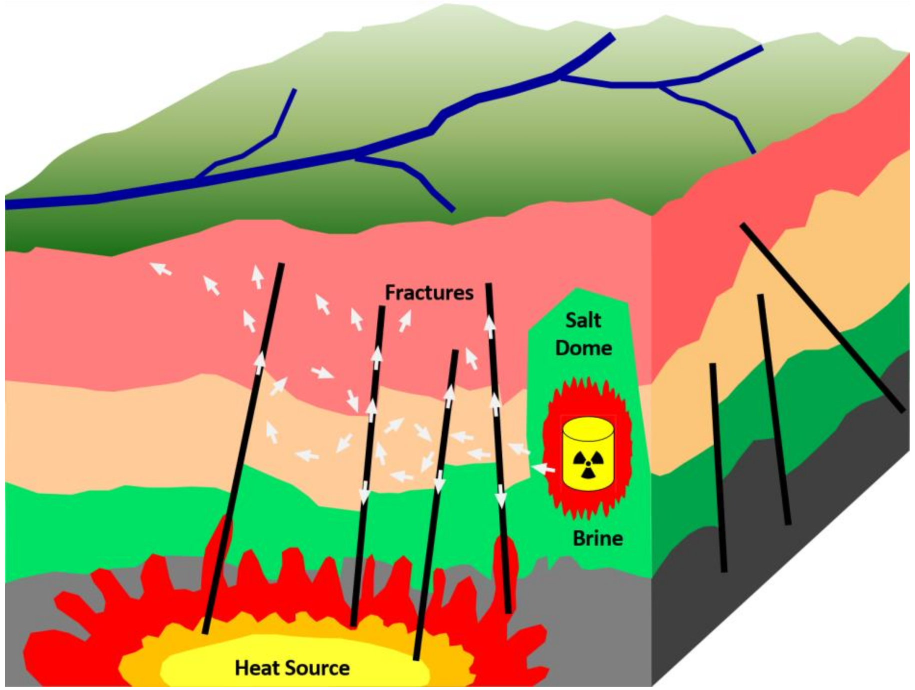


Jonas Suilmann, Andrea Perin

Motivation

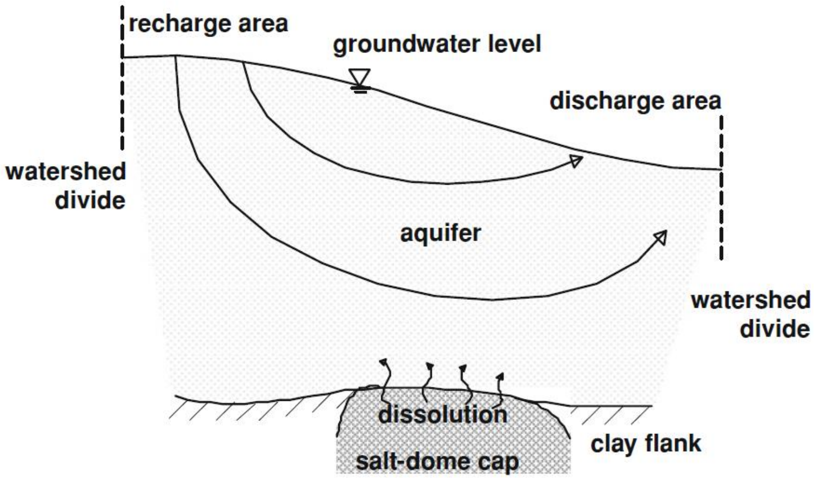
- Relevant processes in far field of salt dome:
  - Density-dependent flow
  - Heat transport (variable viscosity flow)
  - Potential radionuclide migration
  - Groundwater age (as exclusion criterium)



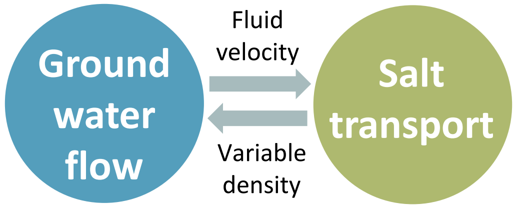


Salt dome problem

- Simplified hydrogeological situation above Gorleben saltdome
- **Density-dependent flow** benchmark problem for numerical codes
- Strong coupling of flow and 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

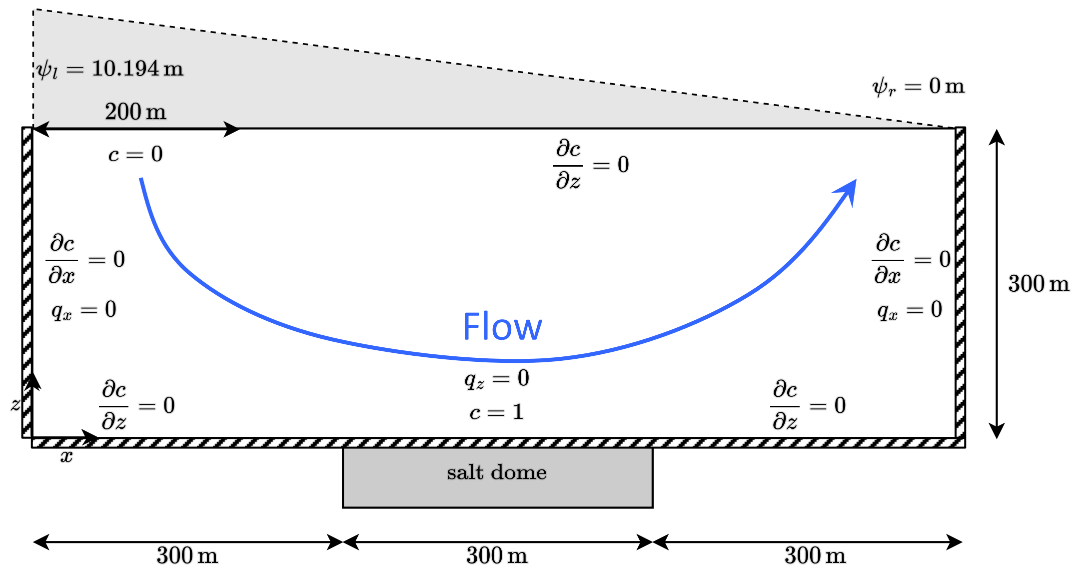


Holzbecher et al. 2010



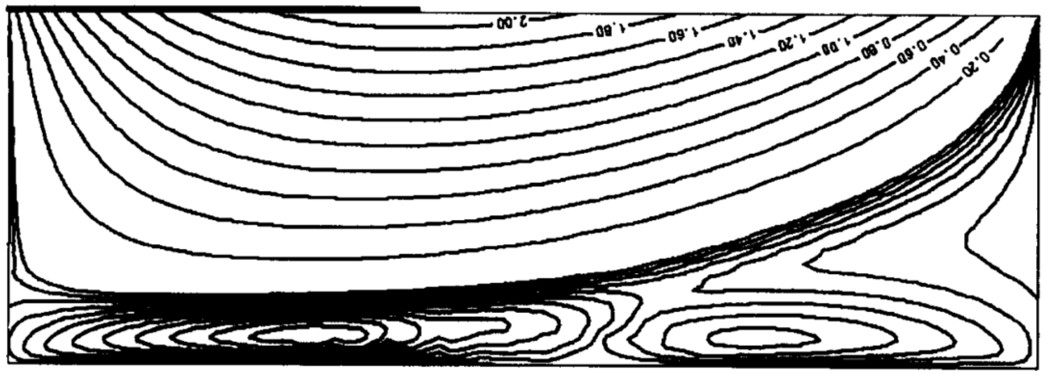
Salt dome Problem

Conceptual model:



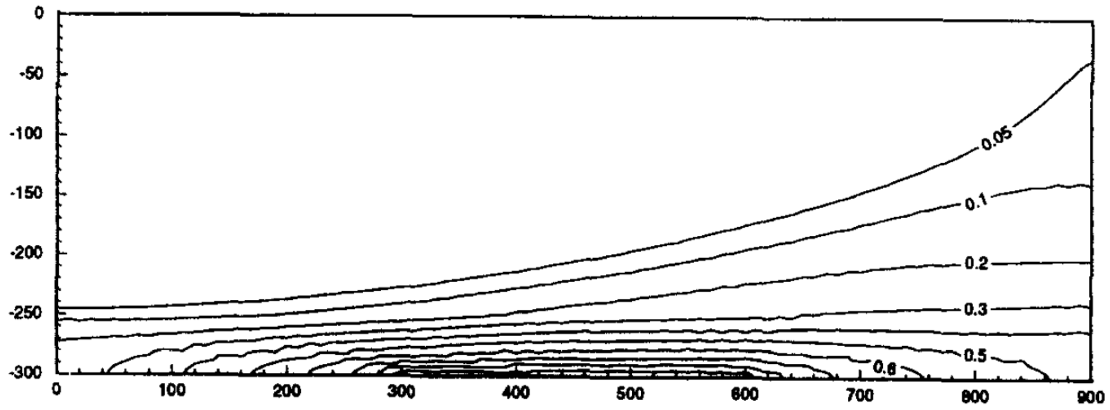
Adapted from Herbert et al. 1988 and Diersch 2013

Flow solution (steady state):



Kolditz et al. 1998

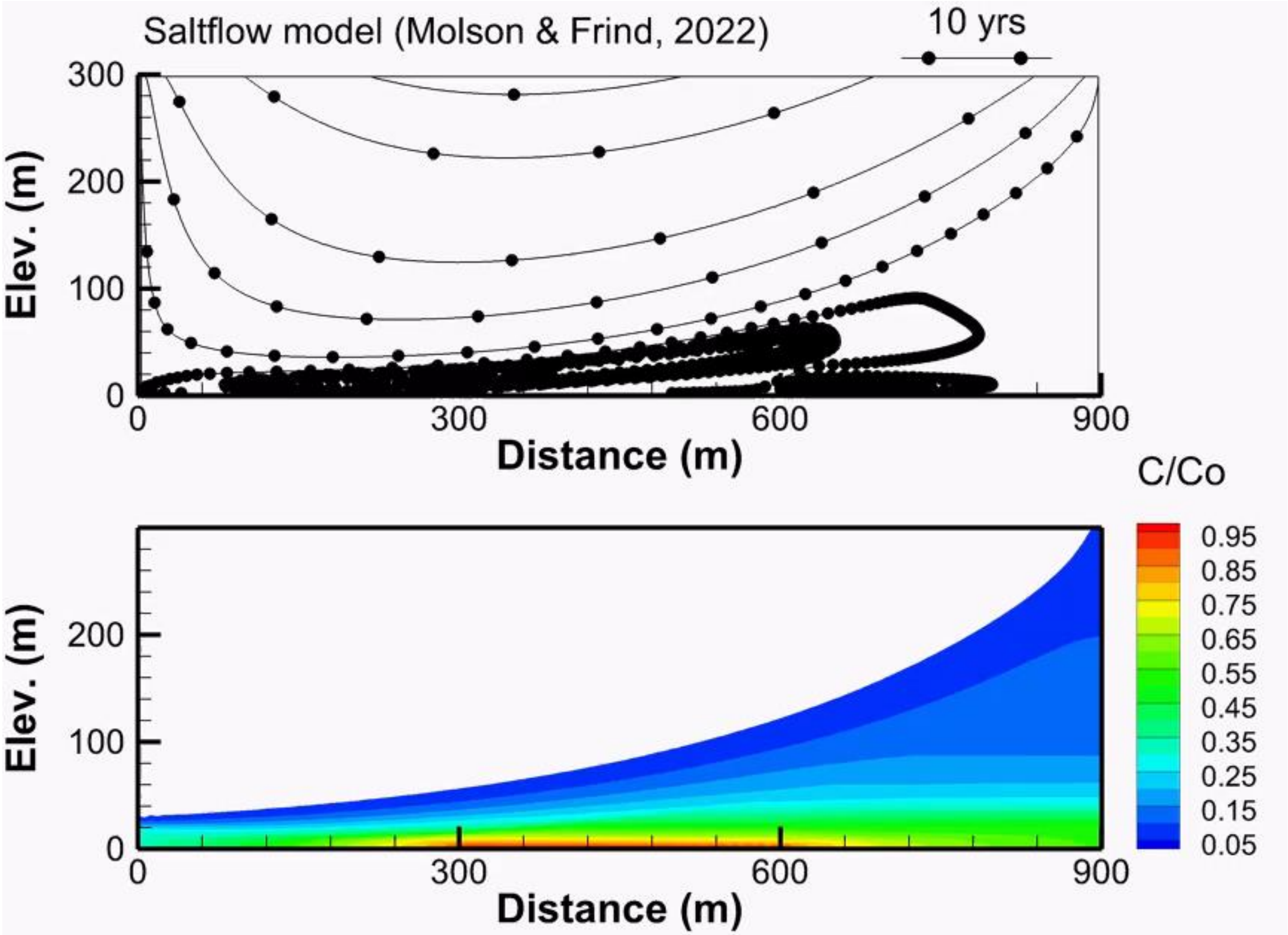
Transport solution (steady state):



Kolditz et al. 1998

Salt Dome Problem

- Base case from literature:
  α_L = 20 m, α_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:

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

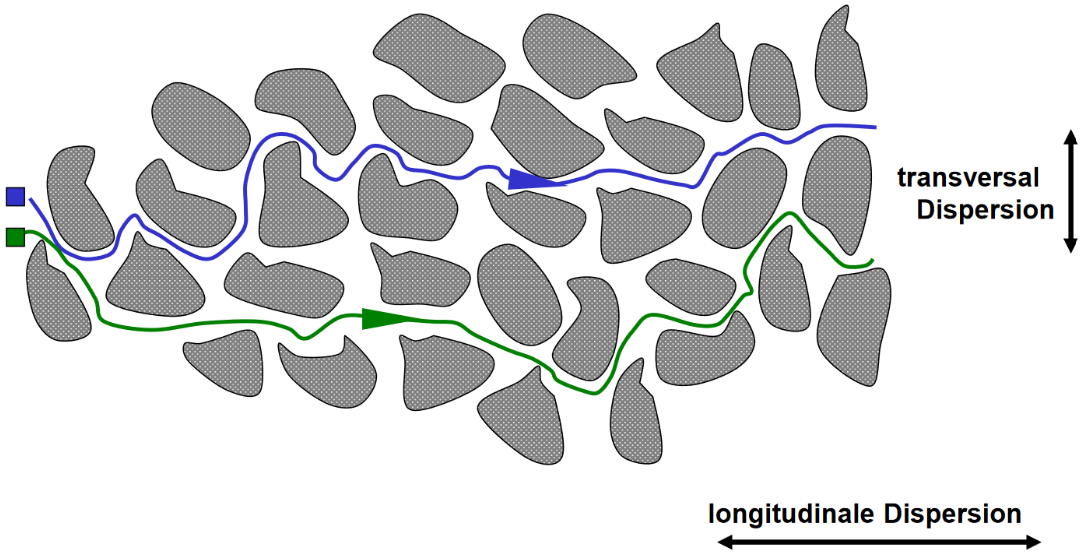
Saltflow code (Molson and Frind 2022)

Methods – Dispersion

- Molecular diffusion
- Dispersion (macroscopic):
  - Mixing effect due to aquifer heterogeneity
  - Different flow paths
  - Dependent on flow velocity

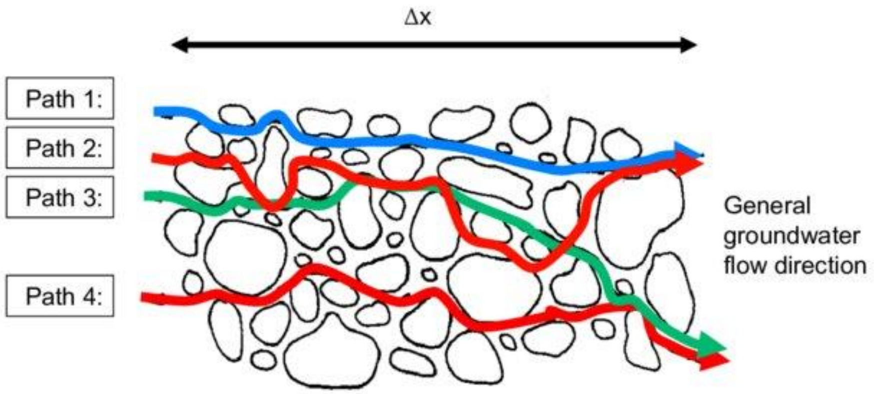
  - Longitudinal dispersivity in flow direction
  - Transverse dispersivity perpendicular to flow

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



Graf 2022: Lecture on Groundwater modeling

Methods – Dispersion formulation

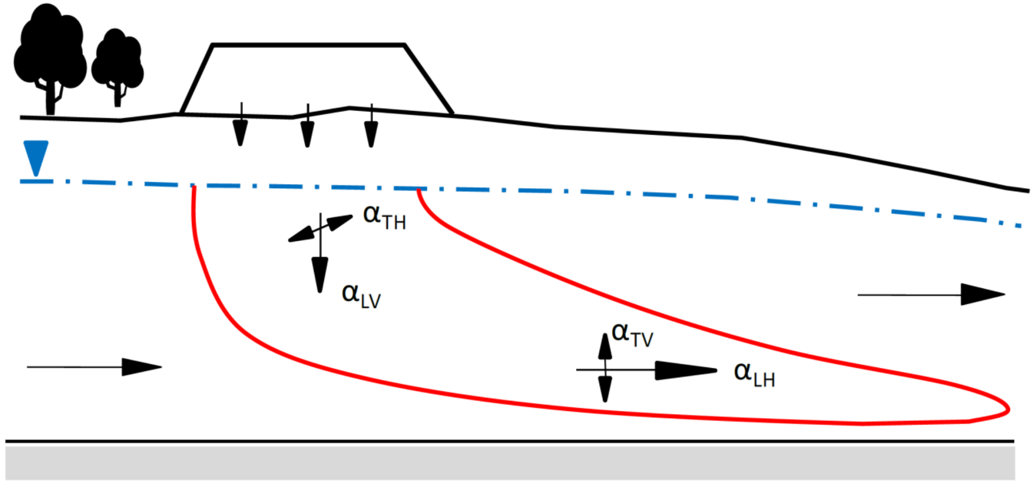


Torgersen et al. 2013

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

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

- BUT, fixed ratios are site-specific
- Chose independently
- Dispersivities are subject of large uncertainty



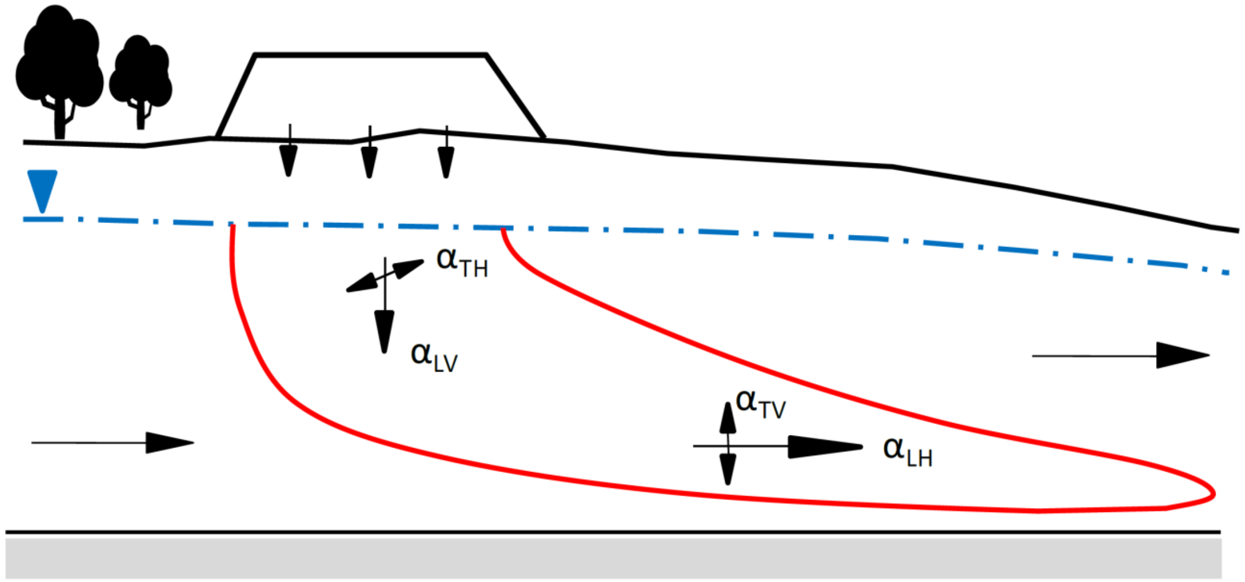
Molson and Frind 2022

Methods – Dispersion formulation

- Lichtner et al. 2002 dispersion formulation

- General approach
  - 2 dispersivities in 2D
  - Longitudinal (flow direction)
  - Vertical (perpendicular to flow)

