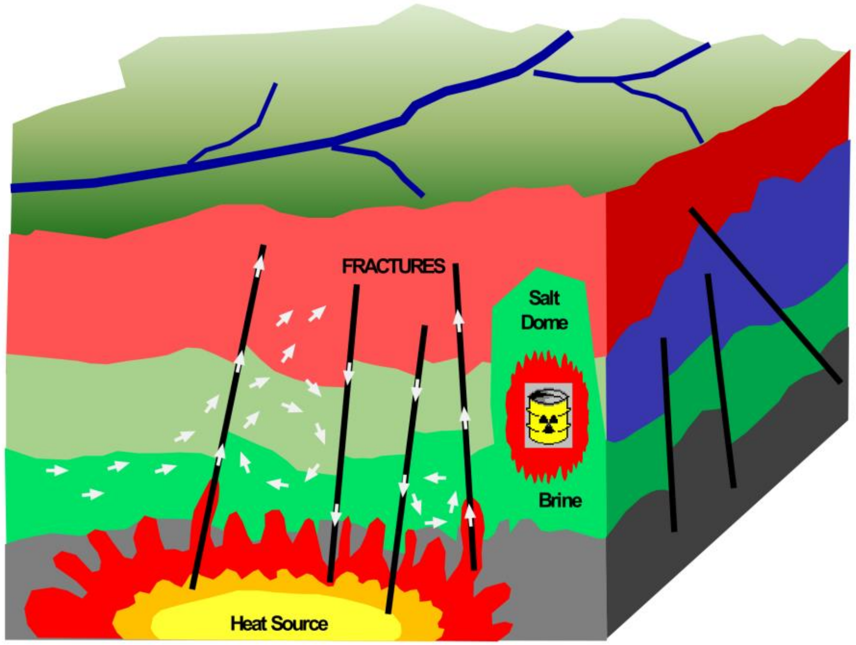
Institute of Fluid Mechanics and
Environmental Physics in Civil Engineering

Leibniz Universität Hannover

RADON – Numerical Simulation of Thermohaline Flow and Salt Transport

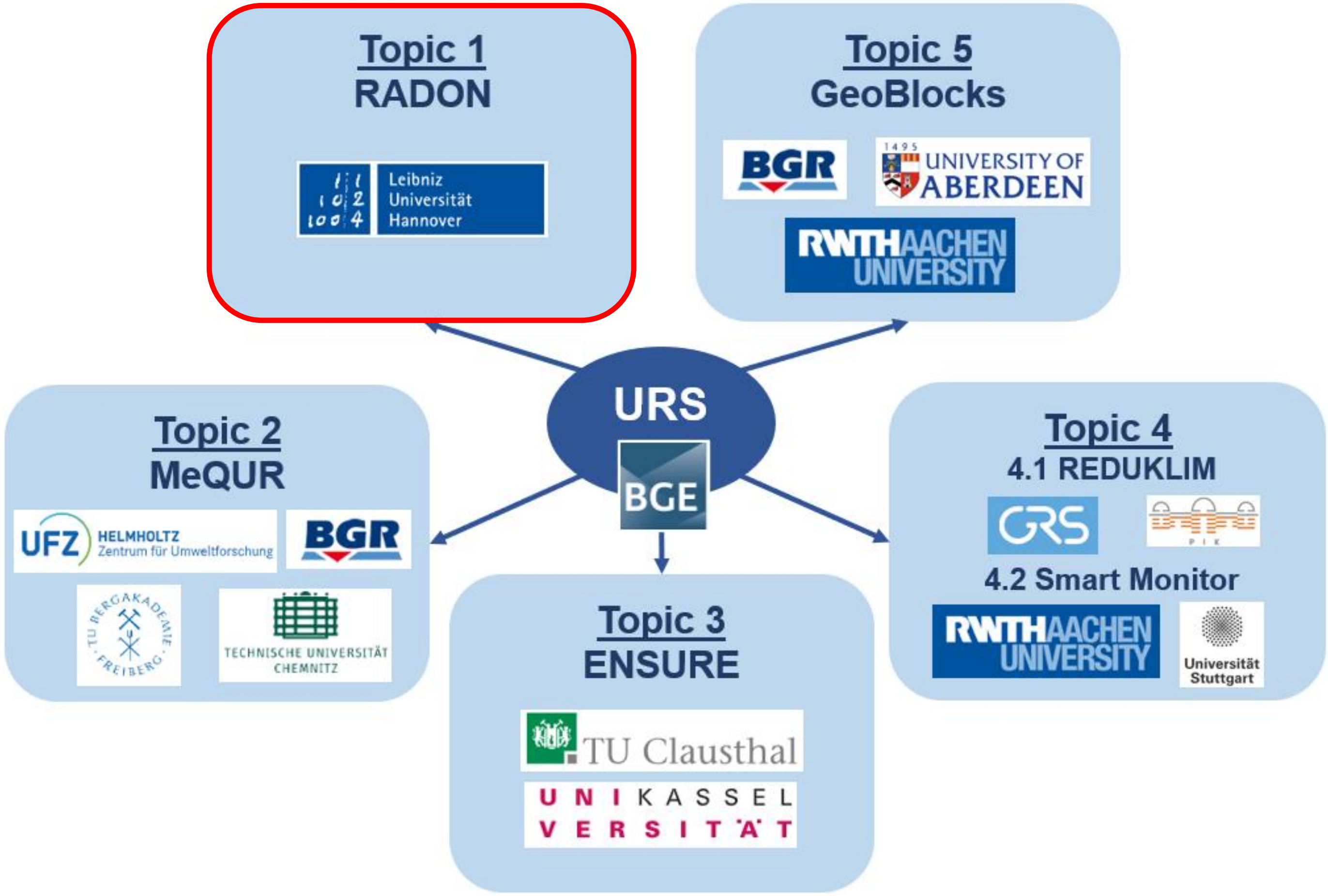


18.04.2023

Thomas Graf

URS 2023 Klausurtagung

Topic Orientation



https://urs.ifgt.tu-freiberg.de/en/home

Co-workers

Inst. of Fluid Mechanics:

Jonas Suilmann (PhD cand.)
Thomas Graf (PI)

Inst. of Risk and Reliability:

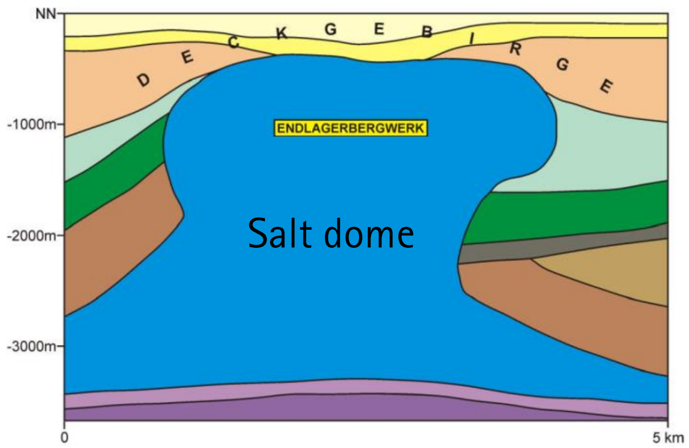
Andrea Perain (PhD cand.)
Matteo Broggi (PI)

