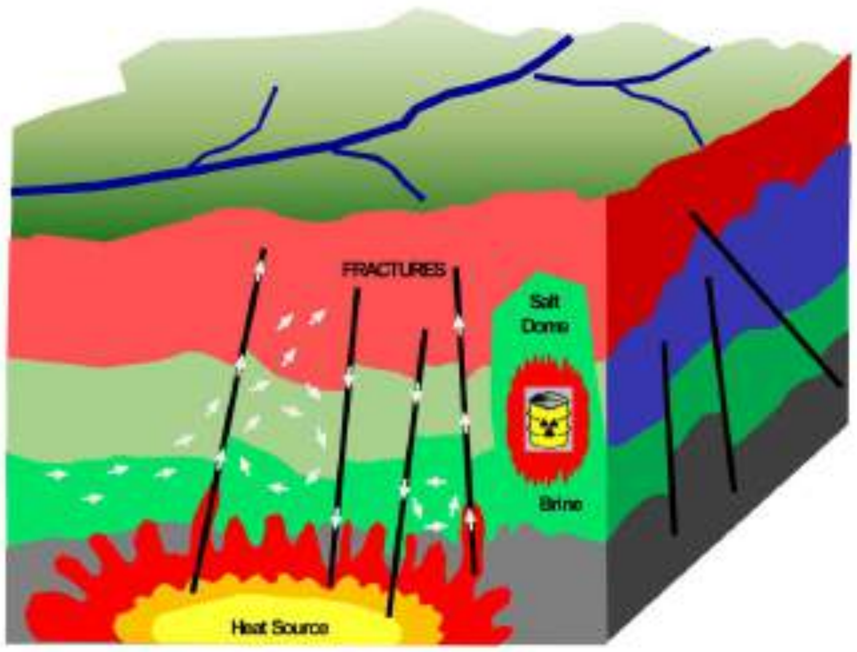
Institute of Fluid Mechanics and
Environmental Physics in Civil Engineering

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:

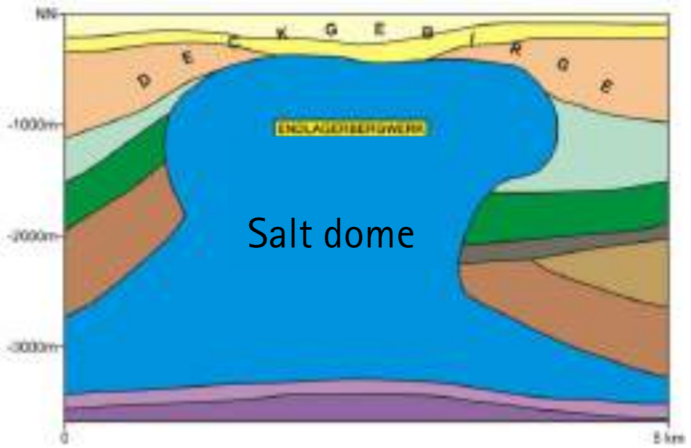
Andrea Perain (PhD cand.)
Matteo Broggi (PI)

All from LU Hannover

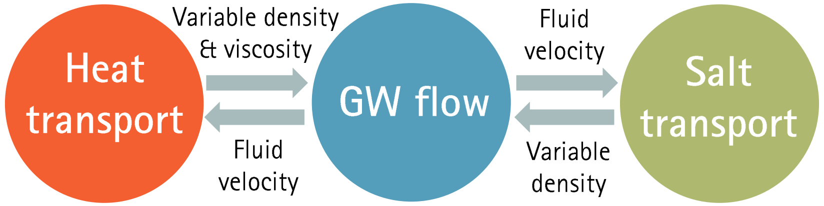
# Motivation

**Goal**: 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)

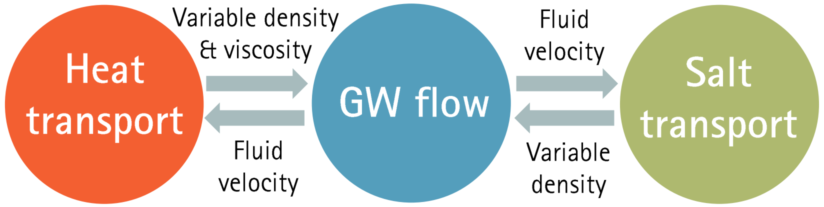


adapted from Brasser et al. 2008



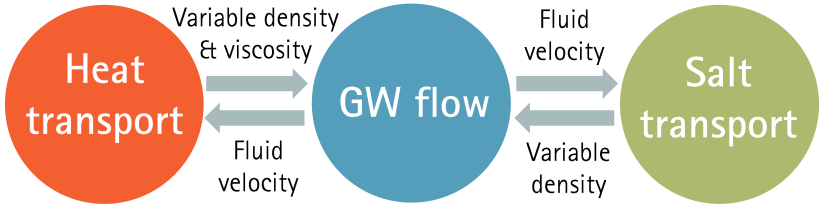
# Numerical Analysis

- 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

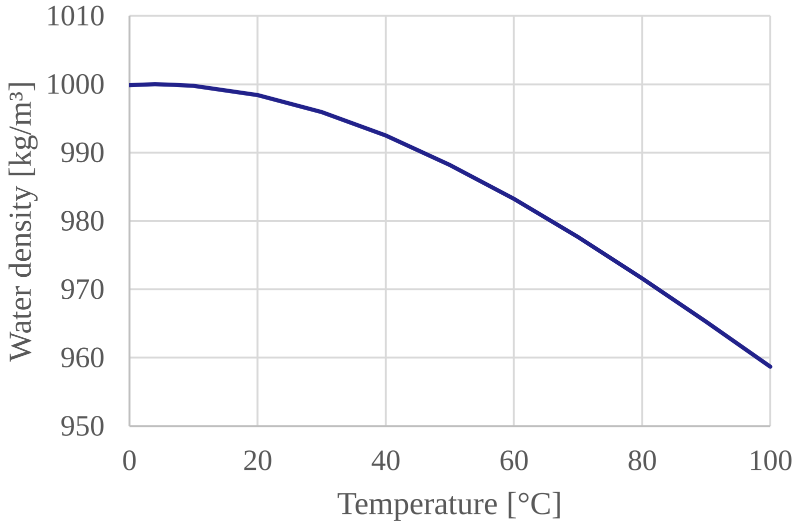
$$\frac{\partial}{\partial x_i}\left[\lambda\frac{\partial T}{\partial x_j}\right] - c^w\rho^w\frac{\partial}{\partial x_i}(v_i T) = c\rho\frac{\partial T}{\partial t}$$