- 4 dispersivities Lichtner formulation
- Flow direction dependent



Molson and Frind 2022

Research objective

- **Global Sensitivity analysis** on direction-dependent dispersivities
  - Conducted for other DDF problems (Younes et al. 2020, Fahs et al. 2022)

- Global Sensitvity Analysis on:
  - Classic DDF salt dome problem (salt concentration)
  - Groundwater age distribution
  - Groundwater life expectancy (LE)
  - Total residence time of Groundwater

Uncertain dispersivity range

	Min	max
α_{LH}	5 m	40 m
α_{LV}	2.5 m	20 m
α_{TH}	0.5 m	4 m
α_{TV}	0.05 m	0.4 m

Understand the effect of uncertain dispersivities on DDF salt dome problem, resulting groundwater age and life expectancy using Global Sensitvity Analysis

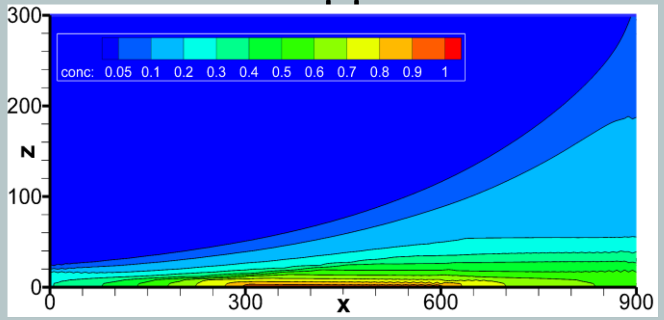
Methods – Groundwater age simulation

Groundwater age simulation with transport equation:

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

Simulation workflow:

Coupled flow & transport solution of salt dome



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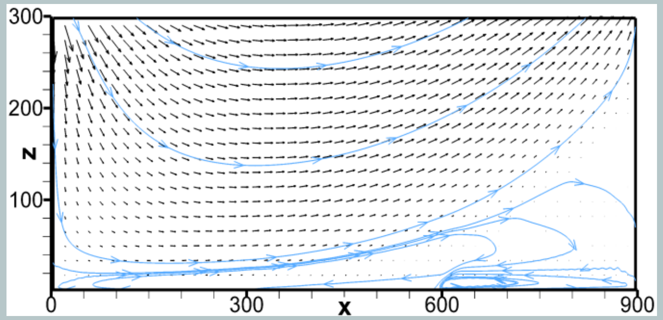
Steady-state flow velocities



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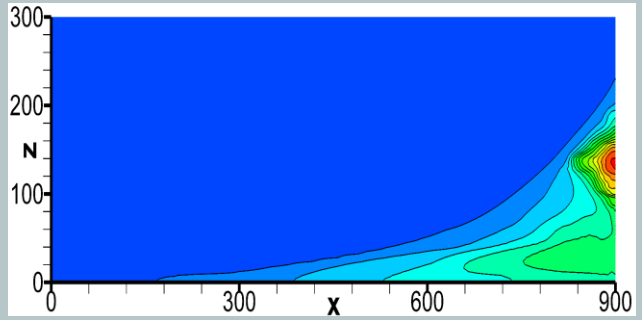
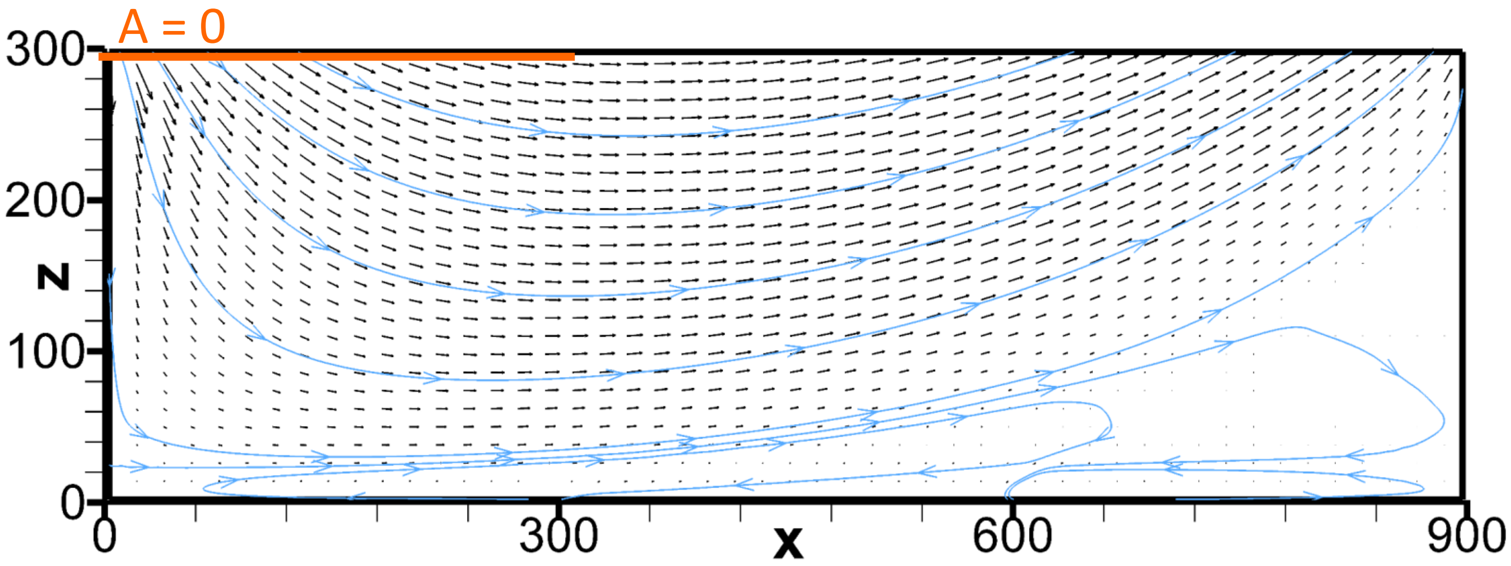
GW-age simulation