All from LU Hannover

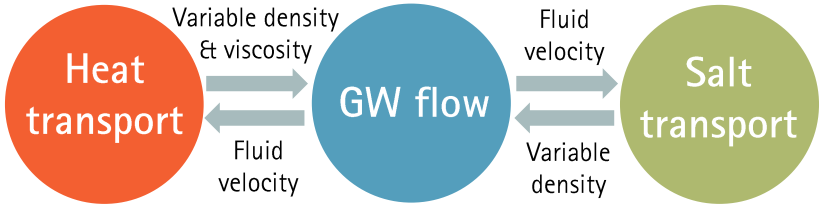
Motivation

<u>Goal</u>: Develop a **numerical framework** for **risk assessment** of hazardous events of a final nuclear waste repository (salt dome)

- Salt rock (salt domes) have been investigated intensively in Germany (Gorleben)
- Numerical model of radionuclide transport in far field
- Groundwater flow
- Heat and salt transport with water density and viscosity effects
- Fractured porous media
- Risk of hazardous events (link to partner-institute)

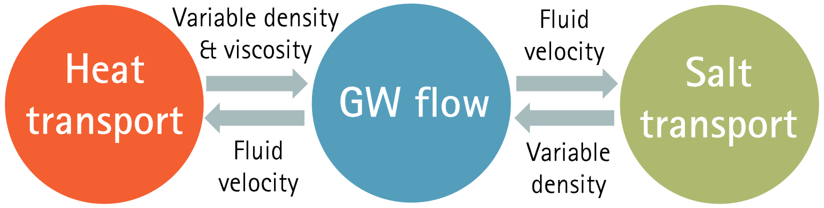


adapted from Brasser et al. 2008



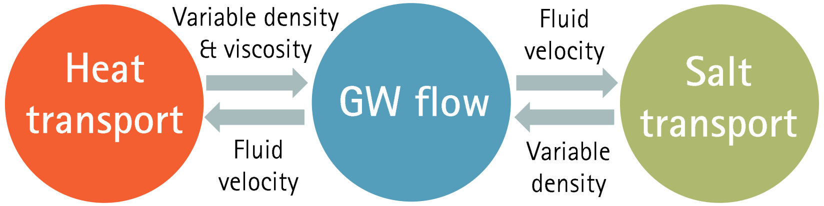
Numerical Analysis

- THC simulations in fractured porous media
- Groundwater flow around salt domes
- Transport of a radionuclide and dissolved salt
- Heat transport due to geothermal gradient and heat generation of waste
- Variable density and viscosity flow: dependency on temperature and salinity
- Coupling of THC processes
- Using **Heatflow smoker** code (Moldon and Frind, 2021; 2023)
- John Molson, Université Laval, Canada



Numerical Analysis

- **Heatflow smoker**
- Standard Galerkin finite element method
- Preconditioned conjugate gradient (PCG) solver for flow & transport
- Second order scheme transport
- Effectively second-order accurate, giving results equivalent to those obtained with a Crank-Nicolson scheme



Governing Equations

Darcy equation

$$q_i = -\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_j}\right)$$

Water flow equation

$$\frac{\partial}{\partial x_i}\left[\frac{k_{ij}}{\mu}\left(\frac{\partial p}{\partial x_j} + \rho g \frac{\partial z}{\partial x_j}\right)\right] = S_s \frac{\partial p}{\partial t}$$

Heat transport equation

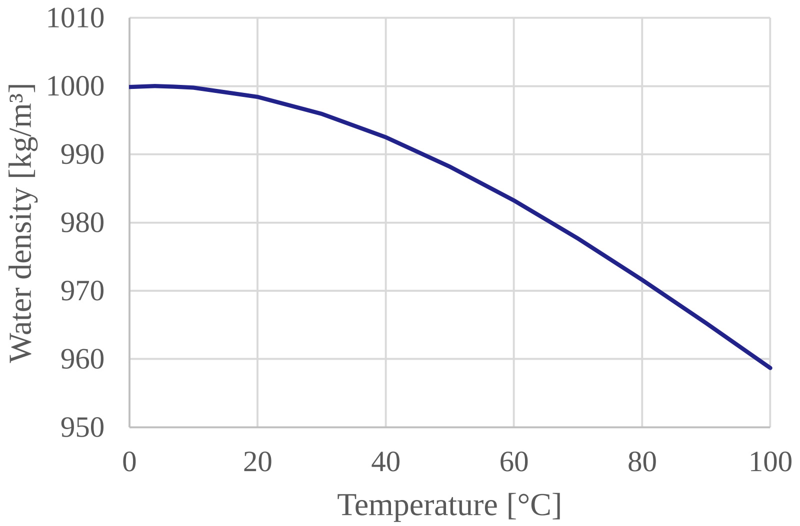
$$\frac{\partial}{\partial x_i}\left[\lambda \frac{\partial T}{\partial x_j}\right] - c^w \rho^w \frac{\partial}{\partial x_i}(v_i T) = c\rho \frac{\partial T}{\partial t}$$

Mass transport equation

$$\frac{\partial}{\partial x_i}\left[D_{ij} \frac{\partial c}{\partial x_j}\right] - \frac{\partial}{\partial x_i}(v_i c) = \frac{\partial c}{\partial t}$$