Mass transport equation

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

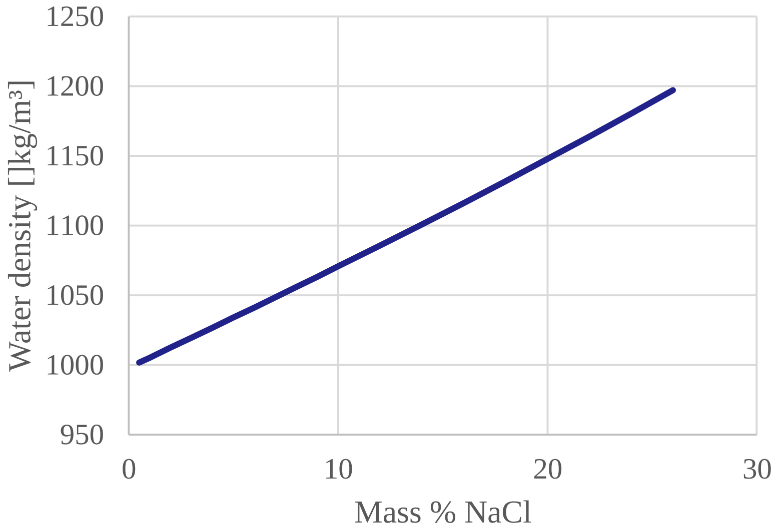
# Constitutive Equations – Density

Temperature




Data from Lide 2005

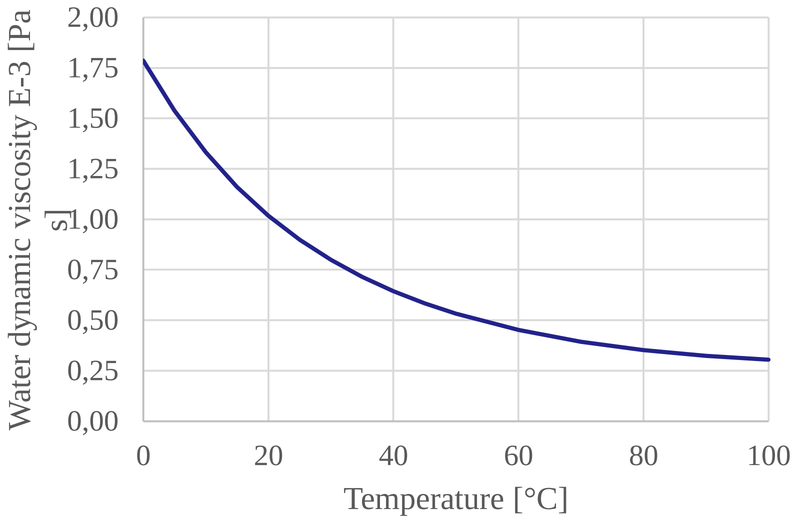
Salt mass %




T = 20 ° C Data from Lide 2005

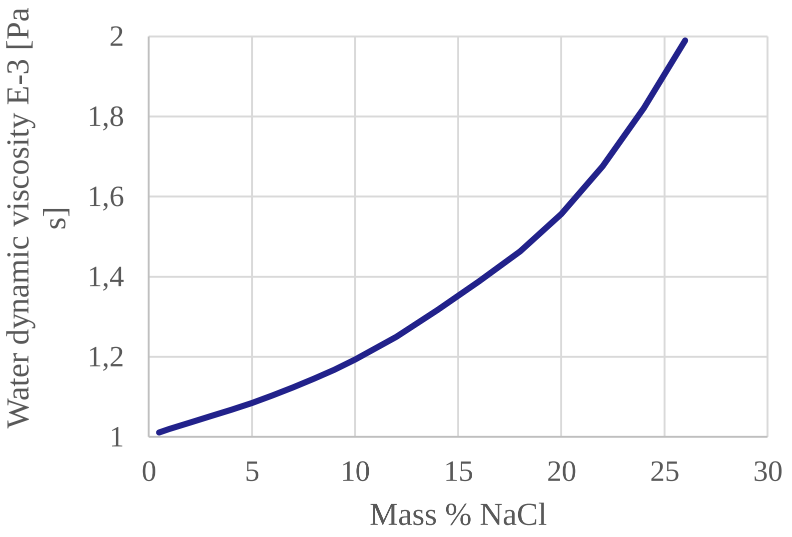
# Constitutive Equations – Viscosity

## Temperature




Data from Lide 2005

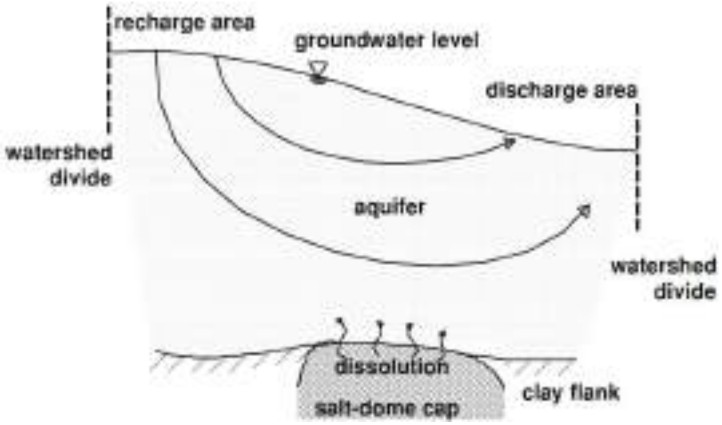
## Salt mass %



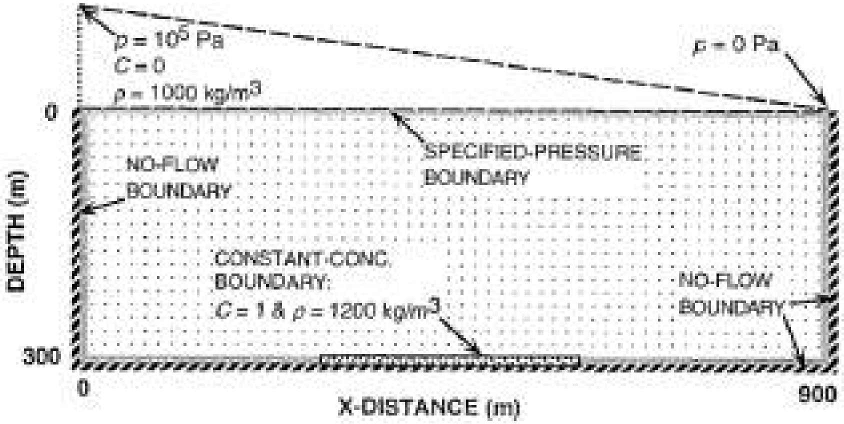

Data from Lide 2005