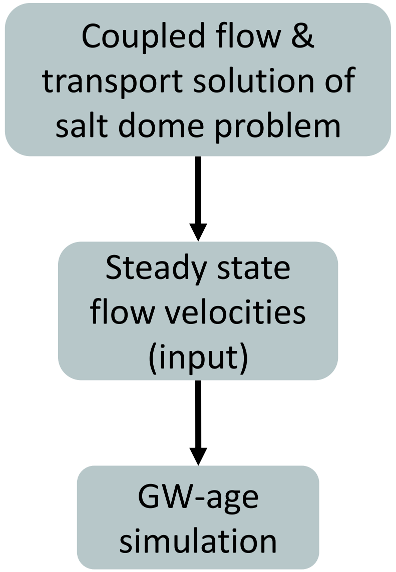


Methods – Groundwater age simulation

- Groundwater age distribution for 150x75 elements
- ($D = 1.39e\text{-}8\ m^2/s$; $\alpha_L = 20\ m$; $\alpha_T = 2\ m$)

- Steady-state flow velocities as input:
- BC at inflow region: A = 0

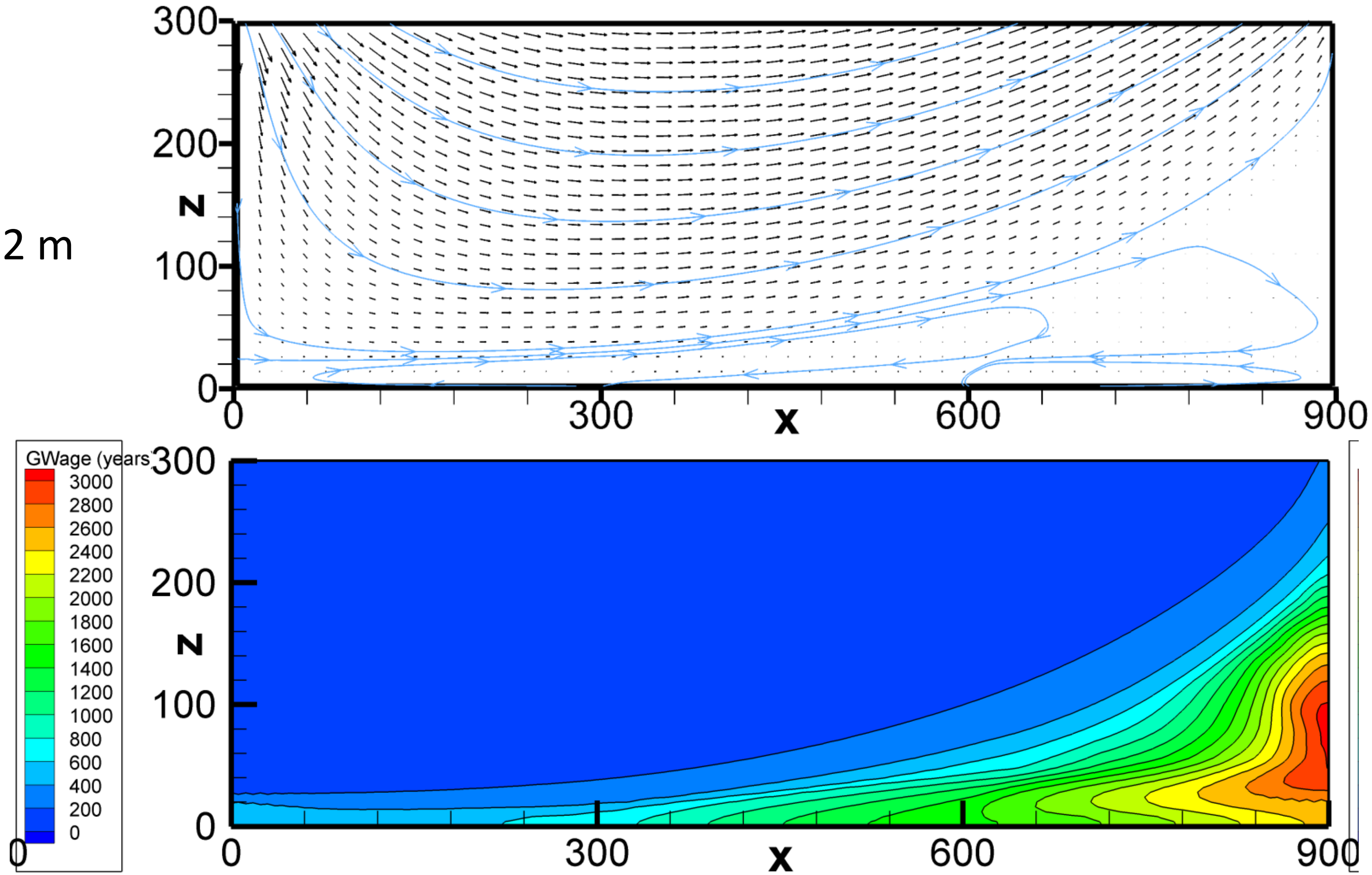




Methods – Groundwater age simulation

- Groundwater age distribution:

- 150x75 elements
- D = 1.39e8 m²/s; α_L = 20 m; α_T = 2 m



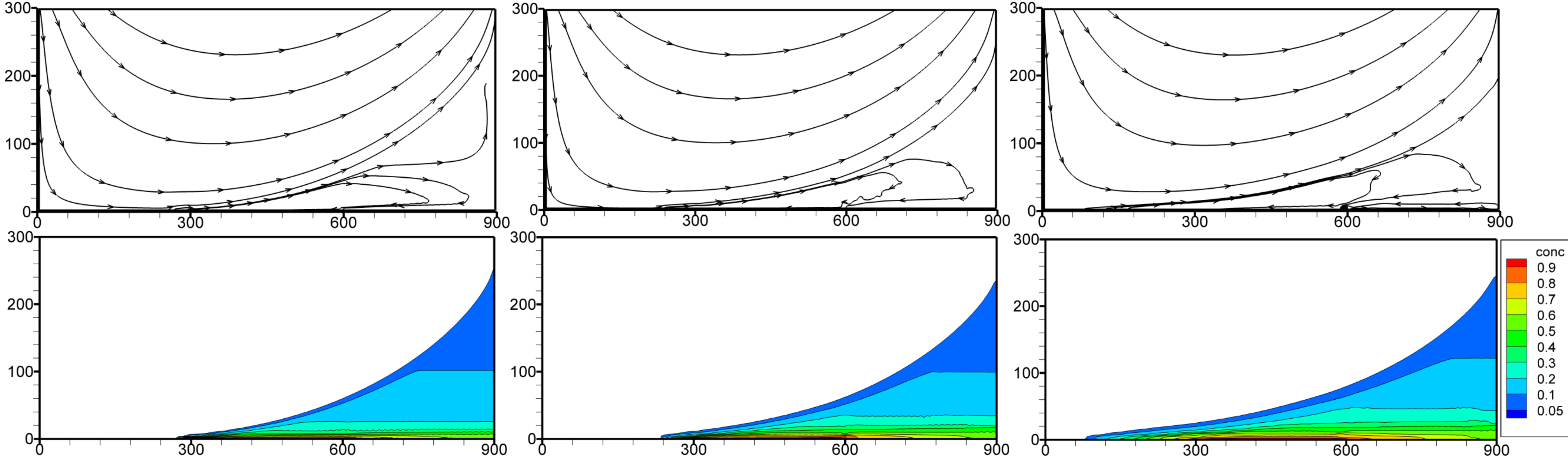
Global Sensitivity analysis on dispersivities – Initial screening