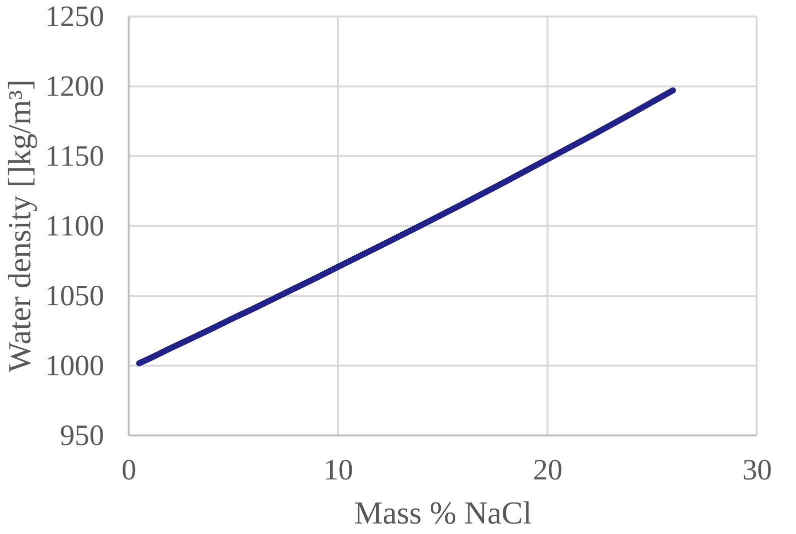
Constitutive Equations – Density

Temperature



Data from Lide 2005

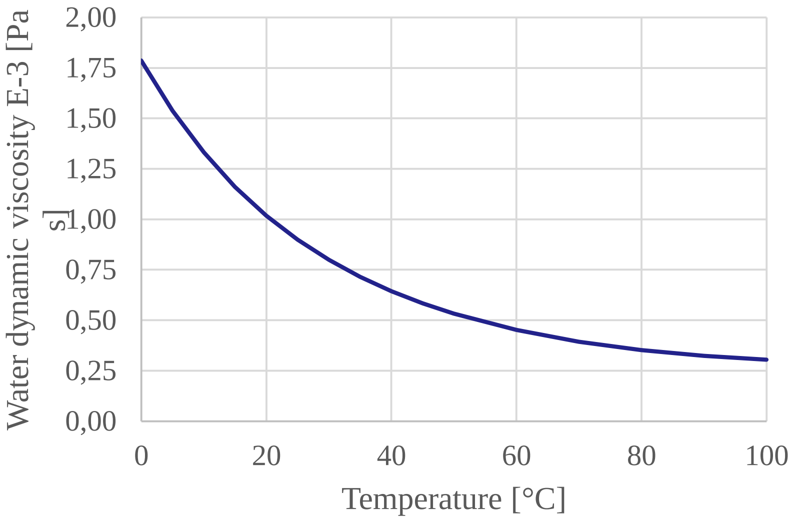
Salt mass %



T = 20 ° C Data from Lide 2005

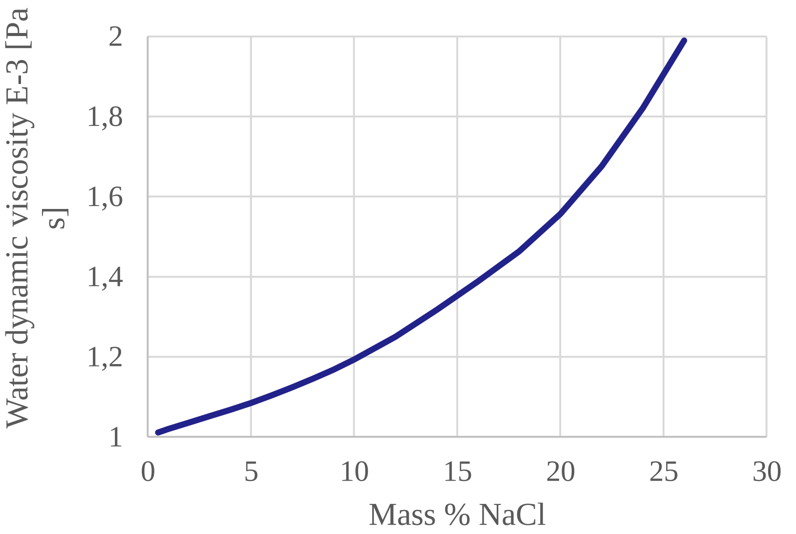
Constitutive Equations – Viscosity

Temperature



Data from Lide 2005

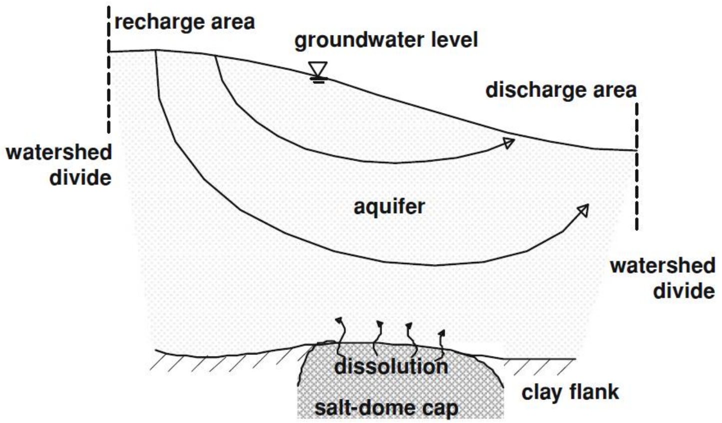
Salt mass %



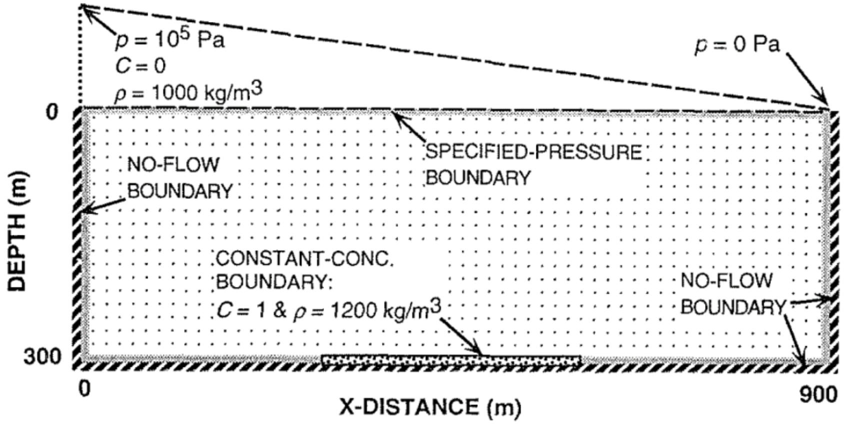
Data from Lide 2005

Salt Dome Problem

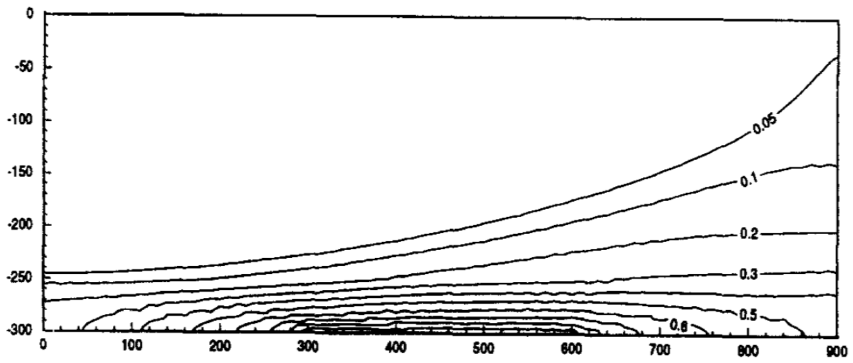
- Test case for variable-density flow numerical codes (Diersch and Kolditz, 1998)
- Strong coupling of flow and transport (density variation of 20 %)
- Hydrogeological situation above Gorleben saltdome
- Intensively investigated in the 80‘s and 90‘s (Herbert et al. 1988, Oldenburg and Pruess 1995, Kolditz et al. 1998, etc.)
- Different diffusion coefficients and long. & trans. dispersivities used