# Salt Dome Problem

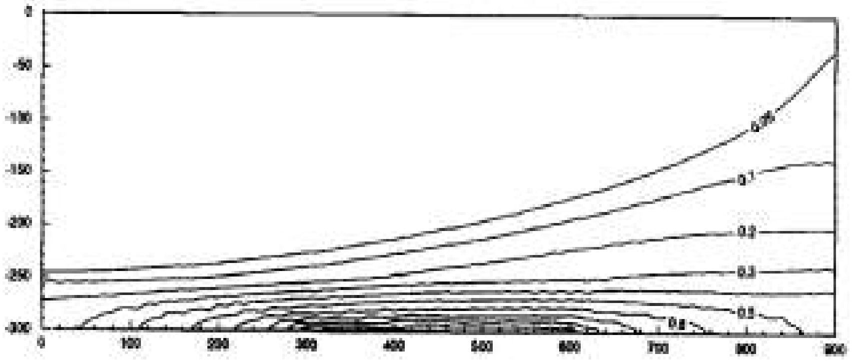
- Test case for variable-density flow numerical codes (Diersch and Kolditz, 1998)
- Strong coupling of flow and transport (density variation of 20 %)
- Hydrogeological situation above Gorleben saltdome
- Intensively investigated in the 80‘s and 90‘s (Herbert et al. 1988, Oldenburg and Pruess 1995, Kolditz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




Holzbecher et al. 2010



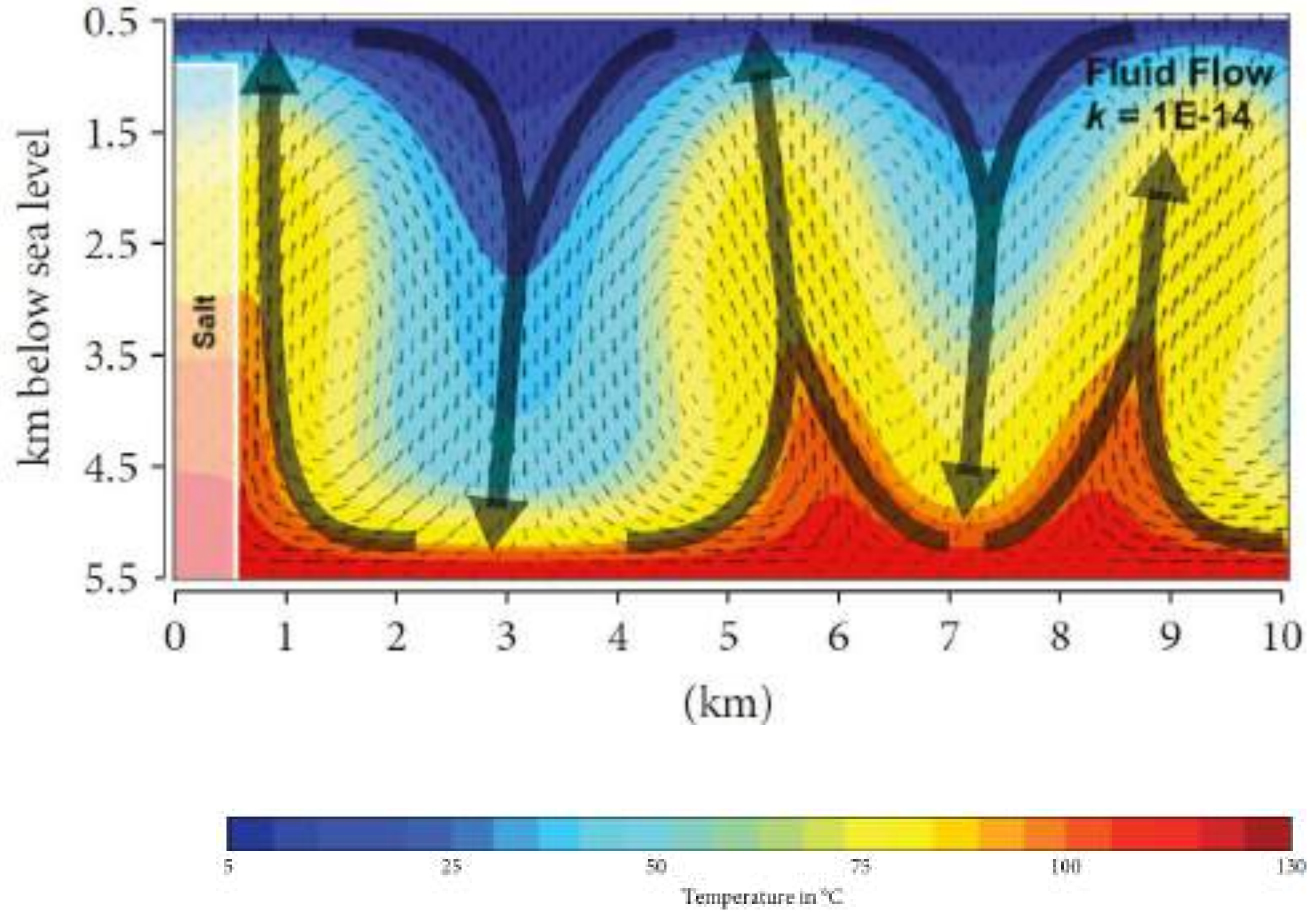

Konikow et al. 1996



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):

