

OpenTHMC
Developer Benchmark Book
BASED ON
OpenGeoSys
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Contributed by

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Chapter 1

Introduction

Scopus

The intention of the Developer Benchmark Book (DBB) is twofold:

- DDB provides a collection of test cases which are used for benchmarking the GeoSys code development.
- We recommend the benchmark collection for users as a starting point for their own GeoSys applications.

RockFlow, GeoSys, OpenTHMC, a historical note ...

Looking back to a more than 20 years lasting scientific project as "RockFlow" is amazing ... and at the same time completely impossible to be comprehensive and to be fair ...

RockFlow-1

Somewhen in the mid eighties Dr. Liedtke with the Federal Institute of Geosciences (BGR) was asking Prof. Zielke (Institute of Hydromechanics, University of Hannover) whether the development of a simulation programm for fractured rock is possible. (Never ask a scientist about impossible things). The idea was born (including some funding from the BGR): the development of a computer code based on multi-dimensional FEM. The first name was DURST, which for Germans is not really a good choice (because it means "thirsty"). Later it was renamed into Rockflow: Flow and associated processes in rock. The pioneering work of RockFlow-1 was done in the following four doctoral dissertations [1], [2], [3], [4].

RockFlow-2

The next stages in the early nineties was related to couple the individual RF-1 modules and improve the computational efficiency, e.g. by introducing iterative equation solver. RockFlow-2 was now used in several application projects as waste deposition and geothermal energy ([5],[6]). A "market" for RockFlow in Applied Geoscience was open. From this time the most cited RockFlow paper so far [7] originated (more than 70 times, which is not so bad for a modeling paper).

RockFlow-3

It turned out that the coupling of the different RF modules needed a new code structure. Moreover for the use of grid-adaptive methods dynamic data structures have been necessary. Consequently, in the late nineties a complete re-organization of RF was started. C experience began ... [8], [9]. Major research topics of the RF group had been multi-phase flow [10], grid adaptation [11], reactive transport [12], and deformation processes [13]. Beside the numerical parts geometric modeling and meshing methods became more and more important [14], [15].

GeoSys/RockFlow-4

Tuebingen: Due to the increasing functionality, the RF code became more and more sophisticated and difficult to handle. Consequently, the introduction of object-oriented methods was necessary. RF-4 or now GeoSys was (again) completely re-designed and rewritten in C++ [16], [17]. Several doctoral theses have been prepared in the fields of geotechnical simulation (DECOVALEX project, [18], [19], [20]), contaminant hydrology (Virtual Aquifer project, [21], [22], [23]), geothermal reservoir modeling (Urach Spa project, [24]). Aside computational mechanics progress had been made as well in the pre-processing for numerical analysis [25], [26], [27]. First GeoSys/RockFlow habilitations appeared [28], [29], [30]. As mentioned in the beginning it is impossible to cite everything, other important works in the Tuebingen era are [31], [32], [33].

GeoSys/OpenTHMC

Leipzig: The new challenge for GeoSys is to continue the development as a distributed open-source project, i.e. sharing and widening the knowledge, as people from the GeoSys group got interesting offers. The number of GeoSys-project partners is already quite large (see cover page). At the Helmholtz Center for Environmental Research a new research platform TESSIN is available, which combines high-performance-computing (HPC) and visualization facilities. Post-processing becomes more and more important as more and more information

becomes available, due to high-resolution measurement techniques and HPC itself [34].

Next ...

Benchmarks coming soon ...

- Matrix diffusion (CMCD, GK)
- Thermal signatures in soils and sediments (JOD)
- Gas flow (OK)
- Heat transport in gas flows (OK)
- Two-phase flow and CO₂ stuff (PCH)
- Biodegradation et al (Kiel: CB, SB)
- More overland flow (EK, SF)
- ...

Chapter 2

Heat Transport – T-Process

2.1 Theory

Heat transfer is the passage of thermal energy from a hot to a cold body. Transfer of thermal energy occurs, when a body and its surroundings have not reached thermal equilibrium yet.

Heat transfer can occur in three different ways:

- Conduction
- Advection
- Radiation

Conduction takes place when there is a temperature gradient in a solid or a stationary fluid medium. The conduction process takes place into the direction of decreasing temperature. The thermal conductivity is defined in order to quantify the ease with which a particular medium conducts. Against it, convection is caused by moving fluids of different temperatures, but in the following only conductive heat flow is considered.

Temperature changes cause a change of fluid density and viscosity which influences again the behaviour of the fluid while flowing through a porous medium and therefore the velocity of heat transport by groundwater flow. The dependence of density on temperature changes is regarded by using the relation given in equation 2.1.1.

$$\rho(T) = \rho_0 \cdot (1 + \beta_T (T - T_0)) \quad (2.1.1)$$

with

ρ_0 – initial density,

β_T – constant,
 T – temperature,
 T_0 – initial temperature.

Heat conduction equation:

$$\frac{\mathbf{p}T}{\mathbf{p}t} = \nabla \cdot (\alpha \nabla T) \quad (2.1.2)$$

where T is temperature, $\alpha = \lambda/c\rho$ is the heat diffusivity coefficient.

Heat transport equation:

$$c\rho \frac{\mathbf{p}T}{\mathbf{p}t} + c\rho \mathbf{v} \cdot \nabla T - \nabla \cdot (\lambda \nabla T) = Q_T \quad (2.1.3)$$

where c is specific heat capacity, ρ is density, \mathbf{v} is advection velocity, λ is thermal conductivity.

2.2 Linear heat diffusion

2.2.1 Problem definition

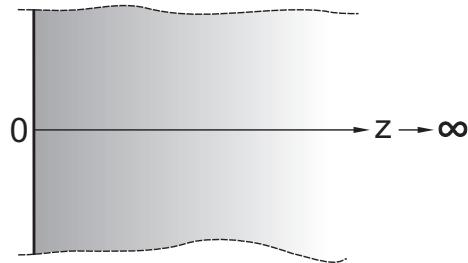


Figure 2.2.1: One side limited domain in cartesian coordinates

2.2.2 Analytical solution

The one dimensional heat transport in a domain limited just by one side can be derived by equation 2.2.1:

$$T(x, t) = T_0 \operatorname{erfc} \left(\frac{x}{\sqrt{4\alpha t}} \right) \quad (2.2.1)$$

where T_0 is the initial temperature and $\alpha = \lambda/c\rho$ is the heat diffusivity coefficient of the used material.

2.2.3 Numerical solution

Model setup

The numerical model consists of 60 line elements connected by 61 nodes along the z-axis (figure 2.2.3). The distances of the nodes Δz is one meter. At $z = 0m$ there is a constant temperature boundary condition.

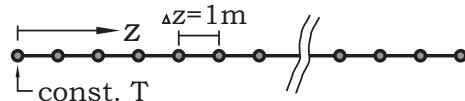


Figure 2.2.2: Spatial discretisation of the numerical model

Parameters

The material parameters for this model setup is given in table 2.2.3:

Table 2.2.1: Material properties

symbol	quantity	value
ρ	density of the solid	$2500 \text{ kg}\cdot\text{m}^{-3}$
c	thermal capacity	$1000 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
λ	thermal conductivity	$3.2 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$

Using these values, the diffusivity constant $\alpha = \lambda/c\rho$ outcomes to $\alpha = 1.28 \cdot 10^{-6} \text{ m}^2/\text{s}$.

Temporal discretisation

The *Neumann* stability criteria has to be restrained so that the temperature gradient can't be inverted by diffusive fluxes. Using equation 2.2.2 the best time step can be estimated:

$$\text{Ne} = \frac{\alpha \Delta t}{(\Delta z)^2} \leq \frac{1}{2} \quad (2.2.2)$$

with $\Delta z = 1 \text{ m}$ and $\alpha = 1.28 \cdot 10^{-6} \text{ m}^2/\text{s}$ the timestep outcomes to $\Delta t \leq 390.625 \text{ s}$ or 4.5 days respectively.

2.2.4 Results

The following figures shows the comparison of the solution of equation 2.2.1 and the numerical simulation results. Figure 2.2.3 shows the temperature distribution along the model domain after 2 months, 1 year, 2 years and 4 years.

Table 2.2.2: Benchmark deposit

Deposit	Version	Date
T\TDiff\TDiff	4.7.03	Jun. 2008

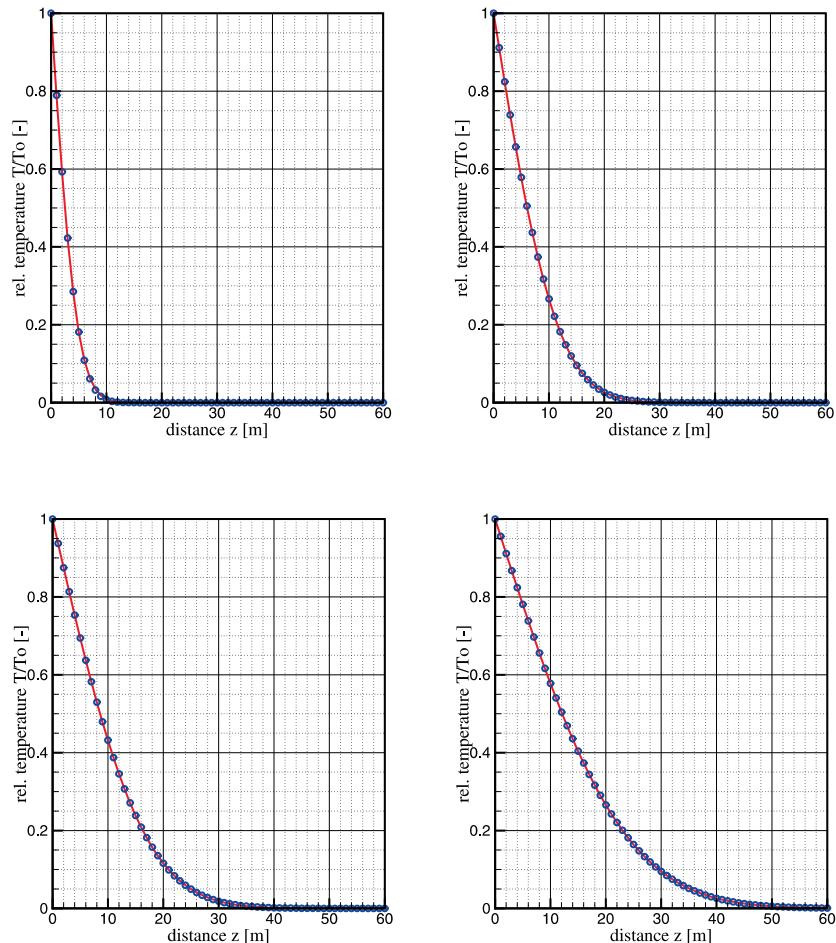


Figure 2.2.3: Temperature distribution along the z-axis after 2 months, 1 year, 2 years and 4 years

2.3 Linear heat diffusion in a wall

2.3.1 Problem definition

In the last example there was a domain limited only by one side with a constant temperature at the boundary. The following problem shows the profile of a homogeneous and isotropic wall with a constant heat flow Q_A on the left and a constant temperature T_L on the right boundary (fig. 2.3.1). This example consists also just of diffusive heat transport.

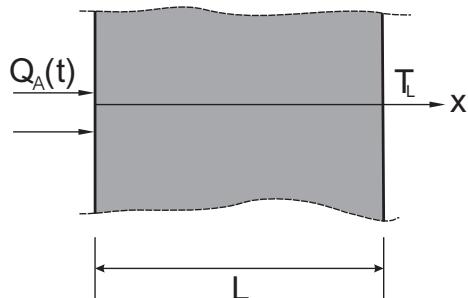


Figure 2.3.1: Heat conduction through a wall

2.3.2 Analytical solution

A solution for this problem can be found by solving the heat conduction equation (eq. 2.1.2) using *Fourier's* method (see [35]). It can be shown:

$$T(x, t) = T_L + \frac{Q_A}{\lambda} (L - x) + \sum_{n=1}^{\infty} -\frac{8L}{(2n-1)^2 \pi^2} \frac{Q_A}{\lambda} \cos \frac{(2n-1)\pi x}{2L} e^{-\frac{(2n-1)^2 \pi^2}{4L^2} \alpha t} \quad (2.3.1)$$

with

T_L – initial temperature,

Q_A – constant heat source,

λ – thermal conductivity,

α – heat diffusivity constant.

Table 2.3.1: Parameters and properties

symbol	quantity	value
Q_A	heat source	$30 \text{ W}\cdot\text{m}^{-2}$
T_L	initial temperature	25°C
L	wall thickness	4 m
ρ	density of the solid	$2000 \text{ kg}\cdot\text{m}^{-3}$
c	thermal capacity	$900 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
λ	thermal conductivity	$5.5 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$

Table 2.3.2: Benchmark deposit

Deposit	Version	Date
T\TDiff-wall\TDiff-wall	4.7.03	Jun. 2008

2.3.3 Numerical solution

Model setup

The numerical model consists of 40 line elements and 41 nodes along the x-axis (fig. 2.3.2). The step size Δz is set to 0.1m. On the left boundary a constant source term is set. The right side obtains a constant temperature.

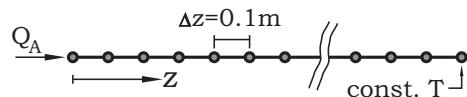


Figure 2.3.2: Boundary conditions and discretisation for the numerical model

Parameters

Table 2.3.3 shows the used parameters and material properties. The diffusivity constant α outcomes to $\alpha = 3.1 \cdot 10^{-6} \text{ m}^2/\text{s}$.

2.3.4 Results

The comparison of analytical and numerical solution is presented in figure 2.3.3. The figure shows the distribution of the temperature along the profile of the wall. Due to the thickness of the wall, the heat transport takes very long, after 5.000.000 seconds (≈ 58 days) the temperature distribution becomes steady-state.

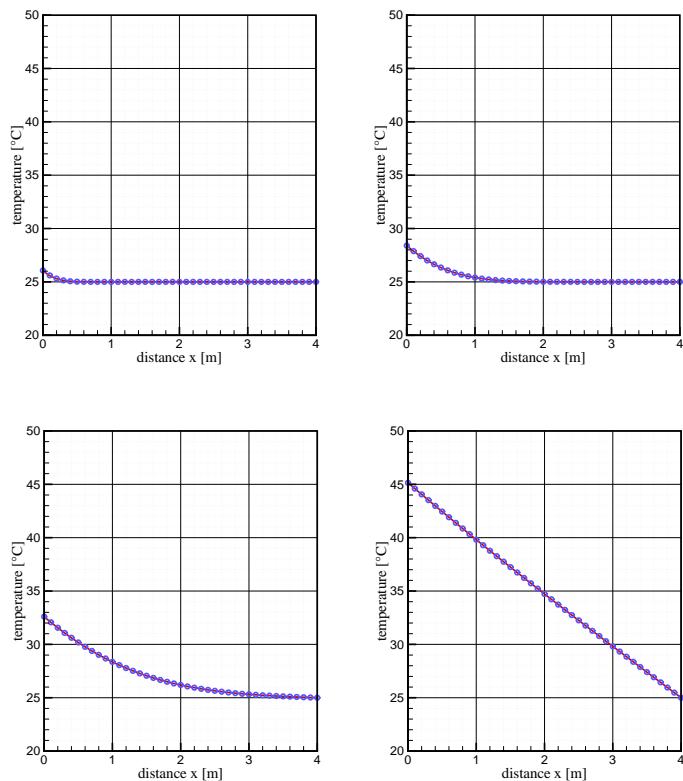


Figure 2.3.3: Temperature distribution along the wall profile after 10.000, 100.000, 500.000 and 5.000.000 seconds

2.4 Radial heat diffusion

2.4.1 Problem definition

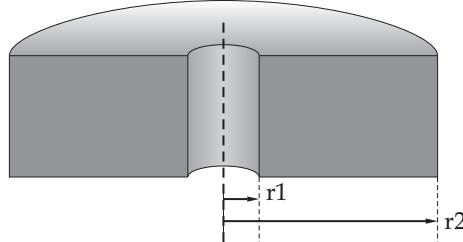


Figure 2.4.1: Calculation area

A slice with a hole in its centre, that means a 2 D annulus, which consists of a solid of a constant temperature is exposed to a higher temperature at the surface of its hole. The aim of this calculation is to simulate the heat transfer through this homogeneous solid by the use of an axisymmetric model. Figure 2.4.1 shows a sketch of the calculation area.

Assumptions

- | | |
|--------------|---|
| Temperature: | constant temperature in the whole body at the beginning,
heating of the slice at the inner surface of the hole |
| Solid: | homogeneous |

2.4.2 Model set-up of the 1 D numerical model

The inner radius R_1 of the axisymmetric model is 1 m and the outer radius R_2 5 m. The numerical model consists of 40 elements and 41 nodes. The initial temperature in the whole area is 25 °C. At the right boundary of the numerical model a thermal boundary condition is set with a constant value of 25 °C. At the left boundary a source term for heat flux of $q = 30 \text{ W/m}^2$ is defined. Thereby the continuous heating of the solid is simulated. The used parameters of the solid are listed in table 2.4.1. The simulation of 5000 time steps with a constant time step length of 1000 s is done.

Table 2.4.1: Used parameters

symbol	quantity	value
ρ	density of the solid	$2.0 \text{ t}\cdot\text{m}^{-3}$
c	thermal capacity	$900 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
λ	thermal conductivity	$5.5 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$

2.4.3 Evaluation method

For the heating of the annulus with the inner radius R_1 and the outer radius R_2 the following analytical solution for temperature in dependency on the radius r was used.

$$T(r) = \frac{R_1 q}{\kappa} \ln \left(\frac{R_2}{r} \right) + T_0 \quad (2.4.1)$$

with

q – heat source (W/m^2)

λ – thermal conductivity ($\text{W}/(\text{m}\cdot\text{K})$)

T_0 – initial temperature ($^\circ\text{C}$)

2.4.4 Results

The results of the analytical equation for the temperature distribution over the model length are compared to those of the numerical simulation by GeoSys/RockFlow. Figure 2.4.2 shows the temperature distribution over the radius of the annulus. Obviously, with the axisymmetric model a GeoSys/RockFlow simulation generates comprehensible results that agree well with the analytic solution.

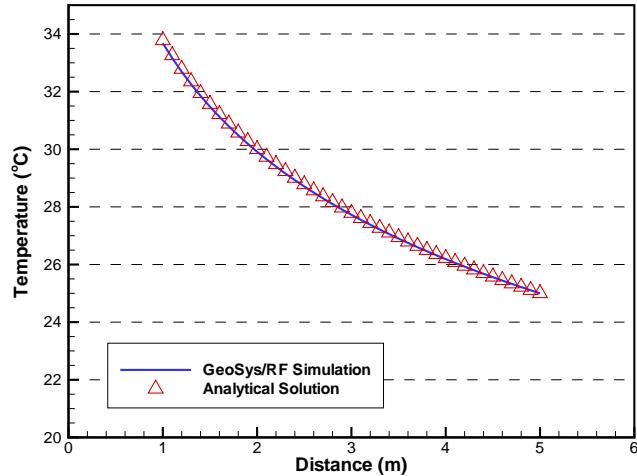


Figure 2.4.2: Temperature distribution over the radius

Table 2.4.2: Benchmark deposit

Deposit	Version	Date
T\heat1d\T_1D_axi	4.7.02	Mar. 2008

2.5 Temperature-dependent thermal properties

for coming version

2.6 Heat transport in a fracture

2.6.1 Problem definition

This problem shows 1D heat transport by advection and diffusion in a 100 m long fracture. The fracture is fully saturated with groundwater, flowing with constant velocity. There is no rock matrix around the fracture which could store heat.

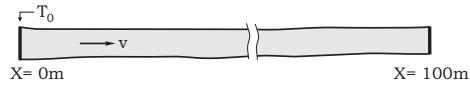


Figure 2.6.1: A fully saturated fracture with flowing groundwater and a constant temperature at the left border.

2.6.2 Parameters

The fracture is described as a porous medium with 100% porosity, so that no solid material influences the heat transport process. The properties of the fluid are given as:

Table 2.6.1: Fluid properties

symbol	quantity	value	unit
ρ	density	1000	$\text{kg}\cdot\text{m}^{-3}$
c	thermal capacity	4000	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
λ	thermal conductivity	0.6	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$

These values gives a diffusivity constant for water of $\alpha = 1.5 \cdot 10^{-7} \text{m}^2/\text{s}$. The groundwater velocity in the fracture is $v = 3.0 \cdot 10^{-7} \text{m}^2/\text{s}$.

2.6.3 Analytical solution

For 1D-advection/diffusive transport, an analytical solution is given by OGATA & BANKS as:

$$T(x, t) = \frac{T_0}{2} \left(\operatorname{erfc} \frac{x - v_x \cdot t}{\sqrt{4\alpha t}} + e^{\frac{v_x \cdot x}{\alpha}} \operatorname{erfc} \frac{x + v_x \cdot t}{\sqrt{4\alpha t}} \right) \quad (2.6.1)$$

Where T_0 is the constant temperature at $x = 0$, v_x is groundwater velocity, α is heat diffusivity coefficient of water (see [35],[36]).

2.6.4 Numerical solution

The mesh for the numerical model consists of 501 nodes combining 500 line elements. The distance between the nodes is $\Delta x = 0.2m$.

Boundary conditions: Left border:

- constant source term (liquid flow) with $Q = 3.0 \cdot 10^{-7} m^3/s$
- constant temperature with $T = 1^\circ C$

Right border:

- constant pressure with $P = 100,000$ kPa

Initial conditions:

- pressure with $P = 100,000.0$ kPa for whole domain
- temperature $T = 0^\circ C$ for whole domain

Time step:

- $\Delta t = 133,333.0$ s

With the given parameters, the NEUMANN criteria (eqn. 2.2.2) results on $Ne = 0.5$ which guarantees the numerical stability of the diffusion part of the transport process. The *Courant* criteria, given by:

$$C = \frac{v_x \cdot \Delta t}{\Delta x} \leq 1 \quad (2.6.2)$$

outcomes to $C = 0.2$.

2.6.5 Results

In Figure 2.6.2 the comparison of analytical and numerical solution is plotted. The figure shows the temperature breakthrough curve at the end of the fracture at $x = 100$ m. The numerical results show an acceptable agreement to the analytical solution. In a further step, the diffusion part of the heat transport process was avoided by minimizing the thermal conductivity of the fluid. Figure 2.6.3 shows the breakthrough curve for only advective heat transport.

Table 2.6.2: Benchmark deposit

Deposit	Version	Date
T\Ogata-Banks\Ogata-Banks	4.7.03	Jul. 2008

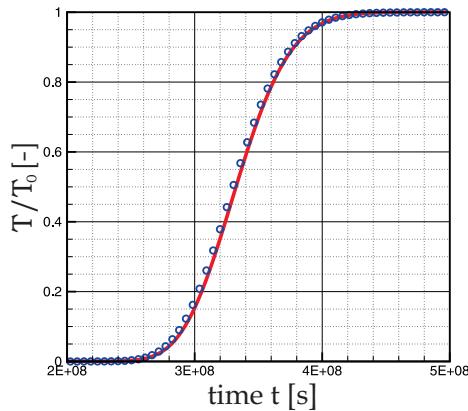


Figure 2.6.2: Temperature breakthrough curve at the point $x = 100$ m.

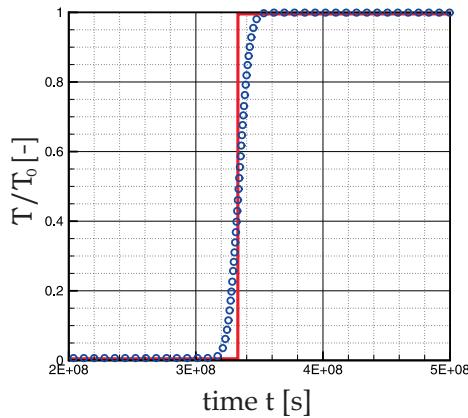


Figure 2.6.3: Temperature breakthrough curve when diffusion is avoided.

2.7 Heat transport in fracture-matrix systems

2.7.1 Problem definition

Based on the last benchmark example, the heat transport by advection and diffusion in a fracture, this problem is extended by heat diffusion through a rock matrix orthogonal to the fracture (fig. 2.7.1).

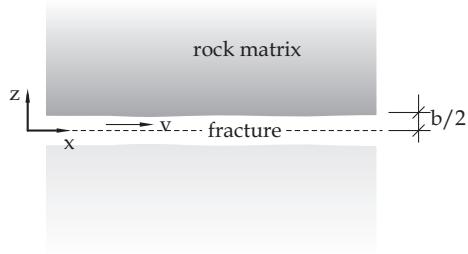


Figure 2.7.1: Heat transport in a fracture-matrix system

2.7.2 Analytical solution

For this problem an analytical solution is given by LAUWERIER (1955) (see [36]) with following restrictions:

- In the fracture, heat is transported just by advection
- In the rock matrix, heat transport takes place by diffusion (only along the z-axis)

The LAUWERIER equation is given by

$$T_D = \begin{cases} 0, & t_D < x_D \\ \operatorname{erfc} \left\{ \frac{\beta}{\sqrt{\alpha(t_D - x_D)}} \left[x_D + \frac{1}{2\beta} (z_D - \frac{1}{2}) \right] \right\}, & t_D > x_D, z_D \geq \frac{1}{2} \end{cases} \quad (2.7.1)$$

with the following dimensionless parameters:

$$t_D = \frac{v_x}{b} t, \quad x_D = \frac{x}{b}, \quad z_D = \frac{z}{b}, \quad \alpha = \frac{\lambda^r}{c^r \rho^r} \frac{1}{b v_x}, \quad \beta = \frac{\lambda^r}{c^w \rho^w} \frac{1}{b v_x}$$

where b is fracture width, λ is thermal conductivity, c is heat capacity, ρ is density and r & w are rock or water material parameters respectively.

2.7.3 Model setup

The LAUWERIER-problem is formed as a coupling of advective 1D heat transport in x -direction and diffusive 1D heat transport in z -direction. This means, that nodes in the rock matrix are not influenced by their left or right neighbors. The matrix elements are connected to the fracture elements orthogonally. Figure 2.7.2 shows a schematical description of the model setup. Because of the symmetry, the numerical model calculates just the domain above the X-axis.

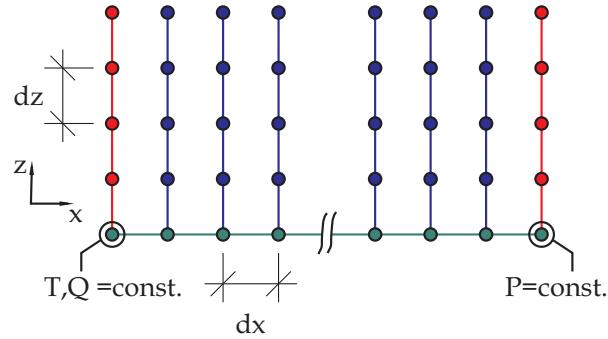


Figure 2.7.2: Alignment of the grid for the numerical model

Figure 2.7.3 shows the positions of observation points which were chosen to evaluate the numerical model by the comparison with analytical solutions.

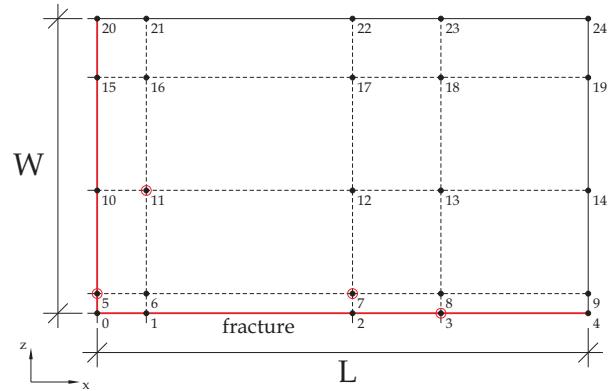


Figure 2.7.3: Positions of observation points for temperature breakthrough curves.

2.7.4 Parameters

The chosen parameters and material properties for this solution are shown in table 2.7.1.

Table 2.7.1: Model parameters for LAUWERIER-problem

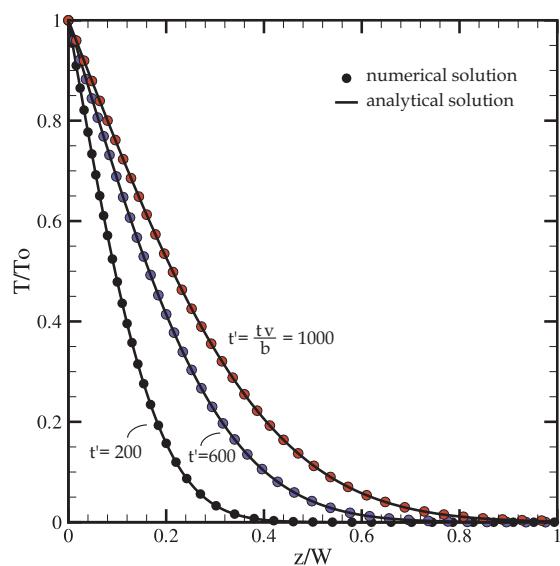
description	symbol	unit	value
<i>spatial discretisation</i>			
fracture length	L	[m]	50
matrix width	W	[m]	63.25
step size X	Δx	[m]	2
step size Z	Δz	[m]	0.1265
half of fracture width	b/2	[m]	$1.0 \cdot 10^{-3}$
groundwater velocity	v_x	[m/s]	$1.0 \cdot 10^{-4}$
<i>temporal discretisation</i>			
timesteps	Δt	[s]	$2.0 \cdot 10^5$
No. of timesteps		[\cdot]	2500
total time		[s]	$5.0 \cdot 10^8$
<i>material properties</i>			
<i>solid</i>			
thermal conductivity	λ	[$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$]	1
heat capacity	c	[$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$]	1000
density	ρ	[$\text{kg} \cdot \text{m}^{-3}$]	2500
<i>fluid</i>			
heat capacity	c	[$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$]	4000
density	ρ	[$\text{kg} \cdot \text{m}^{-3}$]	1000

2.7.5 Results

The quality of the numerical results can be shown by temperature distribution curves for several times in the rock matrix. Figure 2.7.6 shows the temperature profiles for $x = 0$ m at three moments t' . The numerical solution has a very good agreement to the analytical results. Temperature profiles along the fracture at $z = 0$ m are plotted in figure 2.7.5. For long simulation times ($t' = 1000$; $t' = 600$) both solutions fits very well together. For short simulation times, the numerical solution differ slightly from the analytical results. This discrepancy for short simulation times can be examined in figure 2.7.6, where temperature breakthrough cures for certain points (see figure 2.7.3) is plotted.

Table 2.7.2: Benchmark deposit

Deposit	Version	Date
T\Laue\Laue	4.7.03	Jul. 2008

Figure 2.7.4: Temperature distribution orthogonal to the fracture at $x = 0$ at three different times.

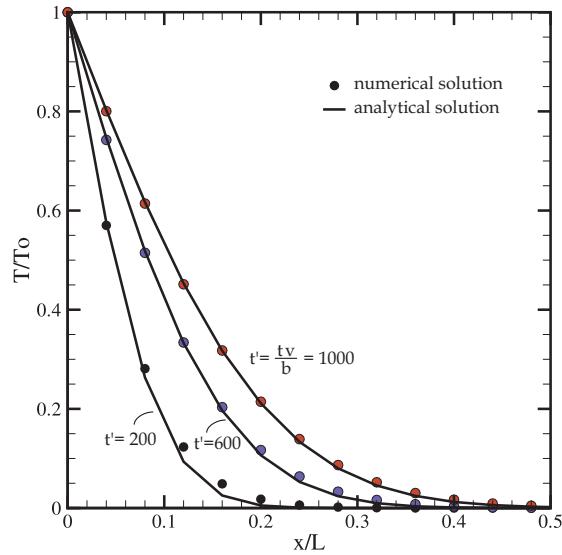


Figure 2.7.5: Temperature distribution along the fracture at three different times.

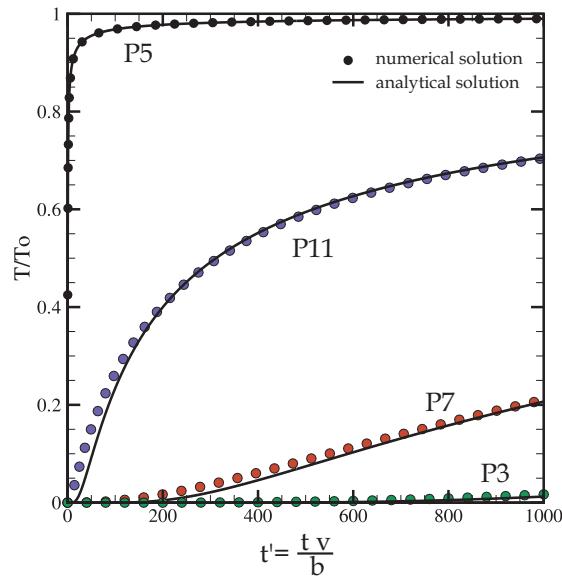


Figure 2.7.6: Temperature breakthrough curves at certain points in the rock matrix.

2.8 Heat transport with temperature dependent fluid properties

2.8.1 Problem definition

A 1 D test example for groundwater flow and simultaneous heat transport in the aquifer is made. The aim of the numerical simulation with GeoSys/RockFlow is to get out if the consideration of varying density with temperature changes is possible.

Assumptions

Aquifer:	homogeneous, saturated, stationary flow
Fluid flow:	incompressible fluid, non-isothermal

2.8.2 Model set-up of the 1 D numerical model

For the 1-dimensional calculation the calculation area is simplified as a line of a length of 5.2 m. The calculation model includes 25 elements and 26 nodes. The initial pressure in the whole area is 100 kPa and the initial temperature 300 K. As boundary condition a constant pressure of 101 kPa is given at the left boundary and of 100 kPa at the right boundary. A constant temperature of 400 K is set at the left boundary. The used soil parameters are listed in table 2.8.1. The fluid density is decreasing with increasing temperature. The viscosity, capacity and conductivity of water are set to constant values. The fluid parameters can be found in table 2.8.2.

Table 2.8.1: Used soil parameters

parameter	value	unit
porosity ϕ	0.01	-
permeability K	$1.0 \cdot 10^{-11}$	m^2
density	2850	$kg \cdot m^{-3}$
heat expansion	$1 \cdot 10^{-5}$	K^{-1}
heat capacity	1000	$J \cdot (kg \cdot K)^{-1}$
heat conductivity	3.2	$W \cdot (m \cdot K)^{-1}$

2.8.3 Validation method

In order to find out whether the consideration of varying water density with temperature changes is possible, one simulation run is done with a constant density of 1000 kg/m^3 which is the initial water density before heating and one

Table 2.8.2: Used fluid parameters

parameter	value	unit
initial density	1000	$\text{kg}\cdot\text{m}^{-3}$
viscosity	0.001	$\text{N}\cdot\text{s}\cdot\text{m}^{-2}$
heat capacity	4000	$\text{J}\cdot(\text{kg}\cdot\text{K})^{-1}$
heat conductivity	0.6	$\text{W}\cdot(\text{m}\cdot\text{K})^{-1}$

run with a constant density of 900 kg/m^3 , the density after the heating process. The temperature results for a heat transport with varying density have to be in between both temperature evolution curves.

2.8.4 Results

The curve for temperature evolution, which is shown in figure 2.8.1 for the right boundary (node 26), shows the expected characteristics. Therefore it can be stated, that the consideration of temperature dependent fluid density is possible.

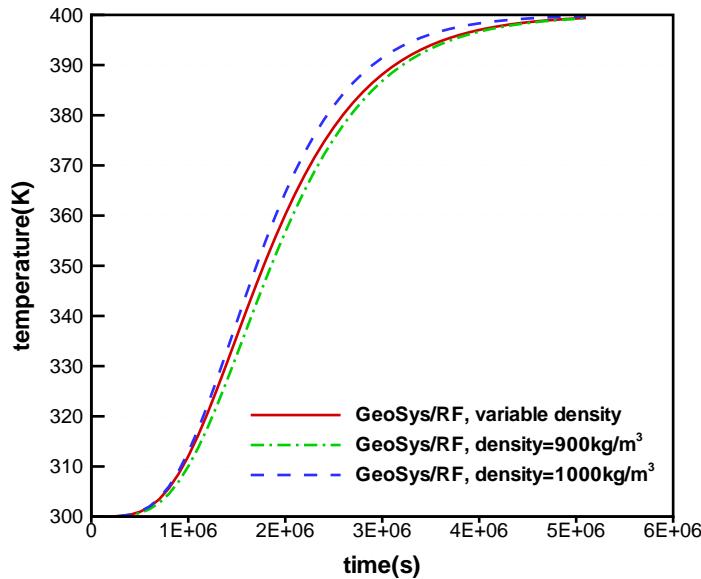


Figure 2.8.1: Temperature evolution with constant and variable fluid densities

Table 2.8.3: Benchmark deposit

Deposit	Version	Date
\HT_var_density_1D	rf4.7.02	March 2008

Chapter 3

Groundwater flow – H-Processe

This chapter deals with saturated subsurface flow. In the aquifer concept balance equations determine strictly horizontal flow and vertical flow can be included by leakage terms through confining beds. The leakage terms add or subtract water from aquifers overlying and underlying a leaky confining bed according to the aquifer's head difference and a confining bed conductivity. An aquifer which contains a water table is termed unconfined and a completely filled aquifer is termed confined. The governing equations for three-dimensional groundwater, confined, and unconfined aquifer flow are introduced in Sec. 3.1. In Sec. 3.3 the benchmarks for confined and in Sec. 3.4 for unconfined aquifers are introduced. Groundwater flow is solved two- and three dimensionally in the benchmark examples.

3.1 Theory

A three-dimensional description of groundwater flow is given by the mass balance equation

$$S_s \frac{\partial h}{\partial t} - \nabla \cdot \frac{\rho g}{\mu} \kappa \nabla h = q^{ex} \quad (3.1.1)$$

where the head h is the primary variable of groundwater flow and S_s is the specific storage which is assumed to be independent of the head neglecting fluid and soil matrix compression. Use of Darcy's law for momentum balance leads to the fluid density ρ , dynamic fluid viscosity μ , gravity constant g , and aquifer permeability matrix κ . Finally q^{ex} denotes external sources and sinks. Depth integration leads to the two-dimensional Boussinesq equation which describes

unconfined aquifers and reads

$$S_y \frac{\partial h}{\partial t} - \nabla \cdot \frac{\rho g h}{\mu} \kappa \nabla h = q^{ex} \quad (3.1.2)$$

where S_y is the specific yield. For confined aquifers Eq. 3.1.2 becomes

$$S \frac{\partial h}{\partial t} - \nabla \cdot \frac{\rho g L}{\mu} \kappa \nabla h = q^{ex} \quad (3.1.3)$$

where S is the storage and L the aquifer thickness. The aquifer thickness L is taken into account by changing the soil permeability κ in the following benchmark examples. A channel source term can be assigned according to

$$q^{ex} = K_A \frac{P}{B} \frac{h^{sur} - h^{sub}}{a} \quad (3.1.4)$$

where K_A is the channel bed conductivity, B the channel width, a the channel bed thickness, and h^{sur} the channel flow head. The wetted perimeter $P = 2(h^{sur} - z^{sur}) + B$ for rectangular channel where z^{sur} is the height of the top of the channel bed. Groundwater head h is taken into account by

$$h^{sub} = \max(h, z^{sur}). \quad (3.1.5)$$

Leakage terms between adjacent aquifers can be defined accordingly.

3.2 Linear groundwater flow

Theory

Water flow in a saturated porous medium is influenced by the pressure gradient over a given distance and the hydraulic conductivity of the aquifer. By Darcy's Law (equ. 3.2.1) the flow rate by considering these influences can be calculated.

$$v_f = k_f \cdot i \quad (3.2.1)$$

with

- v_f – flow rate (m/s),
- k_f – hydraulic conductivity (m/s),
- i – pressure gradient (-).

The hydraulic conductivity is calculated by the following relation.

$$k_f = \frac{\kappa \cdot \rho \cdot g}{\mu} \quad (3.2.2)$$

with

κ – permeability (m^2)

ρ – density of the fluid ($\text{kg}\cdot\text{m}^{-3}$)

g – gravity constant ($\text{m}\cdot\text{s}^{-2}$)

μ – dynamic viscosity of the fluid ($\text{Pa}\cdot\text{s}$)

By using the law of continuity the discharge through a defined cross section can be calculated.

$$Q = v_f \cdot A \quad (3.2.3)$$

with

Q – discharge (m^3/s)

A – cross section (m^2)

Layered soil material is possibly less permeable in one direction than in the direction perpendicular to it. In this case the input of different values for the permeability κ in dependence on the direction of anisotropy is possible in RockFlow.

3.2.1 Flow in an isotropic medium

Problem definition

This test example for groundwater flow is taken from the RockFlow Tutorial A (Maßmann, 2004). The aim of this example is to simulate the stationary groundwater flow in a homogeneous aquifer. Figure 3.2.1 shows a sketch of the calculation area.

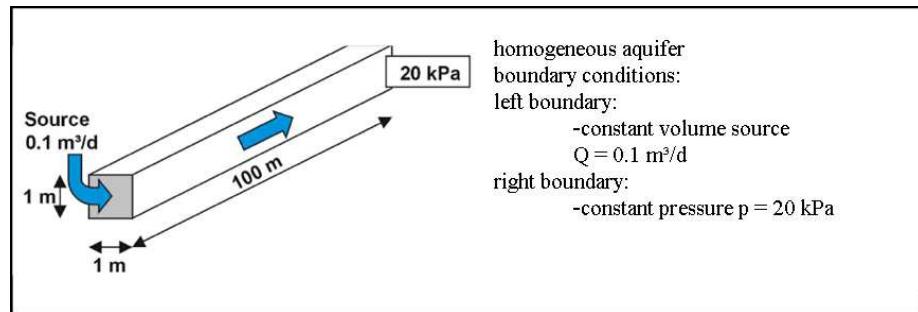


Figure 3.2.1: Calculation area: homogeneous aquifer (Maßmann, 2004)

Assumptions

Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

For the 1-dimensional calculation the calculation area is simplified as a line of a length of 100 m. The calculation model includes 100 elements and 101 nodes. As boundary condition the source volume of the fluid phase of $0.1 \text{ m}^3/\text{d}$ is given at the left border of the calculation area and the constant pressure of 20 kPa at the right boundary. The used parameters of the soil are listed in table 3.2.1.

parameter	value	unit
porosity Φ	0.2	–
permeability κ	$1.0 \cdot 10^{-12}$	m^2

Table 3.2.1: Used parameters

Evaluation method

The constant flow rate v_f is calculated by using equation 3.2.3. In order to calculate the pressure at the left border of the calculation model, Darcy's Law is applied in the following way. The second relation (eq. 3.2.4) shows that the pressure gradient is linear.

$$i = \frac{Q}{k_f \cdot A} = \frac{Q}{K \cdot \frac{\rho \cdot g}{\eta} \cdot A} = \frac{1.157 \cdot 10^{-6} \frac{\text{m}^3}{\text{s}}}{9.81 \cdot 10^{-6} \frac{\text{m}}{\text{s}} \cdot 1 \text{ m}^2} \quad \text{and} \quad p_{\text{left}} = p_{\text{right}} + \rho \cdot g \cdot i \cdot l \quad (3.2.4)$$

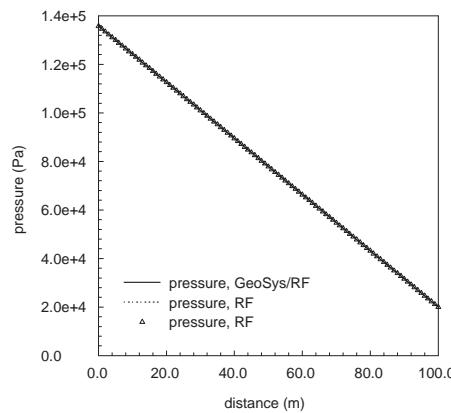


Figure 3.2.2: Pressure distribution over the distance of 100 m

Results

In figure 3.2.2 you can find the pressure distribution over the whole length of the 1 D model that was calculated by GeoSys/RockFlow. In addition, the analytically calculated pressure distribution is depicted in this figure. These pressure values match the numerical results well.