Holzbecher et al. 2010



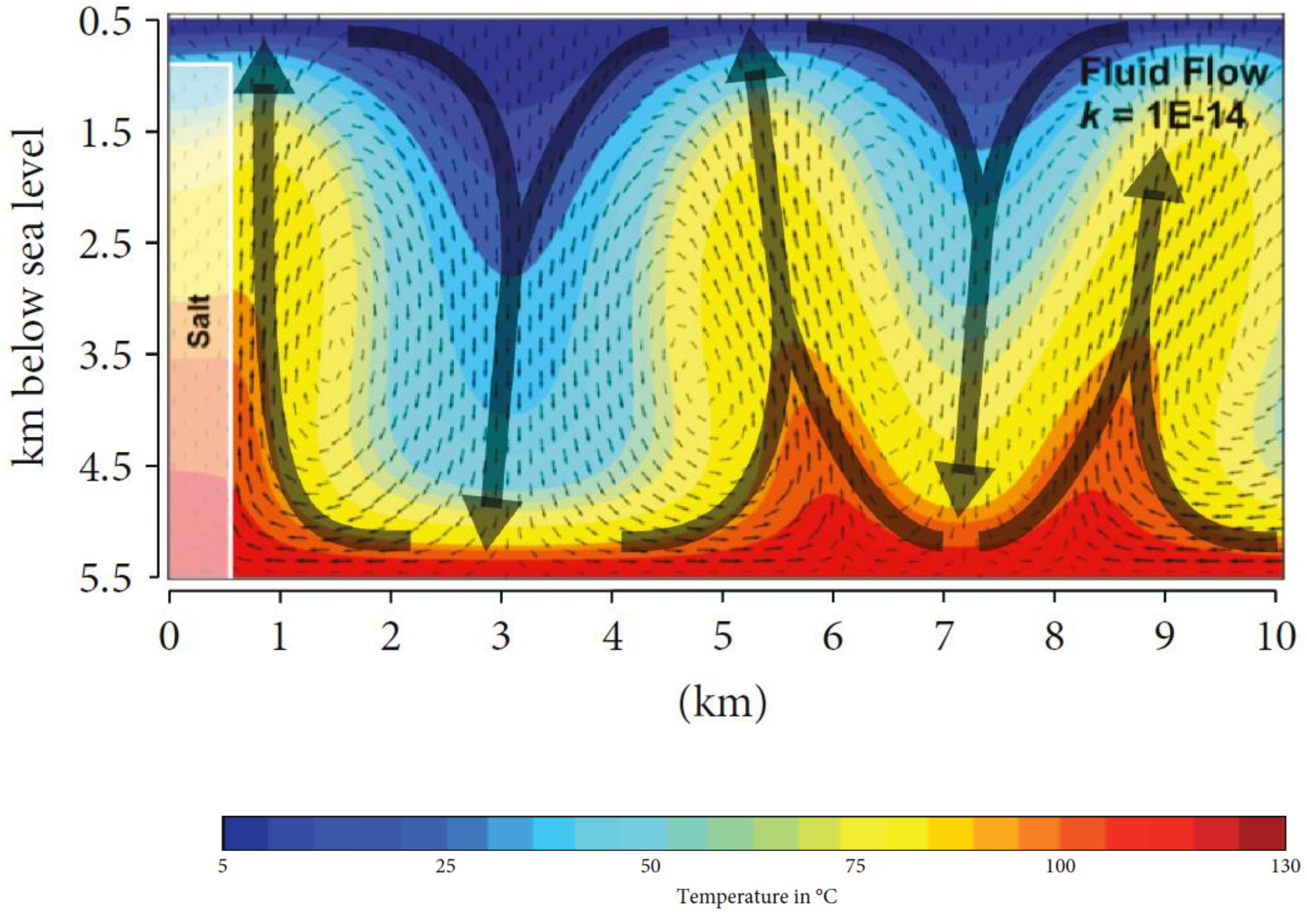
Konikow et al. 1996



Kolditz et al. 1998

Salt Chimney Effect

- Salt chimney effect (Canova et al. 2018)
- Heat transport and water flow next to salt dome
- High thermal conductivity of salt compared to surrounding rock
- Therefore smaller temperature gradients within the salt formation



1. Research Objective: Salt Dome

- Further investigate the salt dome problem in terms of groundwater age
- Calculated as transport equation (steady state):

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial A}{\partial x_j}\right) - v_i\frac{\partial A}{\partial x_i} + 1 = 0 \qquad \text{(Goode 1996)}$$

- Steady state flow velocities of salt dome problem solution as input for GW-age simulation
- Sensitvity of long. & trans. dispersivity on
  - original salt dome problem (salt concentration in model domain) and
  - GW-age distribution in model domain

1. Research Objective: Salt Dome

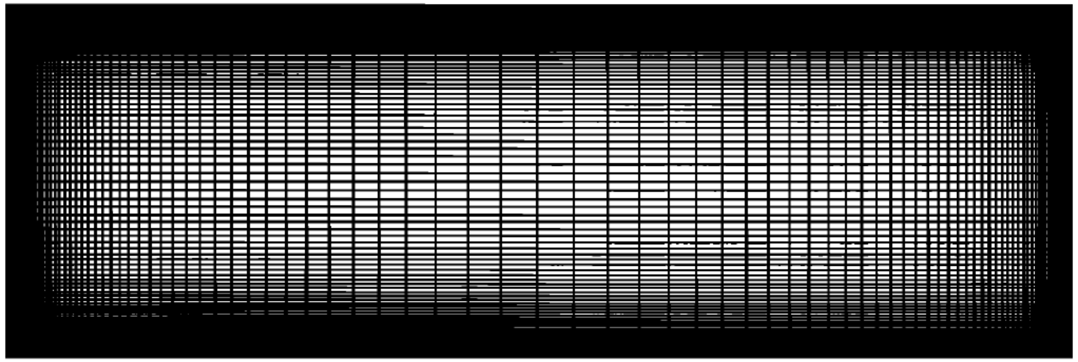
Groundwater age in original and thermohaline salt dome problem

- Investigate
  1. Grid convergence
  2. Flow field & salt distribution
  3. Groundwater age distribution (for steady state flow)
  4. Transport of a radionuclide
- Including
  1. Different dispersivities and diffusion coefficients
  2. Different hydraulic conductivities

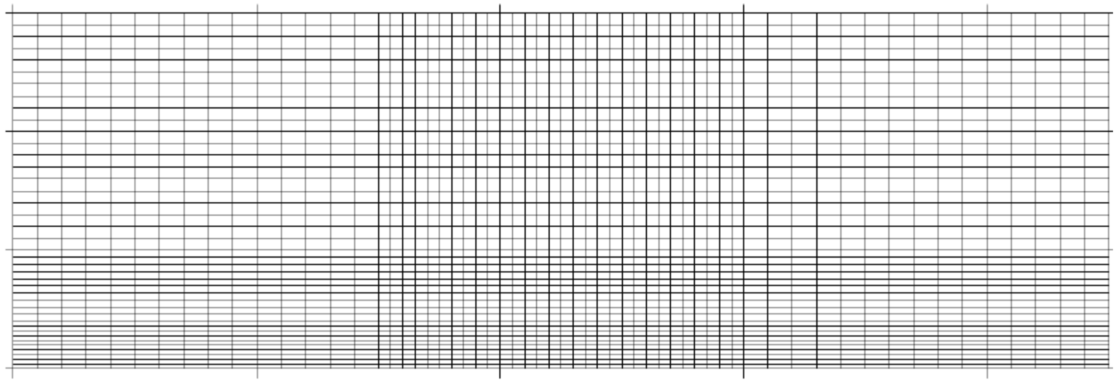
1. Research Objective: Salt Dome

Grid Analysis

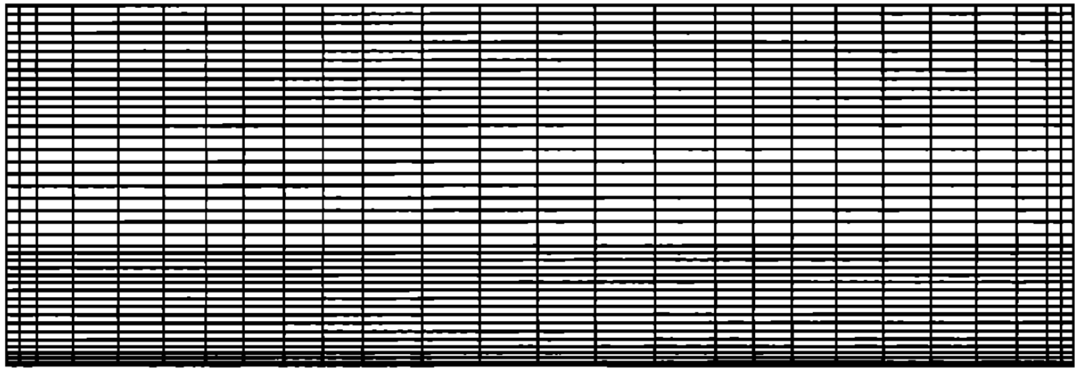
- very different meshes have been used
- systematic grid analysis is absent