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

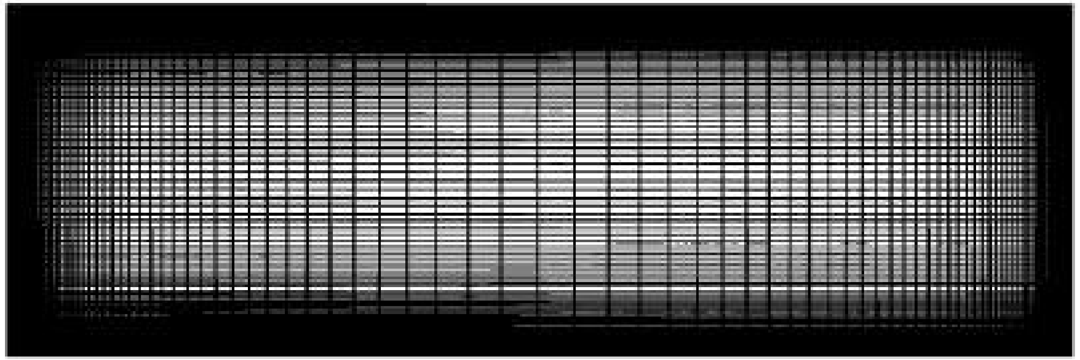
## Groundwater age in original and thermohaline salt dome problem

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

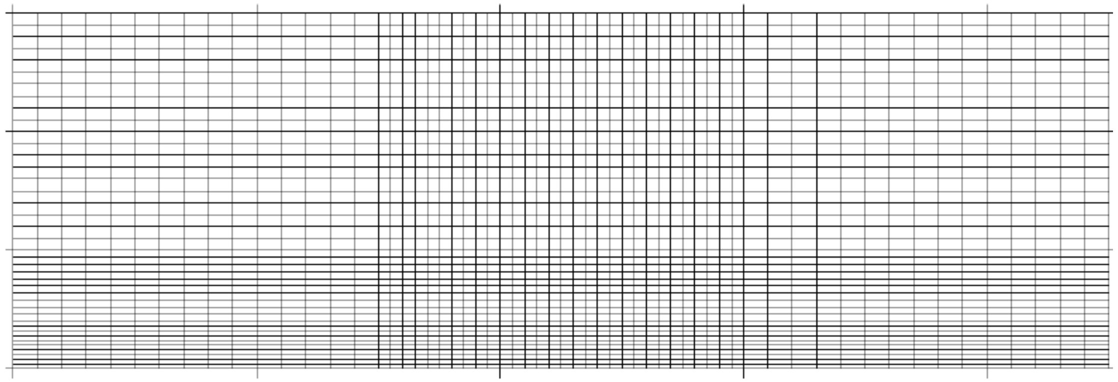
# 1. Research Objective: Salt Dome

## Grid Analysis

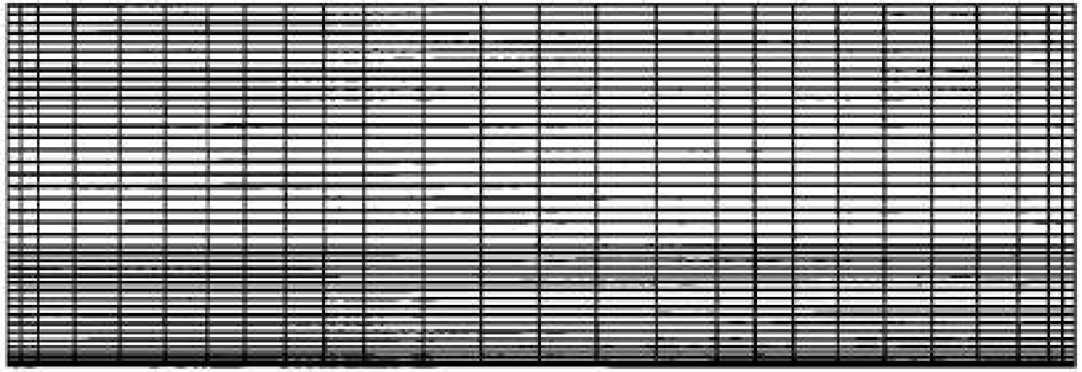
- very different meshes have been used
- systematic grid analysis is absent



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 ($\Delta z$ = 4m, 75 elements)