- Steady state salt concentration & flow

Lowest dispersivity combination
α_{LH} = 5 m, α_{LV} = 2.5 m, α_{TH} = 0.5 m, α_{TV} = 0.05 m

„Base case“ dispersivity combination

Lowest dispersivity combination
α_{LH} = 40 m, α_{LV} = 20 m, α_{TH} = 4 m, α_{TV} = 0.4 m



Global Sensitivity analysis on dispersivities – Initial screening

- Groundwater age

Lowest dispersivity combination

α_{LH} = 5 m, α_{LV} = 2.5 m, α_{TH} = 0.5 m, α_{TV} = 0.05 m

Max GW age: 35,306 yrs

„Base case“ dispersivity combination

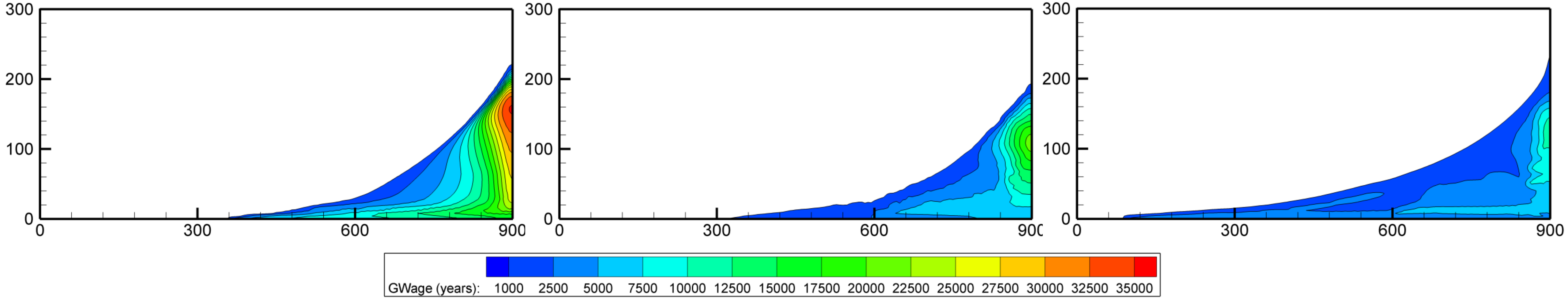
α_{LH} = 20 m, α_{LV} = 10 m, α_{TH} = 2 m, α_{TV} = 0.2 m

Max GW age: 21,028 yrs

Lowest dispersivity combination

α_{LH} = 40 m, α_{LV} = 20 m, α_{TH} = 4 m, α_{TV} = 0.4 m

Max GW age: 11,765 yrs



Research visit – Université Laval, Québec, Canada

- John Molson – developer of software (Saltflow)
- Professor in Hydrogeology

Achievements of intensified cooperation:

- Further benchmarking of code for high density variations (& temperature)
- Reduction of simulation run time
- Reduction of numerical errors (oscillations for small dispersivites)
- Use of 4-component dispersivity formulation (Lichtner et al. 2002)

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Summary & Outlook - Global Sensitivity analysis

- Sensitivity analysis on DDF salt dome problem and resulting Groundwater age
- Understand effects of dispersivities
- Improving general process knowledge

- Conduct simulations for 4 uncertain dispersivity parameters
  - Data collection is work in progress
  - Sobol‘ sequence sampling in parameters space

- Enough data to construct PCE surrogate?
- Calculate Sobol‘ indices and marginal effects from PCE

Thanks for your attention!

Literature

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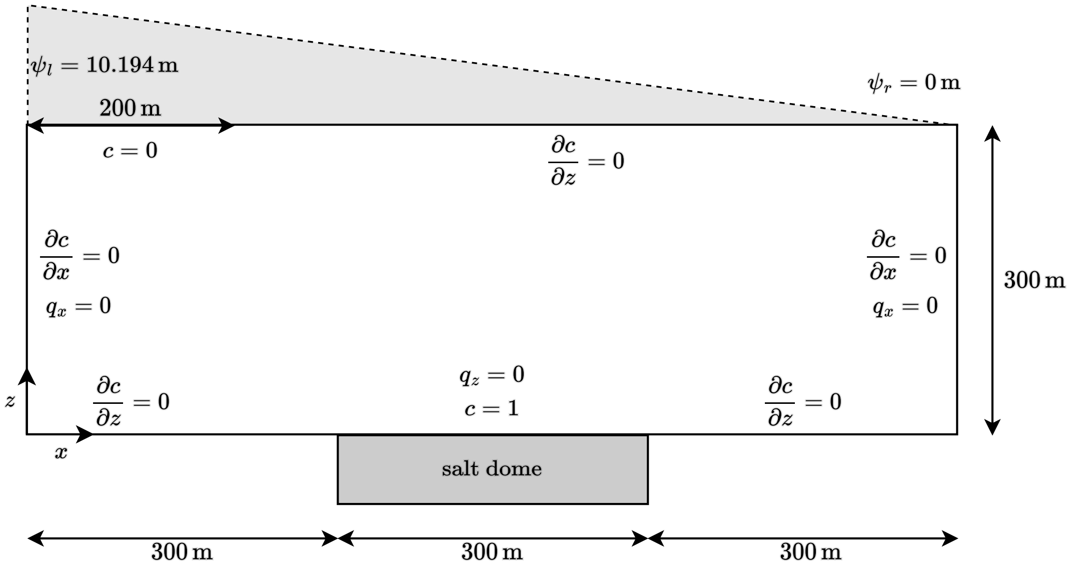
Salt dome problem parameters

Symbol	Parameter	Value	unit
ϕ	porosity	0.2	-
k	permeability	10^{-12}	m^2
μ	dynamic fluid viscosity	10^{-3}	Pa s
ρ_0	freshwater density	1000	kg m^{-3}
ρ_{max}	maximum fluid density	1200	kg m^{-3}
γ	relative density coefficient	0.2	-
g	gravitational acceleration	9.81	m s^{-2}
α_L	longitudinal dispersivity	20	m
α_T	transversal dispersivity	2	m
D_m	molecular diffusion coefficient	$1.39 \cdot 10^{-8}$	m^2 s^{-1}
S_s	specific storage	0	m^{-1}



Hydr. conductivity:

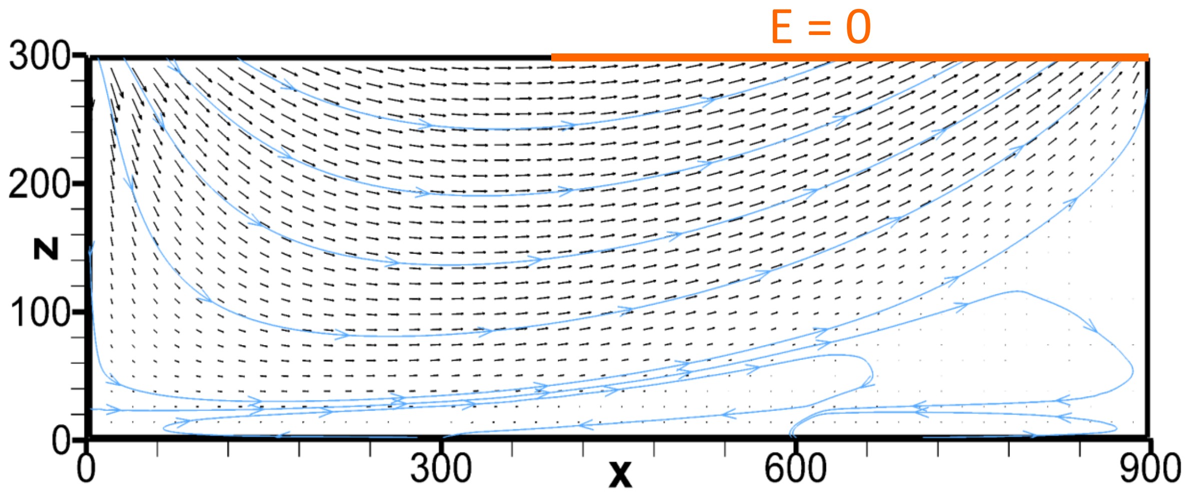
$$K_{ij} = 10^{-12}\,m^2 \cdot \frac{1000\,kg\ m^{-3} \cdot 9.81\,m\ s^{-2}}{10^{-3}\,Pa\ s} = 9.81 \cdot 10^{-6}\,m\ s^{-1}$$

Methods – Groundwater life expectancy simulation

Groundwater life expectancy simulation with transport equation:

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

- Negative velocities as input
- BC: E = 0 for outflow boundary

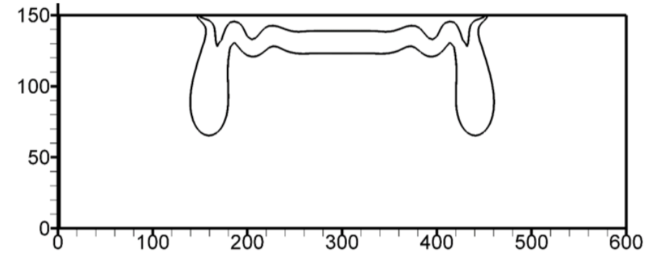


Numerical Software - Benchmarking

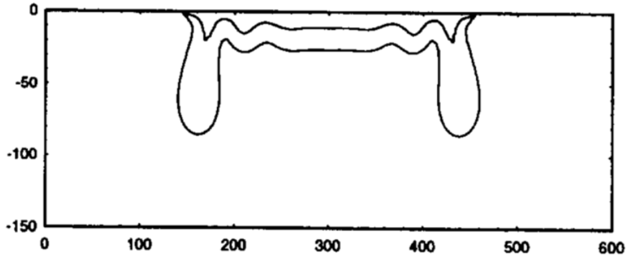
- Solutal Elder Problem (Strongly coupled DDF)

t = 2a

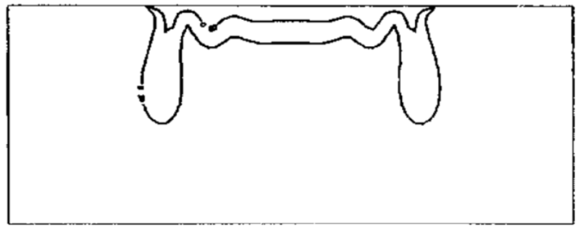
Saltflow



Rockflow (Kolditz et al., 1998)

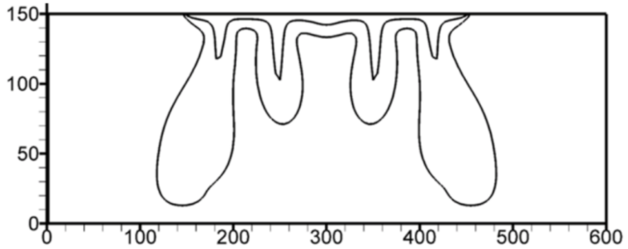


Feflow (Kolditz et al., 1998) 4400 elements used here only

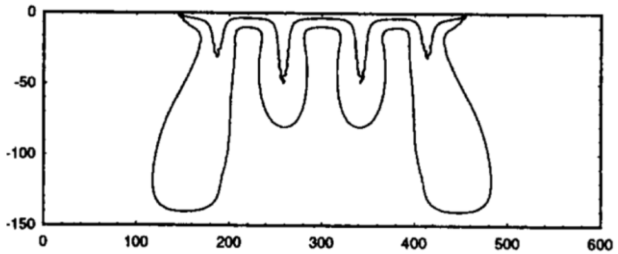


t = 4 a

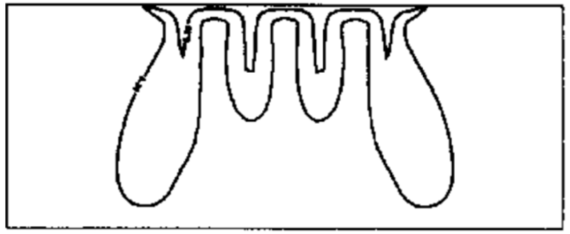
Saltflow



Rockflow (Kolditz et al., 1998)

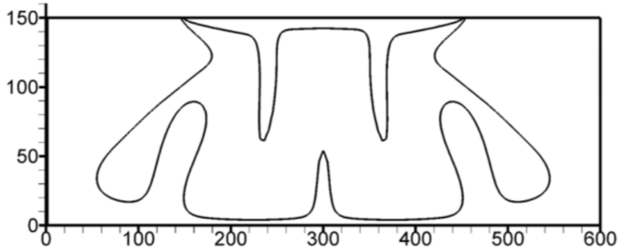


Feflow, high resolution of 9900 used in the following (Kolditz et al., 1998)

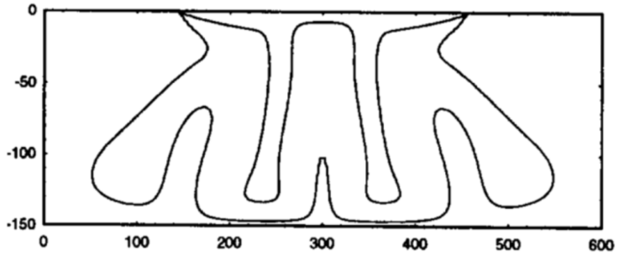


t = 10 a

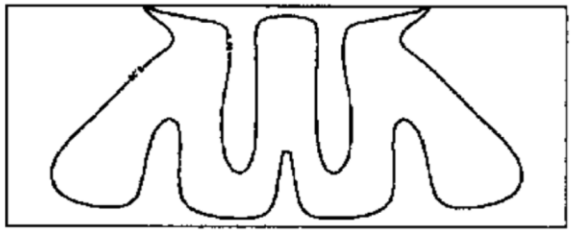
Saltflow



Rockflow (Kolditz et al., 1998)