Johns and Rivera et al. 1996



Younes et al. 1999



Herbert et al. 1988

1. Research Objective: Salt Dome

Grid Analysis

- Graded meshes gave no consistent results → uniform mesh used here
- Assumption: aspect ratio of elements influences result
- Focus aspect ratio of elements
- In literature: z-discretization of 4 m is sufficient for grid convergence
  (Konikow et al. 1996, Oldenburg and Pruess 1995, Younes et al. 1999)
- Determine influence of aspect ratio by changing discretization in x-dimension (Δz = 4m, 75 elements)

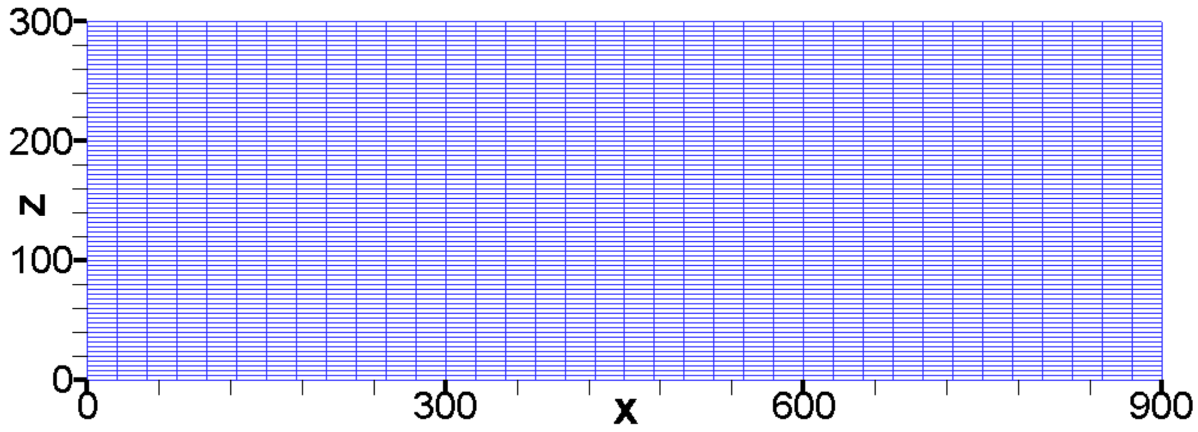
1. Research Objective: Salt Dome

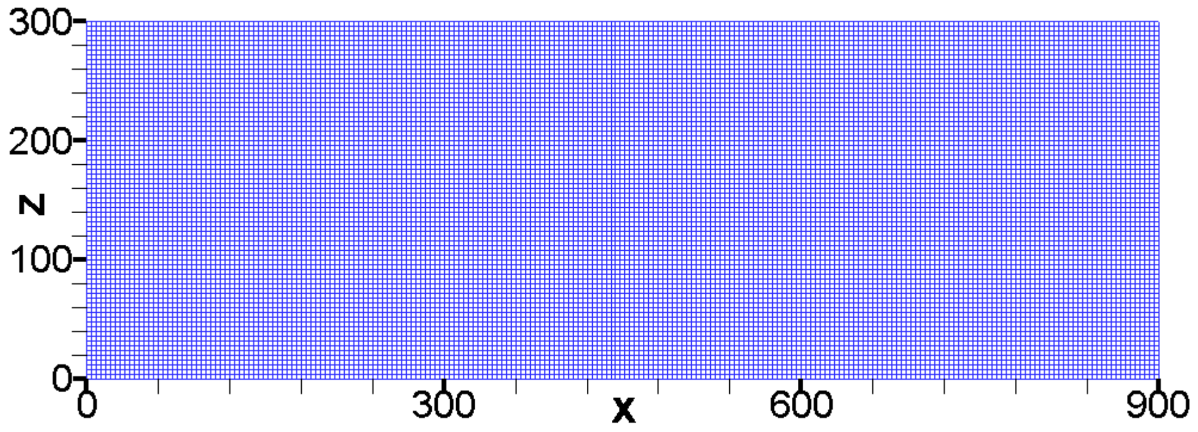
Grid Analysis – Some Results

Stepwise reduction of aspect ratio from

36 x-elements (2700 in total) to **225 x-elements** (16875 in total)