Benchmark	Problem type	Path in benchmark deposit
h_sat_flow_1d	H	benchmarks \H\sat_1D

3.2.2 Flow in an anisotropic medium

Problem definition

The aim of this example is to simulate the stationary groundwater flow in an anisotropic porous medium. In order to consider the anisotropy of permeability, a 2 D numerical model was built which contains a higher permeability in the vertical than in the horizontal direction.

Assumptions

Aquifer: anisotropic, saturated, stationary flow

Model set-up of the 2 D numerical model

For the 2-dimensional simulation, the cube consisting of a porous medium is simplified as a square with an area of 1 m². The calculation model includes 736 triangular elements and 409 nodes. At the left corner at the bottom of the model a constant pressure of 1000 Pa is specified along two polylines of the length of 0.3 m (3.2.3). At the top and the right border the pressure is set to 0 in order to create a pressure gradient. As the porous medium is assumed to be anisotropic, which influences the groundwater flow, the values for permeability are equal to $1.0 \cdot 10^{-15}$ m² in x-direction and $1.0 \cdot 10^{-14}$ m² in y-direction.

parameter	value	unit
porosity Φ	0.2	–
permeability κ_x	$1.0 \cdot 10^{-15}$	m ²
permeability κ_y	$1.0 \cdot 10^{-14}$	m ²

Table 3.2.2: Used parameters

Evaluation method

This test example is not made up to introduce a new process, but it shows the possibility for the GeoSys/RockFlow user to give a specific permeability for each

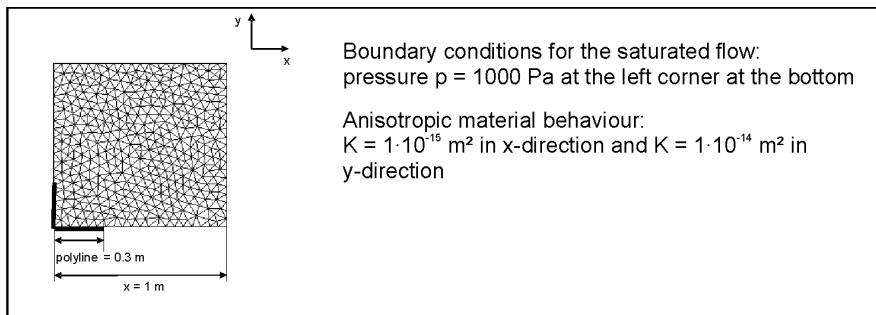


Figure 3.2.3: Calculation model (2 D)

direction. Therefore, the interpretation of GeoSys/RockFlow results comprises merely the comparison between pressure distributions due to anisotropic groundwater flow that were simulated by the use of RockFlow and GeoSys/RockFlow. This comparison is possible because both versions are developed separately concerning anisotropy of soils.

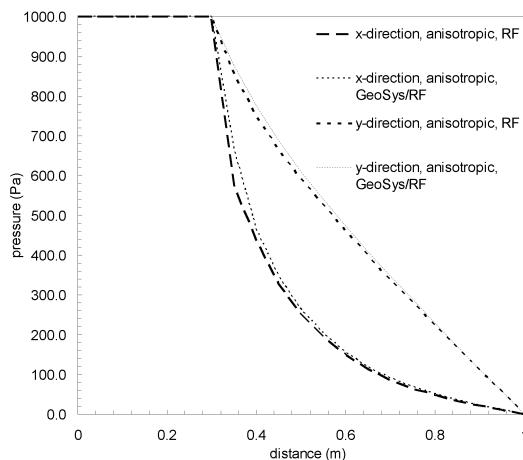


Figure 3.2.4: Pressure distribution caused by anisotropic saturated flow

Results

In figure 3.2.4 the horizontal and vertical pressure distributions of an anisotropic groundwater model which is made using the program code RockFlow are depicted next to the pressure distributions of the described anisotropic model. While presuming an anisotropic medium, an inhomogeneous pressure field is developing, because the groundwater is not able to spread out uniformly. This

can be recognized at the different curve gradients in x- and y-direction. There are slight differences between the curve characteristics of the RockFlow and the GeoSys/RockFlow simulation results. These differences are due to different element types (square in the RockFlow model) and the resulting differing x- or y-coordinates. Therefore, the pressure distributions that are obtained by the simulation with GeoSys/RockFlow are evaluated to be correct.

Benchmark	Problem type	Path in benchmark deposit
H_sat_flow_K_ortho	H	benchmarks \H\sat_2D

3.2.3 Flow in an isotropic and heterogeneous medium

Problem definition

The aim of this example is to simulate the stationary groundwater flow in an isotropic and heterogeneous porous medium. In order to consider the heterogeneous of permeability, a 2 D numerical model was built. The heterogeneous distribution of permeability is showed in 3.2.5.

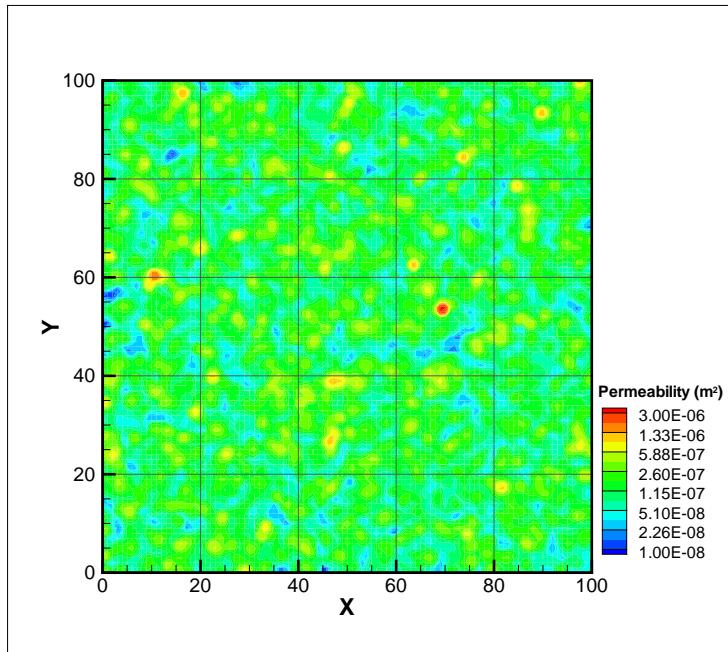


Figure 3.2.5: Calculation model(2 D): heterogeneous permeability distribution

Assumptions

Aquifer: isotropic, heterogeneous, saturated, stationary flow

Model set-up of the 2 D numerical model

For the 2-dimensional simulation, the cube consisting of a porous medium is simplified as a square with an area of 10000 m². The calculation model includes 10000 quad elements and 10201 nodes. At the left boundary a constant head of 10 m and the right boundary a constant head of 9 m are specified in order to create a pressure gradient.

Results

In figure 3.2.6 the horizontal and vertical head distributions of a groundwater flow in a heterogeneous medium are depicted responding to the distribution of the permeability.

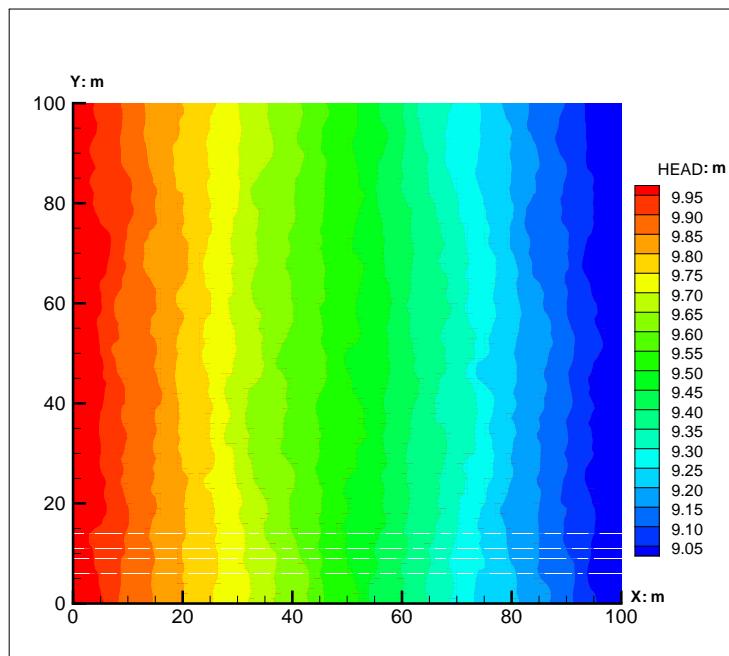


Figure 3.2.6: Head distribution responded to isotropic and heterogeneous medium

Benchmark	Problem type	Path in benchmark deposit
2D1P-GWFlow	H	benchmarks \H\HetGWFlow

3.3 Confined aquifer

3.3.1 Constant source term

Problem definition

These examples deal with an aquifer which is subject to a constant recharge line source. [37] presented an analytical solution for a constant line source on an infinite domain which reads for the groundwater head at the source

$$h = q^{ex} \sqrt{\frac{\mu t}{\pi \rho g k L S_y}}. \quad (3.3.1)$$

The aquifer size is $20m \times 10m$ with the source term at one boundary (See Fig. 3.3.2). The simulation time is $30min$.

Initial and boundary conditions

Initial groundwater head is $0m$. The source term is $2 \times 10^{-4}m/s$, groundwater head is 0 at the opposite boundary, and at the remaining part no-flow is imposed.

Material properties

For the spatial discretization 24×12 quadrants or hexahedra are used. The hexahedra have a height of $1m$. Material parameters are given in Tab. 3.3.1.

Table 3.3.1: Parameters for the constant source term examples

Parameter	Symbol	Setting	Unit
Storage	S	0.2	–
Specific storage	S_s	0.2	$1/m$
Viscosity	μ	1×10^{-3}	$Pa \cdot s$
Thickness	L	1	m

Results

Simulation results are compared with the analytical solution in Fig. 3.3.1

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
q_quad	H	benchmarks\GROUNDWATER_FLOW\
q_hex	H	benchmarks\GROUNDWATER_FLOW\

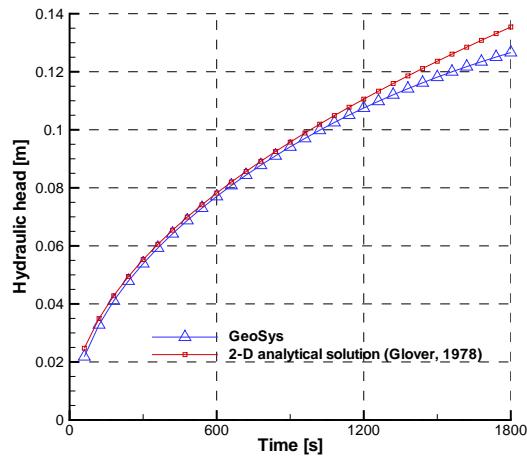


Figure 3.3.1: Results and analytical solution for confined aquifer with line source term

3.3.2 Channel source term

Problem definition

For these examples the source term of the previous examples (Sec. 3.3.1) is substituted by a corresponding channel source term (Eqn. 3.1.4). The channel is assumed to be not affected by the water loss and the exchange flux is independent of the groundwater head. Therefore, the source term represents a steady and uniform channel located above the aquifer. The cross-section of the channel is rectangular. The setup, spatial discretization, and calculated water head are shown in Fig. 3.3.2. The simulation time is 30min.

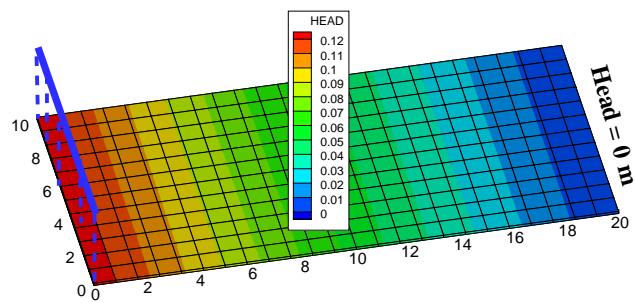


Figure 3.3.2: Computational domain and (channel) source term location

Initial and boundary conditions

The initial groundwater head is $0m$. The channel source term is the boundary condition at one side, at the opposite boundary the head is fixed 0 . At the remaining boundaries no-flow is imposed.

Material properties

For the spatial discretization either 24×12 quadrants or hexahedra are used as well prisms which are generated by cutting the hexahedra in two parts. The hexahedra or prism height is $1m$. The time step is $1min$. Simulation parameters for the aquifer and the channel source term are given in Tab. 3.3.3.

Table 3.3.2: Parameters for channel source term examples

Parameter	Symbol	Setting	Unit
Aquifer			
Storage	S	0.2	–
Specific storage	S_s	0.2	$1/m$
Viscosity	μ	1×10^{-3}	$Pa \cdot s$
Thickness	L	1	m
Channel source term			
Head	h^{sur}	4	m
Bed top location	z^{sur}	1	m
Width	B	14	m
Conductivity	K_A	1×10^{-6}	m/s
Thickness	a	0.3	m

Results

Comparison of simulation results and analytical solution is given in Fig. 3.3.3 for quadrants and in Fig. 3.3.4 for hexahedra.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>riv1_quad</i>	H	benchmarks\GROUNDWATER_FLOW\
<i>riv1_pris</i>	H	benchmarks\GROUNDWATER_FLOW\
<i>riv1_hex</i>	H	benchmarks\GROUNDWATER_FLOW\

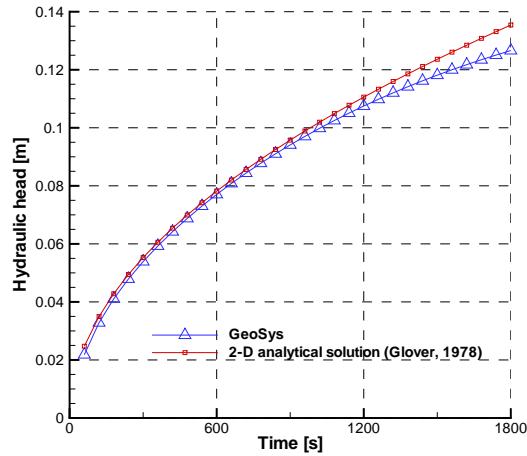


Figure 3.3.3: Results with quadratic elements and analytical solution for confined aquifer below uniform and steady channel

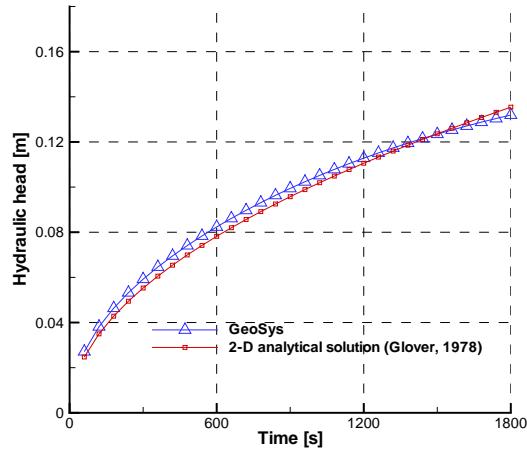


Figure 3.3.4: Results with hexahedral and prismatic elements compared with the analytical solution for confined aquifer below uniform and steady channel

3.3.3 Channel sink term

Problem definition

For this example the channel of the previous examples (Sec. 3.3.2) is located such that flow from the aquifer to the channel takes place. Therefore, the source

term represents a steady and uniform rectangular channel located in the aquifer. The setup is shown in Fig. 3.3.2. The simulation time is 30min .

Initial and boundary conditions

Initial groundwater head is 0m . The channel source term is the boundary condition at one side, at the opposite boundary the head is 0 . At the other boundaries no-flow is imposed.

Material properties

The domain is discretization with 24×12 quadrants. The time step size is 1min . Simulation parameters for the aquifer and the channel source term are given in Tab. 3.3.3.

Table 3.3.3: Parameters for the channel sink term example

Parameter	Symbol	Setting	Unit
Aquifer			
Storage	S	0.2	–
Specific storage	S_s	0.2	$1/\text{m}$
Viscosity	μ	1×10^{-3}	$\text{Pa} \cdot \text{s}$
Thickness	L	1	m
Channel source term			
Head	h_{sur}	-0.5	m
Bed top location	z_{sur}	-0.7	m
Width	B	59.6	m
Bed conductivity	K_A	1×10^{-6}	m/s
Bed thickness	a	0.3	m

Results

Simulation results are shown in Fig. 3.3.5.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>riv2_hex</i>	H	benchmarks\GROUNDWATER_FLOW\

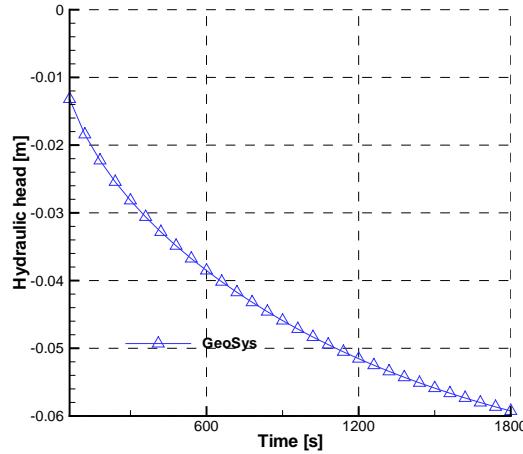


Figure 3.3.5: Results by GeoSys for confined aquifer with a constant channel sink term

3.4 Unconfined aquifer

3.4.1 Steady state case

Problem definition

In these examples the aquifer consists of a small strip with the size of $100m \times 2m$ (see Fig. 3.4.1). At both ends the head is fixed and constant recharge is imposed on the whole domain which leads to steady state flow. This setting allows comparison with an analytical solution.

Initial and boundary conditions

Initial groundwater head is $0m$. At one end of the strip the head is 1 at the other 5 . At the top a source term of $1.0 \times 10^{-8}m/s$ and at the remaining parts no-flow is imposed.

Material properties

For the spatial discretization 100 equal quadrants and 410 triangles or prisms are used. In latter case the three-dimensional groundwater Eqn. 3.1.2 is solved with elements adapting to the water height. One time step with the size of $100s$ is used. The specific storage $S_s = 0m^{-1}$ or specific yield $S_y = 0$ and a permeability κ of $1 \times 10^{-9}m^2$ is used.

Results

Comparison of simulation results for prisms and analytical solution is shown in Fig. 3.4.1.

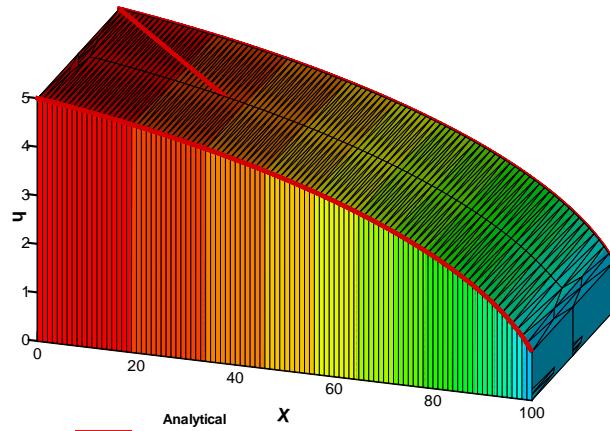


Figure 3.4.1: Results of unconfined aquifer benchmark example by GeoSys with prisms

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>uc_quad</i>	H	benchmarks\GROUNDWATER_FLOW\
<i>uc_tri</i>	H	benchmarks\GROUNDWATER_FLOW\
<i>uc_pris</i>	H	benchmarks\GROUNDWATER_FLOW\

Chapter 4

Fluid property functions

4.1 Theory of thermodynamic and transport properties

4.1.1 Density

In subterranean oil and gas reservoirs, properties of gases and liquids strongly depend from environmental pressure and temperature conditions. Equations of state (EOS) may be used to describe the relationship of volume, pressure and temperature of a real fluid. The knowledge of a fluids volume or its density is essential to estimate further thermodynamic properties. The first EOS for real gases, which was based on the ideal gas law, was presented by Johannes Diderik VAN DER WAALS in 1873 [38]. In 1910 he received the Nobel prize for the development of the equation

$$p = \frac{RT}{V_m - b} - \frac{a}{V_m^2} \quad (4.1.1)$$

where p is the pressure, R is the gas constant, T is the temperature, V_m is the molare volume and a and b are correcting parameters.

Following three different EOS will be described, which are implemented in version GeoSys (4.10.00), based on the VAN DER WAALS-equation (4.1.1).

Redlich-Kwong equation of state (RKEOS) The Equation of REDLICH and KWONG from 1949 (4.1.2) represents just a little improvement of the van der Waals equation [39]. It is given as

$$p = \frac{RT}{V_m - b} - \frac{a}{T^{0.5} V_m (V_m + b)}. \quad (4.1.2)$$

Its results are satisfactory only for temperatures above the critical point (see Tab. 4.1.1).

Table 4.1.1: Fluid properties used in equations of state, where ω is the acentric factor, T_c and p_c are temperature und pressure at the critical point and R ist the gas constant.

substance	ω [-]	T_c [K]	p_c [MPa]	R [J/kg/K]
Carbon dioxide	0.239	304.13	7.38	188.9
Ethane	0.099	305.32	4.87	276.5
Methane	0.011	190.56	4.60	518.3
Water	0.344	647.10	22.06	461.5

Equation (4.1.2) can be recasted as a cubic equation in terms of volume

$$V_m^3 - \frac{RT}{p} V_m^2 - \left(\frac{RTb}{p} - \frac{a}{T^{0.5}p} + b^2 \right) V_m - \frac{ab}{T^{0.5}p} = 0. \quad (4.1.3)$$

This equation yields to one or three real roots depending on the number of phases in the system. In the two-phase region, the largest positive root represents the molar volume of the gas phase while the smallest root corresponds to the volume of the liquid phase. The correcting terms a and b are given as

$$a = 0.4275 \frac{R^2 T_c^{2.5}}{p_c} \quad (4.1.4)$$

and

$$b = 0.0866 \frac{RT_c}{p_c} \quad (4.1.5)$$

where T_c and p_c are Temperature and pressure at the critical point (see Tab. 4.1.1). Figs. 4.1.1 and 4.1.2 show the results of the RKEOS for several substances at four different temperatures in comparison to other equations of state.

Peng-Robinson equation of state (PREOS) D. Y. PENG and D. B. ROBINSON presented an improvement of the RKEOS in 1975 [40]. The proposed equation is also a two-constant van der Waals-Type equation and combines simplicity and accuracy. The PREOS is very simple to solve and gives satisfying results within the whole fluid region of a gas. It is given in the form

$$p = \frac{RT}{V_m - b} - \frac{a(T_c) \cdot \alpha(T_r, \omega)}{V_m^2 + 2 \cdot bV_m - b^2} \quad (4.1.6)$$

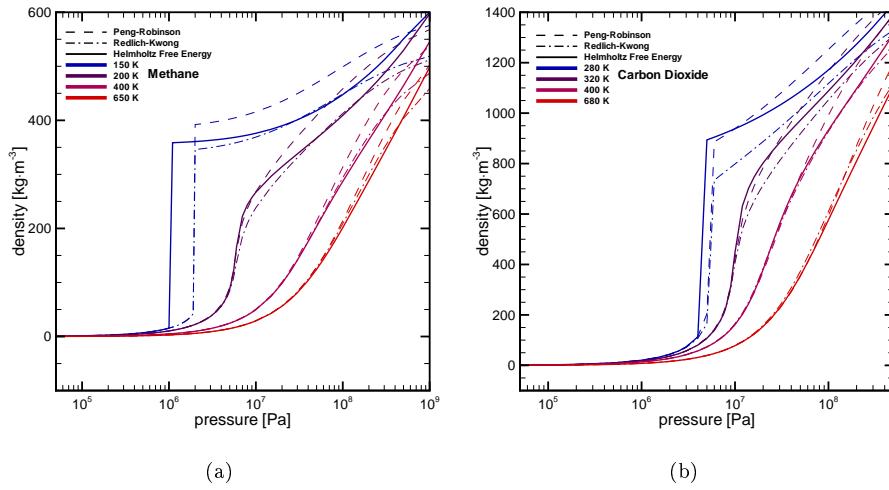


Figure 4.1.1: Density of CH_4 (a) and CO_2 (b) derived by different EOS. There stand — for the HELMHOLTZ Free Energy, - - - for the PREOS and - · - for the RKEOS. The colours refer to different temperatures (blue - 280 K, violet - 320 K, pink - 400 K, red - 680 K).

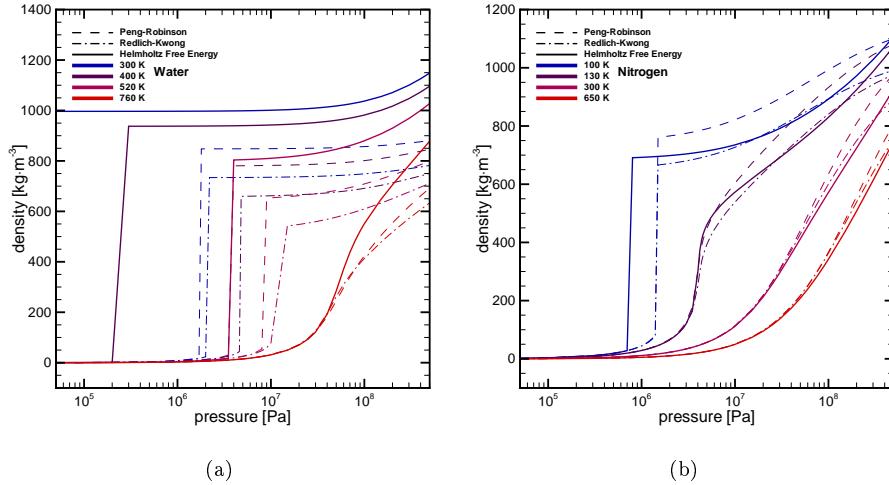


Figure 4.1.2: Density of H_2O (a) and N_2 (b) derived by different EOS. There stand — for the HELMHOLTZ Free Energy, - - - for the PREOS and - · - for the RKEOS. The colours refer to different temperatures (blue - 280 K, violet - 320 K, pink - 400 K, red - 680 K).

where a and b are correcting terms. They can be derived by

$$a(T_c) = 0.45724 \frac{R^2 T_c^2}{p_c} \quad (4.1.7)$$

and

$$b(T_c) = 0.07780 \frac{RT_c}{p_c} \quad (4.1.8)$$

for the particular fluids under specification of pressure and temperature at the critical point. Parameter $\alpha(T_r, \omega)$ is a dimensionless function of reduced temperature T_r and acentric factor ω . It is given as

$$\alpha = (1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5}))^2 \quad (4.1.9)$$

for $\omega \leq 0.49$ and

$$\alpha = (1 + (0.379642 + (1.48503 - (1.164423 - 1.016666\omega)\omega)\omega)(1 - T_r^{0.5}))^2 \quad (4.1.10)$$

for $\omega > 0.49$.

Tab. 4.1.1 shows acentric factors and critical parameters for different real gases. The resulting density distribution of the PREOS is shown in Figs. 4.1.1 and 4.1.2 at four different temperatures.

Fundamental equations For highly precise results it is necessary to adapt fundamental equations based on the free energy. The HELMHOLTZ free energy is given as

$$\frac{f(\rho, T)}{RT} = \phi(\delta, \tau) = \phi^o(\delta, \tau) + \phi^r(\delta, \tau) \quad (4.1.11)$$

in dependence from density ρ and temperature T in its dimensionless form. These dimensionless parts are given as the terms $\delta = \rho/\rho_c$ and $\tau = T_c/T$, whereas ρ_c and T_c are density and temperature at the critical point (see Tab. 4.1.1). The HELMHOLTZ free energy provides relations between density, temperature and all thermodynamic properties of a fluid, which are expressed in the parameter ϕ^o as the ideal gas part and ϕ^r as the residual part. For their derivatives in the short forms like ϕ_δ^r , $\phi_{\delta\delta}^r$, ϕ_τ^r , $\phi_{\tau\tau}^r$, $\phi_{\delta\tau}^r$, ϕ_τ^o , $\phi_{\tau\tau}^o$ it is referred to [41].

Many authors used the approach of HELMHOLTZ free energy to develop EOS for different substances, e. g. :

- SPAN&WAGNER [41], [42], [43] for carbon dioxide and for nitrogen,

- PRUSS&WAGNER [44], [45] for water,
- BÜCKER&WAGNER [46] for ethane and
- SETZMANN&WAGNER [47] for methane.

The fundamental equation (4.1.11) according to WAGNER et al. ([41],[44],[46], and [47]) is one of the most precise EOS at present. The Equation and its derivatives can be used to describe all thermodynamic properties of a pure substance depending on density and temperature. So it is necessary to solve the relationship between density, pressure and temperature iteratively, as (4.1.12) shows

$$\frac{p(\delta, \tau)}{\rho RT} = 1 + \delta \frac{\partial \phi^r}{\partial \delta}. \quad (4.1.12)$$

For water, the equation became international standard for the IAPWS¹ since 1995. Certainly, the equation is complicated to solve and requires long computing time. Therefore, in the version of GeoSys (4.10.00) it is possible to choose between an iterative solving algorithm and an interpolation of density values out of a database.

The semi-empirical fundamental equation (4.1.11) has to be fitted to measurement data by computer algorithms for each substance. Depending on the fluid, there are up to 200 adjusting coefficients to ensure a very accurate fit to the real gas behaviour. For each substance, (4.1.11) has separate ranges of validity, which are shown in Tab. 4.1.2.

Table 4.1.2: Ranges of validity of the free HELMHOLTZ equation (4.1.11) for several fluids valid from the melting point up to the indicated values.

substance	T [K]	p [MPa]	reference
Carbon dioxide	216	1100	[41], [42]
Nitrogen	1000	2200	[43]
Ethane	520	30	[46]
Methane	625	1000	[47]
Water	1273	1000	[44], [45]

4.1.2 Enthalpy

The specific enthalpy h is the whole amount of energy of a fluid. It consists of the internal energy and the volume changing work. It can be expressed by

¹International Association for the Properties of Water and Steam

deviations of the free HELMHOLTZ energy as

$$\frac{h(\delta, \tau)}{RT} = 1 + \tau (\phi_\tau^o + \phi_\tau^r) + \delta \phi_\delta^r. \quad (4.1.13)$$

4.1.3 Entropy

The entropy s represents which plenty of the energy of a system is potentially available to do work and which plenty of it is potentially defined as heat. In classical thermodynamics, the validity for the entropy is the thermodynamical system in equilibrium. The following equation is given for the entropy:

$$\frac{s(\delta, \tau)}{R} = \tau (\phi_\tau^o + \phi_\tau^r) - \phi^o - \phi^r. \quad (4.1.14)$$

4.1.4 Heat capacity

The specific heat capacity of a fluid is defined as the amount of heat which is needed to increase the temperature of a fluid of 1 kg by 1 K. In thermodynamics, it is distinguished between a heat capacity at constant pressure, the isobaric heat capacity, and a heat capacity at constant volume, the isochoric heat capacity. Both can be expressed in terms of free HELMHOLTZ energy, like the following equations show:

isobaric heat capacity

$$\frac{c_p(\delta, \tau)}{R} = -\tau^2 (\phi_{\tau\tau}^o + \phi_{\tau\tau}^r) + \frac{(1 + \delta \phi_\delta^r - \delta \tau \phi_{\delta\tau}^r)^2}{(1 + 2\delta \phi_\delta^r + \delta^2 \phi_{\delta\delta}^r)} \quad (4.1.15)$$

isochoric heat capacity

$$\frac{c_v(\delta, \tau)}{R} = -\tau^2 (\phi_{\tau\tau}^o + \phi_{\tau\tau}^r). \quad (4.1.16)$$

Due to the high number of adjusting coefficients, the properties based on the HELMHOLTZ free energy may be seen as very accurate. On the other hand, the iterative solution of (4.1.12) takes long computing times, so for long-term simulations or for simulations with a high number of elements, it would be better to use the VAN DER WAALS-type equations of REDLICH-KWONG or PENG-ROBINSON. These cubic equations are easy to solve and lead to results very fast. Figs. 4.1.3 and 4.1.4 illustrate, in which range of temperature and pressure those simple EOS may be used. Here, thermodynamical properties of carbon dioxide based on temperature and density are shown calculated by different EOS. In general, if temperature rises while pressure is declining, the behaviour

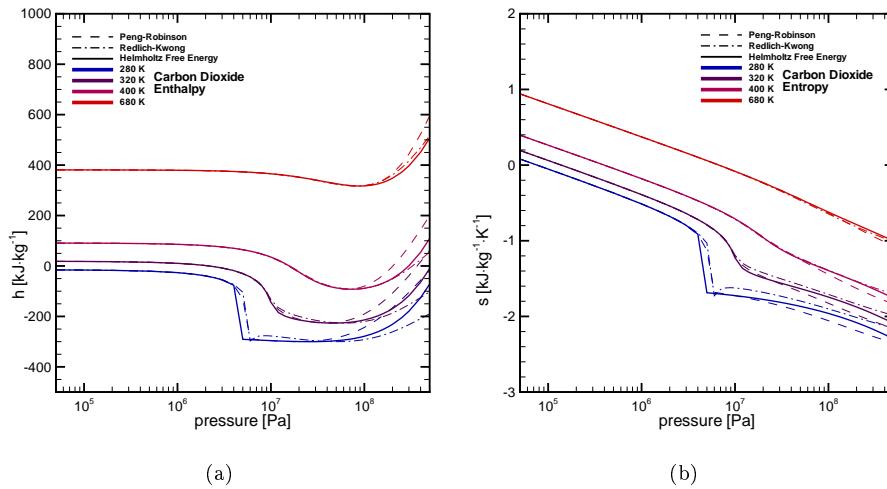


Figure 4.1.3: Enthalpy (a) and entropy (b) of CO₂ based on different EOS. There stand — for the HELMHOLTZ Free Energy, - - - for the PREOS and - · - for the RKEOS. The colours refer to different temperatures (blue - 280 K, violet - 320 K, pink - 400 K, red - 680 K).

of a fluid approaches to that of the ideal gas and the cubic equations of state give suitable results. For instance, the resulting entropy and enthalpy values of carbon dioxide at low pressures and high temperatures are identical, regardless of the density model they are based on (see Fig. 4.3(a) and 4.3(b)). In the liquid and the dense supercritical region, the results based on different EOS diverge increasingly.

In addition, in the vicinity of the saturation curve, the results based on the VAN DER WAALS-type EOS may show large variations compared to the fundamental equation based curves (HELMHOLTZ free energy). Particularly, this becomes apparent from Figs. 4.4(a) and 4.4(b), where the heat capacities of CO₂ are given. The heat capacities at 400 K and 680 K (in the supercritical region of CO₂, where no phase boundary exists) are identical, independent from according density model. Within the two-phase region at 280 K and 320 K, a strong deviation at the phase boundary can be seen.

For water, the cubic EOS are not suitable. Water is a high critical fluid, so its properties are too complex to be described by simple approaches. As we can see in Fig. 4.2(a), the RKEOS, as well as the PREOS equation give viable results only at pressures below 1 MPa and at high temperatures. Therefore it is recommended to use the fundamental equation of the HELMHOLTZ free energy to estimate the density of water.

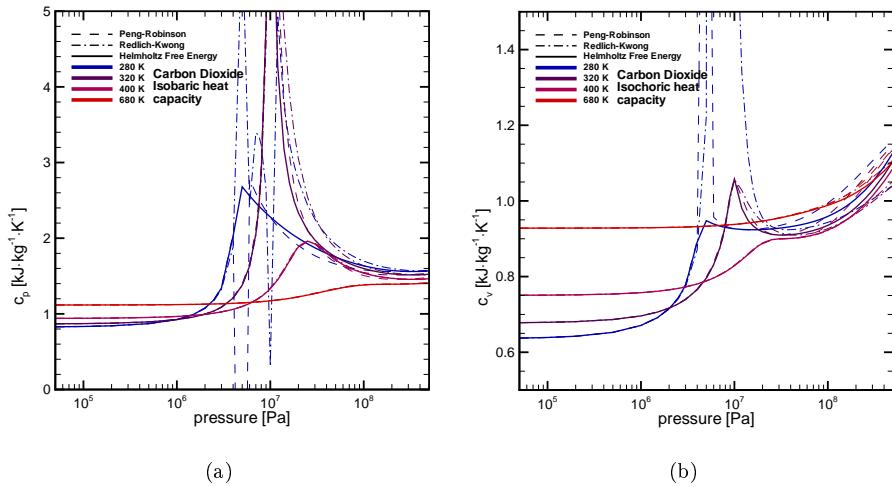


Figure 4.1.4: Isobaric heat capacity (a) and isochoric heat capacity (b) of CO_2 based on different EOS. There stand — for the HELMHOLTZ Free Energy, - - - for the PREOS and - · - for the RKEOS. The colours refer to different temperatures (blue - 280 K, violet - 320 K, pink - 400 K, red - 680 K).

4.1.5 Viscosity

Many authors developed correlation equations for viscosity η of fluids at a density ρ and a temperature T . Those correlation equations may be composed of two or three terms, like

$$\eta(\rho, T) = \eta_0(T) + \eta_{ex}(\rho, T) \quad (4.1.17)$$

or

$$\eta(\rho, T) = \eta_0(T) + \Delta\eta(\rho, T) + \Delta\eta_c(\rho, T). \quad (4.1.18)$$

In the two-term form, the viscosity correlation consists of a zero-density limit viscosity $\eta_0(T)$ at a temperature T , and an excess contribution viscosity $\eta_{ex}(\rho, T)$ at a density ρ and a temperature T . This type of correlation function is used (among others) by FRIEND et al. [48] or STEPHAN et al. [49]. The formulation can be enhanced by a term describing the viscosity in the immediate vicinity of the critical point, $\Delta\eta(\rho, T)$ (4.1.18), as described in FENGHOUR et al. [50] or HUBER et al. [51]. An overview about the used viscosity correlations for several substances is given in Tab. 4.1.3. To show an example, Fig. 4.5(a) portrays the resulting viscosities for carbon dioxide based on densities of different EOS.

Table 4.1.3: Ranges of T and p validity for viscosity correlations for several substances.

substance	T [K]	p [MPa]	reference
Carbon dioxide	200–1500	≤ 300	[50]
Nitrogen	70–1100	≤ 100	[49]
Ethane	90–625	≤ 30	[52]
Methane	91–600	≤ 100	[48]
Water	273–1173	≤ 100	[51]

4.1.6 Thermal conductivity

Similar to the correlations between viscosity and T and p , the thermal conductivity λ can be expressed by an equation consisting of the following three parts (see [53]): A conductivity in the limit of zero-density $\lambda^0(0, T)$, where only two-body interaction occurs, a term $\Delta_c \lambda(\rho, T)$ which enhances the property function in the critical region of the fluid, and finally $\Delta\lambda(\rho, T)$ which represents the contribution of all other effects to the thermal conductivity at elevated densities including many-body collisions, molecular-velocity correlations and collisional transfer. This equation is

$$\lambda(\rho, T) = \lambda^0(T) + \Delta\lambda(\rho) + \Delta_c \lambda(\rho, T). \quad (4.1.19)$$

Fig. 4.5(b) shows the thermal conductivity of carbon dioxide at four temperatures based on different EOS. In Tab. 4.1.4 the ranges for the validity of T and p concerning thermal conductivity correlations for several substances are shown.

Table 4.1.4: Ranges of T and p validity for thermal conductivity correlations for several substances.

substance	T [K]	p [MPa]	Reference
Carbon dioxide	200–1000	≤ 100	[50]
Nitrogen	70–1100	≤ 100	[49]
Ethane	≤ 600	≤ 70	[54]
Methane	≤ 200	≤ 600	[54]
Water	≤ 800	≤ 100	[55]

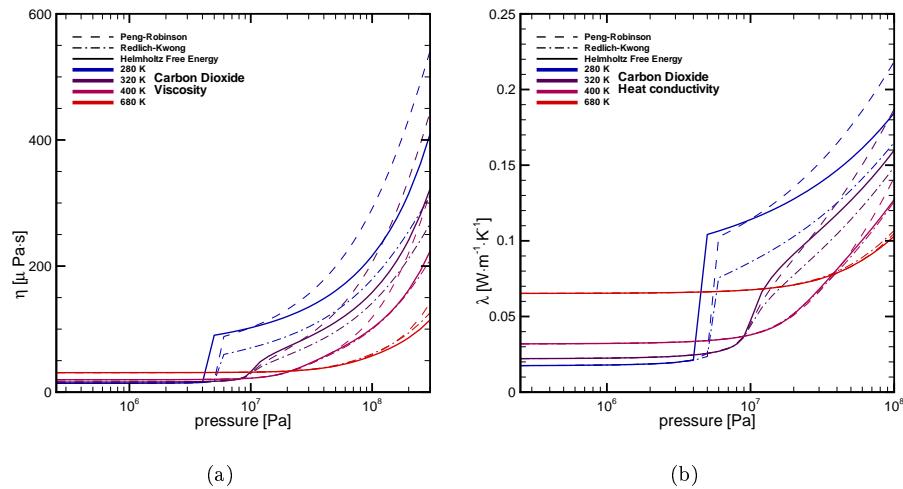


Figure 4.1.5: Viscosity (a) and thermal conductivity (b) of CO₂ based on different EOS. There stand — for the HELMHOLTZ Free Energy, - - - for the PREOS and - · - for the RKEOS. The colours refer to different temperatures (blue - 280 K, violet - 320 K, pink - 400 K, red - 680 K).

4.2 Keywords

4.2.1 Fluid specification

The new fluid property functions are working for specific substances. So, it is necessary to specify the desired fluid in the *.MFP-file. This has the advantage, that there is no need to know or to look-up fluid properties like initial density or viscosity for a specific pressure or temperature condition. The subkeyword **\$FLUID_NAME** identifies the substance. Since GeoSys version 4.10.02, four substances are defined: CO₂, H₂O, CH₄ and N₂. By defining the fluid name, all necessary coefficients, parameters and critical values are called by the source code to solve the EOS and the fluid property functions.

Example: In MFP-file, write:

```
#FLUID_PROPERTIES  
$FLUID_TYPE  
LIQUID  
$FLUID_NAME  
CARBON DIOXIDE
```

The first letter of the fluid name identifies the substance, so 'C' would be sufficient define the substance clearly as CO₂. Table 4.2.1 shows all available substances and their identifiers.

Table 4.2.1: Fluid substances and their identifiers.

Identifier	Substance
W	Water
C	Carbon dioxide
M	Methane
N	Nitrogen

4.2.2 Density model specification

With these specified substances, it is possible to choose between different equations of state, which are described in detail in section 4.1.1. In addition to former ones, a selection of new density models is available since GeoSys version 4.10.00. The referring density model identifiers are shown in table 4.2.2. These density models determine the fluid density depending on pressure and temperature. If multiple phases or components are defined, an optional argument name can be specified behind the density model identifier.

Example: (MFP-file)

```
$FLUID_NAME
CARBON_DIOXIDE
$DENSITY
12 PRESSURE_W TEMPERATURE1
```

This example sets up density model 12 (PREOS), where PRESSURE_W and TEMPERATURE1 serve as property function arguments. If the optional argument specification is omitted, the default argument names are PRESSURE1 and TEMPERATURE1. So, especially for multiphase-flow examples, the declaration of arguments can be important. For isothermal problems, it is possible to define a reference temperature behind the density model identifier.

Example: (MFP-file)

```
$FLUID_NAME
CARBON_DIOXIDE
$DENSITY
13 400 PRESSURE2
```

In this case, the temperature argument for the equation of state is a constant value of 400 K, regardless if heat transport considered or not.

Table 4.2.2: Density model identifiers

Identifier	Density model
10	Lookup-table
11	REDLICH&KWONG
12	PENG&ROBINSON
13	HELMHOLTZ free energy

4.2.3 Viscosity model specification

For viscosity, several correlation functions were presented by different authors (see section 4.1.5), but there is only one new viscosity model identified by no. 9. When viscosity model is 9, the right correlation function is chosen automatically by the fluid name (see section 4.2.1). If no fluid name is specified, the default substance will be carbon dioxide. For viscosity model 9, the same arguments as for density models 11 to 13 can be given.

Example: (MFP-file)

```
#FLUID_PROPERTIES
$FLUID_TYPE
LIQUID
$FLUID_NAME
CARBON_DIOXIDE
$VISCOSITY
9 400 PRESSURE2
```

4.2.4 Thermal conductivity model specification

The thermal conductivity correleations depending on temperature and pressure can be switched on by identifier '3'.