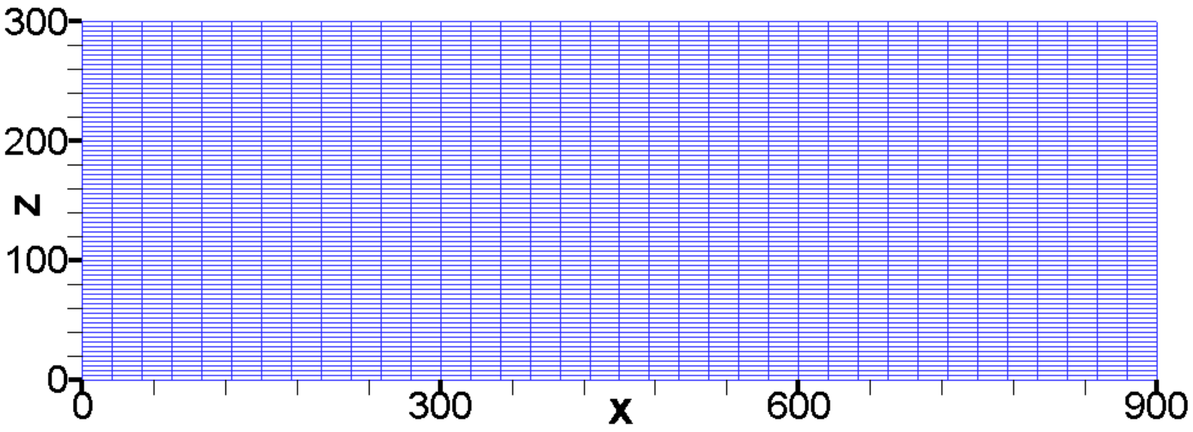
# 1. Research Objective: Salt Dome

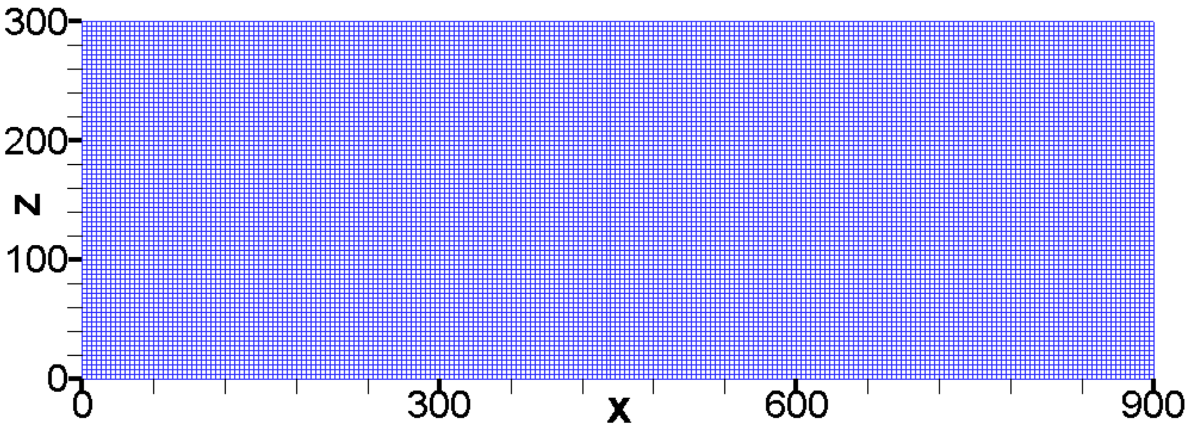
## Grid Analysis – Some Results

Stepwise reduction of aspect ratio from

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

| | |
|---|---|
| **36 x-elements** (2700 in total) | **225 x-elements** (16875 in total) |
| Δx = 25 m | Δx = 4 m |
| Aspect ratio: 6.25 | Aspect ratio: 1 |