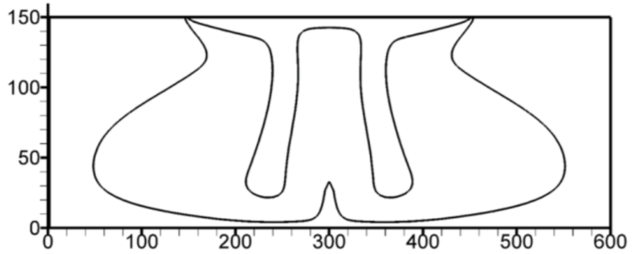


Feflow (Kolditz et al., 1998)

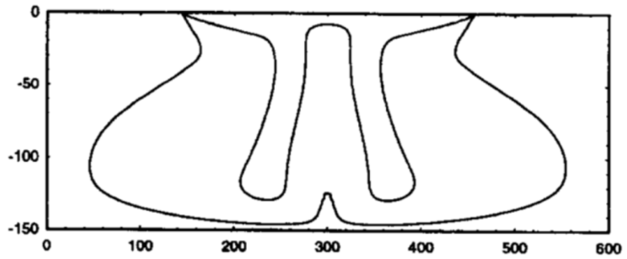


t = 20 a

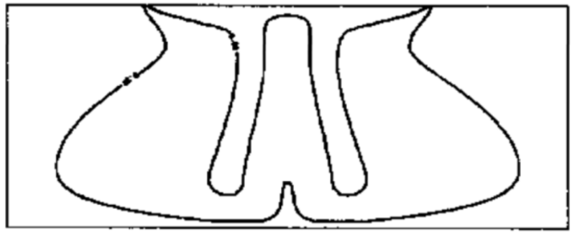
Saltflow



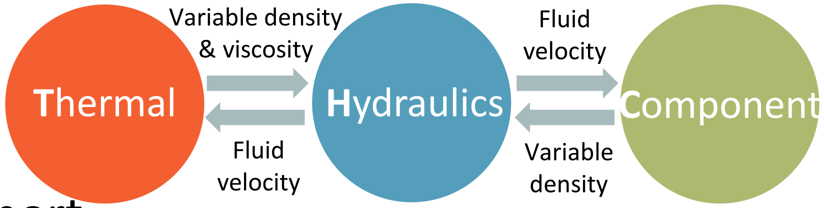
Rockflow (Kolditz et al., 1998)



Feflow (Kolditz et al., 1998)



Numerical Software



- **Heatflow smoker** (Molson & Frind 2023)
- Standard Galerkin finite element method
- Preconditioned conjugate gradient (PCG) solver for flow & transport
- second order scheme transport
- **Leismann time-weighting scheme**
- scheme leads to a symmetric positive-definite coefficient matrix that can be solved with any symmetric-matrix solve
- enabling the use of efficient symmetric matrix solvers
- unconditionally stable
- effectively second-order accurate, giving results equivalent to those obtained with the Crank-Nicolson scheme

Numerical Software

- Heatflow smoker (Molson & Frind 2023)
- **Leismann time-weighting scheme**
- effectively second-order accurate, giving results equivalent to those obtained with the Crank-Nicolson scheme
- Advection & dispersion time weighting terms θ_v, θ_d are augmented with an artificial diffusion term θ_a (that yields a symmetric transport matrix)
- $\theta_v = 0, \;\; \theta_d = 1, \;\; \theta_a = 0.5$
- Advective term is weighted on old time step, dipsersive term on new time step
- Artificial diffusion term is centered in time (Crank-Nicolson)
- Nonlinearities are solved using Picard iterations with max. number or absolute convergence criterium

Methods - Global Sensitivity analysis

- Global Sensitvity Analysis on Dispersivities

- **Variance based sensitivity analysis**
- First-order & total **Sobol‘ indices** (S_i & ST_i)
  - First-order: contribution of one uncertain parameter to output variance
  - Total: remaining output variance after all other uncertain parameters are known
  - Negligible interactions between parameters: $\sum_i S_i = 1,\ S_i = ST_i,\ \forall i$

- Sobol‘ indices for characteristic single values
  - e.g. total salt mass, coordinate of specific salt conc. contour line
  - Mean/ max. Groundwater age etc.
- Marginal effects of parameters

Methods - Global Sensitivity analysis

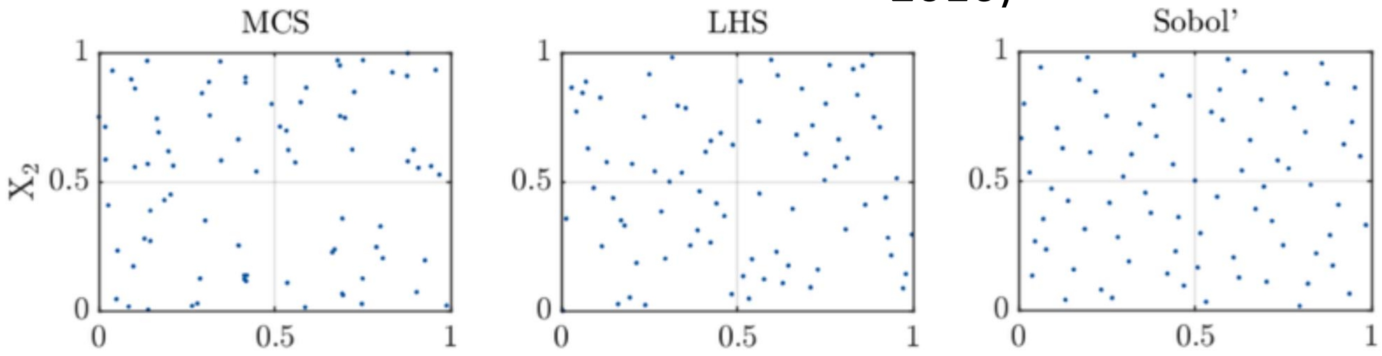
Quasi-Monte Carlo simulations (qMCS)

- Pseudorandom sampling (e.g. Sobol‘ sequence, Latin Hypercube Sampling)
- Many model runs needed (>10^4) for Sobol‘ indices calculation
- Total of $N = n(k + 2)$ simulations
  (n – samples, k – uncertain parameters)

Polynomial Chaos Expansion (PCE)

- **Analytical** calculation of Sobol‘ indices
- 2-3 o. of m. less models runs needed compared to MCS for same accuracy
- Beneficial for comp. demanding models
- Can be constructed from existing data
- Used for DDF (Younes et al. 2020 and Fahs et al. 2022) and LE (Deman et al. 2016)

Sampling strategies



Source: UQLab (https://www.uqlab.com/input-sampling-strategies)