Example: (MFP-file)

```
$HEAT_CONDUCTIVITY
3 PRESSURE2
```

The **heat conductivity model 3** handles the same arguments as **viscosity model 9**. In section ??, the correlation functions for all implemented substances are described and referenced.

4.2.5 Compressibility model specification

Since GeoSys version 4.10.02, a fluid can be considered as compressible or incompressible due to temperature and pressure². The compressibility of a fluid depends on the slope of the density function surface (see (4.3.2) on page 74). This slope can be determined by

- a constant value
- a lookup-table
- the difference quotient
- the analytical derivation of the equation of state

or can be set to zero to treat the fluid as incompressible. In GeoSys version 4.10.02, only the constant value and the difference quotient alternatives are available. This difference quotient is a simple and fast way to approximate the slope of the density function:

$$\frac{\partial \rho_\alpha}{\partial p_\alpha} \approx \frac{\Delta \rho_\alpha}{\Delta p_\alpha} = \frac{\rho_\alpha(p_\alpha + \frac{\Delta p_\alpha}{2}, T) - \rho_\alpha(p_\alpha - \frac{\Delta p_\alpha}{2}, T)}{\Delta p_\alpha}. \quad (4.2.1)$$

A comparable equation determines the slope of the density function in terms of temperature. The compressibility model can be defined for each individual phase. The new subkeyword \$COMPRESSIBILITY requires two lines of arguments: The first line defines the fluids compressibility due to pressure, the second one the compressibility due to temperature. Each argument line has to start with the compressibility model identifier. The meaning of the second argument depends on the chosen identifier (see Table 4.2.3). The following example defines carbon dioxide as compressible due to pressure changes using a numerical approximation of its equation of state (model 3, first line); the pressure difference Δp , which is used to determine the difference quotient (see (4.2.1)) is set to 1 Pa. Furthermore, the example defines the fluid as incompressible due to temperature changes (model 0, second line).

²only in global pressure-saturation formulation

Example: (MFP-file)

```
$FLUID_NAME
CO2
$COMPRESSIBILITY
3 1
0
```

Table 4.2.3: Compressibility model identifiers

Identifier	Argument	Compressibility model
0	-	incompressible
1	$\frac{\Delta\rho}{\Delta p}$ or $\frac{\Delta\rho}{\Delta T}$	constant slope
2	-	lookup-table
3	Δp (eq. 4.2.1) or ΔT	difference quotient
4	-	analytical derivation

4.2.6 Example file

The following listing of an MFP-file defines a two-phase or a two-component scenario with H₂O and CO₂ as involved fluids.

Water is incompressible due to pressure changes, but its density depends on temperature. The chosen equation of state is the fundamental HELHOLTZ free energy equation, which is the only EOS which returns accurate density values for water, but takes long computing time. The viscosity and the thermal conductivity of water is determined by the IAPWS formulation for scientific use [51], [55]. No pressure or temperature argument names are defined for water, so the default PRESSURE1 and TEMPERATURE1 variables are used for fluid no. 1.

The example file considers carbon dioxide as compressible due to pressure and temperature, where the temperature depending density changes are approximated by a constant slope ($2.5 \text{ kg} \cdot \text{m}^{-3} \cdot \text{T}^{-1}$). CO₂ is a much less complex than water, so a simple PREOS is precise enough for density determination. For viscosity and thermal conductivity, the formulations of FENGHOUR et al. [50] are chosen. For this second fluid, the argument name PRESSURE2 has to be declared.

Example: (MFP-file)

```
#FLUID_PROPERTIES
```

```

$FLUID_TYPE
LIQUID
$FLUID_NAME
WATER
$COMPRESSIBILITY
0
3 1
$DENSITY
13
$VISCOSITY
9
$HEAT_CONDUCTIVITY
3
#FLUID_PROPERTIES
$FLUID_TYPE
GAS
$FLUID_NAME
CO2
$COMPRESSIBILITY
3 1
1 2.5
$DENSITY
12 PRESSURE2
$VISCOSITY
9 PRESSURE2
$HEAT_CONDUCTIVITY
3 PRESSURE2
#STOP

```

4.2.7 Fluid property output

Fluid properties can be written in the output-file using the subkeyword \$MFP_VALUES in *.OUT-file. This was only possible for one single phase or component. Since GeoSys version 4.10.02, it is possible to define the number of the phase, whose properties shall be given out. This can be done by writing the phase number directly behind the respective fluid property.

Example: (OUT-file)

```

$MFP_VALUES
DENSITY1
HEAT_CONDUCTIVITY1
DENSITY2
VISCOSITY2

```

This example writes density and thermal conductivity of the first, and density and viscosity of the second defined fluid into the respective output-file.

4.3 Benchmarks

4.3.1 CO₂ flow with pressure dependent density and viscosity (H-process)

Problem definition

This benchmark shows the distribution of pressure along a 1D soil profile for different fluid property models (see Fig. 4.3.1). Two wells, one injection well and one production well are placed with a distance of 400 m. CO₂ is dumped by the injection well at a pressure of 7 MPa, at the production well there is a pressure of 6.5 MPa. The temperature along the profile shall be constant at 400 K.

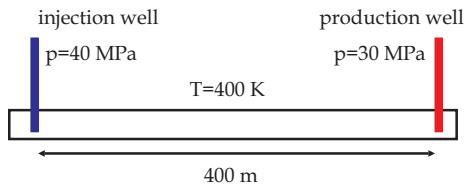


Figure 4.3.1: Problem definition

Model setup

For this case the model area is reduced to a very simple 1D problem. The mesh consists of 200 line elements with a constant length of 2 m. The injection well on the left side is represented as a constant boundary pressure of 40 MPa, the right boundary has a constant pressure of 30 MPa for the whole domain. Initial conditions are a temperature of 400 K and a pressure of 30 MPa. The used material is a porous medium with a porosity of $n_e = 10\%$ and a density of $\rho = 2500 \text{ kg m}^{-3}$.

Fluid properties

Two different cases show the influence of non linear fluid properties. A constant viscosity of $\eta = 0.001 \text{ Pa s}$ in the first simulation is set. For the second simulation, the CO₂ viscosity is calculated by a constant temperature and a pressure depending density. The calculation is based on data tables with $\rho p T$ -data calculated by (4.1.11) and on the data set of $\rho p T$ -data shown in the appendix in Tabs. A to A.0.2.

Results

The pressure distribution for the first simulation with the constant viscosity decreases linearly along the profile. When viscosity and density are variable values the pressure distribution curve shows a non-linear behaviour like in Fig. 4.3.2.

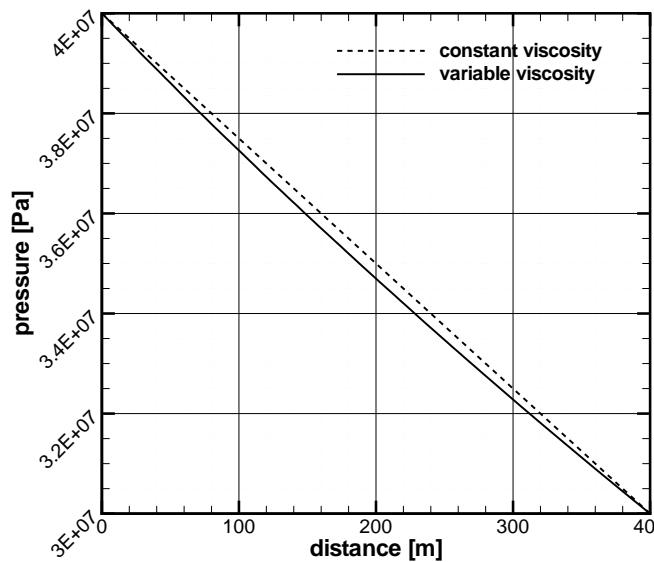


Figure 4.3.2: Pressure distribution along the soil profile

Benchmark deposit

Table 4.3.1: Benchmark location in the repository.

Benchmark	Problem type	Path in benchmark deposit
CO2-FLOW	H	benchmarks\GROUNDWATER_FLOW\C02-FLOW

4.3.2 Non-isothermal single-phase flow of different fluids with variable fluid properties (HT-process)

Problem definition

The aim of this test case is to show the functionality of different equations of state and transport property correlations for different fluids. Because of that, the model setup from section ?? was extended by non-isothermal conditions. At the beginning of the infiltration, the residing fluid within the reservoir has a temperature of 400 K. At the point of injection, a constant temperature of 300 K is defined. During the infiltration process, the reservoir will cool down and the residing fluid will change its properties. In case of CO₂ as working fluid, there will be a phase change during the injection process regarding the CO₂ phase diagram in Fig. 4.3.3. Note that this example shows just the fluid behavior related to temperature and pressure conditions. No physically based phase change is simulated here, only the fluid property functions are tested.

This example is simulated for four different substances (CO₂, CH₄, H₂O, and N₂). For each substance, three different EOS are tested, so that this test case consists of twelve model set ups. Tab. 4.3.2 gives an overview about the used fluid property correlations.

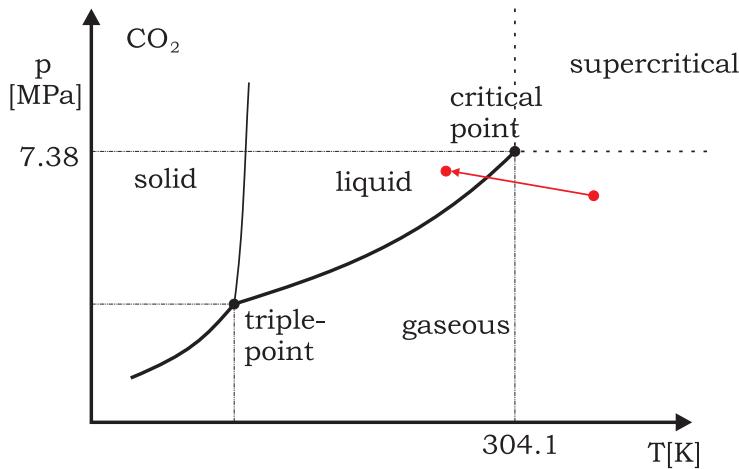


Figure 4.3.3: Phase diagram of carbon dioxide. The two extreme conditions (400 K at 6.5 MPa and 300 K at 7 MPa) are crossing a phase boundary of CO₂, so a phase change from hot gas to liquid state will be forced.

Table 4.3.2: Set-up names and referring correlation functions

working fluid	model name	density	viscosity
Methane CH ₄	CH4-RK	[39]	Friend, 1989 [48]
	CH4-PR	[40]	
	CH4-HE	[47]	
Carbon dioxide CO ₂	CO2-RK	[39]	Fenghour, 1998 [50]
	CO2-PR	[40]	
	CO2-HE	[41]	
Water H ₂ O	H2O-RK	[39]	IAPWS, 1998 [51]
	H2O-PR	[40]	
	H2O-HE	[45]	
Nitrogen N ₂	N2-RK	[39]	Stephan, 1987 [49]
	N2-PR	[40]	
	N2-HE	[43]	

Model setup

The 1D model domain of this test case consists of 200 line elements with a length of 0.5 m. There is an injection well on the left, and a production well on the right side (see Fig. 4.3.4). The thermal properties of the porous medium was all set to zero, so that no heat is stored or transported by the solid material. The fluid pressure on the left hand side (injection point) is $p = 7 \text{ MPa}$, on the right hand side the pressure is $p = 6.5 \text{ MPa}$. Tab. 4.3.3 gives an overview about the model specifications.

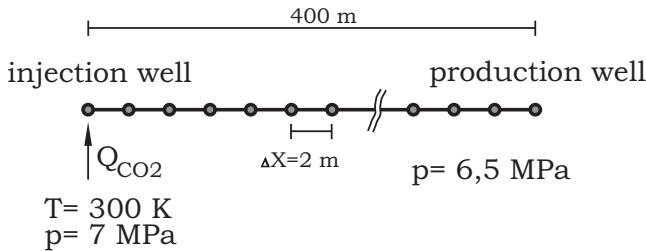


Figure 4.3.4: Model set up

Results

Fig. 4.3.5 shows the distribution of the fluid density and its viscosity after a simulation time of 50 000 seconds. At this time, the phase border has moved 175 m

Table 4.3.3: HT-benchmark specifications

parameter	symbol	value
<i>spatial discretisation</i>		
model dimension:		1D
no. of Elements:		200
length :	L	100 m
step size:	δx	0.5 m
<i>initial conditions</i>		
temperature:	T	400 K
pressure:	p	6.5 MPa
<i>boundary conditions</i>		
pressure (left):	p	7.0 MPa
pressure (right):	p	6.5 MPa
temperature (left):	T	300 K
<i>temporal discretisation</i>		
timesteps:	Δt	10 000 s
no. of timesteps:		30
total time:	t	30 000 s
<i>fluid properties</i>		
density:	ρ	simulated
viscosity:	η	simulated
heat capacity	c	$40 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
heat conductivity	λ	$0.06 \text{ J}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
<i>reservoir properties</i>		
thermal conductivity	λ	-
heat capacity:	c	-
density:	ρ	-

away from the injection well. At this point, the density jumps from $475 \text{ kg} \cdot \text{m}^{-3}$ down to $220 \text{ kg} \cdot \text{m}^{-3}$. The stepwise dropping of density between 175 m and 300 m is caused by the interpolation of database values. A higher resolution of density values in the database should solve this problem. The "saw teeth" and the offset between 60 m and 120 m is also caused by the interpolation, but this time the problem is deeper. Here, the interpolation takes place between liquid and gaseous density values. To solve this problem, the FCT-reading function has to be enhanced by a switch which avoids a interphase interpolation.

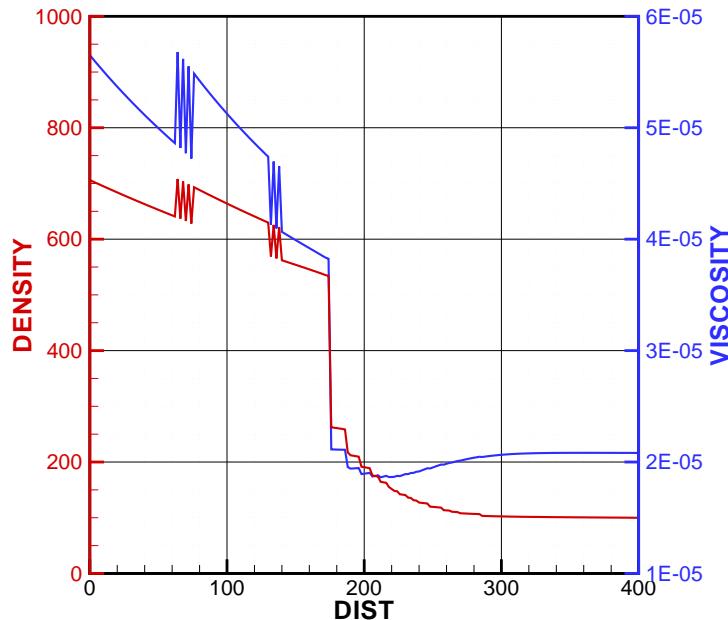


Figure 4.3.5: This is still a dummy graphic, the correct result plot follows soon...

4.3.3 Non-isothermal two-phase flow of compressible fluids (H²T-process)

Intro

In this test case, compressible two-phase flow of real gases is considered. The transport properties of the fluids are determined by accurate constitutive correlations (see sections 4.1.5 and 4.1.6). With the chosen conditions of pressure and temperature, the gases are in a supercritical state. Using equations of state for determining the density changes due to pressure and temperature, the compress-

ibility of the gases can be considered. This test case can be applied for simplified CO_2 storage applications as enhanced gas recovery. CO_2 displaces methane of a depleted gas reservoir (see Fig. 4.3.6). Because of its different chemical polarities, CO_2 and CH_4 are not (completely) miscible (in supercritical state), so two-phase flow can be assumed. Pressure of carbon dioxide and saturation of methane are chosen as independent variables. Different temperatures at the injection point and within the reservoir lead to non-isothermal conditions. The test case show the saturation development of CO_2 in the vicinity of the injection point and the resulting fluid properties of the involved substances due to pressure and temperature conditions.

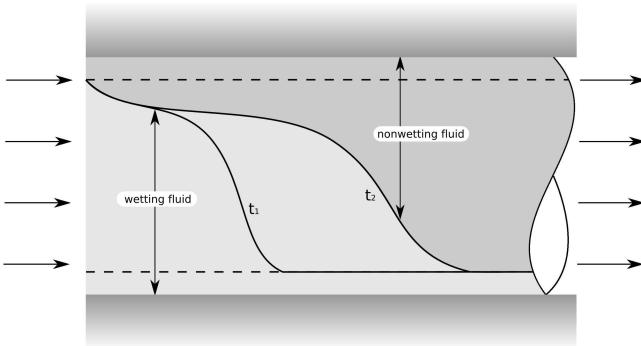


Figure 4.3.6: Schematic drawing of 1D-two phase flow problem: CO_2 is treated as a wetting fluid and displaces the non-wetting methane from the 1D-model domain.

Problem definition

Initially, a 1D gas reservoir in a depth of 3500 m is nearly fully saturated with methane at a pressure of $p_{\text{CH}_4} = 50$ bar and a temperature of $T = 400$ K. The model domain has a length of $L = 5$ m (see Fig. 4.3.7). At $x = 0$ m, CO_2 with a temperature of $T = 350$ K is pumped into the aquifer and displaces the residing methane. To show the influence of temperature to fluid properties clearly, the temperature is forced to grow linearly with the distance from the injection point. Time steps at the beginning of the simulation are very short (0.1 s), and are growing longer up to 100 s. Tab. 4.3.4 shows all relevant model specifications.

Governing equations

The governing equation for two phase flow in porous media can be written as:

Table 4.3.4: Parameters used in the H²T-benchmark test example

parameter	symbol	value
<i>spatial discretisation</i>		
element type		1D
domain length	L	5 m
element number		260
<i>temporal discretisation</i>		
timestep size	Δt	0.1 s to 100 s
timestep number		580 [-]
total time	t	10 000 s
<i>material properties</i>		
density	ρ	2500 kg·m ⁻³
<i>CO₂ properties</i>		
density	$\rho(p, T)$	PREOS [40]
viscosity	$\eta(\rho, T)$	FENGOUR [50]
thermal conductivity	λ	-
<i>CH₄ properties</i>		
density	$\rho(p, T)$	PREOS [40]
viscosity	$\eta(\rho, T)$	FRIEND [48]
thermal conductivity	λ	-
<i>initial conditions</i>		
CH ₄ saturation	S_{CH_4}	0.99 [-]
<i>boundary conditions</i>		
CH ₄ saturation	S_{CH_4}	0 [-]
CO ₂ pressure	p_{CO_2}	5.495 MPa
temperature left	T	380 K
temperature right	T	420 K
(temperature rises linearly from left to right border)		
<i>medium properties</i>		
porosity	ϕ	0.03 [-]
intrinsic permeability	\mathbf{K}	$1 \cdot 10^{-12} \text{ m}^2$
residual CO ₂ saturation	S_{r,CO_2}	0.01 [-]
residual CH ₄ saturation	S_{r,CH_4}	0 [-]
capillary pressure	$p_c(S_{\text{eff}})$	Brooks&Corey
relative permeability	$k_r(S_{\text{eff}})$	Brooks&Corey
soil distribution index	λ	2
entry pressure	p_d	5 000 Pa

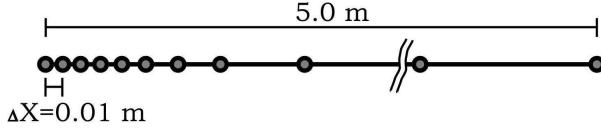


Figure 4.3.7: Model domain consisting of 1D-line elements with growing lengths. The length of the first element (at the injection point) is 1 cm.

$$\phi \frac{\partial S_\alpha \rho_\alpha}{\partial t} = \operatorname{div} \left(\rho_\alpha \frac{k_{r\alpha}}{\mu_\alpha} \mathbf{K} \{ \nabla p_\alpha - \rho \mathbf{g} \} \right) + \rho_\alpha q_\alpha. \quad (4.3.1)$$

In the actual test case, no source terms are considered ($q_\alpha = 0$). Since we consider a horizontal 1D-problem, the z coordinate doesn't change, so the gravity term can be neglected as well. We also handle no changes of porosity due to deformation or precipitation, so porosity ϕ can be treated as constant. Regarding this assumptions, we can expand (4.3.1) to the following formulation:

$$\phi \frac{\partial S_\alpha}{\partial t} + \phi \frac{S_\alpha}{\rho_\alpha} \left(\frac{\partial \rho_\alpha}{\partial p_\alpha} \frac{\partial p_\alpha}{\partial t} + \frac{\partial \rho_\alpha}{\partial T} \frac{\partial T}{\partial t} \right) = \operatorname{div} \left(\rho_\alpha \frac{k_{r\alpha}(S_\alpha)}{\mu_\alpha(p_\alpha, T)} \mathbf{K} \nabla p_\alpha \right) \quad (4.3.2)$$

for both phases α . At the present state, density change due to temperature is not considered yet, so

$$\phi \frac{\partial \rho_\alpha}{\partial T} = 0, \quad (4.3.3)$$

and (4.3.2) reduces to

$$\phi \frac{\partial S_\alpha}{\partial t} + \phi \frac{S_\alpha}{\rho_\alpha} \frac{\partial \rho_\alpha}{\partial p_\alpha} \frac{\partial p_\alpha}{\partial t} = \operatorname{div} \left(\rho_\alpha \frac{k_{r\alpha}(S_\alpha)}{\mu_\alpha(p_\alpha, T)} \mathbf{K} \nabla p_\alpha \right). \quad (4.3.4)$$

The compressibility of fluids due to temperature change will be shown in one of the next benchmarks.

Constitutive equations

A general equation of state for pure substances by PENG&ROBINSON [40] was chosen to determine the densities of carbon dioxide and methane. The viscosity of both fluids is computed by correlations from Fenghour et al. [50] for CO₂ and Friend et al. [48] for CH₄. Both density and viscosity correlations depend on pressure and temperature conditions and are described in detail in sections 4.1.1 and 4.1.5.

Results

The functionality of the fluid property functions can be evaluated by comparing the simulation results with constant fluid property models... In comparison with the H2T-McWhorter problem (sec. X.X.X), the plume of the wetting fluid ...

Table 4.3.5: Benchmark deposit

Deposit	Version	Date
GROUNDWATER_FLOW\EOS\H2T	4.10.02	Oct. 2009

Chapter 5

Richards flow – H-Proceses

5.1 Theory

5.1.1 Single continuum

Richards equations are used to describe water movement in unsaturated zone, which is the portion of the subsurface above the ground water table. Pressure p based formation, that select the unknown primary variable as p , is solved.

$$n \frac{\partial S^l}{\partial p^l} \frac{\partial p^l}{\partial t} - \nabla \cdot \left(- \frac{k_{\text{rel}}^l \mathbf{k}}{\mu^l} (\nabla p^l - \rho^l \mathbf{g}) \right) = \frac{Q_{\rho^l}}{\rho^l} \quad (5.1.1)$$

Constitutive equations are described as:

Saturation:

$$\theta = nS \quad (5.1.2)$$

$$S_{\text{eff}} = \frac{S - S_r}{S_{\max} - S_r} \quad (5.1.3)$$

Pressure:

$$p_c = -p^l \quad (5.1.4)$$

van Genuchten model

$$p_c = \frac{\rho g}{\alpha} (S_{\text{eff}}^{-1/m} - 1)^{1/n} \quad (5.1.5)$$

$$m = 1 - \frac{1}{n} \quad (5.1.6)$$

Permeability: Relationship of hydraulic conductivity and permeability:

$$\mathbf{k} = \frac{\mu}{\rho g} \mathbf{K} \quad (5.1.7)$$

van Genuchten model [van Genuchten, 1980]

$$k_{\text{rel}} = S_{\text{eff}}^{1/2} \left[1 - (1 - S_{\text{eff}}^{1/m})^m \right]^2 \quad (5.1.8)$$

Tangent approximation is applied for capacity coefficient $M = \frac{\partial S^l}{\partial p^l}$, and combined with mass-lumping matrix to reduce oscillation and improve numerical stability. Picard iteration scheme is used for nonlinear iterations.

5.1.2 Dual continua

In structured porous media the water movement can be described by dual-porosity model, which is composed by coupled Richards equations of matrix and fracture continua, respectively, which are combined by additional transfer and specific storage terms.

$$n \frac{\partial S_m^l}{\partial p_m^l} \frac{\partial p_m^l}{\partial t} - \nabla \cdot \left(\frac{k_{\text{rel}}^l \mathbf{k}_m}{\mu^l} (\nabla p_m^l - \rho^l \mathbf{g}) \right) = \frac{Q_{\rho^l m}}{\rho^l} + \frac{\Gamma^l}{w_m} \quad (5.1.9)$$

$$n \frac{\partial S_f^l}{\partial p_f^l} \frac{\partial p_f^l}{\partial t} - \nabla \cdot \left(\frac{k_{\text{rel}}^l \mathbf{k}_f}{\mu^l} (\nabla p_f^l - \rho^l \mathbf{g}) \right) = \frac{Q_{\rho^l f}}{\rho^l} - \frac{\Gamma^l}{w_f} \quad (5.1.10)$$

Relationship of preferential factors w_m and w_f is:

$$w_m + w_f = 1 \quad (5.1.11)$$

Transfer term is given as follows:

$$\Gamma^l = \alpha^* K_\alpha (p_f^l - p_m^l) R^l \quad (5.1.12)$$

The first-order exchange coefficient α^* [1/s] is derived from the properties of the fractures network, which also define the average size and form of the matrix blocks as $A^* \beta / D$, where A^* is the fracture/matrix interface area per bulk volume of rock [m^3/m^3], β is a shape factor, and D is the average fracture spacing [m] (or average matrix block size). K_α is the hydraulic conductivity at the interface between fracture and matrix continua, usually define K_α as the unsaturated hydraulic conductivity of the matrix rock, because the much smaller matrix permeability is the limiting factor for fracture-matrix flow. Interface reduction factor R^l is set to the fracture liquid saturation S_f^l . The saturation of whole system is:

$$S = S_m w_m + S_f w_f \quad (5.1.13)$$

Numerical methods

There are two numerical methods used to solve dual-continua model: partitioned and monolithic, which are given as the following descriptions.

Partitioned

In the partitioned scheme, two coupled Richards equations are solved one after another: one primary variable is given as known value when the other is solved, and the system error is controlled by the first primary variable.

Monolithic

All the primary variables are assembled in one matrix and solved as unknown variables in the same time in monolithic scheme.

5.2 Single Continuum

Single continuum model is based on Eq. 5.1.12.

5.2.1 Infiltration in homogenous soil

Problem definition

This case is a numerical modelling of classical experiment of Warrick et al's(1971)[?]. The solution is Richards equation combining with uniform initial condition, fixed boundary condition without source term, and curve descriptions of homogenous media properties.

As for the dimension extension, triangle and quadrangle mesh are used, and distinctions of different spacial discretization are presented.

Initial and boundary conditions

The uniform initial condition in the whole domain, the saturation is 0.455, and meanwhile the pressure is -21500 Pa. Boundary condition at the top is saturated, accordingly pressure is 0, and pressure equals -21500 Pa at bottom in the simulation period. Details are illustrated in Fig. 5.2.1.

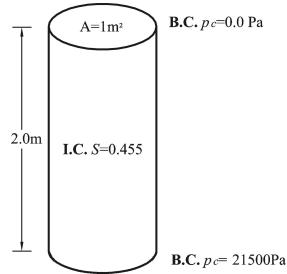


Figure 5.2.1: Illustration of numerical model

Material properties

Homogenous material properties are assumed within the whole domain. Table 5.2.1 gives the parameters.

Table 5.2.1: Parameters in simulation

items	setting
Porosity	0.38
Capillary pressure	$p(S)$ Curve in Fig. 5.2.2(l)
Relative permeability	k_{rel} Curve in Fig. 5.2.2(r)
Permeability tensor (m^2)	9.35e-12

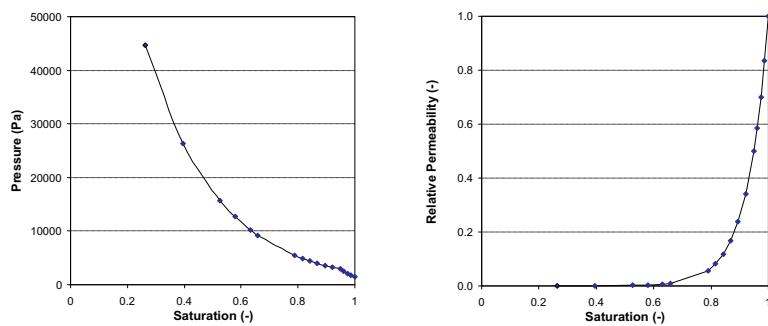


Figure 5.2.2: Relationship of capillary pressure-saturation and relative permeability-saturation

Results

Fig. 5.2.3 shows the distribution of saturation. Symbols in the Fig.5.2.3 are observations of Warrick et al's(1971)[?].

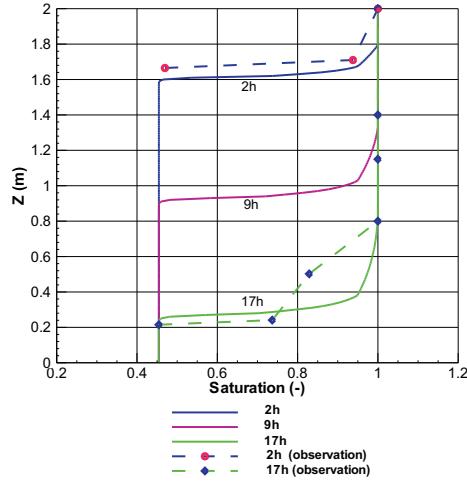


Figure 5.2.3: Saturation comparison of observed (symbol and dashed) and simulated (solid)

Fig. 5.2.4 shows the distribution of saturation by triangle and quadrilateral mesh respectively, the symbol-solid lines are 1D results. When the mesh densities are identical, the results are same; otherwise, there are distinctions.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>h_us_line_warrick</i>	H	benchmarks\h_us\wet\
<i>h_us_quad</i>	H	benchmarks\h_us\wet\
<i>h_us_tri_freebc</i>	H	benchmarks\h_us\wet\

5.2.2 Infiltration in homogenous soil (ST/BC)

Problem definition

Numerical results compare with experimental measurements of Abeele et al.(1981). The soil column is 6m long and the diameter is 3m. The problem is defined as uniform initial condition, continuous infiltration treated as source term at top, van Genuchten homogenous material and constant mesh density.

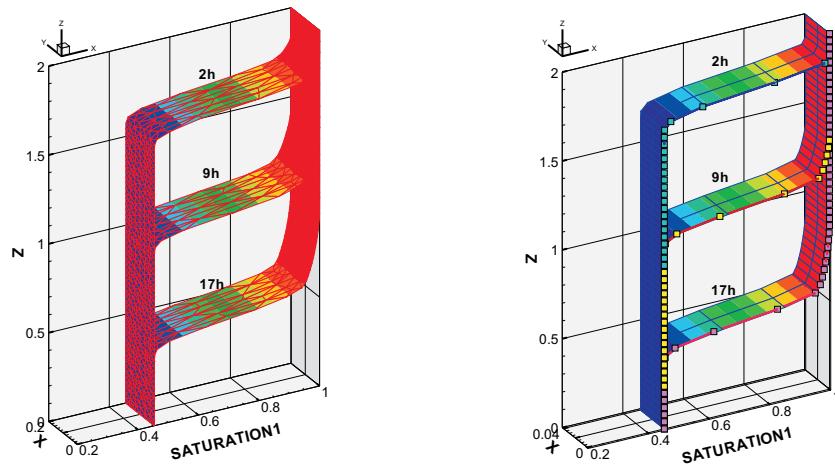


Figure 5.2.4: Saturation simulation by triangle(l) and quadrilateral (r) mesh comparison with 1D mesh (symbol-solid)

Initial, boundary conditions and source term

The initial condition of pressure is -71000pa, and continuous source term at the top is $2.314e-6$ m/s. Details are illustrated in Fig. 5.2.5.

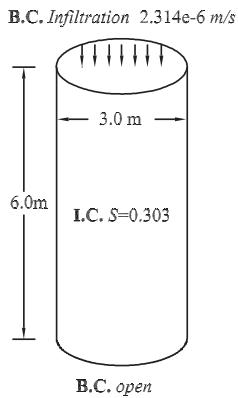


Figure 5.2.5: Illustration of numerical model

Material properties

Homogenous material properties are assumed within the whole domain. Table 5.2.2 gives the parameters.

Table 5.2.2: Parameters in simulation

Parameter	Value	Unit
Porosity	0.33	-
Saturated permeability k_s	2.95e-13	m^2
S_r^l	0.0	-
S_{max}^l	1.0	-
α	1.43	$1/m$
n	1.506	-

Results

Fig. 5.2.6 shows the distribution of saturation. Left side in Fig.5.2.6 is the result of reference [56].

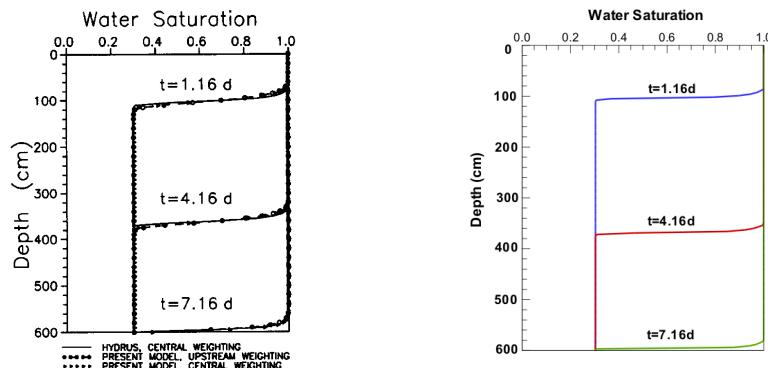


Figure 5.2.6: Saturation simulation by [56] and GeoSys

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>h_us_line_forsyth</i>	H	benchmarks\h_us\wet\

5.2.3 Infiltration in homogenous soil (BC/BC)

Problem definition

Numerical results compare with classical experimental measurements of Celia et al.(1990). The soil column is 0.6m long. The problem is defined as uniform initial condition in water head, fixed water head at top, van Genuchten homogenous material and constant mesh density.

Initial, boundary conditions and source term

The initial condition of pressure is -10m, and boundary conditions at top and bottom are -0.75m and -10m. Details are illustrated in Fig. 5.2.7.

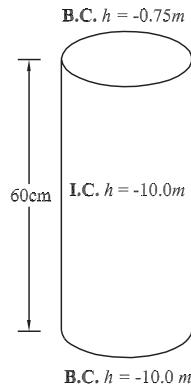


Figure 5.2.7: Illustration of numerical model

Material properties

Homogenous material properties are assumed within the whole domain. Table 5.2.3 gives the parameters.

Table 5.2.3: Parameters in simulation

Parameter	Value	Unit
Porosity	0.368	-
Saturated permeability k_s	9.35247e-12	m^2
S_r^l	0.277	-
S_{max}^l	1.0	-
α	3.35	$1/m$
n	2	-
Gravity constant g	9.807	m/s^2
Liquid density ρ	998.2	kg/m^3

Results

Fig. 5.2.8 shows the distribution of saturation. Left side in Fig.5.2.8 is the result of reference. In GeoSys/RockFlow the tangent approximation is used.

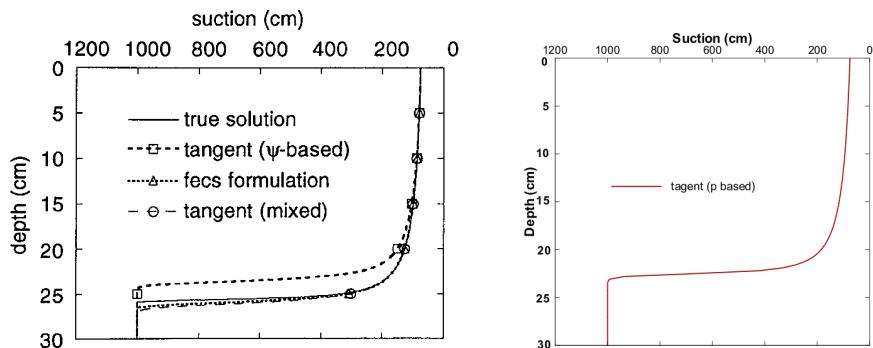


Figure 5.2.8: Suction distribution simulation by [57] and GeoSys at 6 hours

5.2.4 Transient infiltration in homogenous soil

Problem definition

This study case comes from David Kuntz in Tübingen, and it is compared with the numerical solutions of Min3P. It is a 0.25 length soil column with an artificial transient water discharge at top. Three points are selected at different location of the column, and the saturation evolution are presented. The description of model is shown in Fig. 5.2.9.

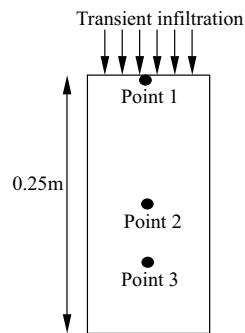


Figure 5.2.9: Illustration of numerical model

Initial, boundary conditions and source term

The initial condition is set by restart file. Artificial transient infiltration source term at top instead of boundary condition, which is shown in Fig. 5.2.10. Fixed boundary condition at bottom as pressure equal -31800Pa.

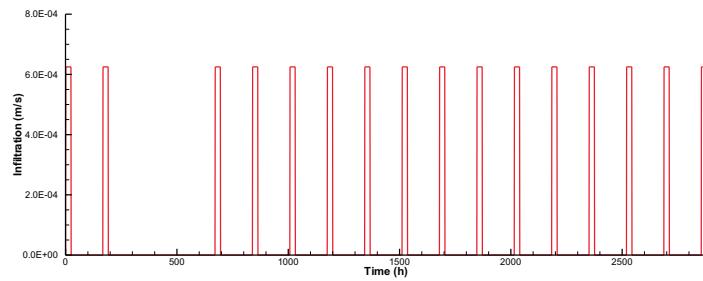


Figure 5.2.10: Discharge serial at the top

Material properties

Homogeneous material is defined by van Genuchten parameters and Table 5.2.4 gives the parameters.

Table 5.2.4: Parameters in simulation

Parameter	Value	Unit
Porosity	0.406	-
Saturated permeability k_s	9.35247e-12	m^2
S_r^l	0.056	-
S_{max}^l	1.0	-
α	4.56	$1/m$
m	0.254	-
Gravity constant g	9.8	m/s^2
Liquid density ρ	1000	kg/m^3

Results

The vertical distributions of saturation at some moments are shown in Fig.5.2.11. Three points, which locate at $(0,0,0.25)$, $(0,0,0.10)$ and $(0,0,0.05)$ respectively,

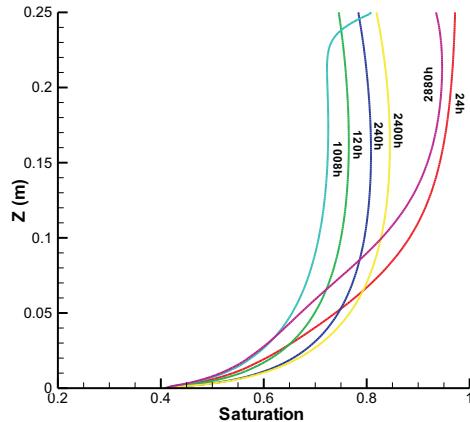


Figure 5.2.11: Saturation distributions

are selected to see the time evolution of saturation and compare with those by Min3p. Fig.5.2.12 shown the results.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>Transient</i>	H	benchmarks\h_us\wet\

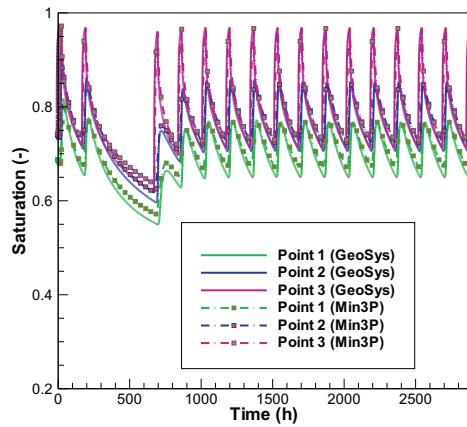


Figure 5.2.12: comparison of saturation time evolutions three points

5.2.5 Nonuniform IC of heterogenous soil column (-/BC)

Problem definition

The case is from DECOVALEX. Heterogenous horizontal soil column starts at nonuniform status, and results show the interruptions at the interface of two material.

Initial and boundary conditions

Heterogeneous initial condition setting is loaded by restart file, and fixed boundary condition is at the end. Details are illustrated in Fig. 5.2.13.

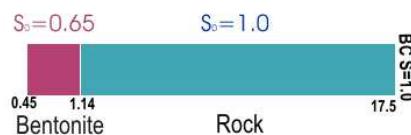


Figure 5.2.13: Illustration of numerical model

Material properties

The heterogeneous soil column consists of two kinds material: bentonite and rock. The van Genuchten parameters of rock are shown in Tab.5.2.5, and as for bentonite the curves in Fig. 5.2.14 are used in the simulation.

Table 5.2.5: Parameters in DECOVALEX

Parameter	Rock	Bentonite	Unit
Porosity	0.41	0.01	-
Saturated permeability k_s	1.03e-17	2.0e-21	m^2
S_r^l	0	-	-
S_{max}^l	1.0	-	-
α	6.673	-	$1/m$
n	0.6	-	-

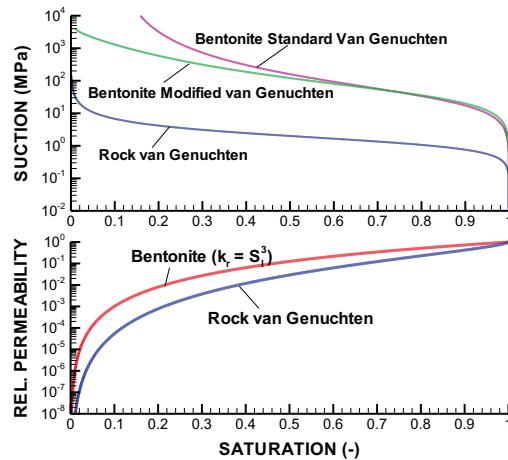


Figure 5.2.14: Characteristic Curves for bentonite and granite rock

Results

Fig. 5.2.15 shows the distribution of saturation and pressure.

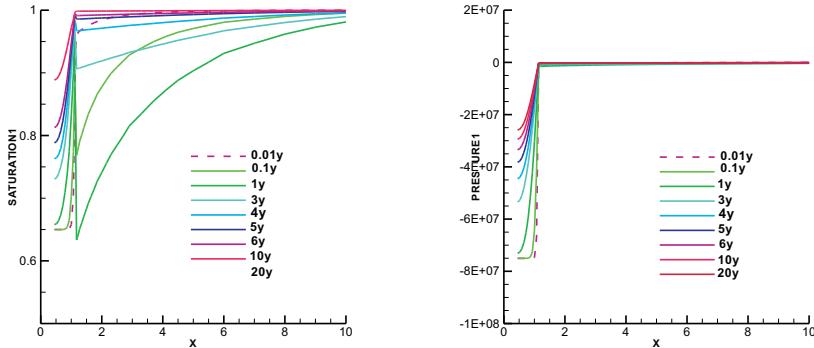


Figure 5.2.15: Saturation and pressure distribution

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
1d_ho	H	benchmarks\h_us\wet\

5.3 Dual continua

Dual continua model is based on Eq. 5.1.9 and 5.1.10.

5.3.1 Comparison with S1D

Problem definition

The simple case is defined by Vogel (2007)[58]. Numerical results compare with HYDRUS for single continua and S1D for dual continua model.

Initial and boundary conditions

The initial conditions for both matrix and fracture continuum are identical as a gradient pressure distribution, which are $p_{top}^l = -27440Pa$ and $p_{bottom}^l = -21560Pa$. The boundary conditions for both continua are also identical as fixed BC at top $p_{top}^l = 98Pa$ and free drainage at bottom. Details are illustrated in Fig. 5.3.4.