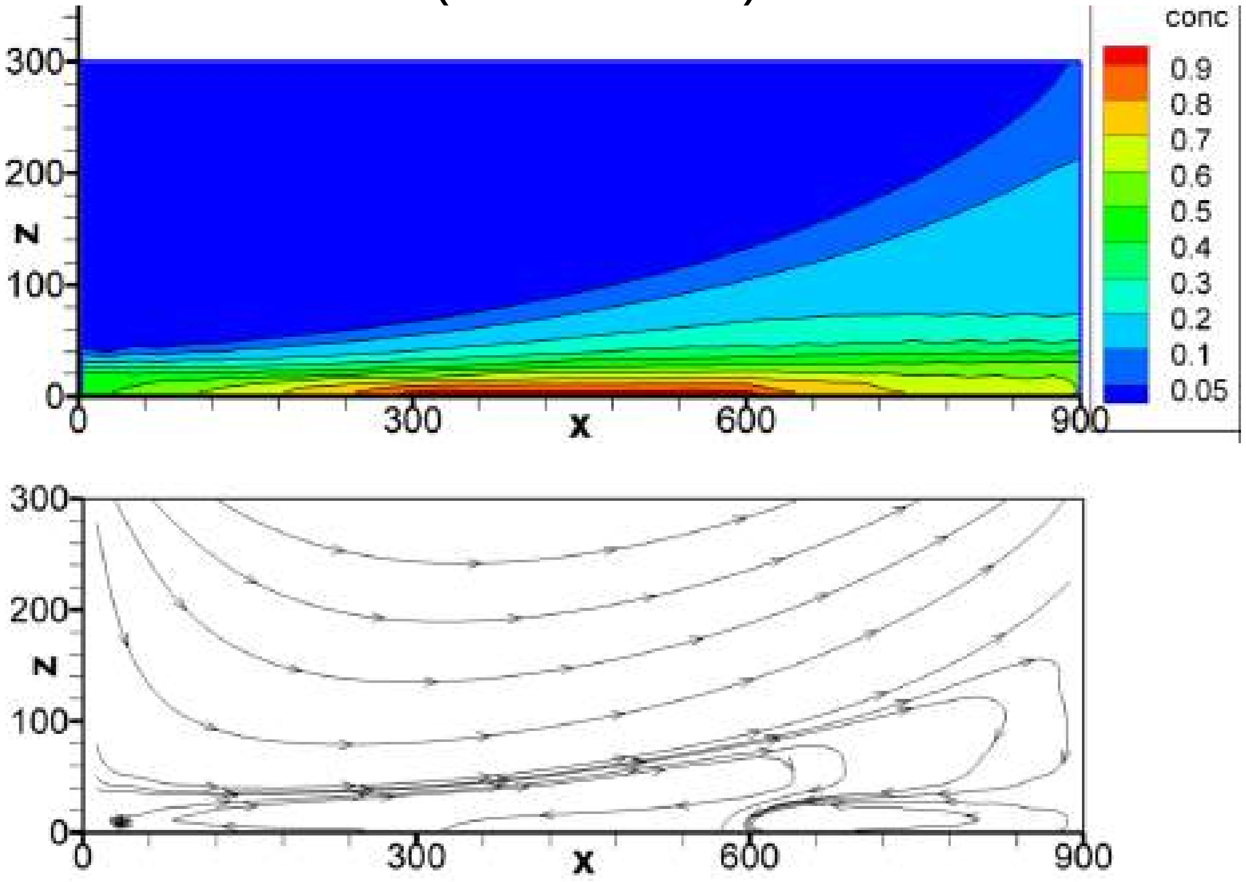


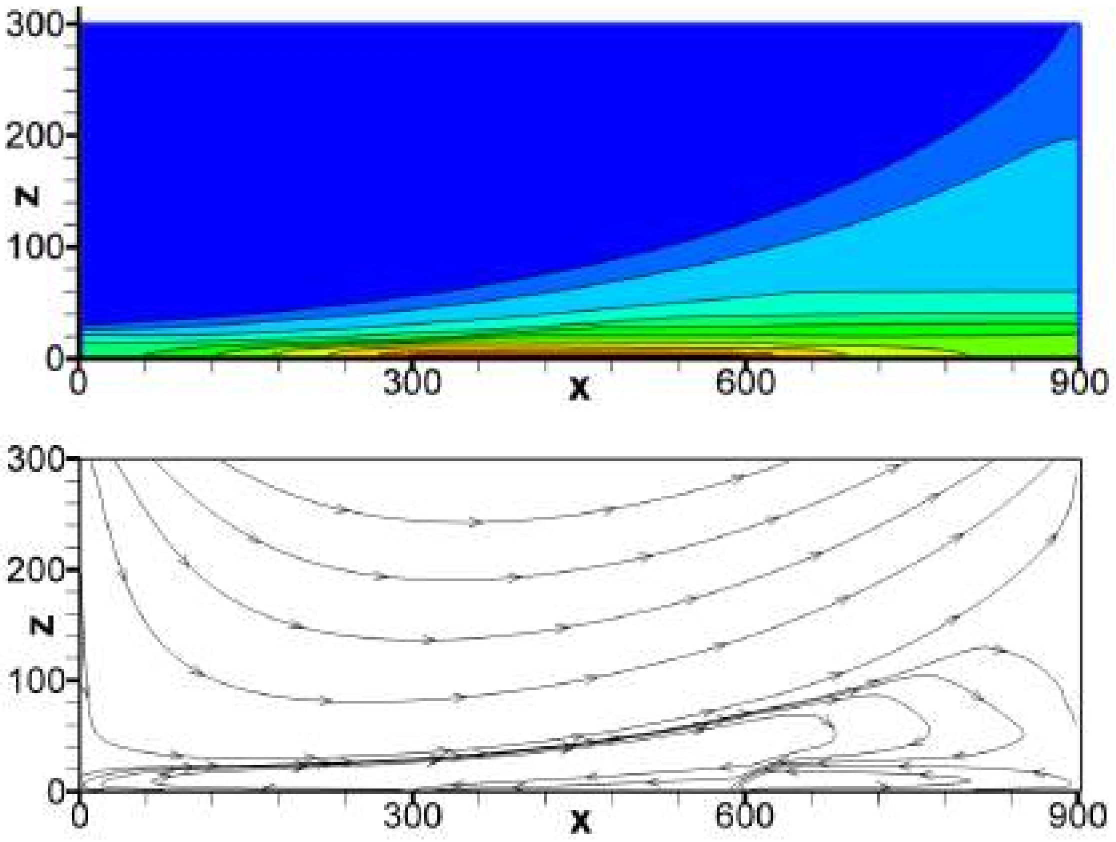
# 1. Research Objective: Salt Dome

## Grid Analysis – Some Results

**36 x-elements** (2700 in total)



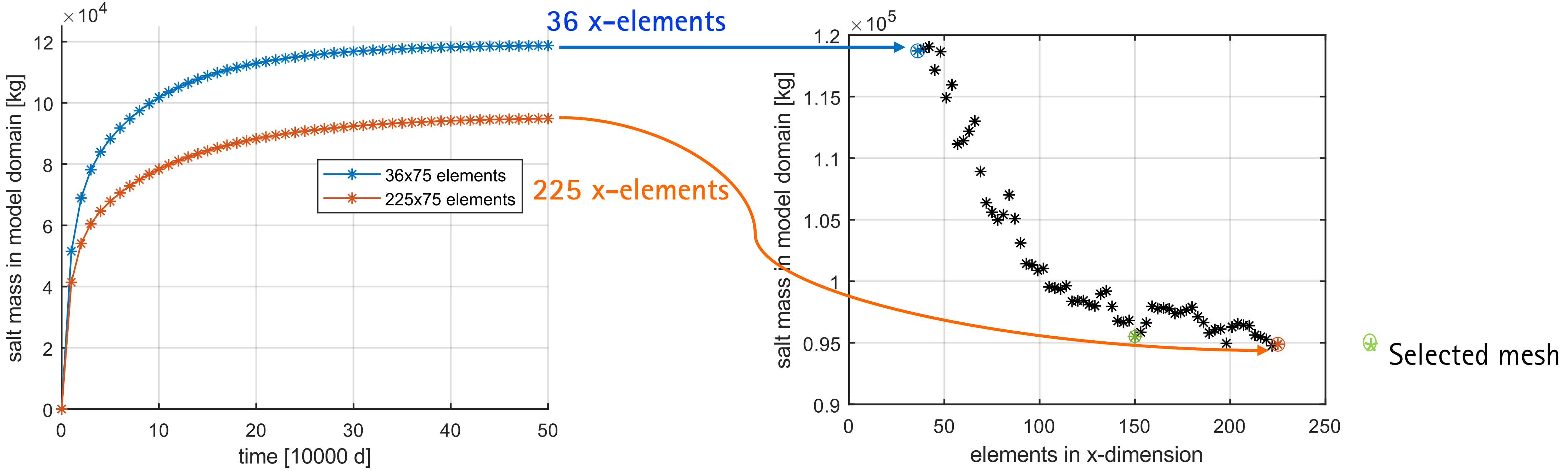

**225 x-elements** (16875 in total)



# 1. Research Objective: Salt Dome

## Grid Analysis – Some Results

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

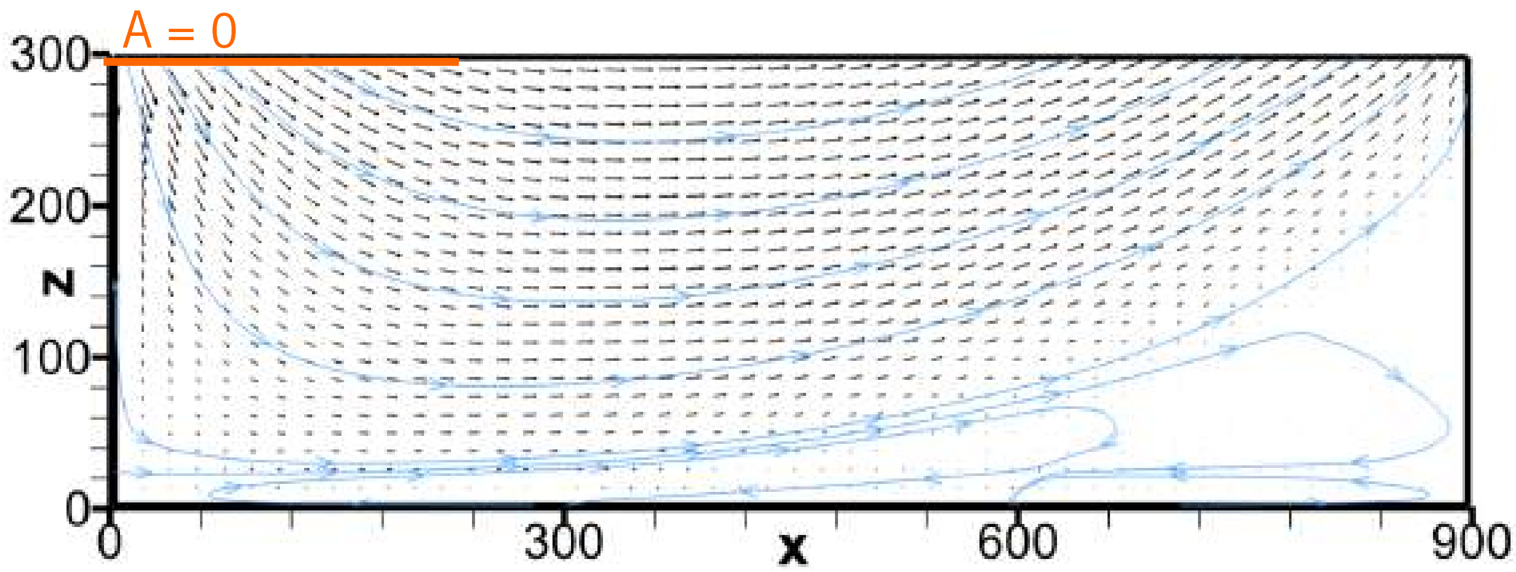


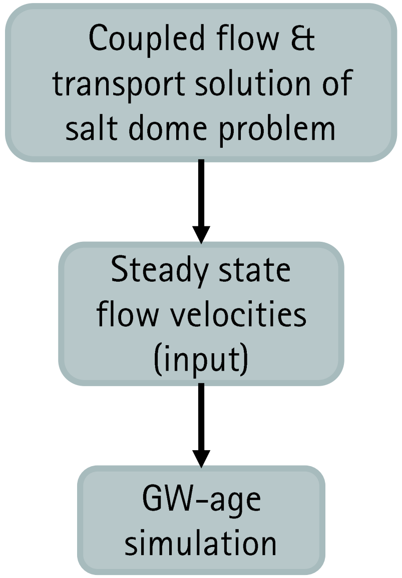

- 150 elements in x-dimension (11250 in total) are chosen (0.79 % deviation in salt mass)
- Aspect ratio 1.5