$\Delta x = 25$ m	$\Delta x = 4$ m
Aspect ratio: 6.25	Aspect ratio: 1

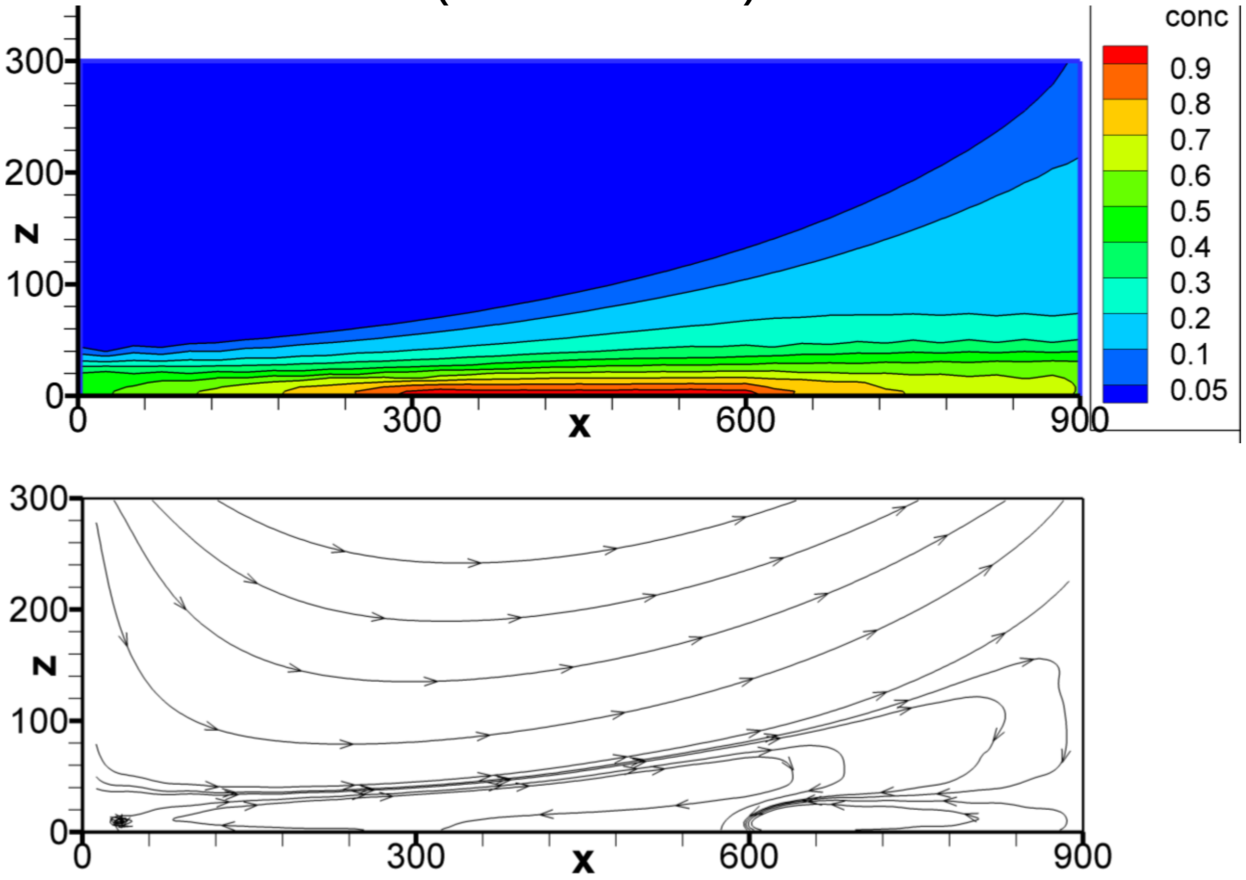




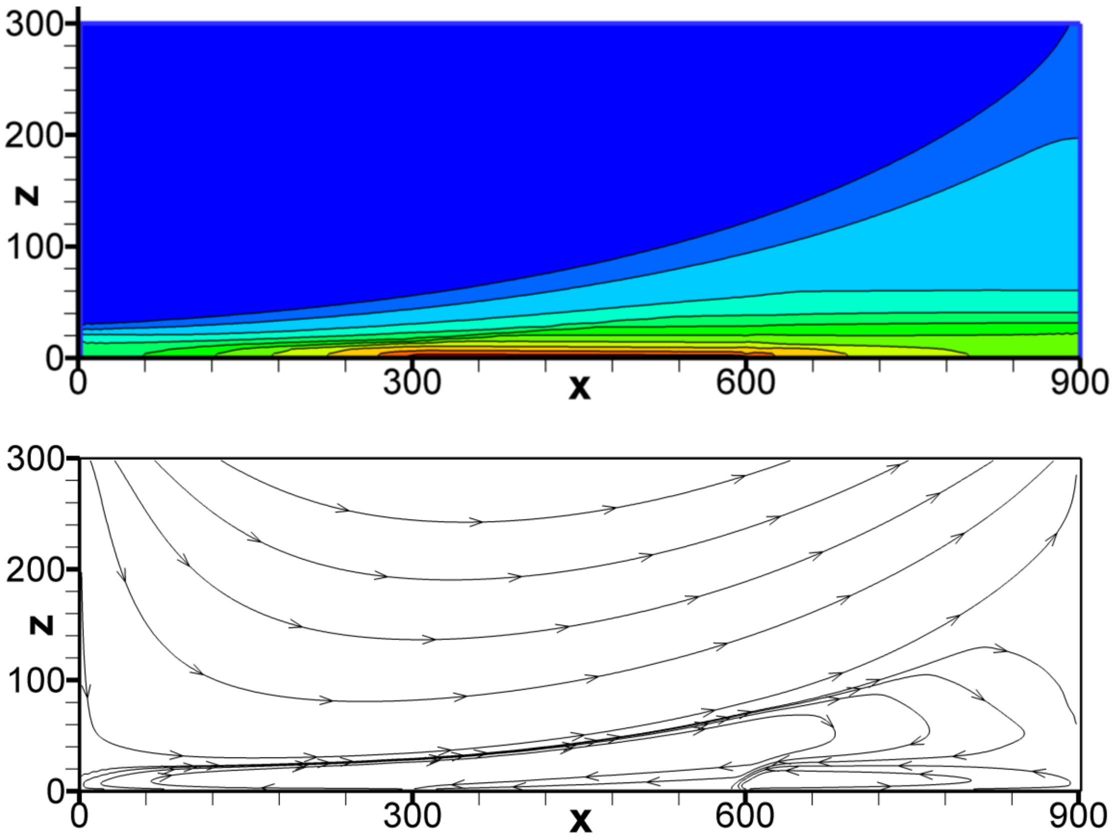
1. Research Objective: Salt Dome

Grid Analysis – Some Results

36 x-elements (2700 in total)



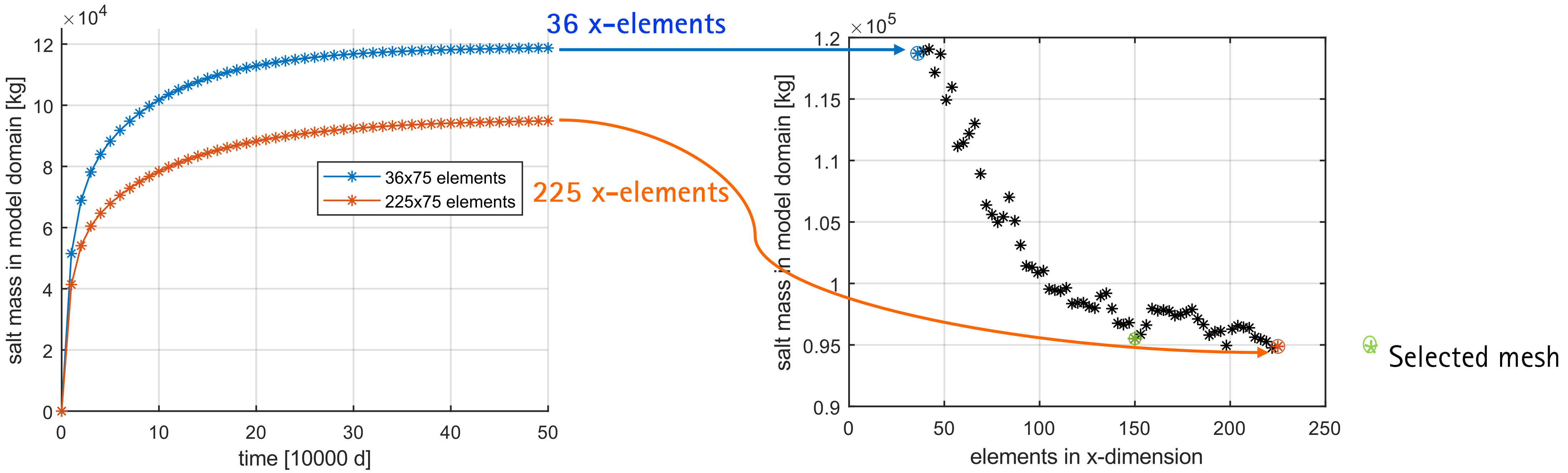
225 x-elements (16875 in total)



1. Research Objective: Salt Dome

Grid Analysis – Some Results

- Results can be compared by total salt mass in model domain

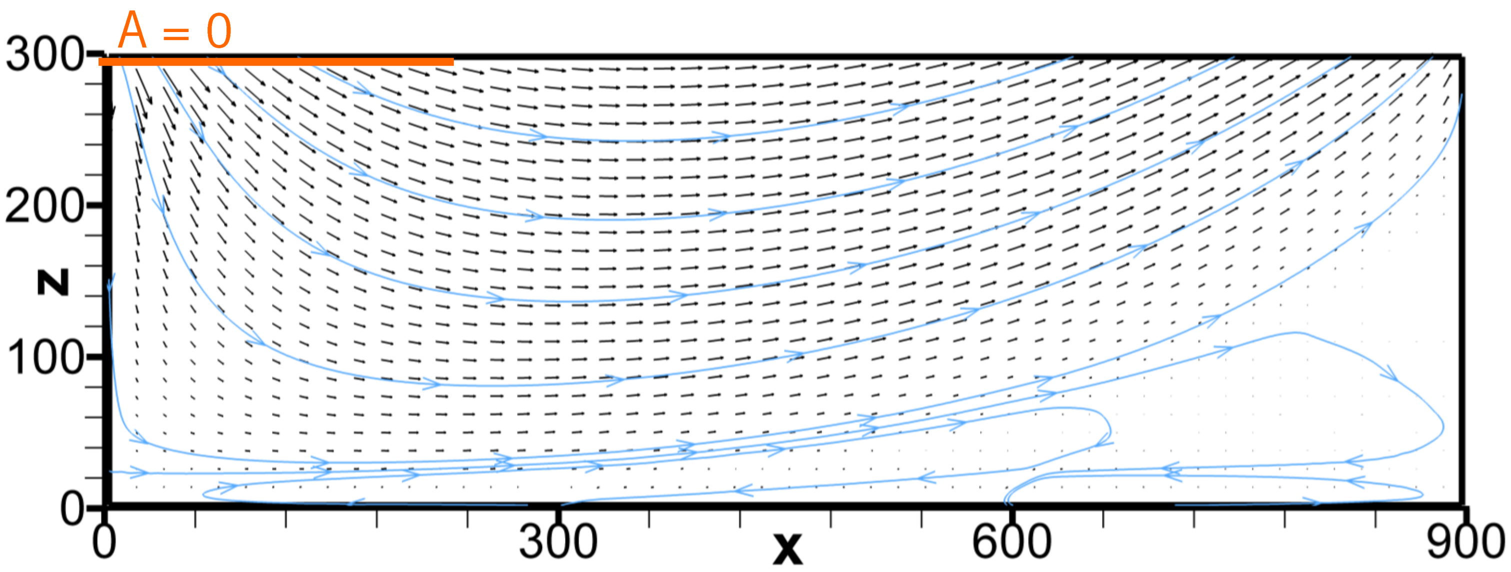


- 150 elements in x-dimension (11250 in total) are chosen (0.79 % deviation in salt mass)
- Aspect ratio 1.5