Material properties

Table 5.3.1 gives the parameters

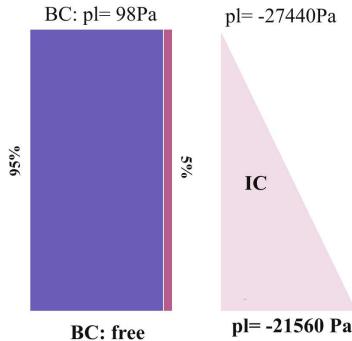


Figure 5.3.1: Illustration of numerical model

Table 5.3.1: Parameters in simulation

Soil type	Items	Setting
Matrix continuum	Preferential factor	0.95
	Porosity	0.498
	S_r^l	0.0
	S_{max}^l	1.0
	α (1/m)	1.8
	n	1.8
	Saturated permeability(1/m ²)	2.32368E-13
Fracture continuum	Preferential factor	0.05
	Porosity	0.6
	S_r^l	0.0833
	S_{max}^l	1.0
	α (1/m)	5.6
	n	2.68
	Saturated permeability(1/m ²)	1.09000E-11
Transfer	Transfer coefficient(1/m ²)	500

Results

Fig. 5.3.2 shows the pressure distribution comparison of single continuum at the time of 20 min and 30 min, which are calculated by GeoSys/RlockFlow (lines) and HYDRUS (symbols) respectively. The solid lines are pressure fronts of matrix, and the dash lines are fracture. The comparisons of dual-continua model results are shown in Fig. 5.3.3. The blue lines are the outcomes without transfer term, and the red lines by GeoSys/RockFlow and symbols by S1D

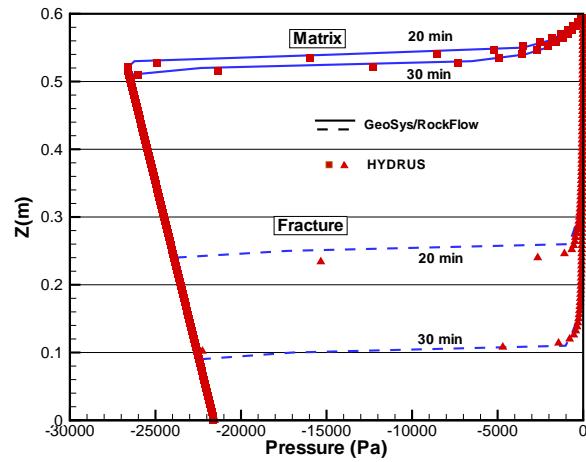


Figure 5.3.2: Pressure comparison of two single continua

show the exchange effects within two continua. Since matrix continuum is the dominant part in whole system, and the influence on matrix is less than that on fracture.

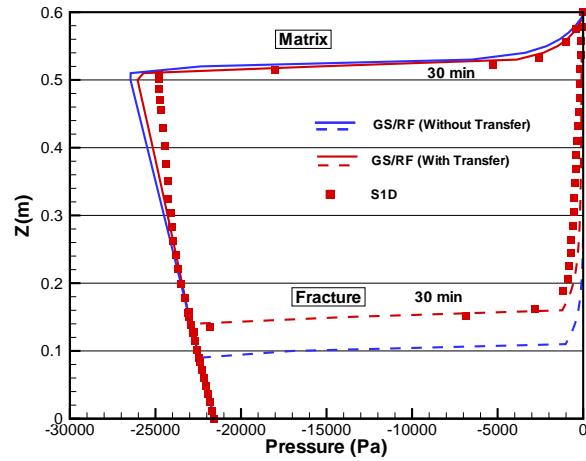


Figure 5.3.3: Pressure comparison of DPM

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>dual.vl</i>	H	benchmarks\h_us\dual\

5.3.2 Classic case: Gerke. etc

Problem definition

The section is a dual continua model comparison of GeoSys/RockFlow with the paper work of Gerke(1993)[59].

Initial and boundary conditions

The initial conditions for both matrix and fracture continuum are identical, which are set as $h_m^l = h_f^l = -10m$ and $p_m^l = p_f^l = -9800Pa$ in GeoSys/RockFlow. The infiltration exclusively goes into the fracture pore part, matrix continuum gets water from transfer. Details are illustrated in Fig. 5.3.4.

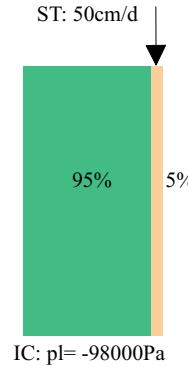


Figure 5.3.4: Illustration of numerical model

Material properties

Table 5.3.2 gives the parameters

Table 5.3.2: Parameters in simulation

Soil type	Items	Setting
Matrix continuum	Preferential factor	0.95
	Porosity	0.5
	S_r^l	0.21052
	S_{max}^l	1.0
	$\alpha (1/m)$	0.05
	n	1.5
Fracture continuum	Saturated permeability($1/m^2$)	1.2419E-14
	Preferential factor	0.05
	Porosity	0.5
	S_r^l	0.0
	S_{max}^l	1.0
	$\alpha (1/m)$	5.6
Transfer	n	10
	Saturated permeability($1/m^2$)	2.3596E-11
	Transfer coefficient($1/m^2$)	$0.01 \times 0.5[K(p_m) + K(p_f)]$

Results

Fig. 5.3.5 shows simulated pressure and saturation profiles during infiltration at some time steps.

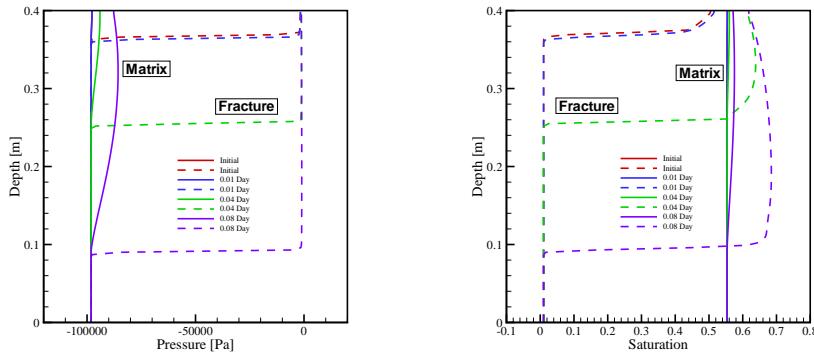


Figure 5.3.5: Simulated pressure and saturation profiles of the matrix (solid lines) and fracture (dashed lines)

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>dual_van</i>	H	benchmarks\h_us\dual\

5.3.3 Discussion

The pressure evolution of fracture continuum in 5.3.1 calculated by GeoSys/RlockFlow is a little slower than that by HYDRUS.

The distributions of saturation and pressure in 5.3.2 are different from the paper. The saturation of fracture is $S \in [0, 0.05]$ in [59].

5.4 Regional soil model

Problem definition

For the large scale area, soil represent significant diversification of moisture content with respect to the meteorologic changing such as precipitation and evapotranspiration as well as its physically-based continuum mechanics. Coupled hydrologic model with global climate model (GCM) is developed to research the impact of climate variabilities to vadose zone. The responses and water budget of alterations in timing and distribution of precipitation on the unsaturated zone are focused on by deterministic physically-based RSM, which is flexible and adaptable to extent one dimensional vertical column to three dimensional spatial area according to the heterogenous characteristics of climatological conditions, soil properties, geographic elevation, which is shown in Fig.5.4.1.

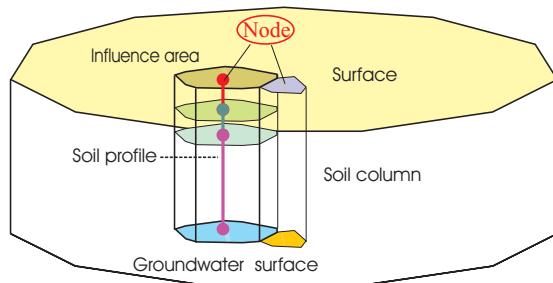


Figure 5.4.1: Concept of regional soil model

Initial and boundary conditions

Initial condition in the whole domain is set as: $P^l = -9000.0 \text{ Pa}$, and the top BC is set as pure infiltration serial in 2000 year in Beerze-Reusel basin, which is described by functions (FCT).

Material properties

The soil materials are from Beerze-Reusel drainage basin. There are several different soil types representing sand, loam and peat soils formed during the pleistocene, and those soil compose 5 kinds of soil profile type, which are defined the vertical structure of soil column. The soil water characteristic curves (SWCC) are given to describe the different soil properties (Fig. 5.4.2, left), for complete SSWC descriptions for the investigation area can be found in [60].

Results

The saturation evolutions of selected soil columns are shown in Fig. 5.4.2 (right).

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
AT_5	H	benchmarks\h_us\RSM

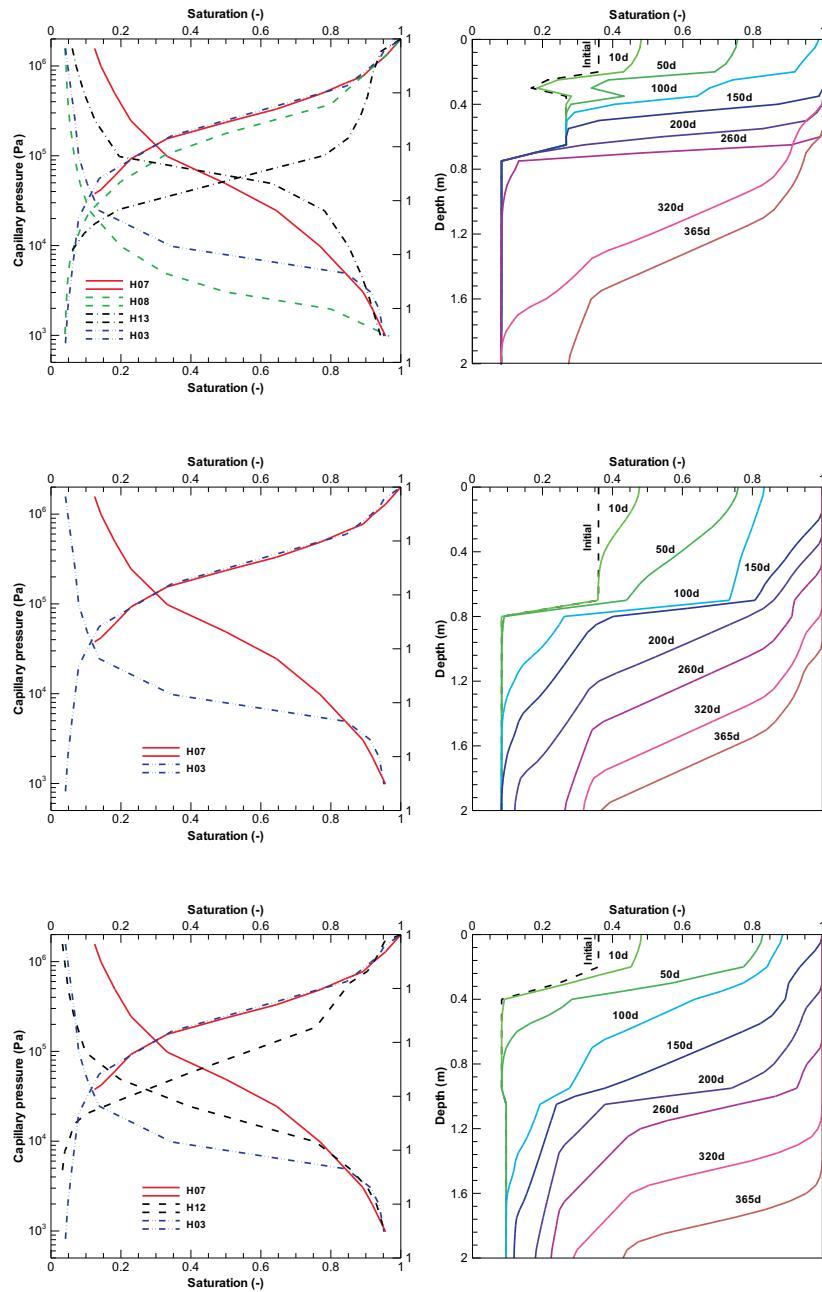


Figure 5.4.2: Soil water characteristic curves (SWCC) (left) and time evolution of water saturation in selected soil columns (right)

Chapter 6

Surface Flow – H-Processes

This chapter deals surface flow, i.e. one- and two-dimensional overland and one-dimensional channel flow. The governing equations are introduced in Sec. 6.1 and the benchmarks in Sec. 6.2.

6.1 Theory

Surface flow is simulated with the diffusive wave approximation of the Saint-Venant equations. Overland flow is calculated one- or two-dimensionally and channel flow one-dimensionally. The governing equation reads

$$\frac{\partial \theta}{\partial t} - \nabla \cdot \frac{CHR_H^m}{|\nabla h|^{1-j}} \nabla h = q^{ex} \quad (6.1.1)$$

where the water height $h = H + z + a$ is the primary variable of surface flow, H the flow depth, z the surface height, a the rill depth, and q^{ex} an external source term. For overland flow surface structure is included with

$$\theta = \frac{(H + \epsilon)^2}{H + a + \epsilon} + \frac{\epsilon^2}{a + \epsilon} \quad (6.1.2)$$

where the parameter ϵ determines the surface structure. Friction is taken into account with a resistance to flow relationship given by

$$u = CS_f^j R_H^m \quad (6.1.3)$$

with the hydraulic radius R_H and the parameters C , j , and m . $j = 1/2$, $m = 2/3$ correspond to the Manning relationship, $j = m = 1/2$ to the turbulent Chézy relationship, and $j = 1$ $m = 2$ to the laminar Chézy relationship. The hydraulic radius R_H is given by

$$R_H = H \quad (6.1.4)$$

$$R_H = \frac{A}{P} \quad (6.1.5)$$

for overland and channel flow, respectively. With use of Eqn. 6.1.4 the resistance to flow relationship 6.1.3 consideres only bottom friction. In Eqn. 6.1.5 channel wall friction is included by taking the ratio between channel cross-section A and the wetted perimeter P . Latter reads for a rectangular channel $P = B + 2H$ where B is the channel width. Normal depth, critical depth, and Green-Ampt infiltration source terms are given by

$$q_{norm}^{ex} = CS_o^j H^m \quad (6.1.6)$$

$$q_{crit}^{ex} = \sqrt{gH^3} \quad (6.1.7)$$

$$q_{GA}^{ex} = K \left(\frac{H - \Psi}{a'} \right) \quad (6.1.8)$$

where S_o is the surface slope, K is related to the soil conductivity, Ψ is the effective capillary drive. The location of the wedging front a' is given by

$$a' = \frac{\int_0^t q^{ga}(s) ds}{\Delta n}. \quad (6.1.9)$$

6.2 Benchmarking examples

6.2.1 Steady state

Problem definition

Flow on a plane and a channel with fixed inflow flux at one boundary and fixed water depth at the outlet are considered. The length of the computational domain is approximately 100m. A flat surface is considered in *a1* whereas in *a2* the slope is $4 \cdot 10^{-4}$.

Initial and boundary conditions

The initial water depth is $4 \cdot 10^{-2} m$. The inflow is $5 \cdot 10^{-2} m/s$ and the water depth at the outlet is $0.1 m$.

Material properties

The domain is spatially discretized by a string of 100 equal line or quadrilateral elements. 10 time steps with a constant step size of 1000s are chosen to ensure the steady state condition. For surface friction the turbulent Chézy resistance to flow relationship is used. Material properties are listed in Tab. 6.2.1

Table 6.2.1: Parameters for steady state examples

Parameter	Symbol	Setting	Unit
Chézy coefficient	C	10	$m^{1/2}/s$
Rill height	a	0	m
Surface structure coefficient	ϵ	0	m
Channel width	B	10	m

Results

Results by GeoSys, Mike11 and a finite difference scheme for $a2$ are compared in Fig. 6.2.1

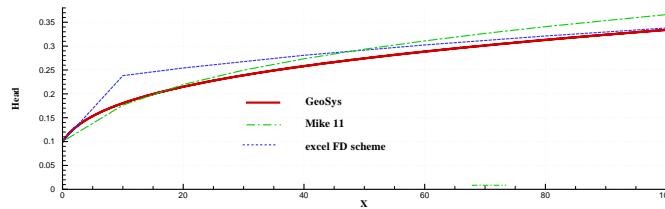


Figure 6.2.1: Water depth calculated by GeoSys, MIKE11, and a FD-scheme for inclined steady state example

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>a1_quad</i>	H	benchmarks\OVERLAND_FLOW\
<i>a2_quad</i>	H	benchmarks\OVERLAND_FLOW\
<i>a2_line</i>	H	benchmarks\OVERLAND_FLOW\
<i>a2_line_channel</i>	H	benchmarks\CHANNEL_FLOW\

6.2.2 One-dimensional precipitation runoff

Problem definition

These examples are based on the study by [61] which compared solutions given by the Saint-Venant equations and its diffusive wave and kinematic wave approximations. The simulation parameters are given by [62]. Constant precipitation is applied for 4min to an initially dry plane with a lenght of 100m and a slope of 0.01. The flow is assumed to continue uniformly at the lower domain boundary.

Initial and boundary conditions

The initial water depth is $1 \cdot 10^{-4} m$. The precipitation value is $4 \cdot 10^{-3} m/s$. A normal depth boundary condition is assigned to the outlet and no-flow to the remaining boundary.

Material properties

The time step size is $1 s$. The domain is discretized with line or quadrilateral elements. The line elements have a length of approximately $1 m$ throughout and the quadrangles $1 m \times 1 m$. For bottom friction Manning's relationship is used. Simulation parameters and fluid characteristics are given in Tab. 6.2.2.

Table 6.2.2: Parameters and fluid characteristics for one-dimensional precipitation runoff examples

Parameter	Symbol	Setting	Unit
Friction coefficient	C	18.25	$m^{1/3}/s$
Corresponding Manning coefficient	$n = 1/C$	$5.48 \cdot 10^{-2}$	$s/m^{1/3}$
Froude number	F_0	0.5	–
Kinematic wave number	K	10	–
Normal depth	H_0	0.4	m
Rill height	a	0	m
Surface structure coefficient	ϵ	0	m

Results

A comparison of GeoSys with HydroSphere and MODFLOW-Surface as well as solutions with the Saint-Venant and kinematic wave equations are shown in Fig. 6.2.2

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>govin_line</i>	H	benchmarks\OVERLAND_FLOW\
<i>govin_quad</i>	H	benchmarks\OVERLAND_FLOW\

6.2.3 One-dimensional precipitation runoff with high slope

Problem definition

These examples deal with one-dimensional flow on a plane with a slope of $S_0 = 0.5$ and a length of approximately $800 m$. Water leaves the domain freely-falling

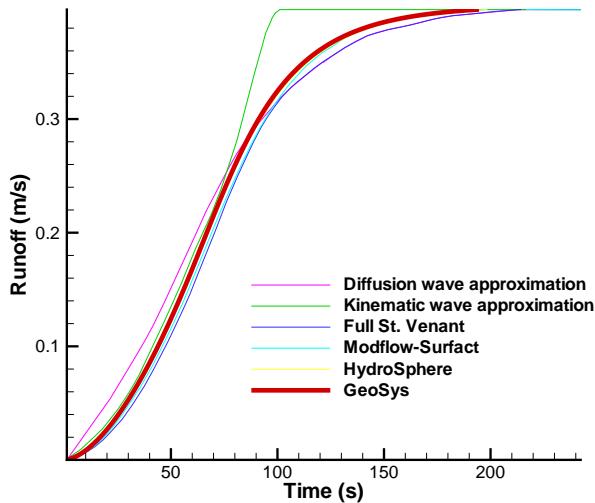


Figure 6.2.2: Results for one-dimensional precipitation runoff examples

at the outlet. Precipitation was applied to the surface for 90min. The total time is 180min. The examples deal with one- and two-dimensional overland flow as well as channel flow. In the one-dimensional cases the width is set 10m and in the two-dimensional the size of the domain is 800m × 100m

Initial and boundary conditions

The initial water depth is $1 \cdot 10^{-3}m$. A critical depth boundary condition is assigned to the outlet and no-flow to the remaining boundary. Precipitation of $4 \cdot 10^{-3}m/s$ is uniformly applied on the surface.

Material properties

The domain is discretized with a string of 10 equal line or rectangular elements. Manning's resistance to flow relationship is used for bottom friction. Parameters are given in Tab. 6.2.3.

Table 6.2.3: Parameters for high slope examples

Parameter	Symbol	Setting	Unit
Friction coefficient	C	66.67	$m^{1/3}/s$
Corresponding Manning coefficient	$n = 1/C$	$1.5 \cdot 10^{-2}$	$s/m^{1/3}$
Rill height	a	0	m
Surface structure coefficient	ϵ	0	m
Channel width	B	10	m

Results

Outflow hydrographs of GeoSys/Rockflow and Hydrosphere are compared in Fig. 6.2.3

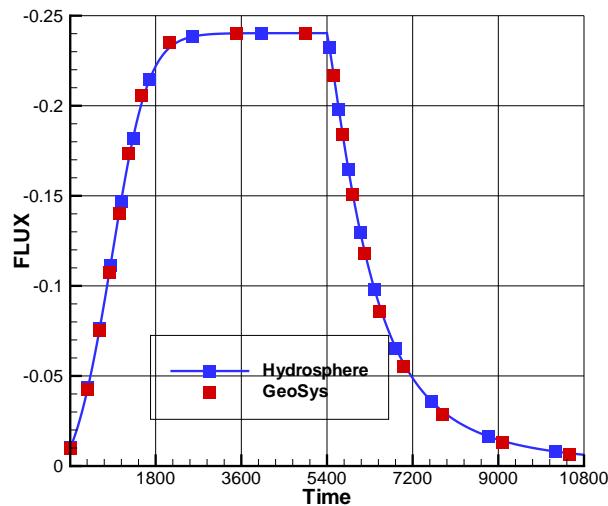


Figure 6.2.3: Outflow hydrographs by GeoSys and Hydrosphere for high slope example

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>v_line</i>	H	benchmarks\OVERLAND_FLOW\
<i>v_quad</i>	H	benchmarks\OVERLAND_FLOW\
<i>v_line_channel</i>	H	benchmarks\CHANNEL_FLOW\

6.2.4 Two-dimensional precipitation runoff

Problem definition

These examples are based on the study by [63] and consider two-dimensional surface flow on a V-catchment subject to constant precipitation for 90min and no-precipitation for additional 90min. At the catchment base the surface roughness is reduced to generate a channel region. At the channel outlet the water is leaving free-falling. Because of symmetry the computational domain involves only one half of the catchment which is a hillslope with the size of 1000m × 800m.

Initial and boundary conditions

The initial water depth is $1 \cdot 10^{-4} m$ and the precipitation $3 \cdot 10^{-6} m/s$. At the channel outlet a critical depth boundary condition and at the residual boundary no-flow is assigned.

Material properties

The domain is discretized with quadrilateral and triangular elements. Former have a size of 100m × 100m and 10m × 100m at the channel region. Triangles are generated by cutting the quadrilaterals into halves. Friction is described by Manning's relationship. The parameters are given in Tab. 6.2.4.

Table 6.2.4: Parameters for two-dimensional precipitation runoff examples

Parameter	Symbol	Setting	Unit
Friction coefficient (Overland)	C	66.67	$m^{1/3}/s$
Corresponding Manning coefficient	$n = 1/C$	$1.5 \cdot 10^{-2}$	$s/m^{1/3}$
Friction coefficient (Channel)	C	6.67	$m^{1/3}/s$
Corresponding Manning coefficient	$n = 1/C$	$1.5 \cdot 10^{-1}$	$s/m^{1/3}$
Rill height	a	0	m
Surface structure coefficient	ϵ	0	m

Results

Results of GeoSys, Hydrosphere and a semianalytical solution are compared in Fig. 6.2.4

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>gian_tri</i>	H	benchmarks\OVERLAND_FLOW\
<i>gian_quad</i>	H	benchmarks\OVERLAND_FLOW\

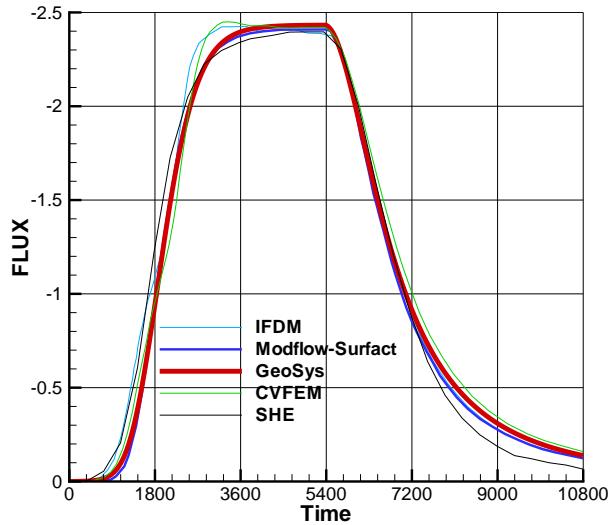


Figure 6.2.4: Results for two-dimensional precipitation runoff example

6.2.5 Infiltration excess (Horton) overland flow

Problem definition

This example is based on the soil flume experiments by [64]. The computational domain consists of an inclined plaine with a length of $12.2m$, a width of $0.051m$ and a slope of 0.01 . Light oil was applied on initially drained sand and generated Horton overland flow. Infiltration is calculated by the Green-Ampt approach for homogeneous soil. The simulation time is $900s$. Sec. 12.2.1 deals with simulations of the experiments by [64] with overland/soil flow coupling.

Initial and boundary conditions

The initial water depth is 1×10^{-6} . Precipitation of $6.944 \times 10^{-5} m/s$ and the Grees-Ampt source term are imposed on the surface. A critical depth boundary condition is assigned at oulet and no-flow at the remaining boundary.

Material properties

For discretization a string of quadrants with a length of $12.2cm$ is used and a time step of $2s$. For bottom friction the laminar Chézy relationship is used. Fluid, surface structure, friction, and infiltration parameters are given in Tab. 6.2.5.

Table 6.2.5: Parameters for Horton overland flow simulation

Parameter	Symbol	Setting	Unit
Kinematic viscosity	ν	1.47×10^{-3}	m^2/s
Density	ρ	755.6	kg/m^3
Laminar Chézy coefficient	C	430000	$1/ms$
Rill depth	a	1×10^{-3}	m
Surface structure parameter	ϵ	1×10^{-3}	m
Conductivity	K	2.3×10^{-5}	m/s
Effective capillary drive	Ψ	0.13	m

Results

The outflow hydrograph by GeoSys is compared with the experimental data in Fig. 6.2.5.

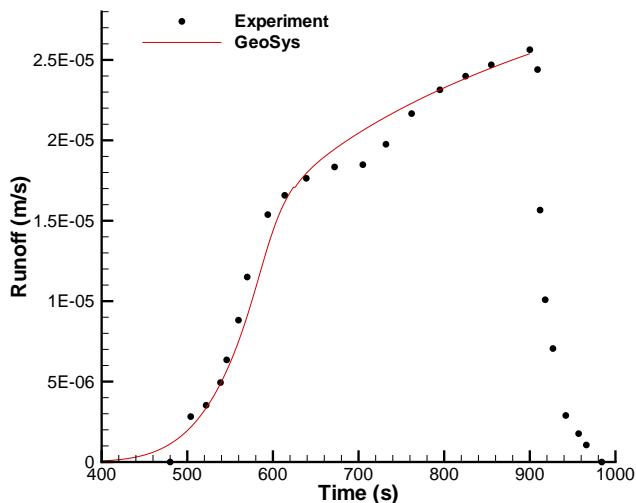


Figure 6.2.5: Measurements and simulation results by Geosys for the outflow hydrograph in the Horton overland flow example

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>Wool_quad</i>	H	benchmarks\OVERLAND_FLOW\

Chapter 7

Fluid Momentum – H-Process dependent

7.1 Theory

7.1.1 Velocity Estimation

For accurate simulation in groundwater, an accurate calculation of the groundwater velocity is a prerequisite. Generally, there are two approaches for calculation of velocities. The first is local element-based, while the second is global-node-based. The first is commonly used in numerical models while the latter is often neglected due to additional computational burden. Several methods based on the first approach have been described in the literature [65, 66, 67, 68]. However, the second approach is much less common and was used by e.g. [69, 70, 71]. In handling continuous velocity estimation on elemental boundaries, the mixed finite element method is also introduced in the literature [70, 72]. In this method, the normal component of the velocity field is continuous at elemental boundaries. Velocity is estimated on each edge of an element. Mixed finite element methods [73, 74] as well as the node-based velocity estimation get increased attention from modelers because of the need for accuracy and continuity. More specifically, the node-based velocity estimation can provide independence from element geometry under the same formation of the FEM's and easiness to interpolate velocity at any location in elements from the known velocity on nodes (i.e., position). In one of the scientific graphical software [75], nodes defined as positions are used for interpolation to have continuous values while elements defined as connections are not used for interpolation so that the values associated to the connections are discrete. Since the velocity estimation can be separated technically from the RWPT method if velocity fields are given, easy adaptation for various types of elements as well as a variety of choices for interpolation

techniques in treating velocity as position-dependent data lead to considerable advantages and become a standard method in scientific graphical software such as OpenDX[75].

The global node based method for velocity interpolation is used, due to the advantages discussed previously. The global-node-based velocity method uses the momentum equation of flow (the Darcy equation) as for the element-based velocity. The momentum balance equation for variable-density fluid flow in a porous medium in terms of hydraulic head, h (L) can be given as [65, 66, 67, 68, 69, 71]

$$\vec{q} = \phi \vec{v} = -\frac{\hat{k} \rho_0 \vec{g}}{\mu} \left(\nabla h + \left(\frac{\rho - \rho_0}{\rho_0} \right) \vec{e} \right) \quad (7.1.1)$$

where \vec{q} is the Darcy velocity vector, ϕ is the porosity, \vec{v} is the velocity vector, \hat{k} is the tensor of permeability of a porous medium, ρ_0 is the reference density, ρ is the density, \vec{g} is the gravitational vector, μ is viscosity, and \vec{e} is the unit vector against the gravitational direction.

Given the hydraulic head and the fluid density at element nodes, the global-node-based velocity can be obtained by applying the Galerkin method to Equation (7.1.1) for each velocity component. This global node based velocity is continuous and smooth so that it can further be used for interpolation at any location inside of elements.

7.1.2 Formulation of Galerkin method to obtain velocity

Equation 7.1.1 can be rewritten in a simplified form as

$$\vec{q} = -\hat{K} (\nabla h + \lambda_C C \vec{e}) \quad (7.1.2)$$

where $\hat{K} = \frac{\hat{k} \rho_0 \vec{g}}{\mu}$ is the hydraulic conductivity, $\lambda_C = \frac{\rho - \rho_0}{\rho_0}$ is the relative density difference term, and C is the relative concentration.

Substitution of the known approximate hydraulic head field and relative density difference term in Equation 7.1.2 yields

$$\begin{aligned}
q_x &= -K_{xx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) - K_{xy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \\
&\quad - K_{xz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \sum_{i=1}^N \hat{C}_k \omega_k \right] \\
q_y &= -K_{yx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) - K_{yy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \\
&\quad - K_{yz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \sum_{i=1}^N \hat{C}_k \omega_k \right] \\
q_z &= -K_{zx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) - K_{zy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \\
&\quad - K_{zz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \sum_{i=1}^N \hat{C}_k \omega_k \right]
\end{aligned} \tag{7.1.3}$$

where w is the basis function and N is the number of nodes in an element.

The residual function for the darcy velocity in x direction in Equation 7.1.3, which is the same for y and z direction, can be written as,

$$\begin{aligned}
R(x, y, z, t) &= q_x + K_{xx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + K_{xy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \\
&\quad + K_{xz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \lambda_C \left(\sum_{i=1}^N \hat{C}_k \omega_k \right) \right]
\end{aligned} \tag{7.1.4}$$

The Galerkin method weighs this residual over the whole domain using basis functions as the weighing function to yield

$$\begin{aligned}
&\int_{\Omega} \left[q_x + K_{xx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + K_{xy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \right. \\
&\quad \left. + K_{xz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \lambda_C \left(\sum_{i=1}^N \hat{C}_k \omega_k \right) \right] \right] \omega_i d\Omega = 0
\end{aligned} \tag{7.1.5}$$

When the approximate solution of each velocity is substituted in the velocity term, the equation yields the following form:

$$\begin{aligned} & \int_{\Omega} \left(\sum_{j=1}^N \hat{q}_x \omega_j \right) \omega_i d\Omega + \int_{\Omega} \left[K_{xx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + K_{xy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \right. \\ & \left. + K_{xz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \lambda_C \left(\sum_{i=1}^N \hat{C}_k \omega_k \right) \right] \right] \omega_i d\Omega = 0 \end{aligned} \quad (7.1.6)$$

The element matrix of integrals can be written in the following form:

$$[\mathbf{A}^e] \{\hat{\mathbf{q}}_x\} = \{\mathbf{B}^e\} \quad (7.1.7)$$

where

$$[\mathbf{A}^e] = \int_{\Omega} \omega_j \omega_i d\Omega^e \quad (7.1.8)$$

$$\begin{aligned} \{\mathbf{B}^e\} = & - \int_{\Omega} \left[K_{xx} \frac{\partial}{\partial x} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + K_{xy} \frac{\partial}{\partial y} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) \right. \\ & \left. + K_{xz} \left[\frac{\partial}{\partial z} \left(\sum_{i=1}^N \hat{h}_k \omega_k \right) + \lambda_C \left(\sum_{i=1}^N \hat{C}_k \omega_k \right) \right] \right] \omega_i d\Omega^e = 0 \end{aligned} \quad (7.1.9)$$

By solving Equation 7.1.7, velocity in each direction for all nodes can be obtained. The same method can also be applied to pressure-based darcy equation. Further, the method is independent of element types and works for one, two, and three dimensions. In this way, the continuous velocity on every node for density-driven flow can be obtained.

7.2 Test problems for various elements

Benchmark name: `1d_line`, `1d_tri`, `1d_quad`, `1d_tet`, `1d_pri`, `1d_hex`.

Purpose: Comparison of the result with simple analytical solution

- one directional constant velocity;
- Homogeneous media: Table ?? gives the parameters;
- fixed BC of 9810 Pa at the left end and 0 Pa at the right end;

Geometry and mesh: a 100m long saturated aquifer.

Table 7.2.1: Parameters in simulation

items	setting
Porosity	1.0
Permeability tensor (m^2)	1.000000e-12
Soil density kg/m^3	2.0e3

Model description: The hydraulic conditions is provided in Fig. 7.2.1

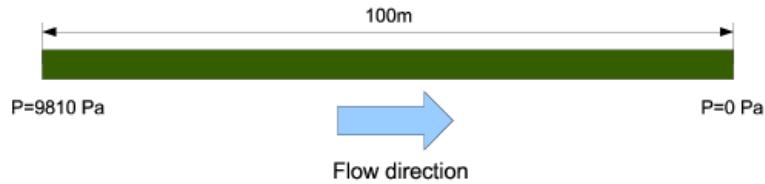


Figure 7.2.1: 1D Flow Description

Results: No matter what element type is used for the problem, the pressure distribution and velocity field should be same as provied in Fig.7.2.2.

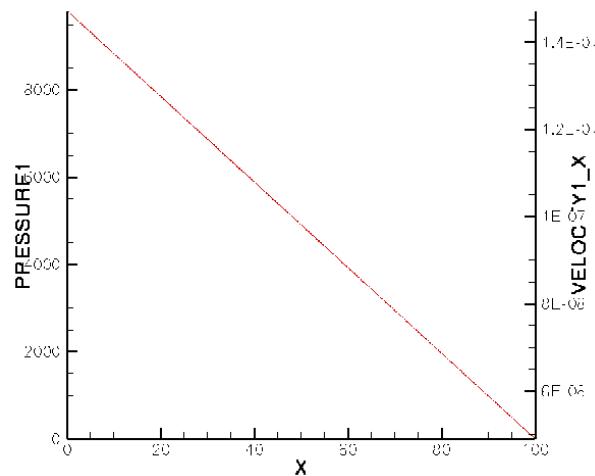


Figure 7.2.2: pressure and velocity

Chapter 8

Deformation – M-Processes

8.1 Theory

Pure deformations in any media can be described by the momentum balance equation in the terms of stress as

$$\nabla \cdot \boldsymbol{\sigma} + \rho g = 0 \quad (8.1.1)$$

where $\boldsymbol{\sigma}$ is stress tensor, ρ is the solid density. In the present implementation, the traditional sign convention for stress and fluid pressure is used. Displacement \mathbf{u} is the primary variable to be solved by substituting the constitutive law for stress-strain behavior

$$\begin{aligned} \boldsymbol{\sigma} &= \mathbb{C}\boldsymbol{\epsilon} \\ \boldsymbol{\epsilon} &= \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \end{aligned} \quad (8.1.2)$$

with \mathbb{C} , a forth order material tensor and $\boldsymbol{\epsilon}$, the strain. Superscript T means the transpose of matrix. The deformation problem can be considered as a boundary value problem with boundary conditions given by

$$\boldsymbol{\sigma} : \mathbf{n} = \mathbf{t} \quad \text{or} \quad \mathbf{u} = \mathbf{u}_\Gamma, \quad \forall \mathbf{x} \in \partial\Omega \quad (8.1.3)$$

where \mathbf{n} is the normal to the portion of domain surface on where the traction boundary condition \mathbf{t} is prescribed, \mathbf{u}_Γ is the described displacement boundary values.

For 2D problems, we restrict the analysis under the assumption of plane strain.

8.2 Elasticity

We consider linear elasticity, i.e. using the generalized Hook's law:

$$\mathbb{C} := \lambda \delta_{ij} \delta_{kl} + 2\mu \delta_{ik} \delta_{jl} \quad (8.2.1)$$

where δ is the Kronecker delta, μ is the shear modulus, $\lambda = 2\mu\nu/(1-2\nu)$ is the so called Lamé constant with Poisson ratio ν .

The elastic deformation is a reversible process. The related material behaviour is called elasticity. The Hooke's linear elastic law (Eqns. 8.2.2 to 8.2.4) describes the elastic behaviour of solids. The elastic strain ε is directly proportional to the effective stress σ .

$$\varepsilon_x = \frac{1}{E} \cdot (\sigma_x - \nu \cdot (\sigma_y + \sigma_z)) \quad (8.2.2)$$

$$\varepsilon_y = \frac{1}{E} \cdot (\sigma_y - \nu \cdot (\sigma_x + \sigma_z)) \quad (8.2.3)$$

$$\varepsilon_z = \frac{1}{E} \cdot (\sigma_z - \nu \cdot (\sigma_x + \sigma_y)) \quad (8.2.4)$$

with

ε_i – strains,

σ_i – stresses in Pa,

E – Young's modulus in Pa,

ν – Poisson's ratio.

The Poisson's number μ can be derived by the following relation.

$$\mu = -\frac{\varepsilon_x}{\varepsilon_x} = -\nu$$

The following examples are utilized to verify the functionality of the software dealing with elastic deformation problems.

8.2.1 Plane strain with uniform loading (2D)

Problem definition

This example deals with calculations of a part of the whole rock mass. This can be done when there are special conditions concerning symmetry, structure of the rock mass and material behaviour. To simulate an initial state of stress in different depths, a pressure at least at one boundary has to be put on which represents the load of the overburden. In addition to this the stresses decrease with depth because of the gravity and the density of the rock mass (Fig. 8.2.1).

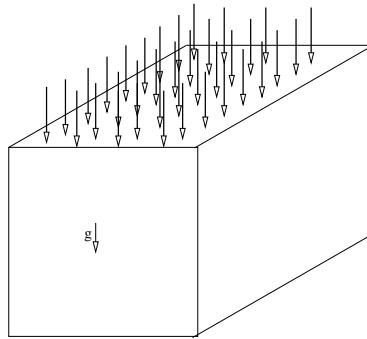


Figure 8.2.1: Conceptual model of elastic foundation

The calculation area has a size of $50m \times 50m$ (length and height) and the problem is simplified under the condition of plane strain. The quadrilateral mesh is illustrated in Fig. 8.2.2, one corner of which is finely meshed in order that it can be used directly to conduct an elastic excavation simulation in a coming example.

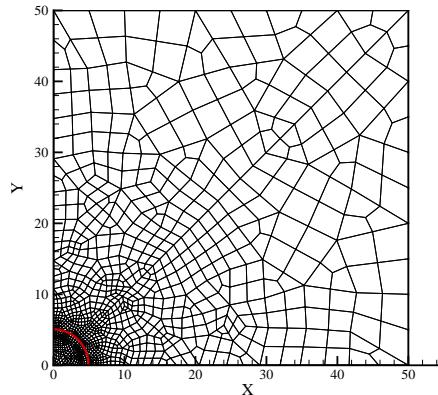


Figure 8.2.2: Special discretization: 1150 quadrilateral elements, 1101 nodes

Initial and boundary conditions

Initial conditions are not required for this problem. As for boundary conditions, the top boundary is prescribed with a uniformly distributed pressure of

23.75 MPa . Such kind of boundary conditions are so called traction boundary in the context of mechanics, they are treated as Neumann type boundary condition. More detailed boundary conditions are illustrated in Fig. 8.2.3.

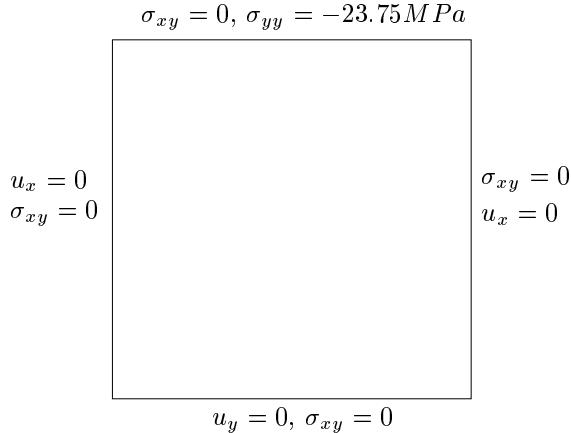


Figure 8.2.3: Boundary conditions

Material properties

Homogeneous material properties are assumed within the whole domain. Table 8.2.1 gives the parameters.

Property	Value	Unit
Young's modulus	25	GPa
Poisson's ratio	0.3	–
Density	2500	kg/m^3

Table 8.2.1: Material parameters

Results

For this simple elastic problem, we have an analytic solution given by

$$\sigma_{yy} = -23.75 - \rho h [\text{MPa}] \quad (8.2.5)$$

where ρ is the solid density and h is the height from top to bottom boundary.

Fig. 8.2.4 (left) shows the distribution of vertical stress in the domain, which implies that the discretization error is very small. Fig. 8.2.4 (right) shows a linear variation of stress σ_{yy} along with height.

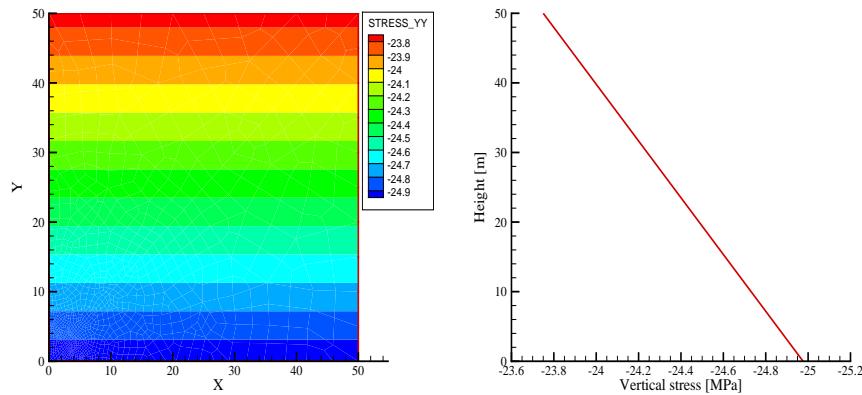


Figure 8.2.4: Result of vertical stress, σ_{yy} (MPa). Left: domain distribution. Right: Vertical profile

The numerical result of σ_{yy} at the bottom boundary is -24.97 MPa, which is very close to the analytic solution, $\sigma_{yy} = -25.0$ MPa. This proves the correctness of the numerical scheme.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_drift</i>	M	benchmarks\M\

8.2.2 Plane strain with uniform loading - Excavation in homogeneous media (2D)

Problem definition

This is the second step of the simulation described in the above section, Section 8.2.1. A long round tunnel is built in the rock mass and this is depicted in Fig. 8.2.5. The deformation due to the excavation is simulated under the assumption of plane strain, same initial condition and material parameters given in Section sec:el2d.