# 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)

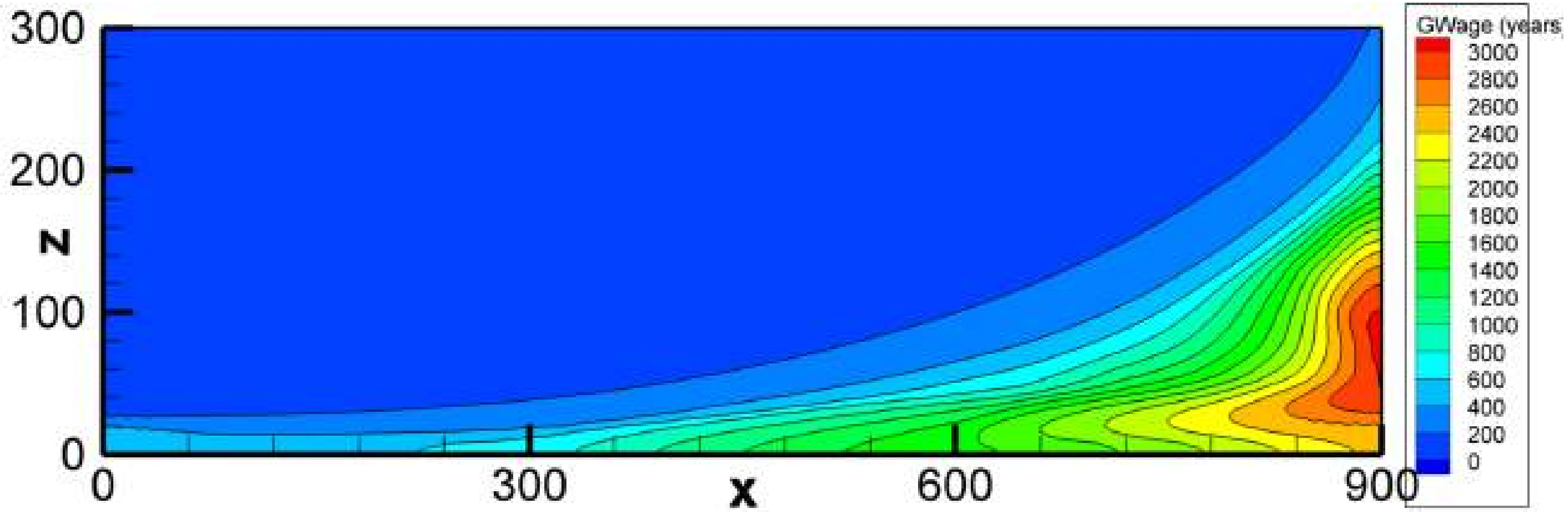


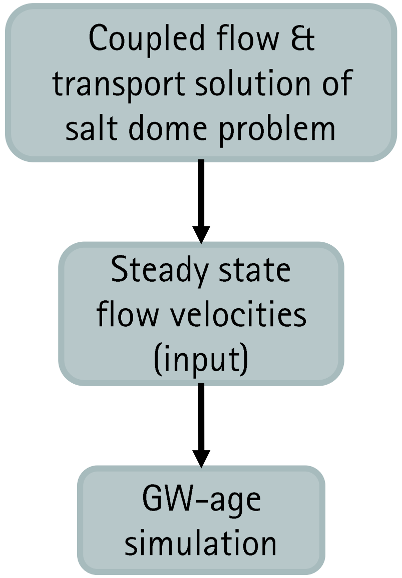



# 1. Research Objective: Salt Dome

## 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: $\alpha_L$ = [3 - 40] m; $\alpha_T$ = [0.3 - 4] m (scale-dependent)
- $\alpha_T$ as a Gaussian distribution with mean of 1/10 of $\alpha_L$
- 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

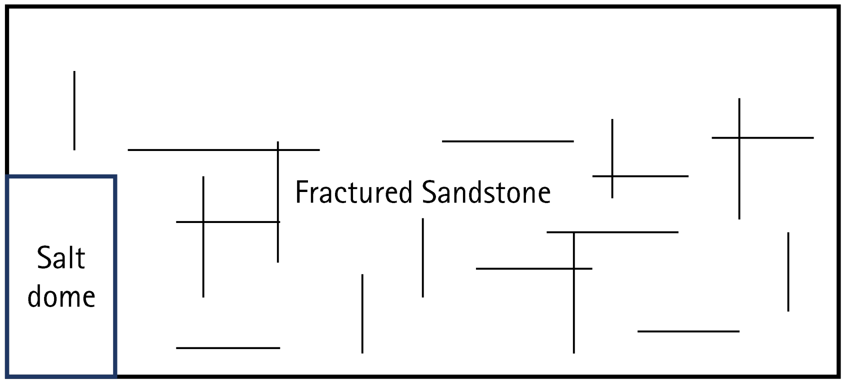
# 2. Research Objective: Salt Chimney Effect

**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

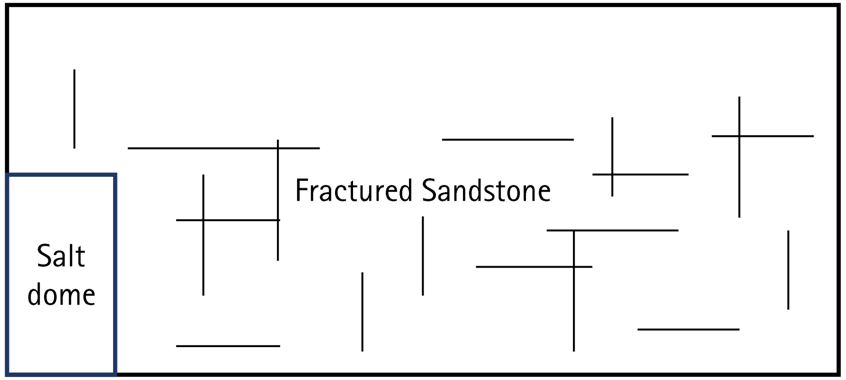


# 3. Research Objective: Implementation of Uncertainty

## 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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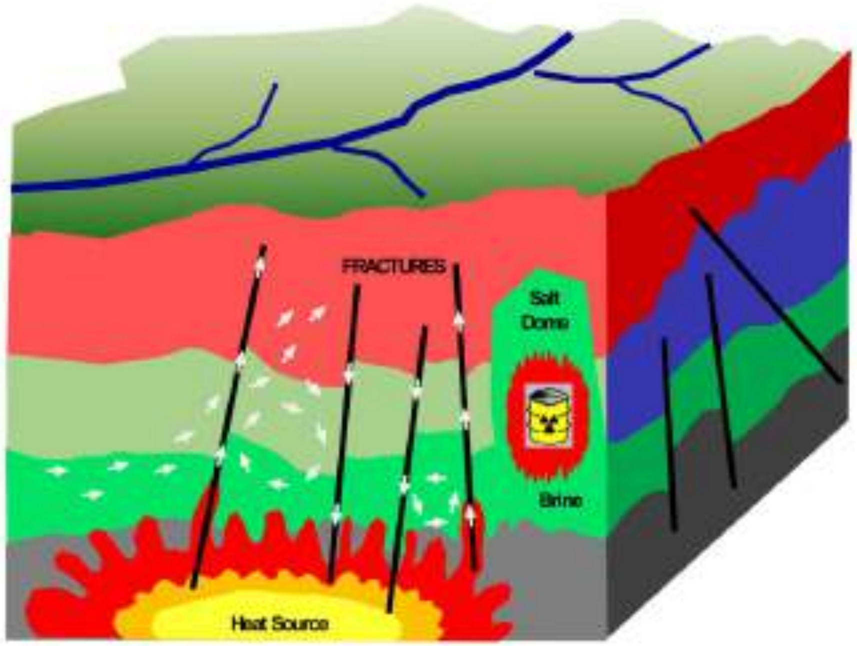
Thank




You !!!



**Thomas Graf**