1. Research Objective: Salt Dome

GW-Age Distribution – Some Results

- GW-Age distribution for 150x75 elements (D = 1.39e8 m²/s; αL = 20 m; αT = 2 m)
- Steady-state flow velocities as input:
- BC at inflow region: A = 0 (necessary)



Coupled flow & transport solution of salt dome problem

↓

Steady state flow velocities (input)

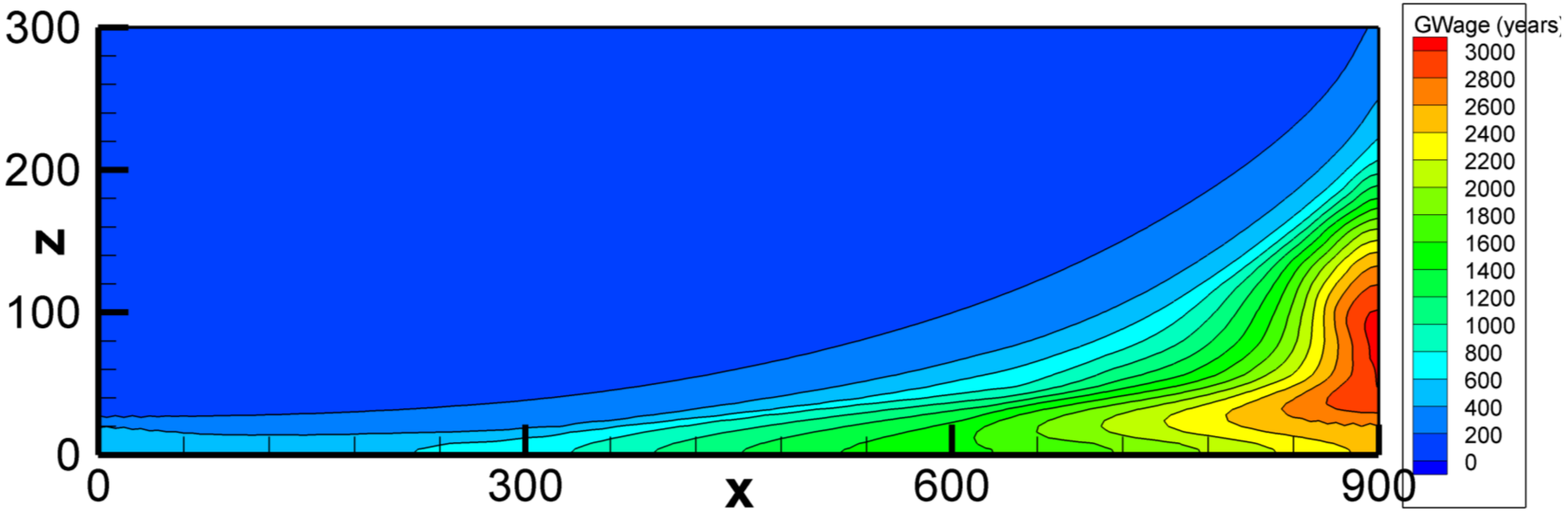
↓

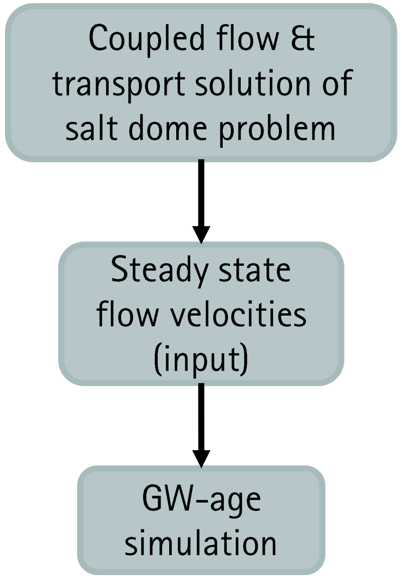
GW-age simulation

1. Research Objective: Salt Dome

GW-Age Distribution – Some Results

- High GW-age in zones with low flow velocities





1. Research Objective: Salt Dome

Outlook

- Sensitvity of long. & trans. dispersivity on
  - Classic salt dome problem (salt concentration in model domain) and
  - GW-age distribution in model domain
- Uncertainty ranges: α_L = [3 - 40] m; α_T = [0.3 - 4] m (scale-dependent)
- α_T as a Gaussian distribution with mean of 1/10 of α_L
- Dispersivities affect steady-state flow solution of salt dome problem
- Dispersivities affect GW-age through flow solution and age transport
- Different GW-age distributions expected

1. Research Objective: Salt Dome

Outlook

- Monte-Carlo-Simulations using Andrea‘s code
- Calculating first-order & total sensitivity
- e.g. total salt mass, coordinate of specific salt conc. contour line
- Or mean GW-age
- High variation of GW-age due to double dependency on dispersivities expected

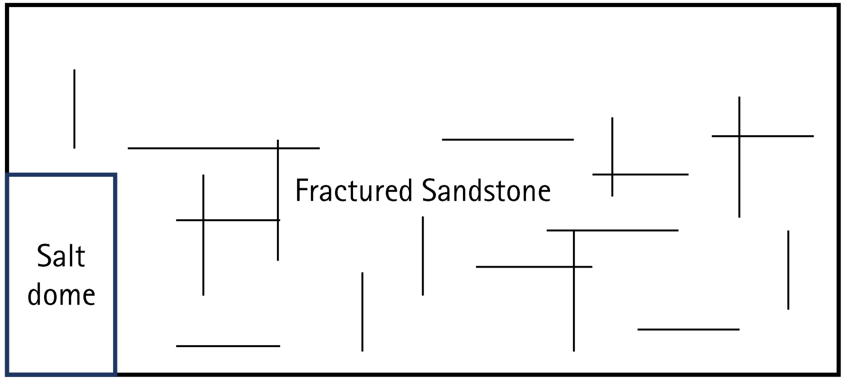
2. Research Objective: Salt Chimney Effect

Role of fractures on salt chimney effect around salt dome

Investigate

1. Influence of regular fractures (and microfractures)
2. Influence of randomly distributed fractures (and fracture connectivity) on:

   – Flow field & salt distribution
   – Groundwater age distribution
     (for steady state flow)
   – Transport of a radionuclide