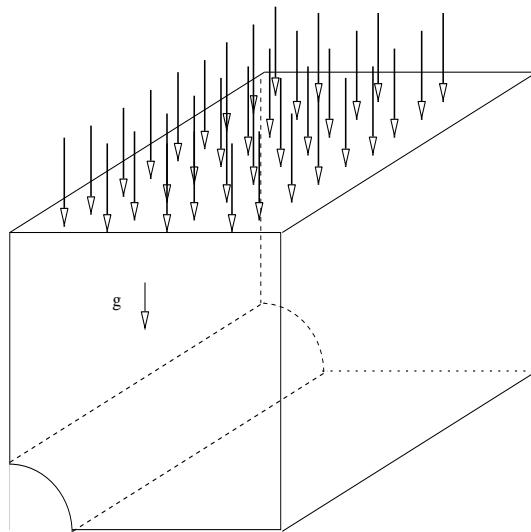


Figure 8.2.5: Excavation in rock mass

Initial and boundary conditions

The tunnel has a radius of 5m. The released loading approach is applied to simulate the excavation.

Results

We use the same mesh as given in the above section to conduct the simulation. Fig. 8.2.7 shows the distribution of vertical displacement and stresses in the domain after excavation.

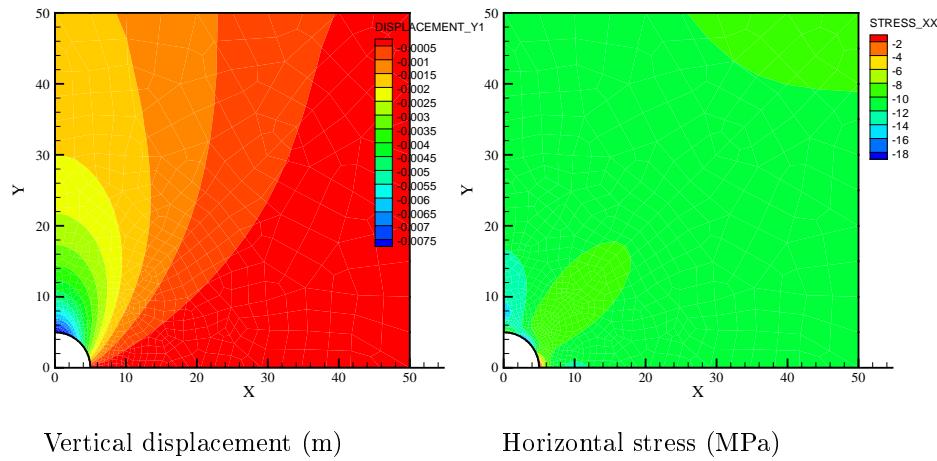


Figure 8.2.6: State variables after excavation

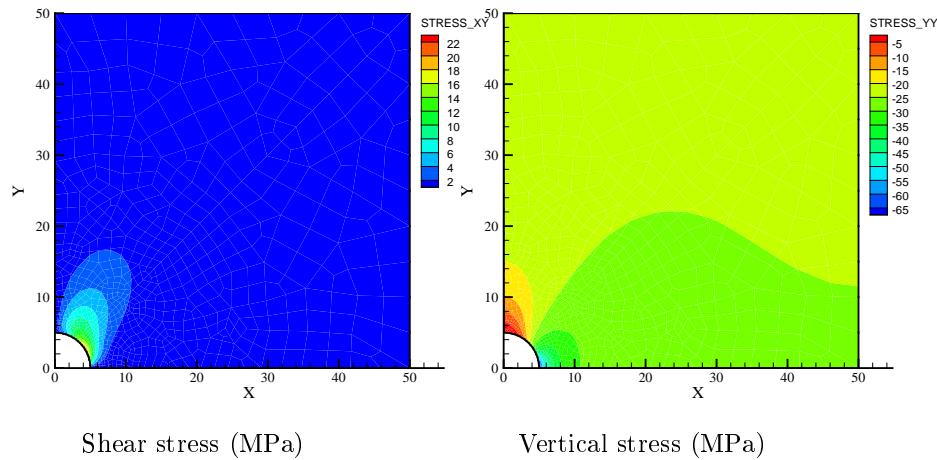


Figure 8.2.7: State variables after excavation

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_drift</i>	M	benchmarks\M\

8.2.3 Plane strain with uniform loading - Excavation in heterogeneous media (2D)

Problem definition

Again, we analyze the deformation of the excavation problem defined in Section 8.2.2. Contrary to homogeneous case, we use function defined initial stress and assume four different material domains make up the geometry (Fig. 8.2.8).

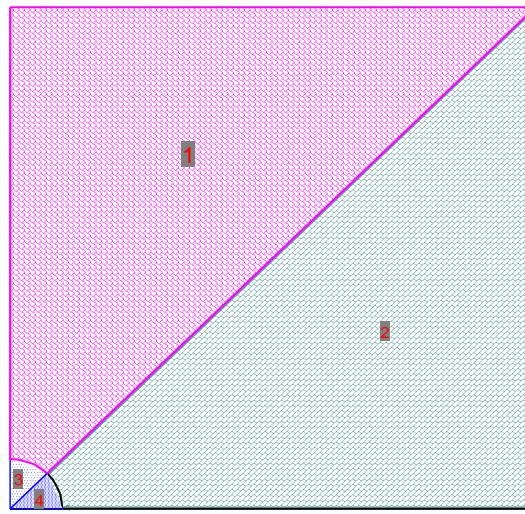


Figure 8.2.8: Excavation in heterogeneous rock mass

Initial and boundary conditions

The initial stresses are assumed linearly distributed within a material domain. The expressions of these distribution are given in

Material (Fig. 8.2.8)	σ_{xx}	σ_{yy}	σ_{zz}
1	$23.75 + 0.2y$	$23.75 + 0.2y$	$23.75 + 0.2y$
2	$24.75 + 0.5y$	$24.75 + 1.3y$	$24.75 + 0.5y$
3	$26.75 + 10.0x + 12.0y$	$26.75 + 20.0x + 16.0y$	$26.75 + 10.0x + 12.0y$
4	$27.75 + 10.0x + 14.0y$	$27.75 + 20.0x + 18.0y$	$27.75 + 10.0x + 14.0y$

Table 8.2.2: Initial stress expression (negative value, kPa)

Material properties

As depicted in Fig. 8.2.8, the domain consists of four different materials denoted by 1, 2, 3 and 4. Hereby, we assume only Young's modulus differs from each other of materials (Table 8.2.3).

Property	Value	Unit
Young's modulus	1:25, 2:26.0, 3:30.0, 4:28.0	GPa
Poisson's ratio	0.3	—
Density	2.5	kg/m^3

Table 8.2.3: Parameters

Results

Fig. 8.2.9 shows the distribution of displacements after excavation. Fig. 8.2.9

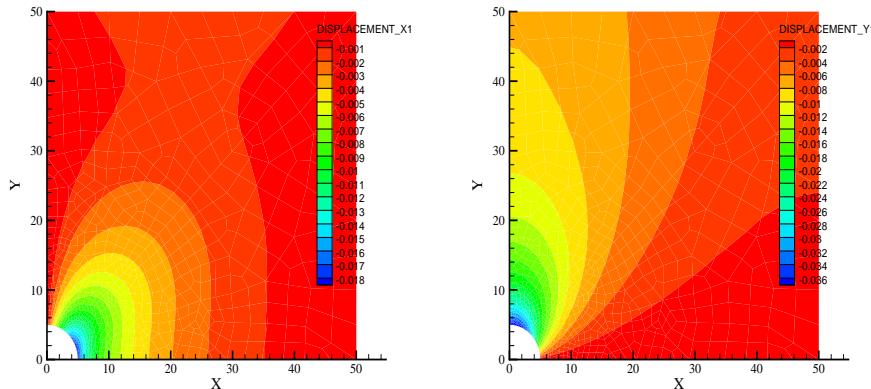


Figure 8.2.9: Distribution of displacement (m)

shows the distribution of stresses after excavation.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_drift_init</i>	M	benchmarks\M\

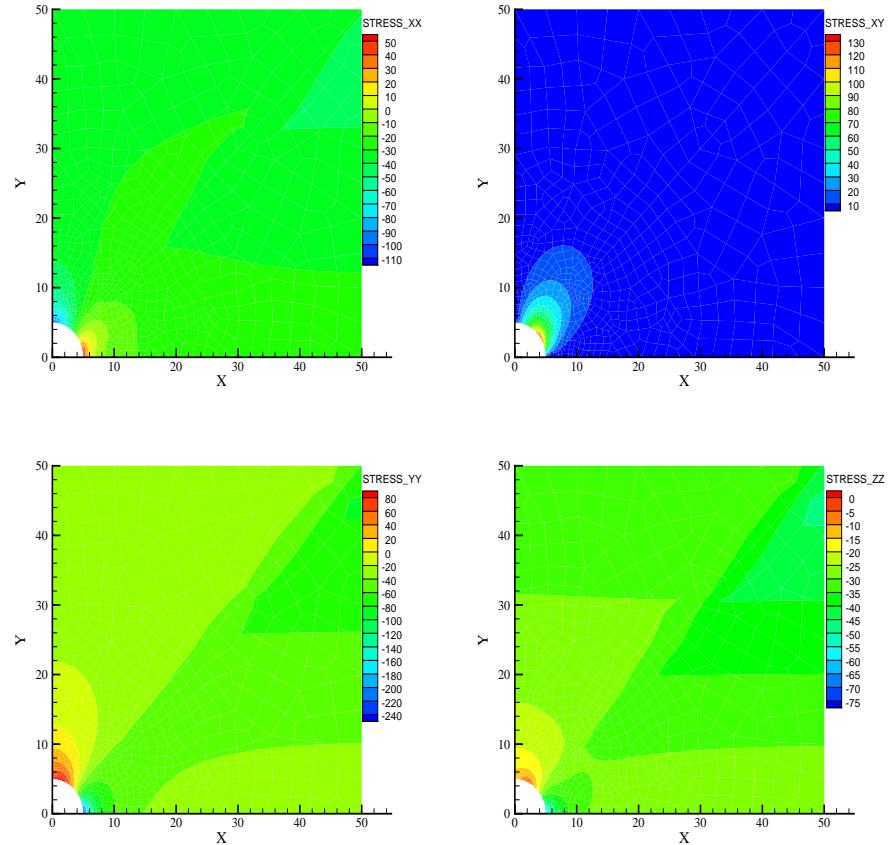


Figure 8.2.10: Distribution of stresses (kPa)

8.2.4 Elastic cube (3D)

Problem definition

We consider deformation in a cubic domain under linearly distributed pressure (Fig. 8.2.11). The size the domain is $1m \times 1m \times 1m$. The deformation is assumed being elastic.

Initial and boundary conditions

Normal translation on the vertical surfaces, which contains vertex A, D and which contains vertex B, C, and on the bottom surface is restricted. On the top

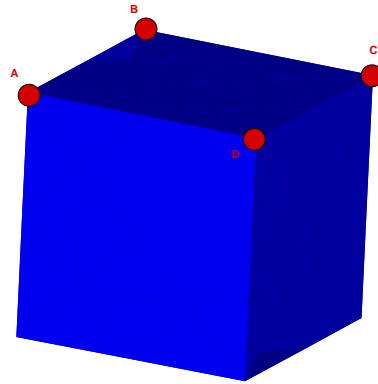


Figure 8.2.11: A block with linear distributed pressure on the top surface

surface, a linear distributed pressure is prescribed in the manner of point-wise as:

- Vertex A: $1.0Pa$
- Vertex B: $1.0Pa$
- Vertex C: $0.0Pa$
- Vertex D: $0.0Pa$

The pressure at any point on the top surface is obtained by a linear interpolation before face integration. This is done by program automatically.

Material properties

The material properties are homogenous with the domain and they are listed in Table 8.2.4

Property	Value	Unit
Young's modulus	2.0×10^7	Pa
Poisson's ratio	0.4	—

Table 8.2.4: Material parameters of cubic domain

Results

A deformed domain is depicted in Fig. 8.2.12, which demonstrated that the results are consistent with the prescribed boundary condition.

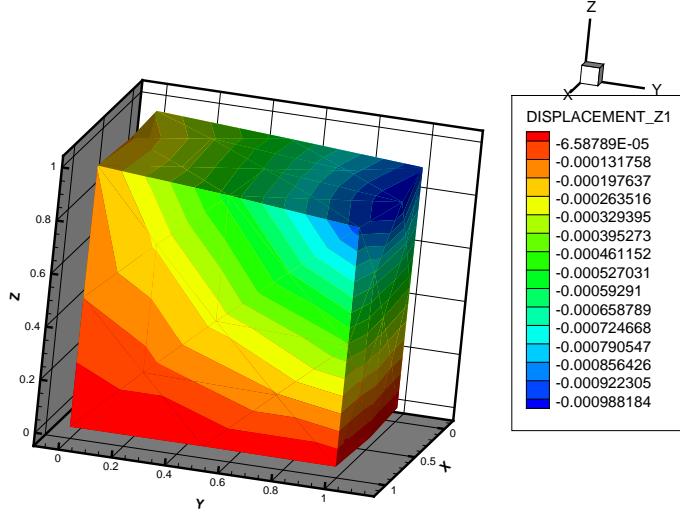


Figure 8.2.12: Deformed cubic domain

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_brick_l</i>	M	benchmarks\M\

8.2.5 Given deformation at the top (3 D)

Problem definition

A quarter of an elastic cylinder is compressed at the top. The deformation that is caused by a uniform vertical stress is given as boundary condition. The aim is to calculate the stress in z -direction which is caused by this deformation and to get to know the resulting deformations in each direction.

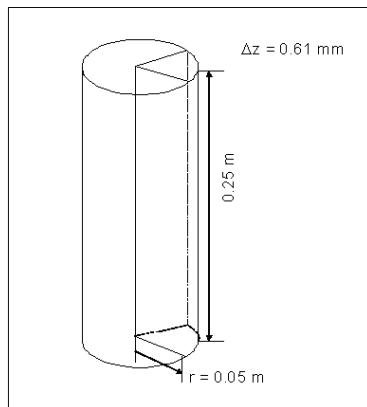


Figure 8.2.13: Calculation area: a quarter of a cylinder

Assumptions

Solid: homogeneous, isotropic, finite dimensions, constant deformation, linear elastic material behaviour

Model set-up of the 3 D numerical model

For the 3-dimensional simulation the calculation area is exclusively out of a quarter of a cylinder. The model includes 4000 elements and 4947 nodes. Deformations in x -direction are suppressed in the $y - z$ -plane. Deformations in y -direction are suppressed in the $x - z$ -plane and deformations in z -direction are inhibited at the bottom of the quarter cylinder. At the top of the model a mechanical boundary condition is set with a constant displacement of 0.61 mm. The elastic deformation of the solid is not time-dependent. The used material parameters are shown in Tab. 8.2.5.

symbol	quantity	value
ρ	density of the solid	$2.5 \text{ t} \cdot \text{m}^{-3}$
E	Young's modulus of the solid	7 GPa
ν	Poisson ratio	0.3

Table 8.2.5: Material parameters

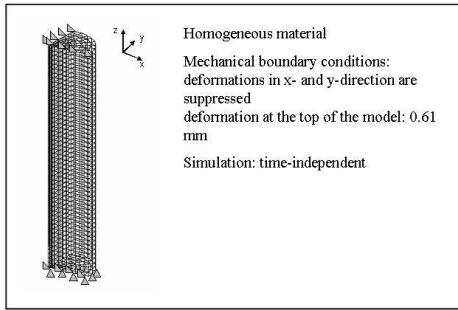


Figure 8.2.14: Calculation model (3D)

Evaluation method

In order to solve the equations of the Hooke's law, there are some constraints that have to be considered: the stresses in x - and y -direction are equal to zero, because the body can expand into radial direction. Thus the Hooke's equations can be simplified as follows:

$$\varepsilon_z = \frac{\Delta z}{z} = \frac{1}{E} \cdot \sigma_z \quad (8.2.6)$$

$$\varepsilon_x = \varepsilon_y = \frac{1}{E} \cdot (-\nu \cdot \sigma_z) \quad (8.2.7)$$

Results

With the given strain in z -direction, the stress σ_z is calculated by Eqn. 8.2.6.

$$\frac{\Delta z}{z} = \frac{-6.1 \cdot 10^{-4} \text{ m}}{0.25 \text{ m}} = -2.44 \cdot 10^{-3} \quad \text{and} \quad \sigma_z = -2.44 \cdot 10^{-3} \cdot 7 \cdot 10^9 \text{ Pa} = -1.71 \cdot 10^7 \text{ Pa}$$

In this way, the strains in x - and y -direction are known.

$$\varepsilon_x = \varepsilon_y = \frac{1}{7 \cdot 10^9 \text{ Pa}} \cdot (-0.3 \cdot -1.71 \cdot 10^7 \text{ Pa}) = 7.32 \cdot 10^{-4}$$

The numerical results meet exactly the analytical solutions. This is sketched in Fig. 8.2.14, where the strains and the resulting stress along a polyline from top to bottom of the quarter cylinder can be found. That means both RockFlow and GeoSys/RockFlow are able to calculate the state of stresses for the 3D elastic deformation.

Path in the benchmark deposit	Used code	Used version	Date of simulation run
\M\elastic_deformation\displacement\displ_Geosys/RF\m_e_displacement_3Du	GeoSys/RockFlow	RockFlow 4, rf4-507	Dec. 2007

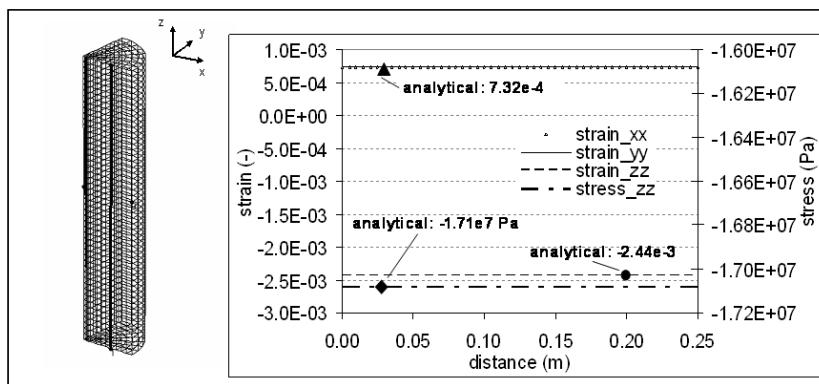


Figure 8.2.15: Strains and stress in z -direction as the result of deformation

8.2.6 Given stress at the top (3 D)

Problem definition

This example is the inverse of the precedent one. The quarter cylinder is deformed by a given stress, while this time the resulting deformation is unknown. In order to check out easily whether the simulated results correspond to the analytical solutions, the value of the effective stress in z -direction on top of the calculation model is the same as in the above described example.

Assumptions

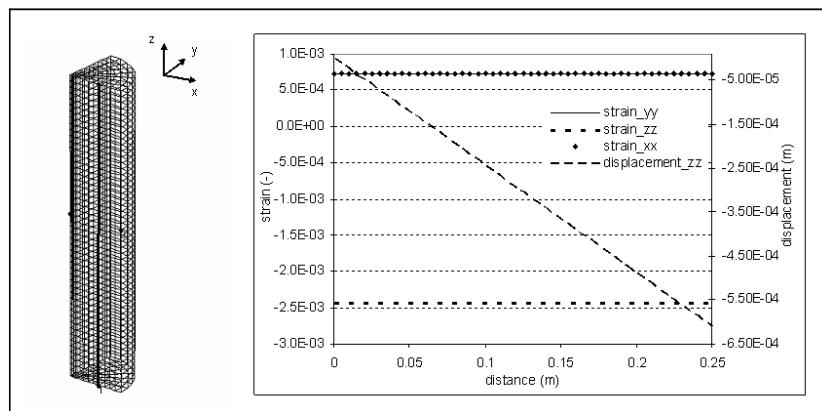
Solid: homogeneous, isotropic, finite dimensions, constant deformation, linear elastic material behaviour

Model set-up of the 3 D numerical model

The calculation model has the same properties as the model of the precedent example. At the top of the model a load of $-1.71 \cdot 10^7$ Pa was set as constant source term. The simulation with both RockFlow and Geosys/RockFlow needs the input of the load as source term in z -direction at the single nodes under consideration of each element node. The input is done as single forces, not as the common stresses. The displacement boundaries are the same as in the precedent example except the z -displacement on the top of the model. The used material parameters are shown in Tab. 8.2.5.

Results

The analytical solution and results are identical to the previous example. The calculated displacement as a result of the constant load on the top amounts to $6.1 \cdot 10^{-4}$ m. The numerical results that are shown in Fig. 8.2.16 meet the analytical solutions well.

Figure 8.2.16: Strains and displacement in z -direction

Path in the benchmark deposit	Used code	Used version	Date of simulation run
\M\elastic_deformation\stress\stress_Geosys RF\m_e_stress_3Du	GeoSys/RockFlow	RockFlow 4, rf4-507	Dec. 2007

8.3 Elasto-plasticity

Plasticity is a property of a material to undergo a non-reversible change of shape in response to an applied force. During the elasto-plastic deformation, the onset of plasticity is determined by a yield criterion and post-yield deformation is governed by the yield criterion and a plastic potential. To illustrate features of elasto-plasticity deformation, we consider a uniaxial test of stress depicted in Fig. 8.3.1.

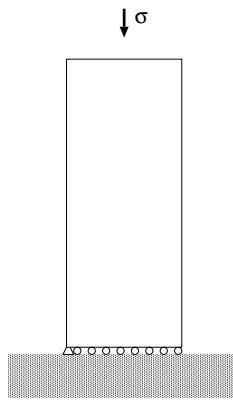


Figure 8.3.1: Uniaxial test

This means only one direction has non-zero stress and strain, e.g. $\sigma = \sigma_{yy}$ and $\epsilon = \gamma_{yy}$. Different material exhibits different elasto-plastic behavior. Fig. 8.3.2 depicts a typical

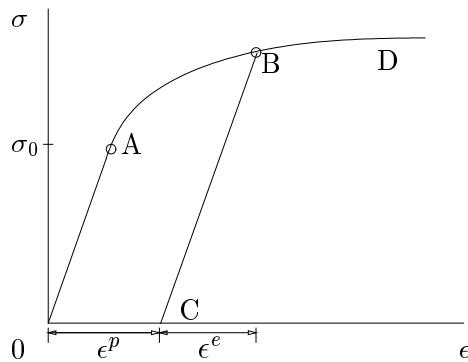


Figure 8.3.2: Stress-strain curve of 1D problems

stress-strain curve of the uniaxial test. If load σ is gradually increased, a corresponding point in (σ, ϵ) plane are moving from 0 to A. Up to A, stress reaches a value σ_0 , so called yield stress. If the load is removed gradually before its

reaches the yield value, the point follows the line from A to 0. On the other hand, if the load is continually increased after stress is bigger than σ_0 , the material experiences plastic deformation. Assuming the curve is extended from A to B during load acting. If we remove the load gradually, the point will not take the way its from, i.e. from B to A to 0. On the contrary, it will move from B to C linearly. Furthermore, if the load is applied again, the point will take the path from C \rightarrow B \rightarrow D.

This implies that: i) The unloading is elastic and there is still strain ϵ^p left after the load being removed, Therefore, the plastic deformation is irreversible; ii) The strain is admissible to be decomposed into several components, e.g. $\epsilon = \epsilon^e + \epsilon^p$; iii) The relationship of stress-strain is history dependent curve. Based on the last point and the Hook's law, the constitutive equation for the 1D deformation problem can be described as

$$\sigma_{yy} = E\epsilon_{yy}^e = E(\epsilon_{yy} - \epsilon_{yy}^p) \quad (8.3.1)$$

where E is so called Young's modulus. If the stress-strain is monotonic increasing after yielding, the material shows hardening behavior. For some porous media, softening behavior may be observed and its stress-strain curve looks like what depicted in Fig. 8.3.3.

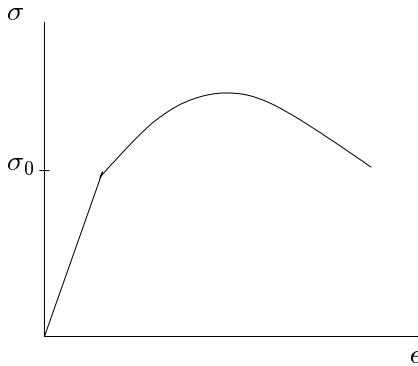


Figure 8.3.3: Softening

For the constitutive equation, the case of more than one direction have non-zero stress and strain are much more complicated. A yield function f and a plastic potential g are introduced to establish a constitutive equation. Normally, the variables of the two functions are the first, second or third stress invariant σ_v , II or III. If we cast the yield functions to the principal stress space, we get the yield surfaces. Fig. 8.3.4 depicts three typical yield surfaces of porous media.

If the stress path of any point locates inside the surface, the point undergoes elastic deformation. Otherwise, the stress status is determined by the Kuhn-Tucker criterion for the loading or unloading:

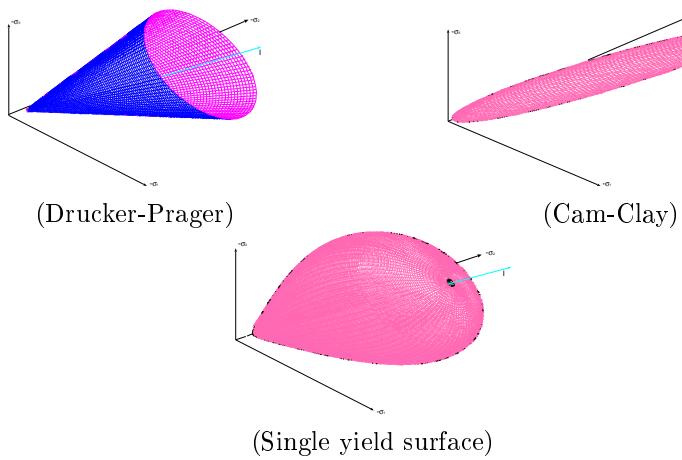


Figure 8.3.4: Yield surface

$$\dot{f} \leq 0, \quad \dot{\lambda}_p f = 0, \text{ or, } \dot{\lambda}_p \geq 0 \quad (8.3.2)$$

is then used to check the yield status.

Since the stress path in plastic deformation is history dependent, we describe the constitutive equations in the sense of increment of stress and strain. Considering the generalized Hook's law (8.2.1), the relationship of incremental stress tensor $d\sigma$ and incremental strain tensor $d\varepsilon$ the relationship of stress and strain obeys the generalized Hook's law:

$$d\sigma = \mathbf{D}d\varepsilon^e = \mathbf{D}(d\varepsilon - d\varepsilon^p) \quad (8.3.3)$$

From the definition of plastic potential surface g , and normality law, it is possible to express the generalized plastic strain increment if the potential surface is smooth. Since $d\varepsilon^p$ lies parallel to the normal to g at σ , we may write

$$d\varepsilon^p = d\lambda_p \frac{\partial g}{\partial \sigma} \quad (8.3.4)$$

where $d\lambda_p$ is non-negative factor, plastic multiplier. Equation (8.3.4) is so called flow rule. Hence, the general elasto-plastic constitutive equation is given by

$$d\sigma = \mathbf{D}d\varepsilon^e = \mathbf{D}(d\varepsilon - d\lambda_p \frac{\partial g}{\partial \sigma}) \quad (8.3.5)$$

The flow rule is associative if $f \equiv g$. Otherwise, it is non-associative. Typical plastic models, i.e. yield functions and plastic potentials are described below.

Drucker-Prager model

This model is a function of the two stress invariants and hardening parameter. Its yield function takes the form

$$f(\boldsymbol{\sigma}, \kappa) = \|\mathbf{s}\| + \alpha\sigma_v - y(\kappa) = 0 \quad (8.3.6)$$

$$g(\boldsymbol{\sigma}, \kappa) = \|\mathbf{s}\| + \beta\sigma_v - y(\kappa) = 0 \quad (8.3.7)$$

where α is a coefficient related to the internal frictional angle, $y(\kappa)$ is the yield stress depending on the hardening parameter.

Cam-Clay model

Similar to the Drucker-Prager model, the Cam-Clay model is a function of both of the first and the second stress invariants. The generalized Cam-Clay model reads:

$$f = q^2 + M^2 p_s (p_s - p_{scn}) = 0 \quad (8.3.8)$$

where $q = \sqrt{3/2} = \|\mathbf{s}\|$, $p_s = \sigma_v/3$ the mean stress, M is the slope of the critical state line in a $q - p_s$ diagram and p_{scn} is the isotropic preconsolidation pressure. The rate of p_{scn} is given by

$$\frac{dp_s}{d\epsilon_v^p} = \frac{(1+e)p_s}{\lambda_c - \kappa_c} \quad (8.3.9)$$

with e the void ratio, ϵ_v^p the volume plastic strain, λ_c the virgin compression index and λ_c the swelling/recompression index.

The model also describes the nonlinear elastic behavior of the clay-like media before plastic yielding occurs, in which the bulk modulus K is dependent of stress status as

$$K = \frac{1+e}{\kappa_c} p_s = 0 \quad (8.3.10)$$

with $\mu = 3(1-2\nu)K/(2(1+\nu))$.

8.3.1 Plastic plate - von Mises plasticity (2D)

Problem definition

This is a typical plane strain benchmark for von Mises plasticity, which is defined in [76]. We first analyze this example to compare the behavior of two approaches on pure plastic deformation problems. In the present simulation, a quarter of plate is taken due to the symmetry of the problem. The model set-up is depicted in Fig. 8.3.5. The radius of the hole is 10mm. Two points as point 1 and point 2 are specified to monitor the evolution of variables. Point 1 is at one third of the distance from point 3 to point 4.

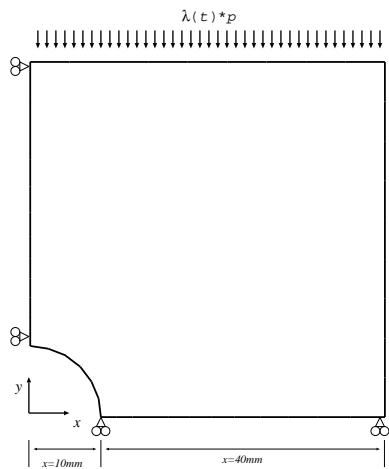


Figure 8.3.5: Stretched steel plate with a hole: one quarter

Boundary conditions

Traction boundary condition, $p = 100 \text{ N/mm}^2 \lambda(t)$ is prescribed on the top with $\lambda(t)$, the time dependent scaling factor. The case of cycling loading is investigated with a scaling function depicted in Fig. 8.3.6, in which, $\lambda_{max} = 4.1$.

The domain is triangulated as depicted in Fig. 8.3.7.

Material properties

The domain is assumed in homogeneous state. Table 8.3.1 gives the material parameters[76].

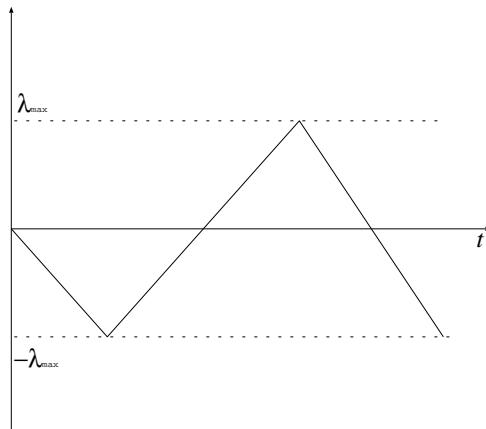


Figure 8.3.6: Time dependent load factor

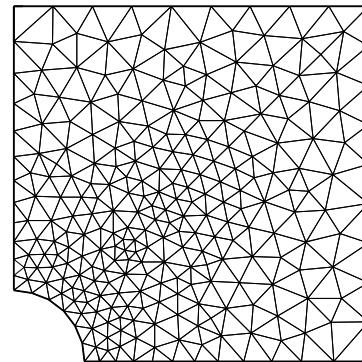


Figure 8.3.7: Mesh: 269 nodes and 484 elements

Table 8.3.1: Material properties

Property	Value	Unit
Young's modulus	206900	N/mm ²
Poisson's ratio	0.29	—
Initial yield stress	450	N/mm ²
Hardening modulus	0.0	kPa

Results

The loading takes 60 steps with constant increment of $\lambda_{max}/10$. The similar distribution of plastic strain and vertical stain given in Fig.8.3.8 shows implies the behavior of von Mises plasticity.

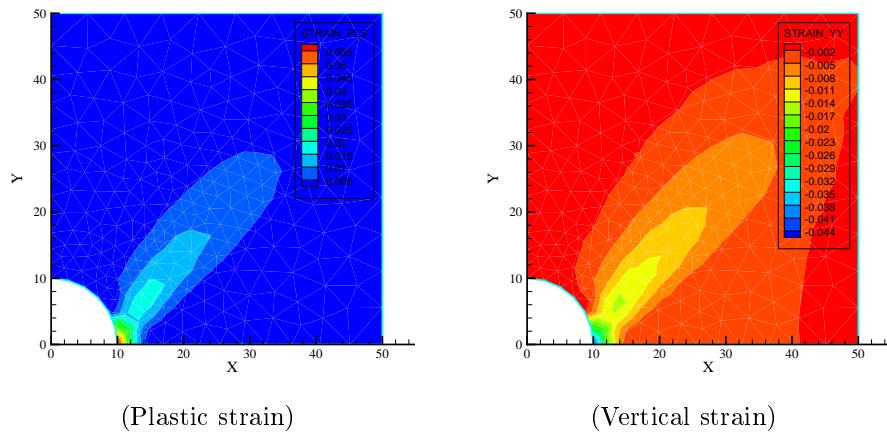


Figure 8.3.8: Distribution of plastic strain and vertical strain at $\lambda_{max}/10$

The evolution of horizontal displacements at point 1 and point 2 along with periodic load factor $\lambda(t)$ are shown on Fig.

8.3.9.

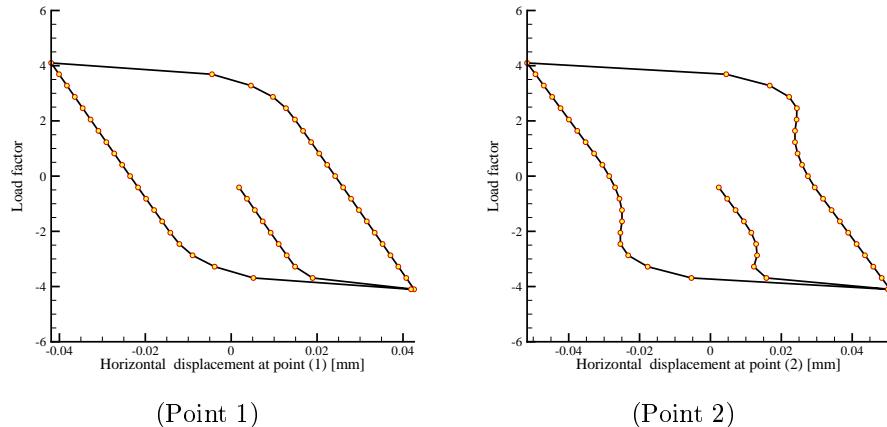


Figure 8.3.9: Evolution of horizontal displacement vs load factor

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_mises</i>	M	benchmarks\M\

8.3.2 Plastic plate - Drucker-Prager plasticity, enhanced strain element (2D)

Problem definition

In this application, we analyze a plane strain biaxial failure deformation problem with triangle and quadrilateral elements, correspondingly. We use an enhanced strain approximation to simulate the displacement discontinuity after failure appears. Neighbor relationships of an element object are essential data for constructing the deforming mesh and to determinate the propagation orientation of the discontinuity in the failure analysis.

From the view point of bifurcation theory, strain localization is a bifurcation phenomenon, which takes place when the velocity field moves away from the branch of continuous solutions and takes a new path of discontinuous solutions. If standard finite element is applied to this problem, we have to refine mesh adaptively near the localization area. Otherwise, the system equation is ill-posed. The strong discontinuity approach with enhanced strain element avoids the ill-posed system equations and therefore avoid mesh sensitive of the analysis [77].

The set-up of the biaxial compression problem as proposed by [78] is shown in Fig. 8.3.10. The geometry of the specimen is simplified to a rectangle with size of $1\text{m} \times 3\text{m}$.

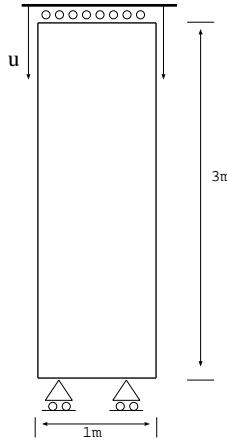


Figure 8.3.10: Plane strain biaxial test

Boundary conditions

The bottom of the specimen is placed on horizontal roll supporters. While the top of it is only allowed to a vertical down movement u_z . Both lateral sides are considered to be traction free.

Material properties

The non-associative flow rule is adopted for the Drucker-Prager model. All material parameters are given in Table (8.3.2)

Parameter	Unit	Value
Young's modulus	kPa	2×10^4
Poisson ratio	-	0.4
Parameter α	-	0.233345 (30° friction angle)
Parameter β	-	0.141421 (16.53° dilatancy angle)
Initial stress σ_0	kPa	29.69 (20 of initial cohesion)
Hardening modulus H	kPa	100
Localized softening modulus H_δ	kPa	-1000, varying

Table 8.3.2: Material parameters of the plane strain biaxial test

Results

Fig. 8.3.11 shows the deformed sample exhibiting localization. Fig. 8.3.12 depicts the stress reaction at the top surface due to the displacement load. The results agrees with what given in [78]

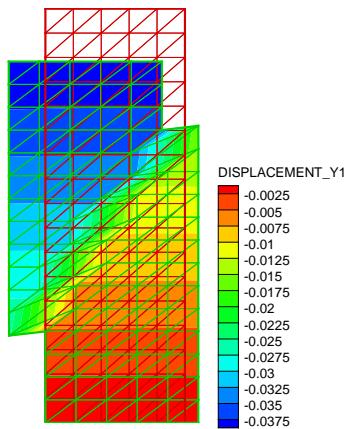


Figure 8.3.11: Vertical reaction of the top

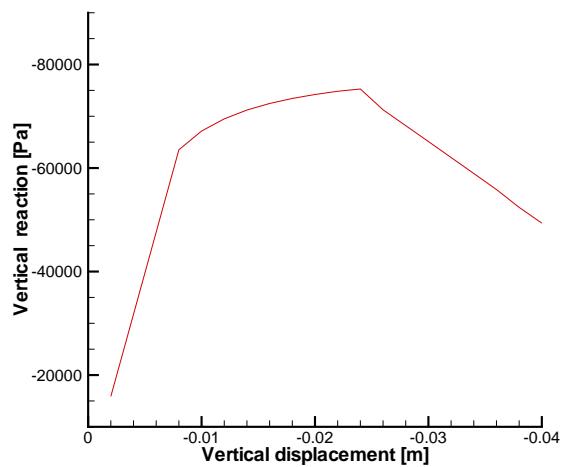


Figure 8.3.12: Vertical reaction of the top

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_sdc</i>	M	benchmarks\M\

8.3.3 Plastic plate - Cam-Clay plasticity (2D)

Problem definition

This example is generally applied to verify a critical state plastic mode, i.e. Cam-Clay model. We consider a quarter of the cylindrical sample of 5cm in diameter and 10cm in length.

Initial and Boundary conditions

The bottom surface is roller supported. A vertical down displacement is prescribed to make an axial strain of 50%. The movement in the radial direction on the top surface is allowed. The cylindrical surface is traction free.

Material properties

Table 8.3.3 shows the material parameters.

Meaning	Value	Unit
Poisson ratio	0.3	—
Slope of the critical state line	1.2	—
Virgin compression index	0.2	—
swelling/recompression index	0.02	—
Initial preconsolidation pressure	60.0	--
Initial void ratio	1.5	--

Table 8.3.3: Solid material properties

Results

The problem is axisymmetrical. A relationship between von Mises type stress, the second stress invariant, and the axial strain is illustrated in Fig. 8.3.13. The results agrees with what given in [79].

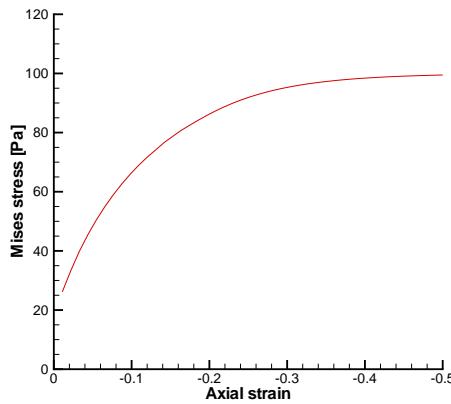


Figure 8.3.13: Axial strain vs von Mises type stress

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_cc_quad_s& m_cc_tri_s</i>	M	benchmarks\M\

8.3.4 Plastic plate - Rotational hardening plasticity (2D)

Problem definition

This example is a plane strain compression test on a material with both isotropic and rotational hardening behaviour.

The geometry of the specimen used is 0.34 m height and 0.1 m width. We denote by σ_x the stress acting on the both lateral sides of the specimen and by σ_y the stress applied to the top side of the specimen. The set-up of the problem is shown in Fig. 8.3.14.

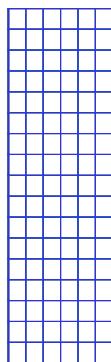


Figure 8.3.14: Plane strain biaxial test: rotational hardening

A vertical down displacement load is applied on the top boundary.

Material properties

Assume all initial stresses are zero. The material properties of the rotational hardening model are defined in Table 8.3.4

Results

The output of the results in a specified point, i.e, a center of a finite element close to the geometrical center of the domain (Fig. 8.3.14), is used to analyze the model behavior. Fig. 8.3.15 shows the varying of vertical stress along with vertical displacement at the top boundary.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_ssy_quad</i>	M	benchmarks\M\

Parameter	Unit	Value
Young's modulus	Pa	1e+08
Poisson ratio	-	0.3
α_0	-	0.0
β_0	-	0.26
δ_0	m^2/N	3.5e-07
ε_0	m^2/N	1.0e-7
κ_0	N/m^2	0.0
γ_0	-	0.0
m_0	-	0.569
$\hat{\alpha}$	-	0.0
$\hat{\beta}_0$	-	0.29
$\hat{\delta}_0$	m^2/N	8.81e-9
$\hat{\varepsilon}_0$	m^2/N	1.5e-8
$\hat{\kappa}_0$	N/m^2	0.0
$\hat{\gamma}_0$	-	0.0
\hat{m}_0	-	1.0
ψ_1	-	0.55
ψ_2	-	-0.26
C_h	-	0.81e-3
C_d	-	0.60e-3
b_r	-	100.0
m_r	-	-3.0

Table 8.3.4: Material parameters of rotational hardening model

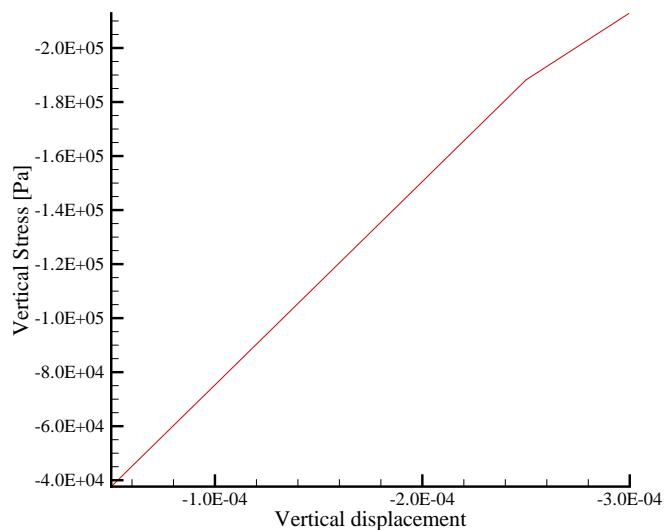


Figure 8.3.15: Vertical stress vs vertical displacement

8.4 Creep

Creep is a time-dependent and/or temperature-dependent deformation process of a solid body under the influence of a constant load. Creep is a phenomenon of time effect to deformation such that the tendency of a material to move or to deform is permanent to relieve stresses. Similar to plastic potential, a creep potential F_c is introduced to describe the constitutive equations.