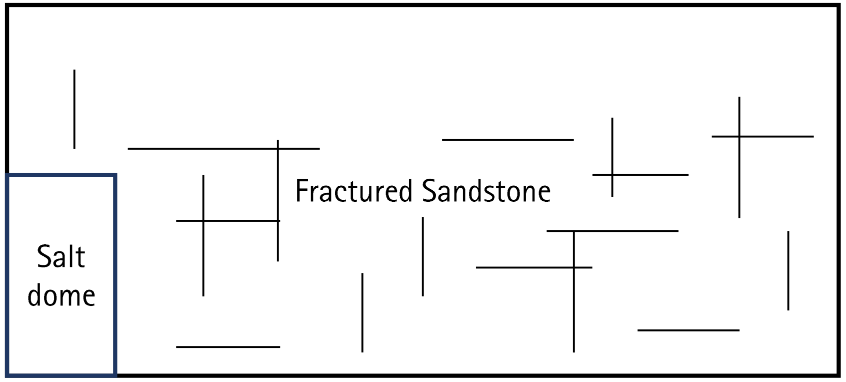


3. Research Objective: Implementation of Uncertainty

Joint ISU – IRZ Project

For the joint project:

- Create 2D test cases including a salt dome and thermohaline effects for the simulation of radionuclide propagation through fractures surrounding rock
- Implementation of uncertainty
  - Time and amount of radionuclide release
  - Unknown fracture location, hydraulic parameters and boundary conditions for flow
- Determination of external events that occur with certain probability and obtain the probabilty distribution of the output of simulations



Literature

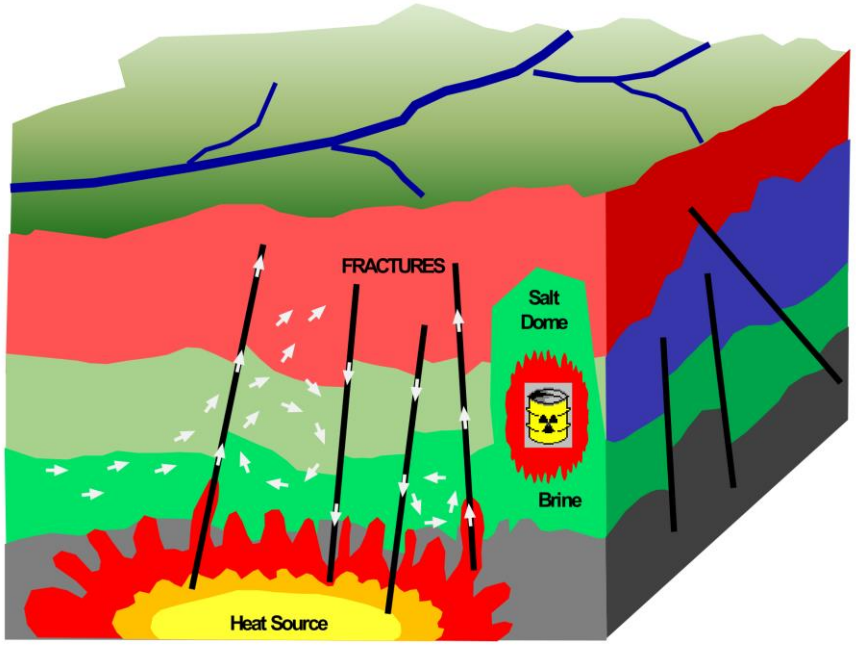
- Brasser, T.; Droste, J.; Müller-Lyda, I.; Neles, J.; Sailer, M.; Schmidt, G.; & Steinhoff, M. (2008): Endlagerung wärmeentwickelnder radioaktiver Abfälle in Deutschland. GRS; Öko-Institut e.V. Braunschweig / Darmstadt.
- Canova, David P.; Fischer, Mark P.; Jayne, Richard S.; Pollyea, Ryan M. (2018): Advective Heat Transport and the Salt Chimney Effect: A Numerical Analysis. In: *Geofluids* 2018, S. 1–18. DOI: 10.1155/2018/2378710.
- Diersch, H.-J.G.; Kolditz, O. (1998): Coupled groundwater flow and transport: 2. Thermohaline and 3D convection systems. In: *Advances in Water Resources* 21 (5), S. 401–425. DOI: 10.1016/S0309-1708(97)00003-1.
- Goode, Daniel J. (1996): Direct Simulation of Groundwater Age. In *Water Resour. Res.* 32 (2), pp. 289–296. DOI: 10.1029/95WR03401.
- Herbert, A. W.; Jackson, C. P.; Lever, D. A. (1988): Coupled groundwater flow and solute transport with fluid density strongly dependent upon concentration. In: *Water Resour. Res.* 24 (10), S. 1781–1795. DOI: 10.1029/WR024i010p01781.
- Holzbecher, E.; Kohfahl, C.; Mazurowski, M.; Bącik, A.; Dobies, M.; Schneider, M. (2010): The Sensitivity of Thermohaline Groundwater Circulation to Flow and Transport Parameters: A Numerical Study Based on Double-Diffusive Convection above a Salt Dome. In: *Transp Porous Med* 83 (3), S. 771–791. DOI: 10.1007/s11242-009-9480-4.
- Johns, Russell T.; Rivera, Alfonso (1996): Comment on “Dispersive Transport Dynamics in a Strongly Coupled Groundwater-Brine Flow System” by Curtis M. Oldenburg and Karsten Pruess. In *Water Resour. Res.* 32 (11), pp. 3405–3410. DOI: 10.1029/96WR02495.
- Kolditz, Olaf; Ratke, Rainer; Diersch, Hans-Jörg G.; Zielke, Werner (1998): Coupled groundwater flow and transport: 1. Verification of variable density flow and transport models. In: *Advances in Water Resources* 21 (1), S. 27–46. DOI: 10.1016/S0309-1708(96)00034-6.
- Konikow, L. F.; P. J. Campbell; W. E. Sanford. (1996): Modelling brine transport in a porous medium: a re-evaluation of the hydrocoin level 1, case 5 problem. In : Calibration and Reliability in Groundwater Modeling, edited by K. Kovar, P. van der Heijde, IAHS Publ. 237, pp. 363–372.
- Lide, David R. (Ed.) (2005): CRC Handbook of Chemistry and Physics. Internet Version 2005. Boca Raton, FL: CRC Press.
- Molson, J. W.; E.O. Frind (2023): HEATFLOW-SMOKER USER GUIDE. Version V3/TC2. Density-dependent flow and advective-dispersive transport of mass, thermal energy or residence time in 3D porous or discretely-fractured porous media. Université Laval & University of Waterloo.
- Molson, J. W.; Frind, E. O. (2021): HEATFLOW - SMOKER. Density-dependent flow and advective-dispersive transport of thermal energy, mass or residence time in three-dimensional porous or discretely-fractured porous media. User Guide, Version 10.0. Université Laval. Quebec City.
- Oldenburg, Curtis M.; Pruess, Karsten (1995): Dispersive Transport Dynamics in a Strongly Coupled Groundwater-Brine Flow System. In: *Water Resour. Res.* 31 (2), S. 289–302. DOI: 10.1029/94WR02272.
- Younes, A.; Ackerer, Ph.; Mose, R. (1999): Modeling Variable Density Flow and Solute Transport in Porous Medium: 2. Re-Evaluation of the Salt Dome Flow Problem. In *Transp Porous Med* 35 (3), pp. 375–394. DOI: 10.1023/A:1006504326005.

Institute of Fluid Mechanics and
Environmental Physics in Civil Engineering

Leibniz Universität Hannover

RADON – Numerical Simulation of Thermohaline Flow and Salt Transport

Thank



You !!!

18.04.2023

Thomas Graf

URS 2023 Klausurtagung