Usually, a stationary creep model is sufficient to describe the creep phenomena in geological media, such as soil and rock. Norton's model reads that the creep potential F_c can be expressed by a function of the first stress invariant σ_v as

$$F_c = \frac{\alpha}{n+1} \sigma_v^{n+1} \quad (8.4.1)$$

where α and n are material parameters, which have to be determined by experiments. Assuming the total strain increment $d\boldsymbol{\varepsilon}$ is admissible to be decomposed in several portions contributed by different physical reactions such elasticity, plasticity and creep, it can be written as

$$d\boldsymbol{\varepsilon} = d\boldsymbol{\varepsilon}^e + d\boldsymbol{\varepsilon}^p + d\boldsymbol{\varepsilon}^c \quad (8.4.2)$$

Similar to the plastic flow rule, we can derive the strain rate resulting from creep as

$$d\boldsymbol{\varepsilon}^c = \frac{\partial F_c}{\partial \boldsymbol{\sigma}} = \left(\frac{3}{2} \right)^{(n+1)/2} \alpha \|\mathbf{s}\|^{n-1} \mathbf{s} \quad (8.4.3)$$

Applying explicit Euler's method to equation (8.4.3), the increment of the strain by creep is obtained from

$$\Delta\boldsymbol{\varepsilon}^c = \left(\frac{3}{2} \right)^{\frac{n+1}{2}} \alpha \|\mathbf{s}^k\|^{n-1} \mathbf{s}^k \Delta t \quad (8.4.4)$$

where \mathbf{s}^k is the deviatoric stress of the previous time step k and Δt is the time step size. Using the generalized Hook's law, the stress change deduced by the creep stain increment is

$$\Delta\boldsymbol{\sigma}^c = \mathbf{D}^e \Delta\boldsymbol{\varepsilon}^c \quad (8.4.5)$$

with \mathbf{D}^e the elastic material tensor.

8.4.1 Creep of a cylindrical sample

Problem definition

In this example, creep is considered in a thick cylinder subjected a constant normal pressure at the inner face. The boundary conditions are as follows: $p = 2.515$ MPa at the inner surface and zero normal stress at the outer surface, no displacements in axial direction. The inner radius of the cylindrical sample is 4

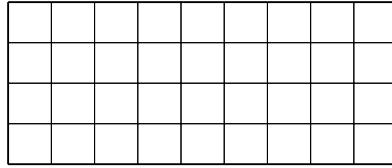


Figure 8.4.1: Mesh for thick cylinder undergoes creep deformation

mm, the outer radius is 6.4 mm and the height is 1 mm. Quadrilateral elements are adopted for meshing (Fig. 8.4.1).

We assume that the initial stress is homogeneously distributed in the domain as $\sigma_r^0 = \sigma_\theta^0 = \sigma_z^0 = -50$ Pa. The parameters of the Norton creep model are given in Tab. 8.4.1.

Symbol	Meaning	Value	Unit
α	Norton model parameter 1	6.415×10^{-10}	–
n	Norton model parameter 2	4	–
ν	Poisson ratio	0.48	–
E	Young's modulus	1.378×10^5	MPa

Table 8.4.1: Material parameters of the Norton creep model

Results

Figs. 8.4.2 and 8.4.3 give the distribution of the first stress invariant and radial displacement along radial direction and the comparison with pure elastic solution. They demonstrated that s at inner surface decreases about 26% after steady state of creep reached. While radial displacements increase about 200%. The results can be compared with Balley's analytical solution, which reads for rate of radial displacement as

$$\dot{u}_r = \alpha \frac{3^{\frac{n+1}{2}}}{2n^n} \frac{r_a^2 r_b^2 p^n}{(r_b^{2/n} - r_a^{2/n})r}$$

and for the steady state of first stress invariant

$$\sigma_v = \frac{2\sqrt{3}}{2n} \frac{p (r_b/r)^{\frac{2}{n}}}{(r_b/r_a)^{2/n} - 1}$$

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>m_crptri</i>	M	benchmarks\M\

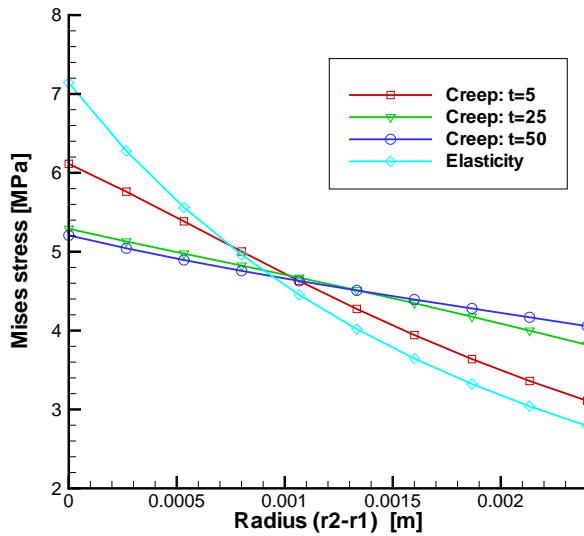


Figure 8.4.2: First stress invariant profiles during creep at different times, $t = 5, 25, 50$ sec, and comparison to elastic solution

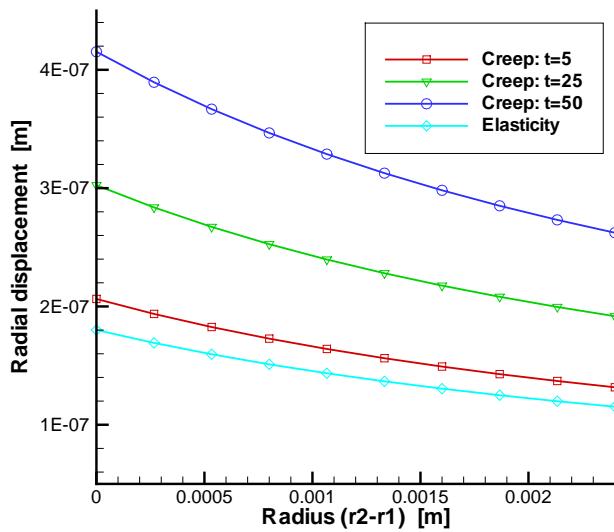


Figure 8.4.3: Radial displacement profiles during creep at different times, $t = 5, 25, 50$ sec, and comparison to elastic solution

8.4.2 Creep in salt rock

Several models exists for the evaluation of the effect of stationary creep in rock salt, i.e the strain variation with time is calculated. One of those models is the BG Ra-model (8.4.6), which is valid for loads between 5 and 25 MPa in a temperature range of 22-200°C (Hunsche and Schulze, 1994).

$$\dot{\varepsilon}^c = A e^{-\frac{Q}{RT}} \left(\frac{\sigma}{\sigma^*} \right)^n \quad (8.4.6)$$

Table 8.4.2 depicts the symbols of equation (8.4.6), their meaning and parameter values.

Symbol	Meaning	Value	Unit
$\dot{\varepsilon}$	Strain rate	1/d	
σ	Effective stress	MPa	
A	Material constant	0.18	1/d
Q	Activation energy	54	kJ/mol
R	Gas constant	8.31447215	J/(K mol)
n	Material constant	5	—
σ^*	Reference effective stress	1	MPa

Table 8.4.2: Creep model, symbols and material values

Example 1: Temperature dropping (relaxation)

Problem definition In a sample of rock salt a stress relaxation is caused by a temperature decrease of 30 K. The aim of the example is to calculate the resulting strain variation with time within the solid body by the use of the stationary creep model BG Ra (8.4.6). The results of the simulation using an axial symmetric calculation model and a 3D model are compared afterwards.

Assumptions	Heat	Constant temperature in the whole body at the beginning (330 K), temperature decrease of 30 K
	Solid	Homogenous, finite dimensions, no deformation at the boundaries in z-direction at the bottom and the top

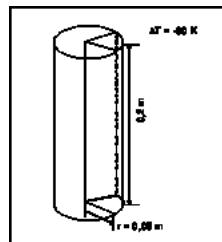


Figure 8.4.4: Core sample model

For the 2D numerical simulation a cylindrical core sample as shown in Fig. 8.4.4 is selected. The 2D numerical model is an axial symmetric one in the x-z-plane (see Fig. 8.4.5). The dimensions of this 2D model are: 0.05 m radius (x-direction) and 0.2 m of height. A relatively coarse mesh consisting of 228 triangular elements and 139 nodes is used. Vertical deformations at the top and the bottom are suppressed (no displacement boundary conditions). The initial temperature in the whole area is 330 K. At the top and the bottom of the model thermal boundary conditions are set with a temperature of 300 K. Thereby the stress relaxation during the cooling down is simulated. The used parameters of the solid represent the material behavior of rock salt are given in Tab. 8.4.2. The calculation is divided in 360 time steps with a constant time step length of 1 day.

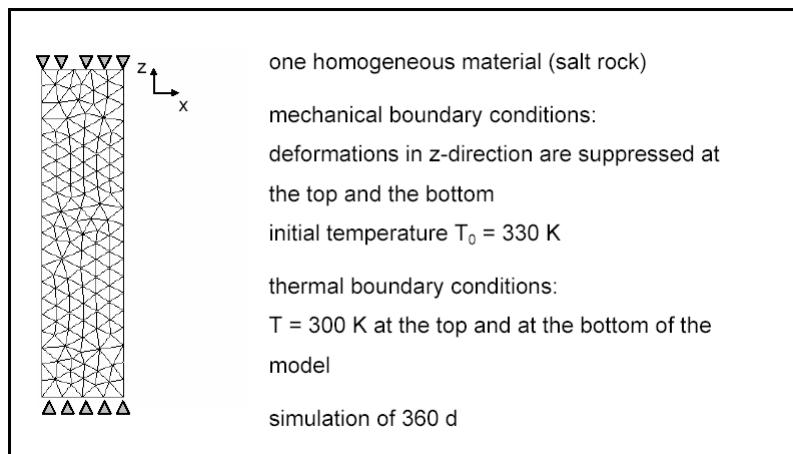


Figure 8.4.5: Numerical axisymmetrical model

Table 8.4.3 depicts the values of material properties for the thermo-mechanical creep model.

Symbol	Meaning	Value	Unit
T_0	Initial temperature (before cooling down)	330	K
T	Temperature after cooling down	300	K
E	Young's modulus	25	GPa
ν	Poisson ratio	0.27	–
α	Thermal expansion coefficient	4×10^{-5}	1/K
c	Thermal capacity	1	J/(kg K)
λ	Thermal conductivity	100	W/(m K)

Table 8.4.3: Material parameters of the thermo-mechanical creep model

Analytical solution In order to evaluate the numerical results of the relaxation problem, the analytical solution of equation (8.4.7) (Eickemeier 2007, personal communication) for the difference of effective stresses within one time step can be applied.

$$\Delta\sigma_{i+1} = \frac{(\dot{\varepsilon}_1^c - A(\sigma/\sigma^*)^n)E_q\Delta t}{1 - E_q/\sigma^*A^*\Delta t\xi n(\sigma/\sigma^*)^{n-1}} \quad (8.4.7)$$

and

$$A^* = Ae^{-Q/RT} \quad (8.4.8)$$

where the initial strain rate $\dot{\varepsilon}_1^c$ in this case is zero, E_q in general is the weighted Young's modulus of the steel plates and the salt rock sample (in this case we consider only salt rock), $\xi = 0.5$.

For the analytical solution of the equation (8.4.7) the vertical stress before the last time step is considered. Time step increment is $\Delta t = 1$ d. The calculation is done for node 705 of the 3D model (Fig. 8.4.6), which is located at point $(x,y,z)=(0.05,0,0.12)$. The calculated stress difference σ_{i+1} has to be identical to the numerical result.

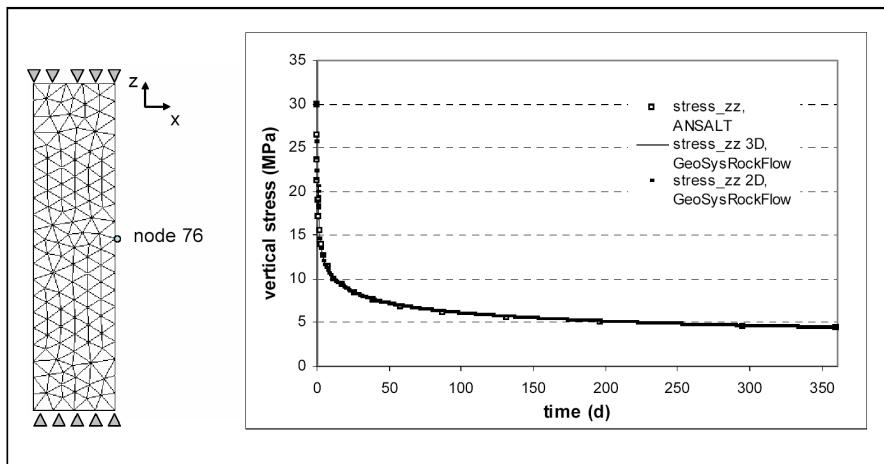


Figure 8.4.6: Comparison of numerical results (GeoSys/RockFlow vs ANSALT) for vertical stresses

Results The comparison of the stress increment σ_{i+1} which was obtained by the use of equation (8.4.7) is identical to the value (of vertical stresses) at node 705 (at the same location as node 76, see Fig. 8.4.6) of the 3D numerical calculation. Both stress increments σ_{i+1} obtained by GS/RF and ANSALT are equal to 3.05×10^{-3} MPa. Additionally, the numerical results for vertical stresses of the 2D simulation at node 76 are compared to the results that were obtained by simulating the creep process by the FE programme ANSALT (Nipp

1988) and also to the results of the 3D simulation with GS/RF at node 705. The comparison of the results of GS/RF in 2D and 3D with the ANSALT findings are depicted in Fig. 8.4.6.

The input data and boundary conditions for each calculation model are identical. Also the results show a good accordance. That means, the creep simulation (2D and 3D) of GS/RF by using the implemented BG Ra model provides correct results.

Benchmark deposit

PCS type	MSH type	Files	Version	Date	Author
TM	axial-symmetry	BGRa	4.4.10(WW)	13.03.07	BGR
TM	axial-symmetry	creep3d	4.4.10(WW)	13.03.07	BGR

Example 2: Creep under constant load

Problem definition In the same example that is described in section 8.4.2 the creep process is now assumed to be caused by a constant load at the bottom of the solid and a constantly high temperature at the same time. The aim of this example is to calculate the resulting strain variation with time by using the stationary creep model BG Ra (8.4.6).

We specify the initial and boundary conditions for the 2D numerical model. For the simulation with GS/RF almost the same calculation models (2D and 3D) as in the precedent creep example were selected. Only the height of the solid is 0.25 m instead of 0.2 m. The initial temperature in the whole area is 373.15 K. There is a constant load of 5 MPa at the bottom of the model as boundary condition. The calculation is divided in 100 time steps with a constant time step length of 1 day.

Analytical solution In order to find out, whether the numerical solutions of GeoSys/RockFlow accord to the results of the BG Ra model (8.4.6), the input parameter A is compared to the A , which results from the simulation run. For this calculation equation (8.4.6) is converted to the following expression.

$$A = \frac{\dot{\varepsilon}^c}{e^{-Q/RT}\sigma_{\text{eff}}} \quad (8.4.9)$$

with

$$\begin{aligned} \sigma_{\text{eff}} &= \frac{1}{\sqrt{2}} \sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2} \\ \dot{\varepsilon} &= \frac{\varepsilon_{\text{eff}}(t + \Delta t) - \varepsilon_{\text{eff}}(t)}{\Delta t} \\ \varepsilon_{\text{eff}} &= \frac{\sqrt{2}}{3} \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + (\varepsilon_2 - \varepsilon_3)^2 + (\varepsilon_3 - \varepsilon_1)^2} \end{aligned} \quad (8.4.10)$$

For these calculation steps the stresses of the regarded time period have to be constant. Equations (8.4.11) are solved for node 25 (see Fig. 8.4.7) of the 2D numerical model. The last time step at $t = 100$ days of the simulation run was considered.

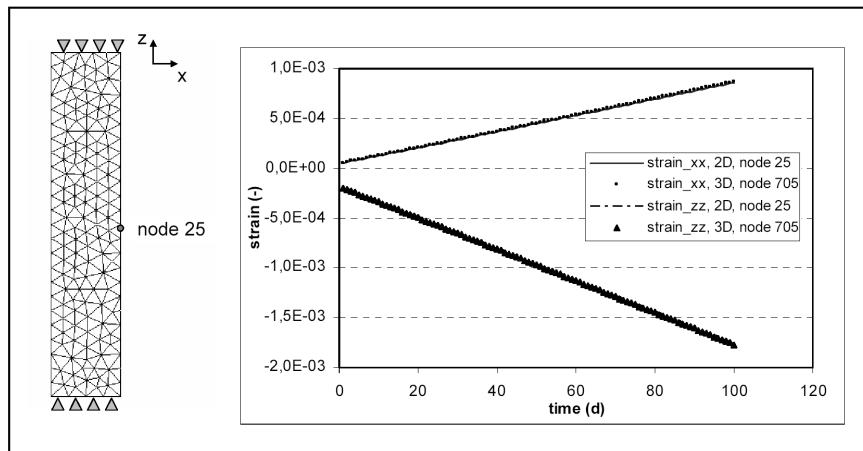


Figure 8.4.7: Comparison of 2D and 3D numerical results for strains (x- and z-directions)

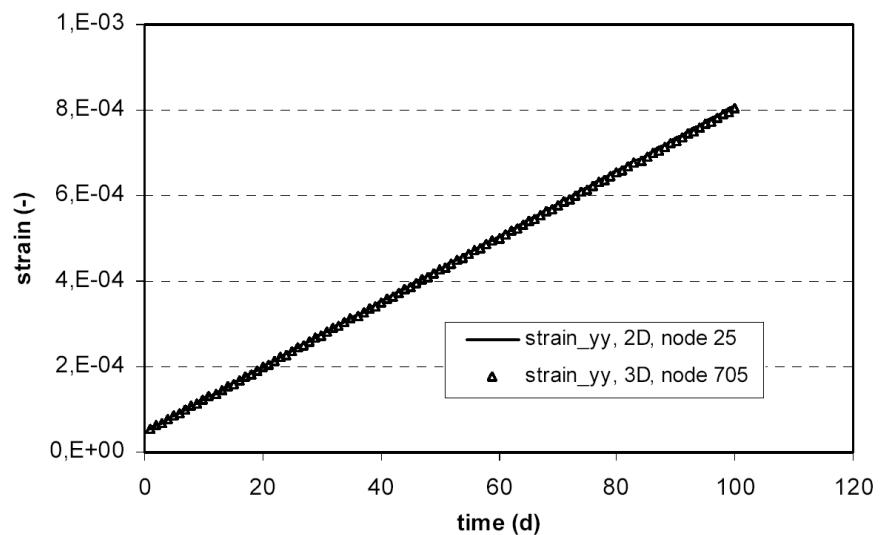


Figure 8.4.8: Comparison of 2D and 3D numerical results for strains (y-direction)

Results The effective stress σ_{eff} at node 25 and for the given time span is 5.03 MPa, which was calculated by the use of equation (8.4.11). The strain of time step 1 is $\varepsilon_{\text{eff}}(t_1) = 1.72 \times 10^{-3}$ and of time step 2: $\varepsilon_{\text{eff}}(t_2) = 1.73 \times 10^{-3}$, calculated by equation (8.4.11), is equal to $1.6 \times 10^{-5} d^{-1}$. After equation (8.4.9) the calculated parameter A is equal to 0.19, which corresponds approximately to the input A of 0.18. Therefore, it can be summarized that the BG Ra creep model is implemented in GeoSys/RockFlow properly. The comparison between the 2D (node 25) and 3D results (node 705) are depicted in Fig. 8.4.7 and Fig. 8.4.8. The 2D and 3D results are identical to each other.

Benchmark deposit

PCS type	MSH type	Files	Version	Date	Author
M	axial-symmetry	uc_creep01	4.4.10(WW)	13.03.07	BGR
M	axial-symmetry	uc_creep3d	4.4.10(WW)	13.03.07	BGR

Chapter 9

Mass Transport – C-Processes

9.1 Theory

The mass transport in a homogeneous, saturated aquifer can be influenced by convection, diffusion, decay and biodegradation, sorption and chemical reactions. For a steady state 1-dimensional flow through a homogeneous isotropic medium with constant material parameters the following differential equation 9.1.1 is applied.

$$\frac{\partial C}{\partial t} + \frac{\rho_b}{R} \cdot \frac{\partial S}{\partial t} + \frac{q}{R} \cdot \frac{\partial C}{\partial x} = D_{xx} \cdot \frac{\partial^2 C}{\partial x^2} - \lambda \cdot C \quad (9.1.1)$$

with

C – dissolved concentration ($\text{kg}\cdot\text{m}^{-3}$),

S – sorbed concentration ($\text{kg}\cdot\text{kg}^{-1}$),

t – time (s),

ρ_b – bulk density ($\text{kg}\cdot\text{m}^{-3}$),

R – retardation factor (-),

q – flow rate ($\text{m}\cdot\text{s}^{-1}$),

x – distance (m),

D_{xx} – dispersion coefficient in x-direction ($\text{m}^2\cdot\text{s}^{-1}$),

λ – decay rate (s^{-1}).

This equation is used to calculate the concentration distribution under consideration of decay and sorption with the linear Henry-isotherm. The retardation

coefficient R for the Henry isotherm is related to the Henry sorption coefficient K_D in the following way (equ. 9.1.2).

$$R = 1 + \frac{\rho_b}{\Phi} K_D = 1 + \frac{1 - \Theta}{\Phi} \rho_s K_D \quad (9.1.2)$$

with

$$\begin{aligned}\Phi &= \text{porosity } (-), \\ \rho_s &= \text{density } (\text{kg} \cdot \text{m}^{-3}),\end{aligned}$$

with the initial and boundary conditions

$$C(x, t = 0) = C_I \quad \forall x$$

with C_I - concentration at time I .

$$C(x = 0, t) = C_0 \quad \forall t, \quad \frac{\partial C}{\partial x}(x \rightarrow \infty, t) = C_I \quad \forall t > 0$$

with C_0 - initial concentration.

The following analytical solution is significant:

$$\begin{aligned}C = C_1 &+ (C_0 - C_1) \cdot \left[\frac{1}{2} \exp \left(\frac{v \cdot x(1 - \gamma)}{2 \cdot D_{xx}} \right) \cdot \operatorname{erfc} \left(\frac{x - v \cdot \gamma \cdot t/R}{2 \cdot \sqrt{D_{xx} \cdot t/R}} \right) \right. \\ &\left. + \exp \left(\frac{v \cdot x(1 + \gamma)}{2 \cdot D_{xx}} \right) \cdot \operatorname{erfc} \left(\frac{x + v \cdot \gamma \cdot t/R}{2 \cdot \sqrt{D_{xx} \cdot t/R}} \right) \right] \quad (9.1.3)\end{aligned}$$

with v - velocity

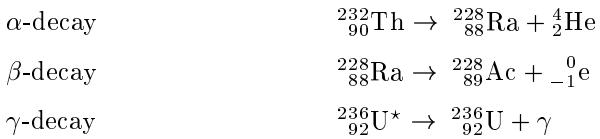
$$\gamma = \sqrt{1 + 4 \cdot \lambda \cdot R \cdot D_{xx} / v^2}. \quad (9.1.4)$$

Equation 9.1.3 is the basis for the verification of the RockFlow-simulation results for the 1-dimensional mass transport. All described equations and all analytical solutions of equation 9.1.3 are taken from [12].

9.2 Solute transport with decay

Theory

Radioactive decay is the change in the composition of a core by emitting particles and/or electro-magnetic radiation. Different kinds of radioactive decay are i.e. decay as a result of emission of negatrons or positrons and decay under emission of γ -rays.



The above given examples show that the radioactive decay is an irreversible process. The following differential equation describes the decay as first order reaction (without chain development):

$$\frac{\partial C}{\partial t} = -\lambda \cdot C \quad (9.2.1)$$

with λ - decay rate (s^{-1}).

The integration of this equation causes an exponential decay term in the following form.

$$C(t) = C_0 \cdot e^{-\lambda \cdot t} \quad (9.2.2)$$

with C_0 - initial concentration ($\text{kg} \cdot \text{m}^{-3}$).

The decay values are commonly expressed as the so-called half life ($t_{1/2}$). This is the point of time when half of the substance is degraded. The relation between the half-life T and the decay rate results from:

$$e^{-\lambda \cdot t} = \frac{1}{2} \Rightarrow \lambda = \frac{\ln(2)}{T} \cong \frac{0.693}{T} \quad (9.2.3)$$

Problem definition

The aim of this example is to simulate the mass transport with the influence of decay, but without any sorption. At the left side of the considered aquifer there is a volume source of $0.1 \text{ m}^3/\text{d}$, at the right side there is a constant water pressure of 20 kPa . The tracer substance in the source volume is distributed by a stationary flow in the homogeneous aquifer. The mass distribution after 100 days has to be calculated. Figure 9.2.1 shows a sketch of the calculation area.

Assumptions

Component: no sorption, exclusively decay
 Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

For the 1-dimensional calculation the calculation area is simplified as a line of a length of 100 m with 100 elements and 101 nodes. As boundary conditions the relative concentration amounts 1 and the source volume of the fluid phase with $0.1 \text{ m}^3/\text{d}$ is given at the left border of the calculation area and a constant

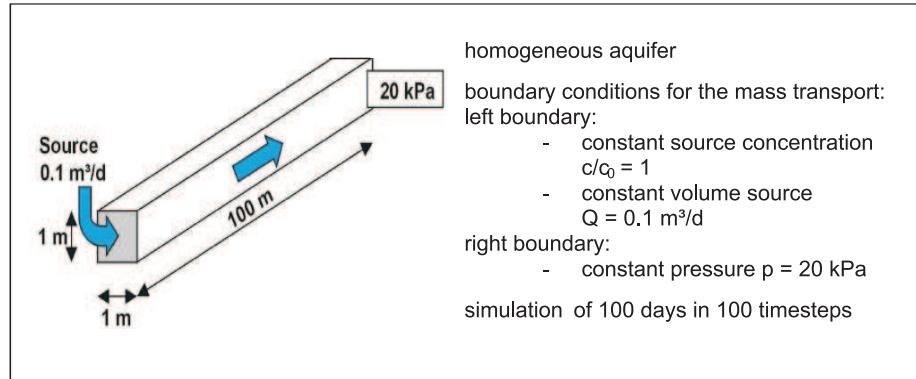


Figure 9.2.1: Calculation area: homogeneous aquifer

pressure of 20 kPa at the right boundary. The used parameters of the soil are listed in table 9.2.1. The calculation is divided into 100 time steps with a constant time step length of 1 day. That means, the flow and transport processes in the aquifer within 100 days are simulated.

parameter	value	unit
porosity Φ	0.2	–
permeability K	$1.0 \cdot 10^{-12}$	m^2
density water ρ	1000	$\text{kg} \cdot \text{m}^{-3}$
viscosity water η	0.001	$\text{Pa} \cdot \text{s}$
dispersion length α_l	5.0	m
decay in solved phase λ	$2.0 \cdot 10^{-7}$	s^{-2}

Table 9.2.1: Used parameters

Evaluation method

The concentration distribution at a special point in time and over a given distance is calculated by equation 9.1.3. Hereby the retardation coefficient is set equal to 1. The analytical solutions are depicted in figure 9.2.2 as single symbols.

Results

In figure 9.2.2 you can find the concentration distribution over the whole length of the 1 D model at the final simulation time of 100 days. Obviously, the numerical results meet well the analytical solutions.

Benchmark	Problem type	Path in benchmark deposit
hc_decay_1Du	HC	benchmarks \HC\decay

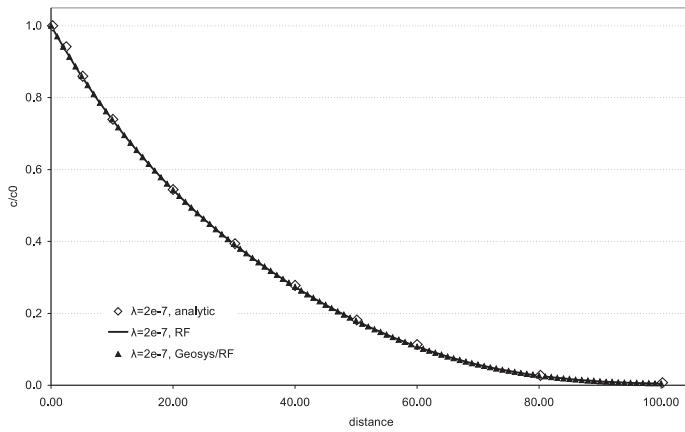


Figure 9.2.2: Concentration distribution after 100 d (decay)

9.3 Solute transport with sorption

Theory

Exchange processes, like sorption, between the solid and the liquid phase in the multiphase system of an aquifer can be caused by physical (Van-der-Waals-forces) or chemical bonds. Sorption processes can be reversible (adsorption-desorption) if the chemical environment is changing. When the transport in a multiphase system is simulated, the mass exchange between the liquid and the solid phase has to be included. The equations that describe the sorption processes are called sorption isotherms. Sorption isotherms describe the relation between the substance that is adsorbed on the solid matrix and the one which is dissolved in the fluid phase. Those equations are only valid under isothermal conditions. The isotherms that are listed below, base on the assumption that the adsorbed substance and the dissolved one are in the state of equilibrium.

$$\text{Henry : } S = K_D \cdot C \quad (9.3.1)$$

$$\text{Freundlich : } S = K_1 \cdot C^{K_2} \quad (9.3.2)$$

$$\text{Langmuir : } S = \frac{K_1 \cdot C}{1 + K_2 \cdot C} \quad (9.3.3)$$

with

K_D , K_1 , K_2 - distribution coefficients,

S - concentration of the adsorbed species (kg/kg),

C - concentration of the dissolved species (kg/m^3).

The distribution coefficients are dependent on the substance and the specific soil properties like the pH. The linear Henry-isotherm is often used when there are low concentrations. Non-linear sorption processes are reproduced by the Freudlich or the Langmuir isotherm. Then the retardation is dependent on the solute concentration. In addition, the use of the Langmuir isotherm assumes a constant amount of sorption space at the solid surface. A maximum concentration for the adsorbed substance on the solid matrix is exclusively considered by the Langmuir isotherm (Habbar, 2001). This maximum concentration c_{\max} is included in the distribution coefficient K_1 ($K_1 = c_{\max} \cdot K_2$). The distribution coefficient K_2 of the Langmuir isotherm stands for the affinity between solid and sorbed solute. The distribution coefficients do not have comparable values: each sorption isotherm has to be considered separately with its specific constants.

9.3.1 Sorption with linear isotherm (Henry isotherm)

Problem definition

The aim of this example is to simulate the solute transport in an aquifer by convection with the influence of retardation as a result of sorption. The solute transport is influenced by linear sorption processes. That means, the Henry-isotherm is relevant to calculate the solute concentration. The calculation area and boundary conditions are the same as described for the precedent example.

Assumptions

Component: exclusively linear sorption (Henry isotherm), no decay
 Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

See chapter 9.2.

The soil parameters are the same as listed in table 9.2.1, but decay is not considered during these simulation runs. For the different simulation runs the Henry-sorption coefficients are varied as listed in table 9.3.1 in order to evaluate the influence of sorption on the mass transport. The retardation coefficients R are calculated by solving equation 9.1.2.

Evaluation method

The concentration distribution at a special point in time and over a given distance is calculated by equation 9.1.3. Hereby the decay term γ is set equal to 1. The analytical solutions are depicted in figure 9.3.1 as single symbols.

K_D -value [m^3/kg]	retardation coefficient [-]
0	1
$6.8 \cdot 10^{-6}$	1.05
$6.8 \cdot 10^{-5}$	1.54
$6.8 \cdot 10^{-4}$	6.44

Table 9.3.1: Variation of K_D -values and retardation coefficients as input variables

Results

In figure 9.3.1 you can find the concentration distribution over the whole length of the 1 D model at the final simulation time of 100 days. Obviously, the numerical results meet well the analytical solutions.

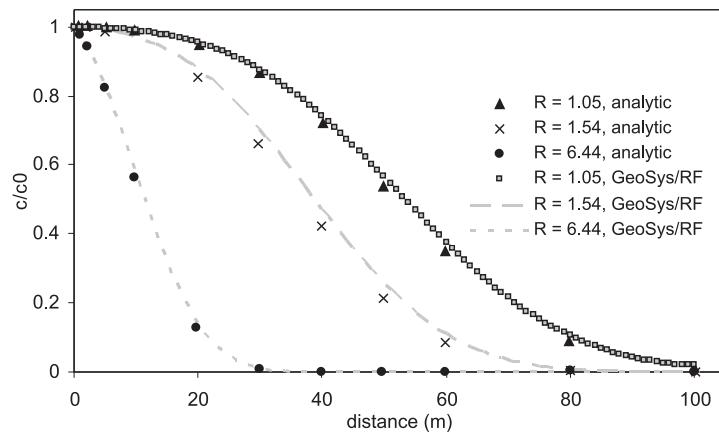


Figure 9.3.1: Concentration distribution after 100 d (Henry sorption)

Benchmark	Problem type	Path in benchmark deposit
hc_sorp_henry_1D	HC	benchmarks \HC\Sorption\Henry

9.3.2 Non-linear sorption with Freundlich isotherm

Problem definition

The non-linear Freundlich isotherm is often used to describe real sorption processes. Therefore, in this example, the transport process by including the Freundlich isotherm is calculated in the same way as in the precedent example (same model and boundary conditions). As there exists no opportunity to calculate analytically the solute transport with non-linear sorption, the results of

the simulation have to be compared with solutions of the transport equation with linear sorption in order to evaluate the simulation results.

Assumptions

Component: non-linear sorption (Freundlich isotherm), no decay
 Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

See chapter 9.2

The soil parameters are the same as listed in table 9.2.1(except decay). For the different simulation runs the Freundlich-sorption coefficients (K_1) are varied in the same way as the K_D -values that are listed in table 9.4.1. The exponent K_2 was constant with a value of 1.

Evaluation method

The dependence of sorbed molecules on the amount of molecules in dilution is given by equation 9.3.3. The concentration distribution at a special point in time and over a given distance cannot be calculated analytically by equation 9.1.3 when a non-linear sorption process is assumed. A possibility to test the correctness of the simulation results for transport with Freundlich sorption is to choose values of distribution coefficients in order to create a concentration distribution which is approximately linear and must therefore almost be equal to the results of transport by use of the Henry isotherm.

Results

As the values for the Freundlich coefficients were chosen in that way, that the concentration distribution between sorbed and solute concentrations is almost linear, the results of the simulation runs have to be equal to the results that are obtained by using the linear Henry isotherm. In figure 9.3.2 the concentration distribution of the solute over the model length of 100 m is shown. As the concentrations of the transport simulation by using the Freundlich isotherm match those of the simulation runs with linear sorption, these results for non-linear sorption are reasonable. Additionally to this test, the values for the constant K_2 were changed to 0.8 in order to prove a difference between linear and non-linear sorption. The results of the comparison are shown in figure 9.3.3. These numerical results show the effect of the application of a non-linear sorption isotherm: the higher the influence of sorption (large value of sorption coefficient K_D resp. K_1) the higher the difference of solute concentration values

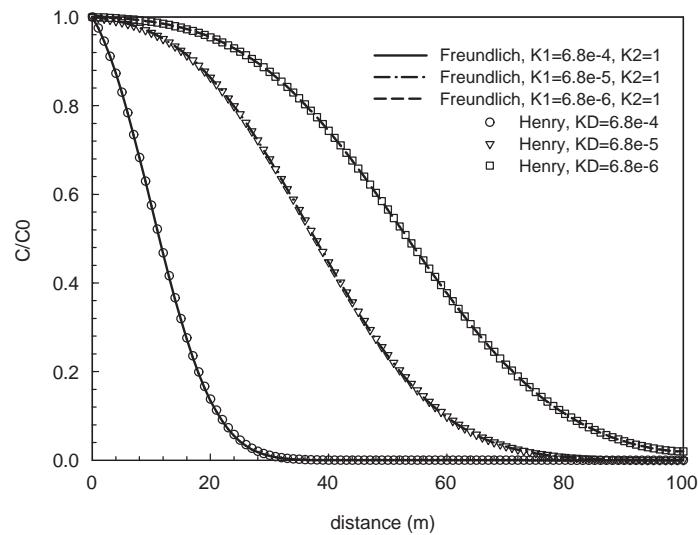


Figure 9.3.2: Concentration distribution after 100 d (Freundlich compared to Henry sorption)

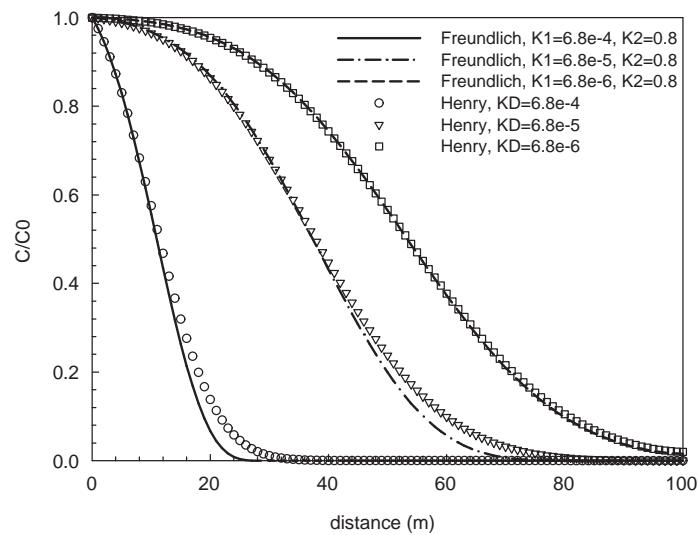


Figure 9.3.3: Different concentration distributions after 100 d (Freundlich compared to Henry sorption)

between non-linear and linear sorption. However, the results for both isotherms were not evaluated quantitatively.

Benchmark	Problem type	Path in benchmark deposit
hc_sorp_Freundl_1D	HC	benchmarks \HC\Sorption\Freundlich

9.3.3 Non linear sorption with Langmuir isotherm

Problem definition

The non-linear Langmuir isotherm is used to describe sorption processes that are restricted by a maximum concentration of sorbed molecules. In this example, the transport process by including the Langmuir isotherm is calculated in the same way as in the precedent examples for mass transport. As there exists no opportunity to calculate analytically the solute transport with non-linear sorption, the results of the simulation have to be compared with solutions of the transport equation with linear sorption in order to evaluate the simulation results.

Assumptions

Component: non-linear sorption with maximum concentration (Langmuir isotherm)
no decay

Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

See chapter 9.2

The soil parameters are the same as listed in table 9.2.1(except decay). In order to create a Langmuir equation which has almost the same linear characteristic as the Henry equation, the Langmuir sorption coefficients, K_1 , were varied in the same way as the Henry coefficients (K_D values in table 9.3.1) for the different simulation runs. The K_2 coefficients stand for the affinity between solid and sorbed solute. Thus, the K_2 value can not be set equal to 0, because this would cause a transport without any sorption. When K_2 equals 1, there is no effect on the binding affinity. Therefore, the coefficient K_2 was set constant with a value of 1 in order to approximate the linear characteristic of the Henry equation (9.3.2).

Evaluation method

The dependence of sorbed molecules on the amount of molecules in dilution is given by equation 9.3.3. The concentration distribution at a special point in time and over a given distance cannot be calculated analytically by equation

?? when a non-linear sorption process is assumed. Therefore, the simulation results are compared with the results for the mass transport by using the linear Henry isotherm. The non-linear Langmuir isotherm was forced to be almost linear in the way as described above. Now the results of the transport by using the Langmuir isotherm can be compared with the results that were obtained by the transport simulation with the linear Henry isotherm.

Results

In figure 9.3.4 the concentration distributions over the whole model length by using the linear Henry isotherm and the non-linear Langmuir isotherm are depicted. Obviously, the results for each specified distribution constant are almost equal. This result is correct, because it was provoked by the choice of the sorption coefficients.

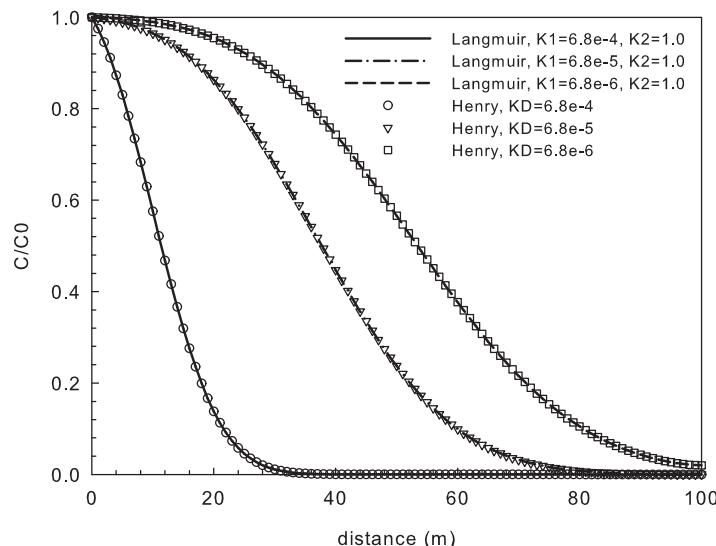


Figure 9.3.4: Concentration distribution after 100 d (Langmuir compared to Henry sorption)

In order to show that the results by the use of the Langmuir isotherm are actually different to those by using the Henry isotherm, the K_2 values were changed to a value of 0.8, so that the Langmuir isotherm got a real non-linear gradient. As the results show (fig. 9.3.5), the differences between the concentration distributions are evident.

Benchmark	Problem type	Path in benchmark deposit
hc_sorp_langmuir_1D	HC	benchmarks \HC\Sorption\Langmuir

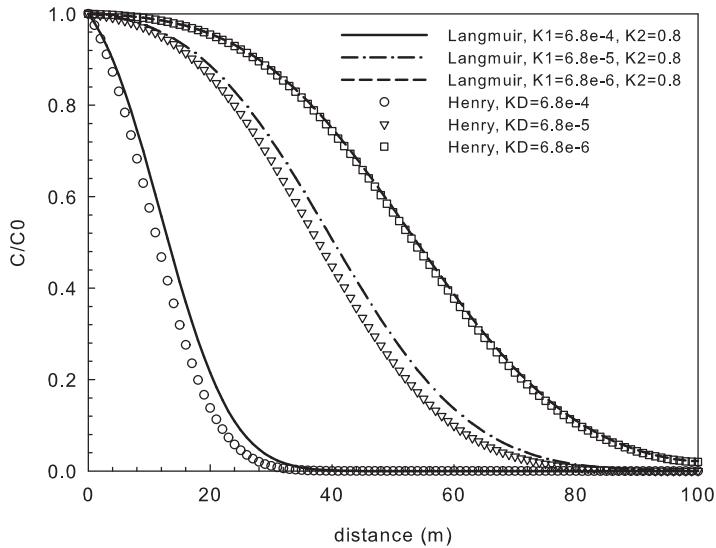


Figure 9.3.5: Different concentration distributions after 100 d (Langmuir compared to Henry sorption)

9.3.4 Solute transport with sorption and decay

Problem definition

The aim of this example is to simulate the solute transport in an aquifer by convection with the influence of retardation as a result of sorption. Additionally, the transported mass will be degraded. The calculation area and boundary conditions are the same as described in chapter 9.2.

Assumptions

Component: linear sorption, decay

Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

See chapter 9.2

The soil parameters are the same as listed in table 9.2.1. The decay rate λ is $2 \cdot 10^{-7} \text{ s}^{-1}$. For the different simulation runs the Henry sorption coefficients are varied as listed in table 9.3.1 to evaluate again the influence of sorption on mass transport.

Evaluation method

The concentration distribution at a special point in time and over a given distance is calculated by equation 9.1.3. The analytical solutions are depicted in figure 9.3.6 as single symbols.

Results

The influence of radioactive decay on the transport process can be recognised at the typical declining exponential curves in figure 9.3.6. According to the different sorption coefficients the transport is retarded. Obviously, the numerical results (lines) meet well the analytical solutions. Therefore, it can be summarised that the transport under the combined consideration of both decay and sorption can be reproduced by the simulation with RockFlow.

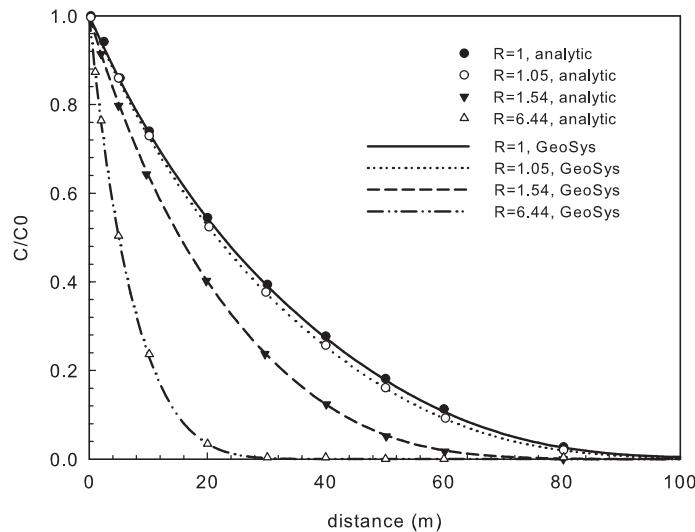


Figure 9.3.6: Concentration distributions after 100 d (sorption and decay)

Benchmark	Problem type	Path in benchmark deposit
hc_decay_sorp_henry_1Du	HC	benchmarks \HC\sorption_decay

9.4 Solute transport by diffusion

Theory

Diffusion is a process that equates concentration differences of gaseous or dissolved matter or energy. The particles move from higher to lower concentrations by Brownian movement in dependence on the temperature. In an aquifer, diffusive transport appears when convective transport is not that relevant (small velocities).

The extent of diffusion is also dependent on the diffusing substance and the medium. In addition, diffusion in soils is influenced by other factors, e.g. tortuosity. The finer a soil the stronger are the interacting forces between the soil matrix and the diffusing molecules. The diffusion coefficient which has to be given in GeoSys/RockFlow is the so-called apparent diffusion coefficient (eq. 9.4.1).

$$D_a = \frac{D_e}{\Phi} \quad (9.4.1)$$

with D_e - effective diffusion coefficient.

9.4.1 Diffusion: axisymmetric model

Problem definition

This diffusion model is built to reproduce a field study in clay. This in situ test consists of a borehole where a solution is circulated that contains tracer substances like HTO. These tracers diffuse into the adjacent clay. The aim of the investigation is to simulate the HTO distribution after 300 d, the final test time, and to compare the simulation results of GeoSys/RockFlow to those that are calculated by HYDRUS 1 D (Simunek et al.) and PHAST (Parkhurst et al.).

Model set-up of the 1 D axisymmetric model

To build a proper model of the tracer test, a one-dimensional axisymmetric model with 3.8 cm of borehole radius and 21.2 cm horizontal distance in the clay soil is created. As initial condition a constant pressure of 0 was specified in the whole model and the concentration relation c/c_0 of 1 within the distance of the borehole radius and of 0 within the clay domain. The pressure boundary condition corresponds to the initial condition. The calculation model includes 310 elements and 311 nodes. Table 9.4.1 shows the used parameters for the clay and the apparent diffusion constant D_a of HTO. The calculation is performed for the test duration of 300 days with fitted time step lengths from 0.001 d to 1 d (Bahr, 2007). The porosity in the modelled borehole is assumed to be 1 in order to evoke the simulation of a tracer reservoir that supplies the tracer solution into the clay.

parameter	value	unit
density ρ	2.5	$t \cdot m^{-3}$
porosity Φ	0.15	—
permeability K	$1.0 \cdot 10^{-11}$	m^2
diffusion coefficient D_a	$3.6 \cdot 10^{-10}$	$m^2 \cdot s^{-1}$

Table 9.4.1: Parameters

Evaluation method

The aim of the presented calculation example is the evaluation of the GeoSys/RockFlow-simulation results by comparing them with numerical results of two other simulation programmes. The comparison is made by the use of Hydrus 1 D, which is a one-dimensional transport model especially for the solute transport in soils. The second programme, PHAST, is linked to the chemical software PHREEQC. The simulation with both programmes was made under consideration of the same boundary conditions and parameters (Bahr, 2007).

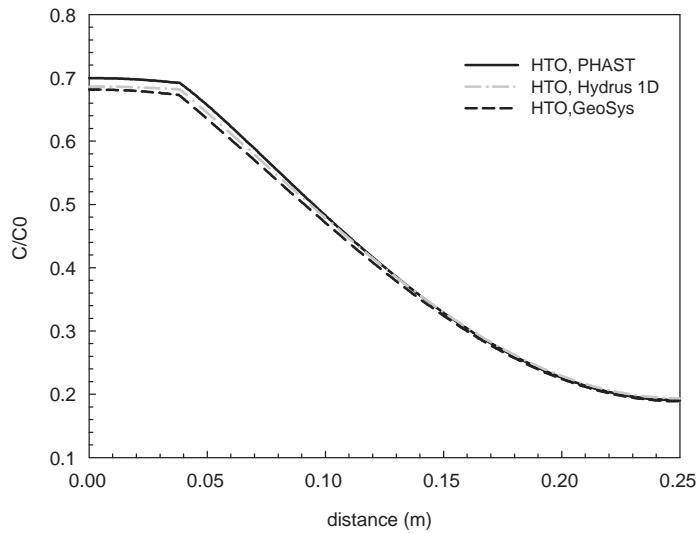


Figure 9.4.1: Concentration distributions after 300 d

Results

In figure 9.4.1 you can find the concentration distributions over the width of 0.25 m after a simulation time of 300 days that were calculated by means of

GeoSys/RockFlow, PHAST and Hydrus 1D (Bahr, 2007). The numerical results accord well to each other. Thus, the comparison shows that the diffusion process can be well reproduced by the use of an axisymmetric GeoSys/RockFlow model.

Benchmark	Problem type	Path in benchmark deposit
Diff_HTO_test	HC	benchmarks \HC\Diffusion\

9.4.2 Diffusion in an anisotropic medium (2 D simulation)

Problem definition

The aim of this example is to simulate the transport of a tracer by molecular diffusion in an anisotropic porous medium. The side length of the square numerical model is 1 m. At the left corner at the bottom of the model a constant concentration is diffusing into the calculation area. Diffusion is the only process for tracer transport, there are no pressure differences in the whole area. Because of the anisotropy of the soil material the tracer has to diffuse much faster in x-direction than in vertical direction. This has to be evaluated by comparing the concentration distributions in both directions.

Model set-up of the 2 D numerical model

As initial condition the pressure and tracer concentration were set to 0 in the whole area. At the left corner at the bottom of the model a concentration relation c/c_0 of 1 is specified along two polylines of the length of 0.3 m. The boundary conditions correspond to the initial conditions. The calculation model includes 736 triangular elements and 409 nodes. Table 9.4.2 shows the used parameters for the simulation. As the porous medium is assumed to be anisotropic, which influences diffusion, the value for tortuosity is set equal to 1 in x-direction and 0.1 in y-direction.

parameter	value	unit
porosity Φ	0.4	–
permeability K	$1.0 \cdot 10^{-15}$	m^2
density water ρ	1000	kg/m^3
viscosity water η	0.001	$Pa \cdot s$
dispersion length	10.0	m
diffusion coefficient D_a	$6.0 \cdot 10^{-10}$	m^2/s

Table 9.4.2: Used parameters

The calculation is made for 30 time steps with a length of $1 \cdot 10^7$ seconds. The calculation model is sketched in figure 9.4.2.

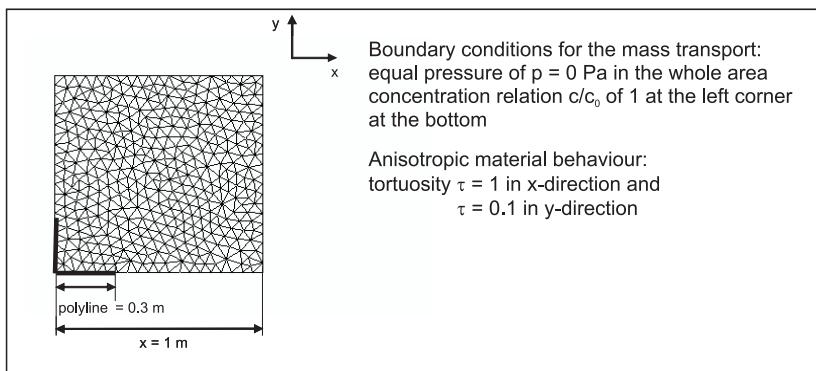


Figure 9.4.2: Calculation model (2D)

Evaluation method

As the process of diffusion is dependent on the actual concentration in the porous medium and on the point in time, an analytical solution for the present calculation model is not possible. Therefore, the results of the RockFlow simulation are solely evaluated in a qualitative way by comparing the concentration distributions in horizontal and vertical direction.

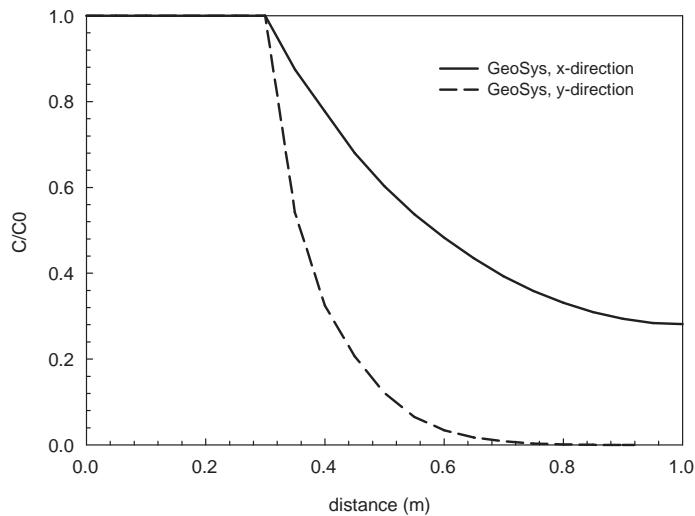


Figure 9.4.3: Concentration distributions in x- and y-direction

Results

In figure 9.4.3 you can find the concentration distributions over the model side length of 1 m in x- and y-direction, respectively, after a simulation time of $1 \cdot 10^8$ seconds. Assuming a small tortuosity of 0.1, the component is not yet transported over the whole transport length of 1 m in vertical direction, while in horizontal direction the concentration relation equals approximately 0.3 at the opposite border of the model. The shown trend in the change of diffusion velocity by assuming different tortuosities in x- and y-direction in order to specify anisotropic material behaviour for molecular diffusion has a comprehensible characteristic.

Benchmark	Problem type	Path in benchmark deposit
diff_aniso	HC	benchmarks \HC\Diffusion\

9.4.3 Solute transport with matrix diffusion

Problem definition

This benchmark is introduced to verify the matrix diffusion function developed by Chris McDermott and Georg Kosakowski. It simulates advective-dispersive transport of a solute in an one-dimensional fracture with constant aperture, with and without the effect of matrix-diffusion. The geometry and the material parameters are chosen to fit the parameters extracted from experiments conducted during the Colloid Radionuclide Retardation Experiment at Nagra's Grimsel test site ???. The result from GS/RF is compared with that from PICNIC, and they fit well.

Model set-up of the 1D domain

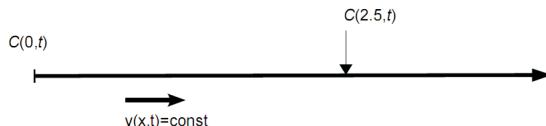


Figure 9.4.4: Conceptual setup of the 1D problem

The geometry and material parameters in PICNIC and GS/RF are summarized in Table 9.4.3 and the conceptual model is shown in Figure 9.4.4. PICNIC solves the one-dimensional problem, whereas in GS/RF a two-dimensional discretization was chosen. A rectangular domain of $5.2\text{m} \times 0.5\text{m}$ was discretized with 1155 nodes and 2080 triangular elements. One of the shorter domain edges was chosen as inflow boundary and fluid was injected at the boundary-nodes in such a way, that the resulting fluid velocity matches exactly the value from 9.4.3.

The concentration is fixed at the inflow boundary. In 2.5m distance the breakthrough curve is recorded. The outflow boundary is assumed to be far away and should not influence the observed breakthrough curve. Picnic V2.2 and GS/RF Rev. 1535 from the subversion server were used for testing.

As defining exactly the same transport boundary conditions in GS/RF and PICNIC is not possible, the following procedure was used to get the inflow boundary condition as similar as possible:

- 1) The system was calculated for injecting a pulse of solute with a constant flux for a time length of 50s with PICNIC. The concentration vs. time was recorded for the inflow-leg.
- 2) The concentrations vs. time extracted from PICNIC's inflow-leg were applied (fixed) to the inflow boundary of the GS/RF system.

These procedures work, as long as advective fluxes are much higher than the dispersive-diffusive fluxes over the boundary.

The outflow boundary condition is set to infinity, i.e. a semi-infinite problem is calculated. In GS/RF the domain is set to 5m, double the distance between inflow boundary and observation point. This prevents the outflow boundary condition to influence the tracer breakthrough at the observation point.

Symbol	Unit	Description	Value
L	m	Distance between boundary and observation points	2.5
α_T	m	Trans. dispersion (GS/RF only)	—
ρ	kg/m^3	Bulk matrix density	2670
$2b$	m	Fracture aperture	0.55×10^{-3}
v	m/s	Fluid velocity	7.05×10^{-4}
α_L	m	Long. dispersion (GS/RF only)	0.1
Pe	—	Peclet number (PICNIC only)	25
ε_p	—	Matrix porosity	0.3
D_p	m^2/s	Diffusion constant in rock matrix	7.4×10^{-11}

Table 9.4.3: Geometry and material properties for the simulations

Results

For the investigated two cases, advection and dispersion(ADE) only and ADE plus matrix diffusion(MD), the PICNIC and GS/RF solutions are in general very similar (see Figure 9.4.5).

Benchmark	Problem type	Path in benchmark deposit
<i>matrix_diffusion</i>	C	benchmarks\C\matrix_diffusion\

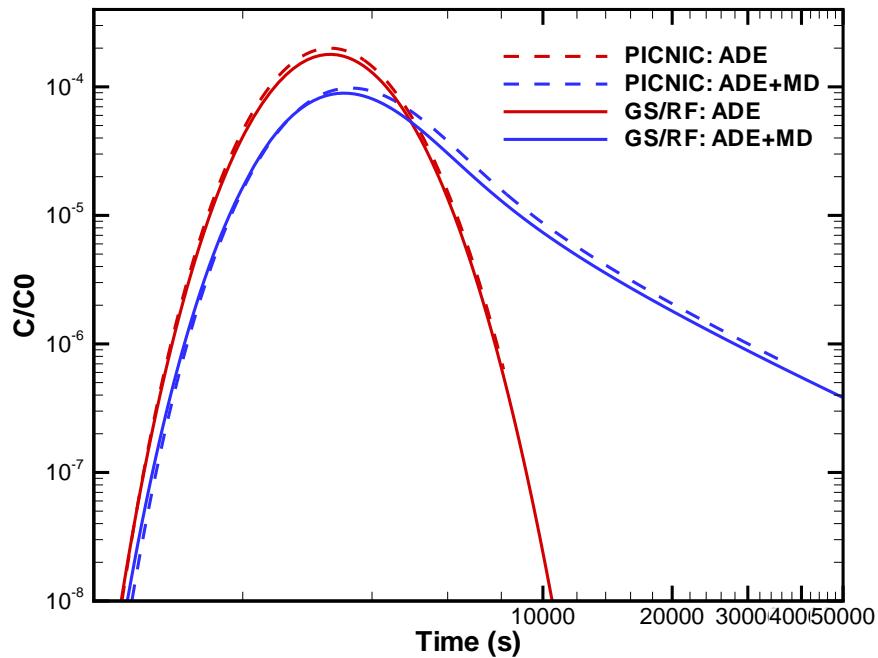


Figure 9.4.5: Breakthrough of the ADE and the ADE+MD solutions calculated with PICNIC and GS/RF

9.4.4 Solute transport with cation exchange

Theory

In contrast to sorption the ion exchange is the replacement of one chemical for another one at the solid surface, the so called ion exchanger. Ion exchange equations do explicitly account for all ions which compete for the exchange sites. The exchange of ions is limited by the exchange capacity, which is the sum of exchangeable ions in the soil and fluctuates with the change of pH in the soil solution. The ion exchanger can be unselective or can have binding preferences for certain ions or classes of ions, depending on their chemical structure (Appelo and Postma, 1996).

Problem definition

This test example is taken from the PHREEQC User's Guide (Parkhurst and Appelo, 1999), a manual for a computer program that is applicable for chemical reactions and transport processes. The simulation is made in order to reproduce the transport of solutes by saturated flow with the influence of cation exchange. The aim of the example is to check out the correctness of the coupling between GeoSys/RockFlow and PHREEQC by comparing the results of the simulations of both programs. With the calculation model the chemical composition of the effluent from a column containing a cation exchanger and a sodium-potassium-nitrate-solution is simulated. This column is flushed with 3 pore volumes of calcium chloride solution.

Assumptions

Components: calcium, potassium and sodium react to equilibrium with cation exchanger at all times

Aquifer: homogeneous, saturated, stationary flow

Model set-up of the 1 D numerical model

The 8.2 cm long column contains a sodium-potassium-nitrate solution that is in equilibrium with a cation exchanger. For the one-dimensional calculation the calculation area is simplified as a line of a length of 8.2 cm. The calculation model includes 82 elements and 83 nodes. As initial condition the water head in the whole domain is given with 2 m. The initial state of the solution is given in table 9.4.4.

parameter	value	unit
Ca	0	–
Cl	0	–
K	$2.0 \cdot 10^{-4}$	mol/kgw
Na	$1.0 \cdot 10^{-3}$	mol/kgw
N(5)	$1.2 \cdot 10^{-3}$	mol/kgw
pH	7	–
pe	12.5	–
Na-X	$5.493 \cdot 10^{-4}$	mol/kgw
K-X	$5.507 \cdot 10^{-4}$	mol/kgw
Ca-X ₂	0	–

Table 9.4.4: Used parameters

with

pe - redox potential

X - ion exchanger
 kgw - kilogram of water.

At the right border of the model the constant head is given with 2 m. At the left border a constant flux of $1.388 \cdot 10^{-6} \text{ m}^3/\text{s}$ is defined as source term. The concentrations of this infiltrating CaCl_2 -solution as well as the pH and pe are given in table 9.4.5.

parameter	value	unit
Ca	$6.0 \cdot 10^{-4}$	mol/kgw
Cl	$1.2 \cdot 10^{-3}$	mol/kgw
pH	7	–
pe	12.5	–

Table 9.4.5: State of the infiltration solution

The soil material is specified by the parameters in table ???. The dispersion of the transported solutes in this soil is set equal to $2 \cdot 10^{-3} \text{ m}$. The calculation is divided in 480 time steps with a constant time step length of 180 seconds. That means, the flow and transport processes in the aquifer within 1 day are simulated.

density ρ	2000	kg/m^{-3}
porosity Φ	0.5	–
permeability K	$1.157 \cdot 10^{-5}$	m^2

Table 9.4.6: Soil parameters

Evaluation method

As this test example has the aim to validate the coupling of GeoSys/RockFlow and PHREEQC, merely the comparison between the simulation results of both programs has to be accomplished.

Results

The numerical results are shown in figure 9.4.6. The time-dependent concentrations are the values of the compared GeoSys/RockFlow and PHREEQC models at the end node and end cell, respectively. Within the calculation time of one day the pore volume of the column model is exchanged three times. As chloride is a conservative tracer it arrives already after the exchange of about one pore volume in the effluent. As long as the exchanger contains sodium this component is eluted. Sodium is initially present in the column and exchanges

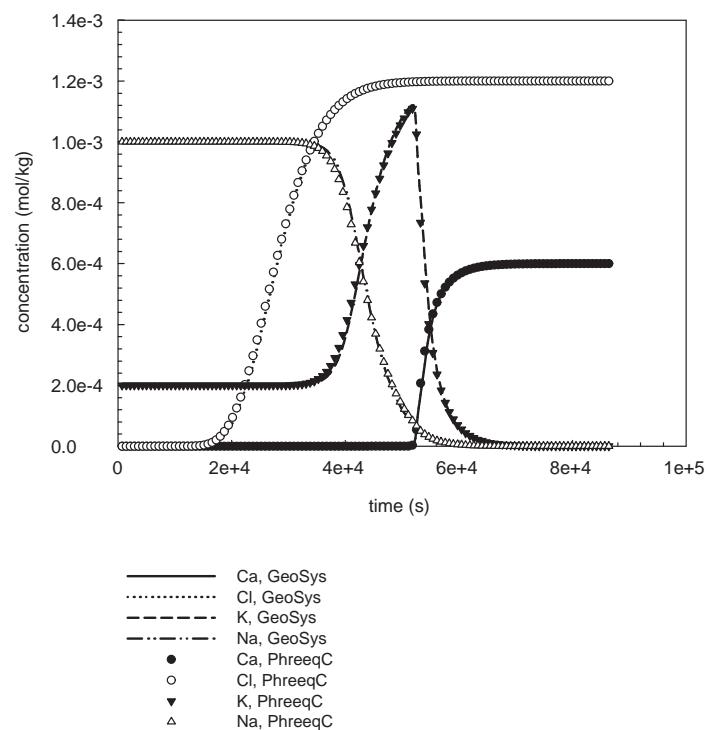


Figure 9.4.6: Effluent concentrations with time of the GeoSys/RockFlow and PHREEQC simulations

with the incoming calcium. Potassium is released after sodium. When all of the potassium has been released, the concentration of calcium increases to a steady-state value. As depicted in figure 9.4.6, between the GeoSys/RockFlow and the PHREEQC simulation results there are no differences.

Benchmark	Problem type	Path in benchmark deposit
pqc1	HC	benchmarks \HC\ion_exchange

9.4.5 Multi-component transport through a one-dimensional column with dissolution and precipitation, using PHREEQC, ChemApp, and GEMIPM2K chemical solver

Problem definition

In this example, a one-dimensional column that initially contains calcite is continuously flushed by water that contains magnesium chloride (Fig. 9.4.7). With the movement of water front, calcite starts to dissolve and dolomite is formed temporarily.

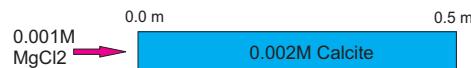


Figure 9.4.7: Model domain

Media Properties

The media properties of this model is listed in Table 9.4.7.

Property	Value	Unit
Column length	0.5	m
Effective porosity	0.32	–
Bulk density	1.8×10^3	kg/m ³
Longitudinal dispersivity	0.0067	m
Pore velocity	9.375×10^{-6}	m/sec
Flow rate	3×10^{-6}	m ³ /sec

Table 9.4.7: Material properties

Initial and Boundary conditions

For GS/RF-GEMIPM2K calculation, all the possible chemical species need to be explicitly set up for initial and boundary conditions. In this example, all

concentration values are given in the unit of *mol/kgwater*. Detailed values can be get from the *.ic and *.bc files in the corresponding benchmark folder.

Results

This model can be simulated by GS/RF-PHREEQC, GS/RF-ChemApp, and GS/RF-GEMIPM2K. In these benchmarks, we use the Nagra/PSI database [80], which provides same thermodynamic data for all three calculations. Fig. 9.4.8 shows the three simulation results. Solid lines are for GS/RF-PHREEQC, symbols "+" are for GS/RF-GEMIPM2K, and triangles are for GS/RF-ChemApp.

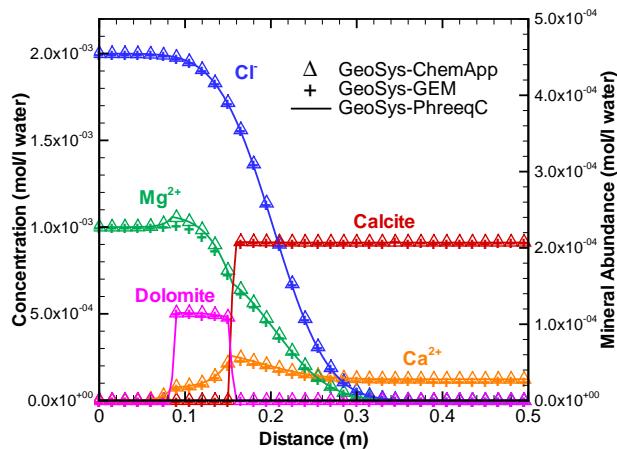


Figure 9.4.8: Benchmark results from GS/RF-ChemApp, GS/RF-PHREEQC, and GS/RF-GEMIPM2K

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>calcite_gems</i>	C	benchmarks\C\calcite_gems\
<i>calcite_pqc</i>	C	benchmarks\C\calcite_pqc\
<i>calcite_chemapp</i>	C	benchmarks\C\calcite_ChemApp\

9.5 1D and 2D conservative transport

9.5.1 1D reactive transport with comparison to analytical solution

This benchmark describes reactive and conservative mass transport in a one-dimensional aquifer and has two aims. Firstly, a conservative component, a linearly retarded component and a component decaying according to a first order decay are transported and profiles as well as breakthrough curves are compared with the corresponding analytical solution. This comparison is possible only using these simplified reaction types. Secondly, the benchmark is set up in a way that allows to test all element types in this simplified "quasi" one-dimensional setup.

The model aquifer has a length of 100 m in x-direction and 1 m in both y and z direction. Discretization is in element sizes of 1 m in x direction, yielding 100 elements and 101 nodes for the line elements, 100 elements and 202 nodes for the quad elements, 200 elements and 202 nodes for the triangular elements, 100 elements and 404 nodes for the hexahedra elements, 200 elements and 404 nodes for the prism elements and 600 elements and 404 nodes for the tetrahedra elements. To make the boundary conditions consistent with all element types, surfaces in the y-z plane are used to define the boundary conditions at x=0 m and x=100 m.

The hydraulic conductivity is assumed to be isotropic and constant in the whole aquifer. Flow is from the left to the right (small to large x), induced by fixed head boundary conditions at x=0 and x=100 and a total head difference of 1 m. All components have initial conditions of 0 and a constant concentration boundary condition of 1 at x=0. For the purpose of this benchmark, the concentration units are arbitrary and are therefore normalized. Transport velocity corresponds to 1 m d^{-1} , thus time step length is chosen accordingly as 86400 s (corresponding to 1 d). Total simulation time is 100 d. Thus the Courant number $Co = 1.0$ and the grid Peclet number $Pe_g = 4$, keeping effects of numerical dispersion as well as oscillations sufficiently small. All parameters used in this simulation are given in table Tab. 9.5.2.

Three components are used in this benchmark: The component **ConsTracer** denotes the conservative tracer, for which the advection - dispersion equation is solved. Component **Decay** is transported according to the advection - dispersion equation with a first order decay rate λ . Component **SorbLin** is transported according to the advection - dispersion equation with a linear instantaneous sorption, which corresponds to a retardation of $R = 1 + \frac{1-n}{n} \rho_s K_d = 1 + \frac{0.5}{0.5} \cdot 2000 \cdot 0.001 = 3$. All components have the same aqueous phase diffusion coefficient.

Table 9.5.1: Parameters used for benchmark HC\1d_analyt

parameter	value	unit
porosity $\Phi = n$	0.5	–
hydraulic conductivity K	$5.787037 \cdot 10^{-4}$	m s^{-1}
storage coefficient S	0.0	s^{-1}
solid density ρ_s	2000	kg m^{-3}
density of water ρ_w	1000	kg m^{-3}
viscosity water η	0.001	Pa s
dispersion length α_l	0.25	m
component diffusion coefficient D	$1.0 \cdot 10^{-9}$	$\text{m}^2 \text{s}^{-1}$
first order decay rate in water λ	$1.0 \cdot 10^{-7}$	s^{-1}
distribution coefficient K_d	$1.0 \cdot 10^{-3}$	$\text{m}^3 \text{kg}^{-1}$

Evaluation method

Model results are compared to the analytical solution for component profiles along x after a simulation time of 75 days, as well as for breakthrough curves at x=50 m for all components. To facilitate testing of all elements, a batch-file is provided (1D.all.bat) which reruns the benchmark for all element types by replacing the mesh file accordingly. Results can be viewed using the corresponding layout files by Tecplot. `companaProfile_*.lay` is used for displaying the profile results and `companaBTC_*.lay` is used for displaying the breakthrough curve results for element type *. The files `companalytBTC.1pk` and `companaProfile.1pk` save the simulation results for both types from an earlier GeoSys/RockFlow version for reference.

Results

Results of the simulation and the comparison with the analytical solution are shown in Fig. 9.5.1 for the profiles and in Fig. 9.5.2 for the breakthrough curves. Numerical results using GeoSys/RockFlow are denoted by symbols, the analytical solution is denoted by the full lines. Correspondence is very good in both cases.

Benchmark	Type	Path
1d_analyt	HC	benchmarks\C\1d_analyt

9.5.2 2D conservative transport with comparison to analytical solution

This benchmark describes the conservative mass transport in a two-dimensional homogeneous aquifer. The main purpose is to compare the numerical results of a

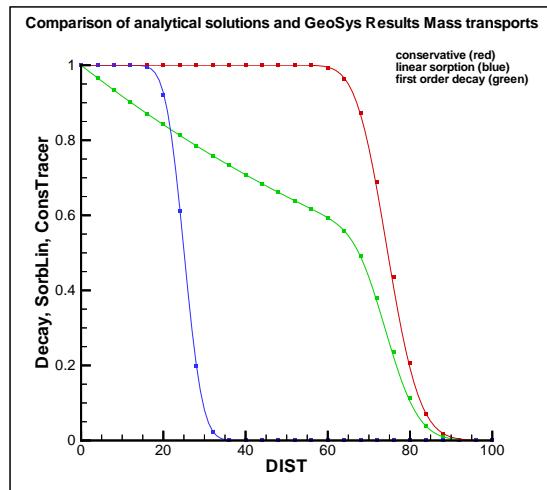


Figure 9.5.1: Concentration profiles after 100 d

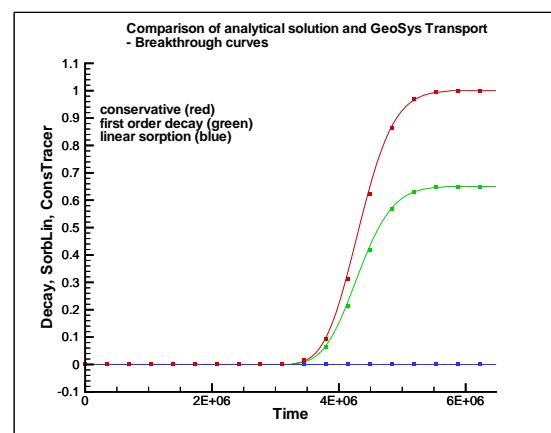


Figure 9.5.2: Concentration breakthrough curves at $x=50$ m

conservative mass transport simulation without any reactions with the suitable analytical solution.

The model aquifer has a length of 100 m in the x-direction, 50 m in the y-direction and 1 m in the z direction. The whole domain is discretized into 10560 triangular elements with a constant x and y dimension of 1 m (this value guarantees a Peclet number = 4), except at the boundaries of the injection area where a finer grid is chosen.

The aquifer is assumed to have a homogeneous and isotropic hydraulic conductivity and the constant head boundary conditions on the left (piezometric surface of 2 m) and right side (piezometric surface of 1 m) produce a steady state flow in the right direction. As the material has a constant porosity of 0.5 the resulting flow velocity is $1.1574074 \cdot 10^{-3} \text{ m s}^{-1}$. Both longitudinal and transversal dispersivity have a value of 0.25, consequently the total simulation time of 80 days is divided into 160 time steps to insure a Courant number lower than 1. The constant tracer is injected with a relative concentration value of 1.0 from a source 8 m wide set on the left boundary of the aquifer, while the initial concentration of the tracer is zero all over the aquifer domain.

Table 9.5.2: Parameters used for benchmark HC\2d_analyt

parameter	value	unit
porosity $\Phi = n$	0.5	—
hydraulic conductivity K	$5.787037 \cdot 10^{-5}$	ms^{-1}
storage coefficient S	0.0	s^{-1}
solid density ρ_s	2000	$\text{kg} \cdot \text{m}^{-3}$
density of water ρ_w	1000	$\text{kg} \cdot \text{m}^{-3}$
viscosity water η	0.001	$\text{Pa} \cdot \text{s}$
longitudinal dispersivity α_l	0.25	m
transversal dispersivity α_t	0.25	m
component diffusion coefficient D	$1.0 \cdot 10^{-9}$	$\text{m}^2 \text{s}^{-1}$

Evaluation method

Model results are compared to the Hewson analytical solution (Hewson, Thomas, 1976, Simulation of leachate movement in the areal plane-A finite element approach: Princeton University, B.S. thesis, 150 p.) for a x-y planar view of the model domain as well as for breakthrough curves at $x=60$ m and $x=80$ m after a simulation time of 80 days. The Hewson solution is more desirable for comparison of this benchmark than the Domenico (1978) solution, because it was developed for a finite width aquifer while the one of Domenico refers to an infinite width aquifer.

Results

Results of the simulation and the comparison with the analytical solution are shown in Fig. 9.5.3 for the profiles at 60 m and 80 m, and in Fig. 9.5.4 for the planar view. Numerical results using GeoSys/RockFlow are represented by the black line, while the Hewson analytical solution is denoted by the red line. Correspondence is very good in both cases and observing the x-y view we can also point out that the numerical simulation is able to properly reproduce lateral and transversal spreading of the constant tracer.

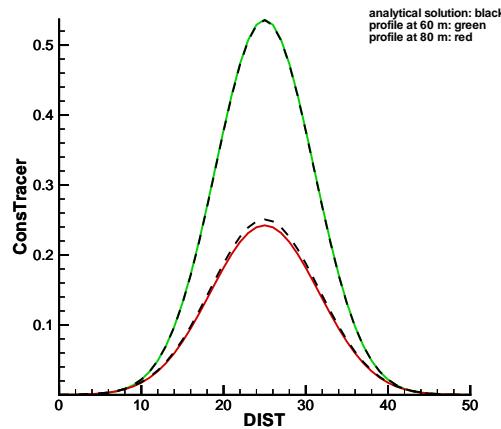


Figure 9.5.3: Profiles at 60 m and 80 m after 80 d. Comparison of analytical solution and GeoSys/RockFlow results.

Benchmark	Type	Path
2d_analyt	HC	benchmarks\{C\}2d_analyt

9.6 Reactive Transport

9.6.1 1D reactive transport: Xylene degradation with multiple monod kinetics, exchange kinetics and biomass growth

This benchmark describes the reactive transport of xylene in a homogeneous aquifer. The main purpose is to document the ongoing reactions, which are xylene degradation under aerobic, sulfate reducing and iron reducing conditions, considering growth of the respective biomasses. Also included is the rate limited

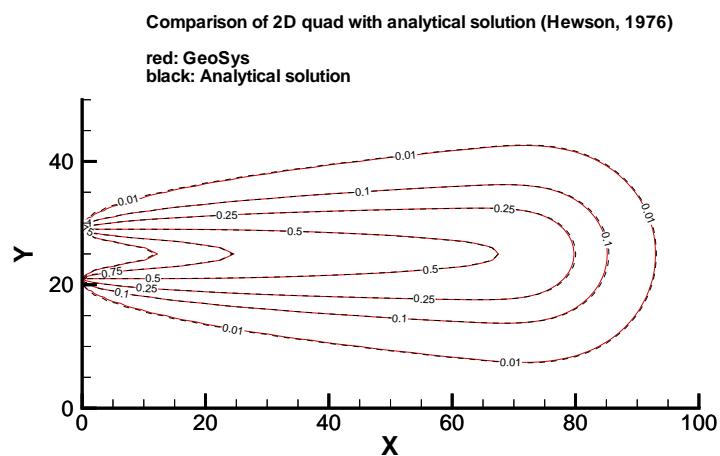


Figure 9.5.4: Planar x-y view after 80 d. Comparison of analytical solution and GeoSys/RockFlow results.

exchange of iron goethite into bioavailable iron. The aquifer is represented by a one-dimensional model of 50 m length in the x-direction and 1 m in the y- and z directions, respectively. The model is discretized by 100 line elements of constant 0.5 m length in x direction. With an isotropic hydraulic conductivity K of $2.13 \cdot 10^{-3} \text{ m s}^{-1}$, a porosity of 0.24 and a hydraulic gradient I of $1.3 \cdot 10^{-4}$, the steady state transport velocity v_a is 0.1 m d^{-1} . Longitudinal dispersivity α_L is set to 0.25 m, the diffusion coefficient D_a is set to $1.0 \cdot 10^{-9} \text{ m}^2 \text{ s}^{-1}$. The physical aquifer parameters are summarized in Tab. 9.6.1. The transport simulation is run for a period of 1000 d with a time step length of 5 d.

The model aquifer has a length of 50 m in the x-direction, 1 m in the y-direction and 1 m in the z direction. The whole domain is discretized into 100 line elements with a constant x and y dimension of 1 m. The aquifer is assumed to have a homogeneous and isotropic hydraulic conductivity. Using a gradient of $1.23 \cdot 10^{-4}$ and a porosity of 0.24 produces a steady state transport velocity of 0.10 m d^{-1} .

Xylene degradation is simulated according to the typical redox sequence.

Table 9.6.1: Parameters used for benchmark HC\1d_xylene_degradation

parameter	value	unit
porosity $\Phi = n$	0.24	–
matrix volume fraction VOL_{MAT}	0.75	–
biomass volume fraction VOL_{BIO}	0.01	–
hydraulic conductivity K	$2.13 \cdot 10^{-3}$	ms^{-1}
storage coefficient S	0.0	s^{-1}
solid density ρ_s	2000	$\text{kg} \cdot \text{m}^{-3}$
density of water ρ_w	1000	$\text{kg} \cdot \text{m}^{-3}$
viscosity water η	0.001	$\text{Pa} \cdot \text{s}$
longitudinal dispersivity α_l	0.25	m
component diffusion coefficient D	$1.0 \cdot 10^{-9}$	$\text{m}^2 \text{s}^{-1}$

Evaluation method

Model results are compared an older version of GeoSys/RockFlow.

Results

Results of the simulation are shown in Fig. 9.6.1 for xylene, the electron acceptors oxygen and sulfate, as well as for the biomass of the aerobic microorganisms, the sulfate reducers and the iron reducers simulation time steps of 100 days. For simulation time $t < 500$ d, one can see the advancing xylene front, a reduction of xylene concentrations is only visible for later times, when xylene concentrations reduce to about 90% of the inflow concentration. Also shown is the increasing

consumption of oxygen with time, accompanied by the growth of the aerobic reducers at the inflow (left) end of the model area. After approximately 800 d, oxygen concentrations in the inflowing groundwater are reduced to almost zero within the first 20 m of the aquifer. Sulfate reducers initially decay from their initial amount, as growth is inhibited throughout the column by the still high concentrations of oxygen. Once oxygen is used up, however, sulfate reducers start to grow downstream of the oxygen reducers and sulfate concentrations in the groundwater reduce accordingly. The iron reducers decay from their initial values and start to grow only for late times $t > 80$ d and $x > 30$ m, as xylene degradation from iron reduction is inhibited by both, oxygen as well as sulfate, which is still present in concentrations larger than the inhibition concentration for iron reducers. Accordingly, the spatial distribution of bioavailable iron is still almost uniform throughout the aquifer.

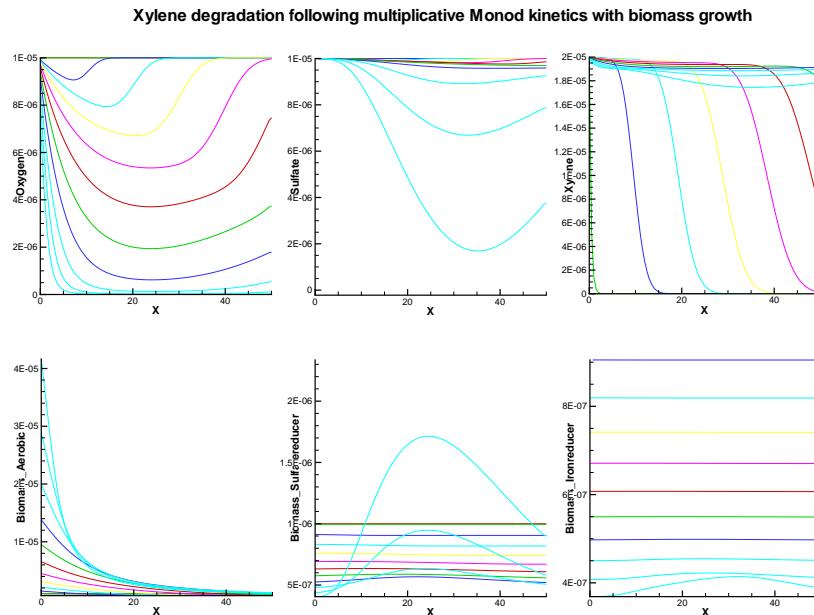


Figure 9.6.1: Profiles of oxygen, sulfate and xylene (top row, from left) and aerobic reducers, sulfate reducers and iron reducers at different times during the 1000 d simulation period.

Benchmark	Type	Path
1d_xylene_degradation	HC	benchmarks\C\1d_xylene_degradation

9.6.2 1D reactive transport: Competition of TCE- and cis-DCE-degradation for the zero valent iron surface

This example simulation demonstrates the use of GeoSys/RockFlow for simulation of multi-species kinetic reactions. The reaction system was set up by D. Schäfer and published in Schäfer et al. (2003) (Schäfer, D., R. Köber and A. Dahmke (2003): Competing TCE- and cis-DCE-degradation kinetics by zero-valent iron - experimental results and numerical simulation. Journal of Contaminant Hydrology, 65(3-4): 183-202). Further, it was used for model verification of the newly implemented and developed kinetic reaction module in GeoSys/RockFlow. The example considers flow in a one-dimensional column of 1 m length, resembling the thickness of a reactive iron barrier perpendicular to the flow direction. It involves 19 species and 16 different geochemical reactions, both first-order degradation reactions of adsorbed substances and kinetic sorption reactions of the langmuir-type, considering competition for the available sorption sites.

The model set up consists of a 1d column with saturated ground water flow with a darcy velocity of $5.0 \cdot 10^{-4}$ m d⁻¹ from left to right. Geochemical species are added to the inflowing water, and their sorption and degradation behavior is modeled. For a complete description of input parameters see the paper by Schäfer et al. (2003). Every degradation reaction follows a Langmuir-Hinshelwood-Hougen-Watson kinetics with a limited number of sites for the adsorption and desorption of chlorinated hydrocarbons on the reactive iron surface. Since all the reactive substances involved have to adsorb onto the reactive iron surface in order to be degraded, a competition for the surface sites occurs. This competition has been investigated in column studies and the observed concentration profiles were simulated with the numerical model TBC (Schäfer et al., 2003).

Evaluation method

Model results are compared an older version of GeoSys/RockFlow, which was compared to the original TBC simulations.

Results

Results of the simulation are shown in Fig. 9.6.2, where profiles of the dissolved species are shown. TCE and cis-DCE are added to the inflowing water. They compete for the sorption sites, and when sorbed degrade according to a first order degradation reaction. The retardation of the reactive species compared to the conservative tracer mobile is clearly visible. Also, just downstream of the concentration decrease of TCE or cis-DCE, the degradation products ethane and C4-containing molecules increase. These species are again mobile and are transported with the water, so an instationary behaviour is observed in Fig. 9.6.2.

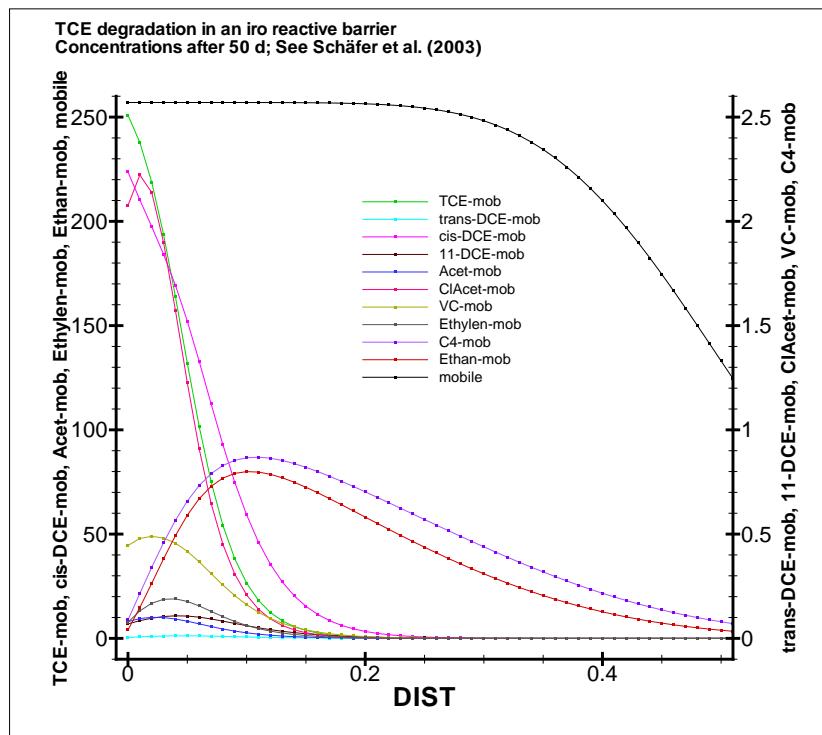


Figure 9.6.2: Concentration profiles of TCE, trans-DCE, cis-DCE, 1,1-DCE, Acetylene, chloroacetylene, C4, VC, ethene and ethane as well as the conservative tracer mobile after 50 d simulation time.

Benchmark	Type	Path
1d_TCEonIon	HC	benchmarks\1d_TCEonIon

9.6.3 1D reactive transport: degradation of organic contaminants in a sand column experiment by five bacterial groups forming a degradation network

The Biogeochemical Reaction Network Simulator (BRNS, [81, 82]) is coupled to GeoSys following a sequential non-iterative operator splitting scheme yielding the reactive transport model GeoSysBRNS. The technical coupling is sketched in Fig. 9.6.3.

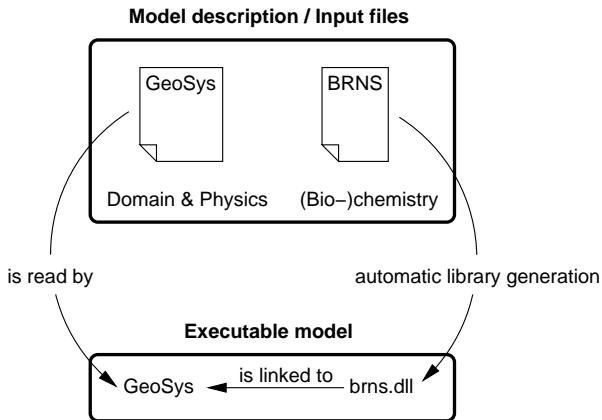


Figure 9.6.3: The setup of GeoSysBRNS. The model description is divided into two parts: the model domain definition, physical parameters, hydrogeological flow, and discretization parameters in GeoSys format, and the description of the coupled (bio-)chemical reaction processes in BRNS format. The latter is compiled into a problem specific library that is accessed by GeoSys at runtime.

The Model

An experimental study by [83] has been used to validate the reactive transport models TBC [84] and the stand-alone 1D version of BRNS [85]. Both models could reproduce the experimental data set. Here, we use the same simulation scenario to validate GeoSysBRNS and compare simulation results to BRNS results.

In the example referred to as “Scenario 1” in [85], a sand column of 29 centimeters length is constantly flushed with water containing lactate as electron donor, and oxygen, nitrate, and sulfate as terminal electron acceptors (TEAs). Manganese and iron oxyhydroxides are bound to the sand matrix in solid phases and act as two additional TEAs. Five distinct microbial groups, which catalyze the reduction of each TEA to sustain their growth, are considered in the model. The experimental results suggest that lactate is concomitantly mineralized into

dissolved inorganic carbon (DIC) and fermented to acetate and propionate, with the latter being further oxidized into DIC. In addition to these microbial degradation pathways, reactive species concentrations are influenced by a set of abiotic reactions (Fig. 9.6.4). The complete reaction network of the model consists of 21 mobile and 18 immobile reactive species. The dynamics of the system is determined by 24 kinetically controlled chemical reactions and nine equilibrium reactions describing acid base dissociations.

- phase exchange (matrix, biophase, pore water)
- oxidation of sulfide by Fe(III)
- precipitation and dissolution of calcite and Fe(II) minerals
- acid-base reactions for carbonates, sulfides, lactate, propionate, acetate

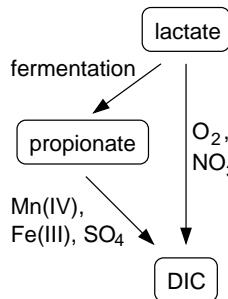


Figure 9.6.4: Modeling organic carbon degradation in a sand column experiment. Coupled abiotic processes considered in the model (left), and microbial degradation pathways with corresponding TAEs (right).

Evaluation method

The coupling of the BRNS to GeoSys is shown to be correct by comparing simulation results of GeoSysBRNS to BRNS results [86].

Results

We simulate the experiment with GeoSysBRNS using two spatial resolutions and three different temporal resolutions per spatial setting, ensuring Courant numbers smaller than 1.0 in all cases. As in previous studies [85, 84], we choose 48 days as the target time for comparing the results of the coupled model to those obtained with the BRNS model using the same set of spatio-temporal resolution settings. At this target time, the system is still in the transient phase.

The simulation results of GeoSysBRNS and BRNS agree very well for all 39 reactive species at the highest spatial and temporal resolution (see selected species in Figs. 9.6.5, 9.6.6). Decreasing the spatial resolution leads to slightly different results, with the coupled model generally staying closer to the high resolution result than the stand-alone version of BRNS (Figs. 9.6.5, 9.6.6).

When the time step size is increased, the numerical results of both models diverge from the high resolution result (Fig. 9.6.7). While increasing the time

step from 4 s to 43.2 s does not lead to significant changes for both models and both spatial resolutions, a noticeable deviation is observed when the time step size is further increased to 108 s for the high, and to 216 s for the low spatial resolution. For these larger time step sizes, the results of GeoSysBRNS are again generally closer to the high resolution result than the BRNS solutions. The observed differences can be attributed to the different numerical schemes used by BRNS (finite differences) and GeoSysBRNS (finite elements). Further details of the GeoSysBRNS and its performance can be found in [86].

Benchmark	Type	Path
1d_degradation_network	C	benchmarks\1d_degradation_network

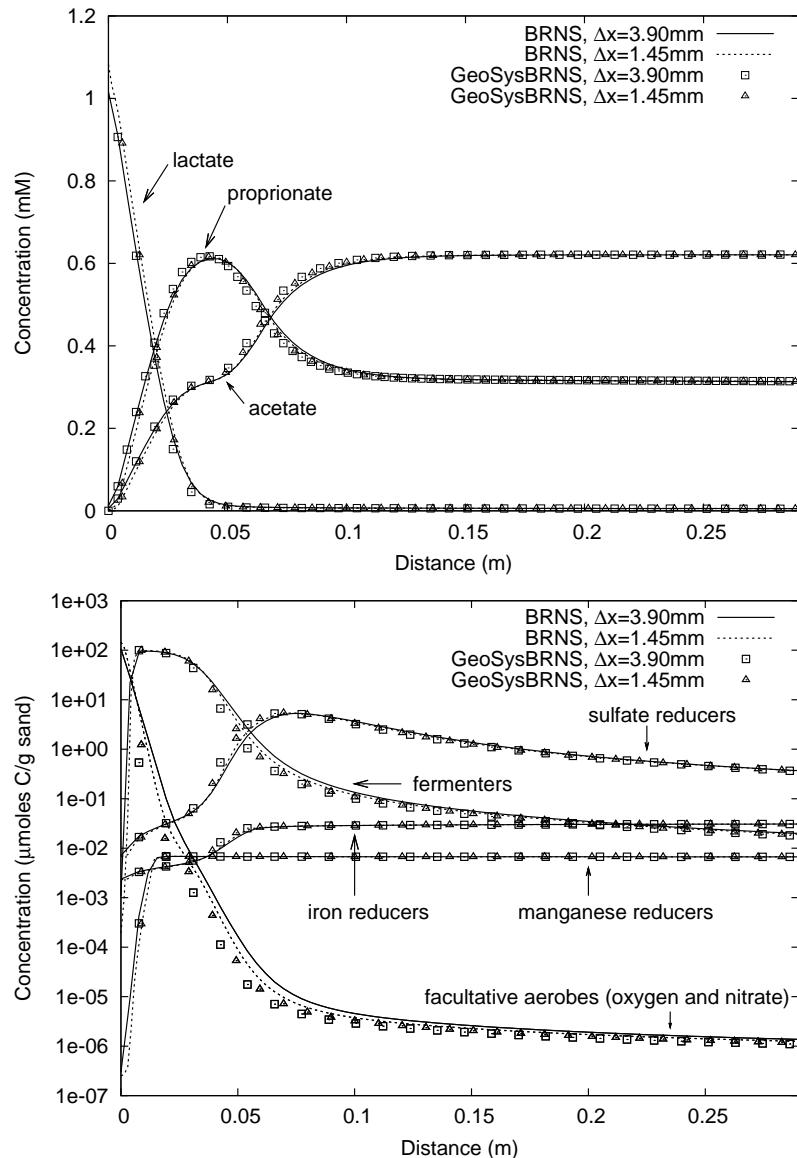


Figure 9.6.5: Comparison of simulation results obtained with BRNS (lines) and GeoSysBRNS (symbols): organic species (top) and all five bacterial groups (bottom) at day 48 using the highest temporal resolution ($\Delta t=4\text{ s}$) and two spatial resolutions.

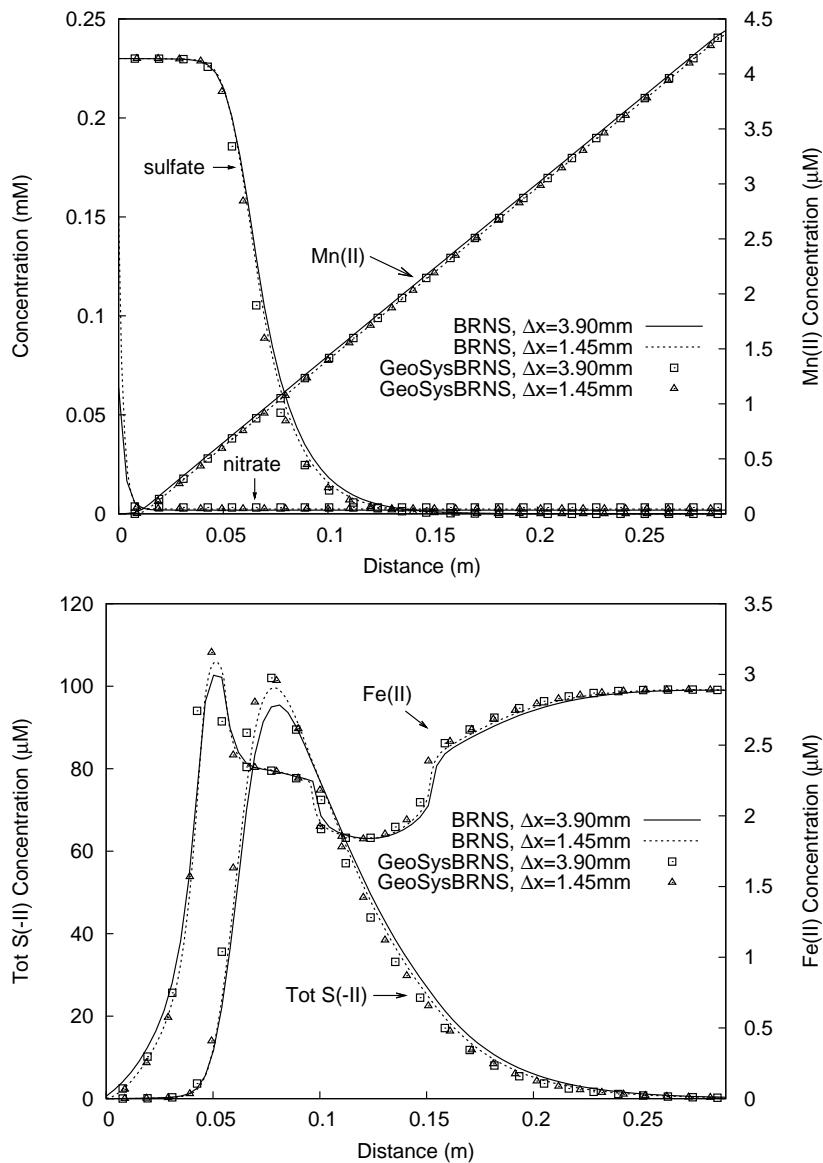


Figure 9.6.6: Comparison of simulation results obtained with BRNS (lines) and GeoSysBRNS (symbols): inorganic species at day 48 using the highest temporal resolution ($\Delta t=4\text{ s}$) and two spatial resolutions.

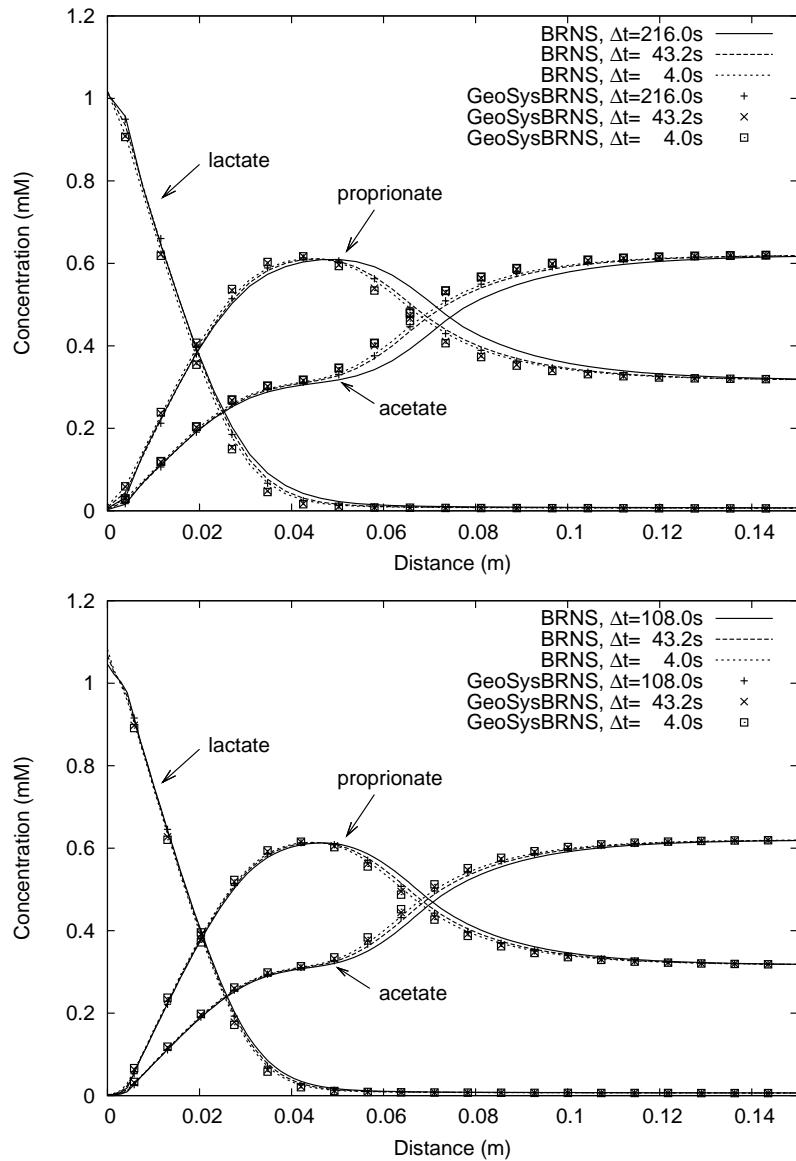


Figure 9.6.7: Comparison of simulation results obtained with BRNS (lines) and GeoSysBRNS (symbols) at day 48 using two spatial resolutions (top: $\Delta x = 3.9 \text{ mm}$, bottom: $\Delta x = 1.45 \text{ mm}$) and different time step sizes for lactate, propionate, and acetate.

9.6.4 Mixing Controlled Bioreactive Transport

Problem definition

For contaminated groundwater, the natural remediation process is usually limited by the availability of substrates acting as a carbon source for soil bacteria and the availability of electron acceptors. The transport of these chemical compounds is controlled by the dispersion length of the flow system. Recently, [87] presented an analytical solution for the steady state of a two-dimensional scenario dominated by transversal mixing. This example serves as a first multidimensional benchmark to validate GeoSysBRNS. [87] provide analytical solutions for double-monod kinetics with first-order biomass decay.

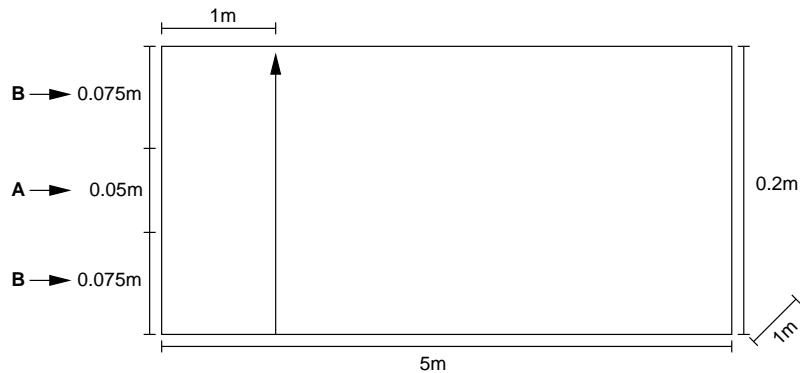


Figure 9.6.8: The simulation domain. Simulation results are compared using concentration profiles along a transect at a distance of one meter from the inflow boundary, indicated by the arrow.

Parameters

In this scenario, bacterial growth is modeled using double-monod terms for the substrates. Biomass decays with a constant decay rate d . The overall dynamics is described by four differential equations, with the dynamics of species A, B, and C directly linked to the biomass growth r via yield factor Y :

$$\frac{\partial C_{bio}}{\partial t} = \underbrace{\frac{C_A}{K_A + C_A} \cdot \frac{C_B}{K_B + C_B} \cdot \mu_{max} \cdot C_{bio} - d \cdot C_{bio}}_r \quad (9.6.1)$$

$$\frac{\partial C_A}{\partial t} = -\frac{1}{Y} \cdot r \quad (9.6.2)$$

$$\frac{\partial C_B}{\partial t} = -\frac{1}{Y} \cdot r \quad (9.6.3)$$

$$\frac{\partial C_C}{\partial t} = +\frac{1}{Y} \cdot r. \quad (9.6.4)$$

The chemical parameters and their values are listed in Table 9.6.2.

Table 9.6.2: Reaction parameters and values.

Symbol	Parameter	Value	Unit
K_A	monod constant substrate A	8.33×10^{-5}	mol/l
K_B	monod constant substrate B	3.13×10^{-5}	mol/l
μ_{max}	maximum growth rate	0.1	d^{-1}
d	biomass death rate	1.0	d^{-1}
Y	yield coefficient	1.0	g/mol

Using GeoSysBRNS, here we simulate the case as a transient state groundwater flow process coupled with biodegradation. The numerical solutions are compared to the analytical steady state solutions.

The model domain is five meters long and 20 centimeters wide (see Figure 9.6.8). Groundwater flows from left to right with a velocity of 1 m/d. The transport parameters are listed in Table 9.6.3. Two substrates are continuously emitted at the left inflow boundary throughout the simulation period. Substrate A is centrally injected over a width of five centimeters with a concentration of 3.3×10^{-4} mol/l, while substrate B is emitted at the remaining part of the boundary with a concentration of 2.5×10^{-4} mol/l. Initially, the concentration in the whole simulation domain is zero for substrate A, 2.5×10^{-4} mol/l for substrate B, and 1.0×10^{-6} g/l for biomass. Biomass is considered to be immobile.

In the presence of both species A and B, with A representing a generic organic contaminant acting as a carbon source and B representing a generic electron acceptor, the biomass grows, and a waste product C is formed.

Results

For the numerical simulation, a grid spacing of 2.5 cm in flow, and 0.5 cm transversal to the flow direction is used. Temporal discretization of 2min is employed. The concentrations of the conservative tracer fit well with the analytical solution, indicating that the flow field is properly modeled. However,

Table 9.6.3: Transport parameters and values.

Parameter	Value	Unit
v seepage velocity	1.0	m/d
D_t transversal dispersion coefficient	2.5	cm ² /d
D_l longitudinal dispersion coefficient	0.0 ^a	cm ² /d

^a As a zero value cannot be used in the numerical simulation, the value $2.5 \times 10^2 \text{ cm}^2/\text{d}$ was used instead. When the numerical simulation reaches steady state, this difference can be neglected.

a discrepancy is found for the component A, B, C, and biomass concentration (see Figure 9.6.9). This is due to an necessary but insufficient ω criterion used to produce analytical solution. Detailed discussions can be found in [88].

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>calcite_gems</i>	C	benchmarks\C\monod2d\

9.7 Conservative mass transport in unsaturated media

Problem definition

This case is a simulation of classical experiment of Warrick et al's(1971)[?]. The solution is Richards equation combining mass transport equation. For the hydraulic, it is define as section 5.2.1. For the mass transport, the tracer component goes into the soil column from top,

Initial and boundary conditions

Details of hydraulic are illustrated in Fig. 5.2.1. The initial concentration of each component is 0, and concentration at the top is in Fig. 9.7.1.

Material properties

Homogenous material properties are assumed within the whole domain. Table 5.2.1 gives the parameters.

Component properties

Component properties are in Table 9.7.1.

Table 9.7.1: Parameters of component properties (mcp)

component	items	setting
tracer	mobile	1
	transport phase water	0
	diffusion coefficient	6.0e-10
adsorb	mobile	1
	transport phase water	0
	diffusion coefficient	6.0e-10
	Sorption: $C_s = K_D C^e$	K_D 1e-3 e 0.9

Results

The hydraulic features are in Fig.5.2.3. Fig. 9.7.2 shows the distribution of concentration. Points in the Fig.9.7.2 are observations.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>ust_line</i>	C	benchmarks\C\1d_ust_line\

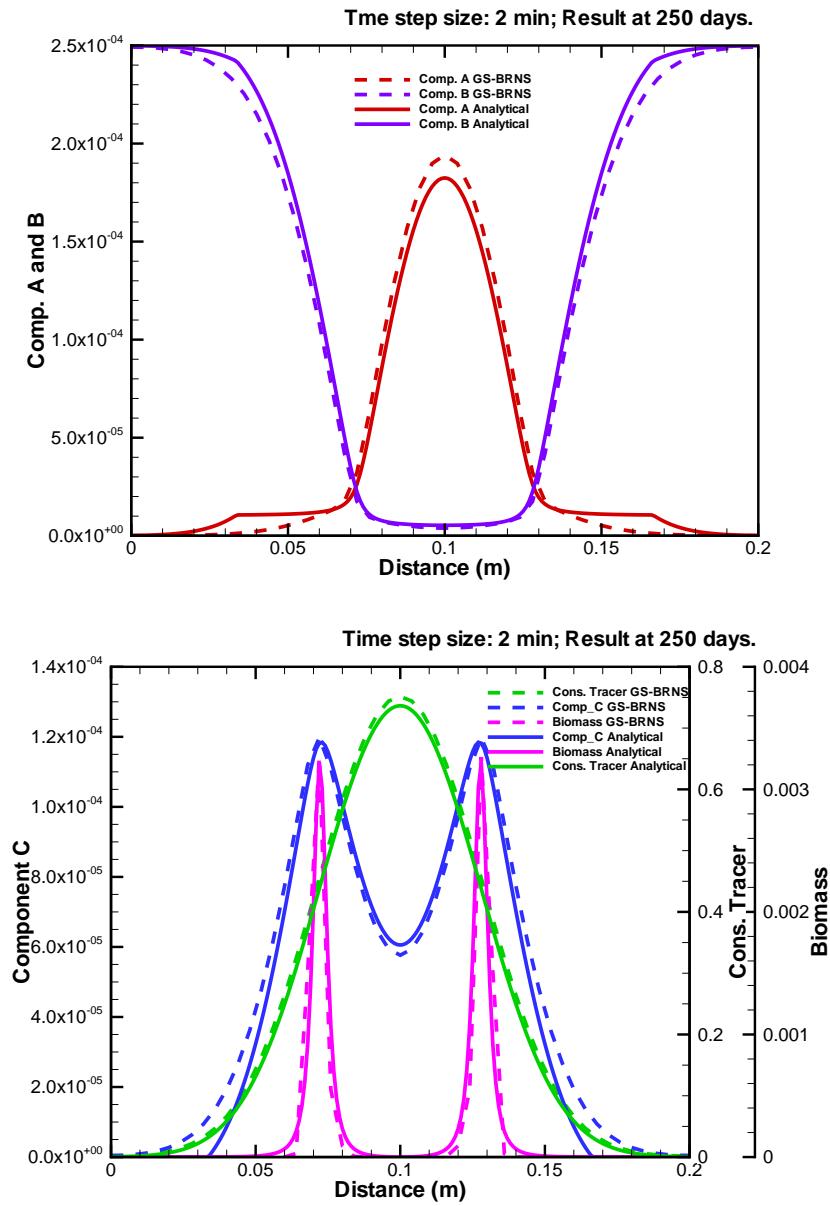


Figure 9.6.9: Simulation results for the transversal mixing model, using the kinetic approach and the finest temporal and spatial resolution. Analytical solution as solid lines, numerical simulation result as dashed lines.

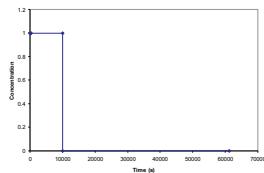


Figure 9.7.1: BC of component

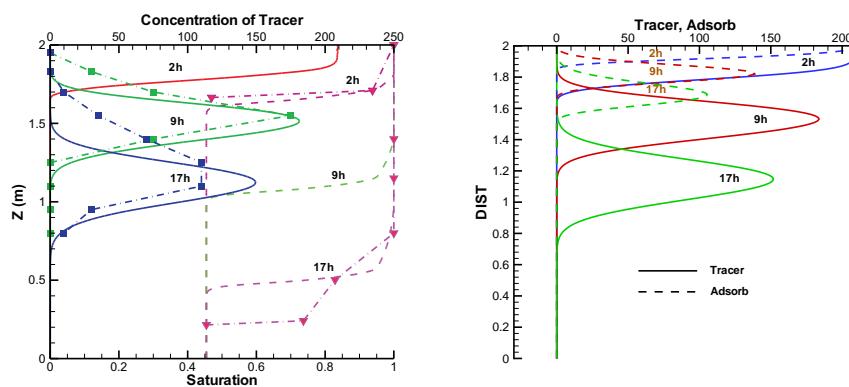


Figure 9.7.2: Distribution of saturation and concentrations

Chapter 10

Random Walk Particle Tracking – H- and Fluid Momentum- Process dependent

10.1 Theory

10.1.1 Governing Equation

The classical advection-dispersion equation of a conservative solute in porous media can be written as [89]

$$\frac{\partial C}{\partial t} = -\nabla(\mathbf{V}C) + \nabla(\mathbf{D}\nabla C) \quad (10.1.1)$$

where C is the concentration (ML^{-3}), \mathbf{V} is the pore velocity vector (ML^{-1}), and \mathbf{D} is the hydrodynamic dispersion tensor (L^2T^{-1}), t is time (T^2) and ∇ is the differential operator.

The modified velocity [90] and the dispersion tensor [89] are expressed as

$$V_i^* = V_i + \sum_{j=1}^3 \frac{\partial D_{ij}}{\partial x_j} \quad (10.1.2)$$

$$D_{ij} = \alpha_T |\mathbf{V}| \delta_{ij} + (\alpha_L - \alpha_T) \frac{V_i V_j}{|\mathbf{V}|} + D_{ii}^d \quad (10.1.3)$$

where δ_{ij} is the Kronecker symbol, α_L is the longitudinal dispersivity, α_T is the transverse dispersivity, D_{ij}^d is the tensor of molecular diffusion coefficient, and V_i is the component of the mean pore velocity in the i th direction.

The stochastic differential equation equivalent to (10.1.1) in three dimensional problems can be written as [91, 92, 93]

$$\begin{aligned} x_{t+\Delta t} &= x_t + \left(V_x(x_t, y_t, z_t, t) + \frac{\partial D_{xx}}{\partial x} + \frac{\partial D_{xy}}{\partial y} + \frac{\partial D_{xz}}{\partial z} \right) \Delta t \\ &\quad + \sqrt{2D_{xx}\Delta t} Z_1 + \sqrt{2D_{xy}\Delta t} Z_2 + \sqrt{2D_{xz}\Delta t} Z_3 \\ y_{t+\Delta t} &= y_t + \left(V_y(x_t, y_t, z_t, t) + \frac{\partial D_{yx}}{\partial x} + \frac{\partial D_{yy}}{\partial y} + \frac{\partial D_{yz}}{\partial z} \right) \Delta t \\ &\quad + \sqrt{2D_{yx}\Delta t} Z_1 + \sqrt{2D_{yy}\Delta t} Z_2 + \sqrt{2D_{yz}\Delta t} Z_3 \\ z_{t+\Delta t} &= z_t + \left(V_z(x_t, y_t, z_t, t) + \frac{\partial D_{zx}}{\partial x} + \frac{\partial D_{zy}}{\partial y} + \frac{\partial D_{zz}}{\partial z} \right) \Delta t \\ &\quad + \sqrt{2D_{zx}\Delta t} Z_1 + \sqrt{2D_{zy}\Delta t} Z_2 + \sqrt{2D_{zz}\Delta t} Z_3 \end{aligned} \quad (10.1.4)$$

where x , y , and z are the coordinates of the particle location, Δt is the time step, and Z_i is a random number whose mean is zero and variance is unit.

In equation (10.1.4), the spatial derivatives of the dispersion coefficients are introduced from the modified velocity [90]. Together with equation (10.1.3), the spatial derivatives of the dispersion coefficients can be expressed as a function of the derivatives of velocity. Note that to obtain the derivatives of velocity, velocity has to be continuous mathematically. For this end, we interpolate velocity at any location in an element from the known velocity at the element nodes. The velocity estimation and the interpolation method are provided in section 7.1.1.

Since the proposed RWPT method makes use of the FEM for velocity estimation, the derivative of velocity within each element is computed as in Figure 10.1.1 and written as

$$\begin{aligned} \frac{\partial V_x}{\partial x} &= \frac{V(x_R) - V(x_L)}{l_x}, \quad \frac{\partial V_y}{\partial y} = \frac{V(y_U) - V(y_D)}{l_y}, \quad \frac{\partial V_z}{\partial z} = \frac{V(z_N) - V(z_S)}{l_z} \\ \frac{\partial V_x}{\partial y} &= \frac{\partial V_x}{\partial z} = \frac{\partial V_y}{\partial z} = \frac{\partial V_y}{\partial x} = \frac{\partial V_z}{\partial x} = \frac{\partial V_z}{\partial y} \simeq 0 \end{aligned} \quad (10.1.5)$$

where x_L and x_R are the intersectional points of the element edges with an extension of a line parallel to the global x axis at which velocities are $V(x_L)$ and $V(x_R)$, y_D and y_U are the intersectional points of the element edge from down to up with extension of the line parallel to the global y axis at which velocities are $V(y_D)$ and $V(y_U)$, z_S and z_N are the intersectional points of the element edge from south to north with extension of the line parallel to the global z axis at which velocities are $V(z_S)$ and $V(z_N)$, and l_x , l_y , and l_z are the length of each intersectional line respectively.

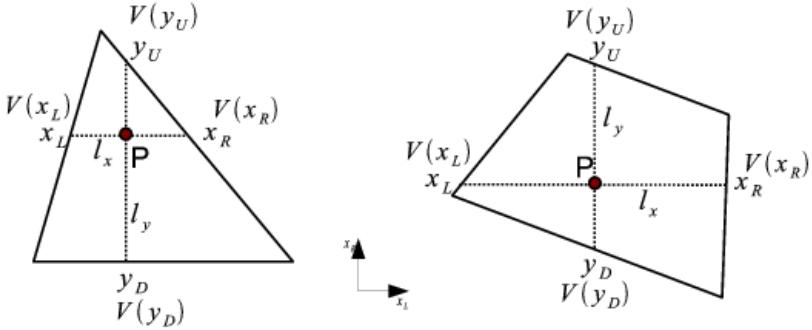


Figure 10.1.1: Spatial derivatives of velocity for a particle in triangular and quadrilateral elements: x_L and x_R are the intersectional points of the element edges with an extension of a line parallel to the global x axis at which velocities are $V(x_L)$ and $V(x_R)$, y_D and y_U are the intersectional points of the element edge from down to up with extension of the line parallel to the global y axis at which velocities are $V(y_D)$ and $V(y_U)$, z_S and z_N are the intersectional points of the element edge from south to north with extension of the line parallel to the global z axis at which velocities are $V(z_S)$ and $V(z_N)$, and l_x , l_y , and l_z are the length of each intersectional line respectively

Thus, the derivatives of the dispersion coefficients are as follows [94]

$$\begin{aligned} \frac{\partial D_{xx}}{\partial x} &= V_x \frac{\partial V_x}{\partial x} \left[\alpha_L \left(\frac{2}{V} - \frac{V_x^2}{V^3} \right) - \alpha_T \frac{V_y^2 + V_z^2}{V^3} \right] \\ \frac{\partial D_{xy}}{\partial y} &= (\alpha_L - \alpha_T) \left[\frac{\partial V_y}{\partial y} \frac{V_x}{V} - \frac{V_x V_y^2}{V^3} \frac{\partial V_y}{\partial y} \right] \\ \frac{\partial D_{xz}}{\partial z} &= (\alpha_L - \alpha_T) \left[\frac{\partial V_z}{\partial z} \frac{V_x}{V} - \frac{V_x V_z^2}{V^3} \frac{\partial V_z}{\partial z} \right] \\ \frac{\partial D_{yy}}{\partial y} &= V_y \frac{\partial V_y}{\partial y} \left[\alpha_L \left(\frac{2}{V} - \frac{V_y^2}{V^3} \right) - \alpha_T \frac{V_x^2 + V_z^2}{V^3} \right] \\ \frac{\partial D_{yx}}{\partial x} &= (\alpha_L - \alpha_T) \left[\frac{\partial V_x}{\partial x} \frac{V_y}{V} - \frac{V_y V_x^2}{V^3} \frac{\partial V_x}{\partial x} \right] \\ \frac{\partial D_{yz}}{\partial z} &= (\alpha_L - \alpha_T) \left[\frac{\partial V_z}{\partial z} \frac{V_y}{V} - \frac{V_y V_z^2}{V^3} \frac{\partial V_z}{\partial z} \right] \\ \frac{\partial D_{zz}}{\partial z} &= V_z \frac{\partial V_z}{\partial z} \left[\alpha_L \left(\frac{2}{V} - \frac{V_z^2}{V^3} \right) - \alpha_T \frac{V_x^2 + V_y^2}{V^3} \right] \\ \frac{\partial D_{zx}}{\partial x} &= (\alpha_L - \alpha_T) \left[\frac{\partial V_x}{\partial x} \frac{V_z}{V} - \frac{V_z V_x^2}{V^3} \frac{\partial V_x}{\partial x} \right] \\ \frac{\partial D_{zy}}{\partial y} &= (\alpha_L - \alpha_T) \left[\frac{\partial V_y}{\partial y} \frac{V_z}{V} - \frac{V_z V_y^2}{V^3} \frac{\partial V_y}{\partial y} \right] \end{aligned} \quad (10.1.6)$$

Because velocity is not derivable at the interface of two adjacent element in a nonuniform flow, computing dispersion coefficient derivatives by using a finite element approach would yield erroneous values [94]. To prevent the errors, a particle is coded to have information of an element index and the velocity estimation is continuous even at the elemental boundaries in this method. Thus,

the derivatives of dispersion coefficients will be computed accordingly. This is an improved approach from the work by [94].

10.2 Transport: Advection and Dispersion

Benchmark name: *Veri1000*.

Purpose: To verify advective dispersive transport, a two-dimensional homogeneous aquifer is chosen to test the proposed RWPT method and the simulated particle distribution is converted to concentration contours.

Model description: The dimension of the model domain is 100 m by 60 m where the uniform velocity field is held constant at 0.5 md^{-1} in the x direction. The hydraulic conductivity is set as $10^{-5} md^{-1}$ and the head gradient of one in the x direction is set by assigning two constant boundary conditions along both left and right sides. The longitudinal and transverse dispersivities are chosen to be isotropic with a length of 0.1 m . This converts to isotropic dispersion coefficients of 0.05 $m^2 d^{-1}$. The initial source load is applied to an area with dimensions of 0.1 m by 0.1 m to have an initial concentration of $C_0 = 1 kgm^{-3}$. Figure 10.2.1 provides a schematic description of the test problem for the two-dimensional homogeneous aquifer. The domain is discretized with quadrilateral elements of 0.5 m by 0.5 m . The same grid density is also used for converting particle distributions to element concentrations.

The stated problem can be solved with an analytical solution provided by [95].

$$C(x, y, t) = \frac{C_0 A}{4\pi t \sqrt{D_{xx} + D_{yy}}} \exp \left[-\frac{(x - x_0)^2}{4D_{xx}t} - \frac{(y - y_0)^2}{4D_{yy}t} \right] \quad (10.2.1)$$

This allows to evaluate the computational accuracy of the proposed method.

Results: The comparison with the analytical solution is provided in Figure 10.2.2. As can be seen, the result of the RWPT method shows good agreement with the analytical solution. The number of particles used for this simulation is 50000. This is significantly less than the number of particles reported by [96], who reported that up to 2.5 million particles were necessary to achieve smoothness of the solution due to oscillations around the contours. As the oscillations observed here for the method proposed are smaller than reported by [96], the proposed method allows to dramatically reduce the number of particles required for a smooth solution by about two orders of magnitude. This shows that the proposed method is both accurate and efficient. In addition, the several numbers of particles used to solve the same problem produces particle clouds as in Fig. 10.2.3. However, the problem for only 1000 particles is used for the purpose of the benchmark test to reduce computation time.

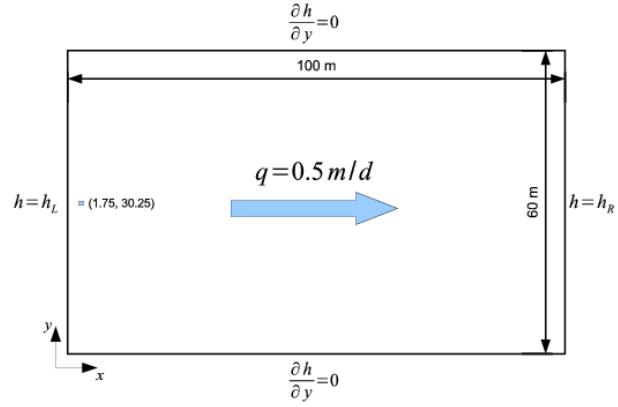


Figure 10.2.1: Schematic description of the two-dimensional aquifer and the boundary conditions of the flow system

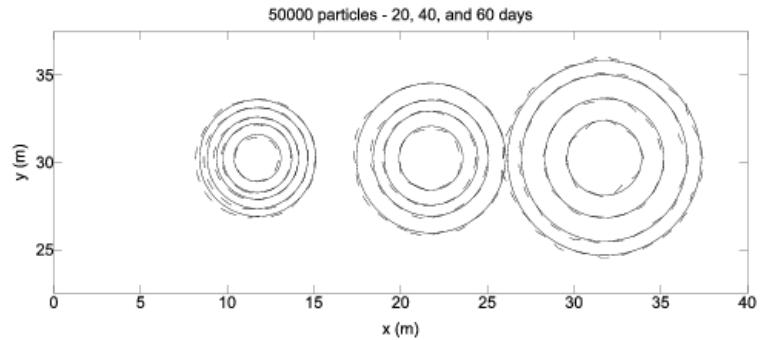


Figure 10.2.2: Transport results of the RWPT method compared with the analytical solution [95] for 50000 particles at 20, 40, and 60 days: The solid line is the analytical solution, the dotted line is the RWPT result. Contour lines are shown for $C = 2.6e^{-4}, 1.6e^{-4}, 1.0e^{-4}, \text{ and } 4e^{-5}$.

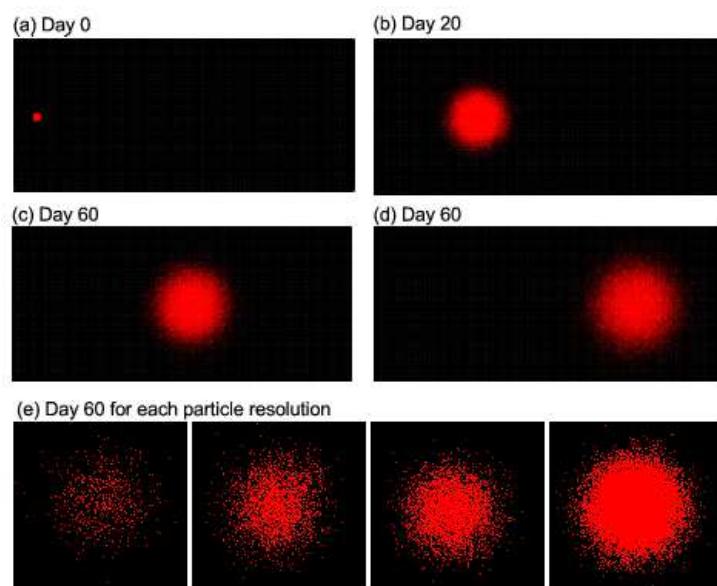


Figure 10.2.3: (a-d)Particle clouds of 50000 particles at 0, 20, 40, and 60 days, (e) Particle clouds of 1000, 5000, 10000, and 50000 at 60 days

Chapter 11

Anisotropy – H or C or HC

11.1 Theory

There are situations where the coordinate directions do not align easily with the directions of anisotropy of the medium. In that case, the governing equation of the flow should be written in the more general form.

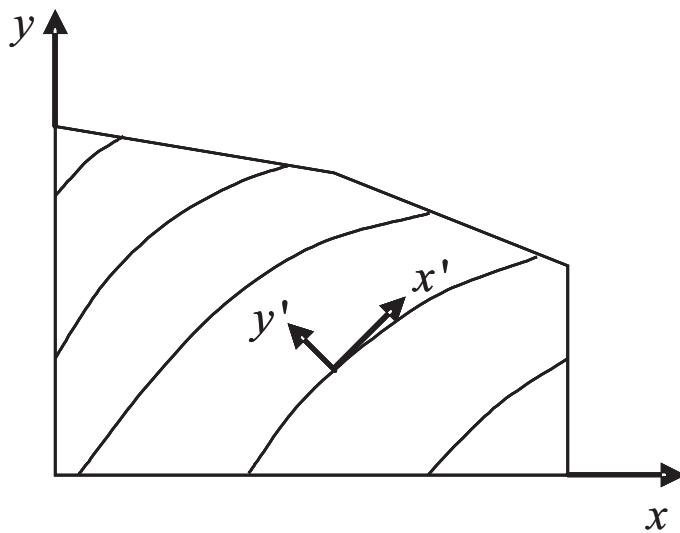


Figure 11.1.1: General anisotropy system

Assumption:

1. The material is isotropic

or

2. The coordinate axes coincide with the principal directions of anisotropy.

For the general case that the coordinate axes do not coincide with the principal directions, the continuity equation is of the form:

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial u}{\partial x_j} \right) = S \frac{\partial u}{\partial t} \quad (11.1.1)$$

where K is the hydraulic conductivity tensor. Equation 11.1.1 can be expanded as to:

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial x} \left(K_{xy} \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left(K_{yx} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial u}{\partial x} \right) = S \frac{\partial u}{\partial t} \quad (11.1.2)$$

For a valid solution of the general case, these terms must be included in the numerical procedure, and in finite differences this would be the only available option. In finite elements, we have a second option, which is to rotate the local coordinate axes into the principal directions of hydraulic conductivity. The second option is computationally more efficient, since the terms in the finite element equation are kept to a minimum. This option is preferred where the principal directions are invariant in time, and where the rotation is easily accomplished, as for example in 2D flow problems. Note that the principal directions can be different for each element. This feature is particularly useful for cross-sectional systems with complex stratification.

The rotation is performed for each element individually. The nodal coordinates on the element are rotated (Figure 11.1.2) according to:

$$\begin{Bmatrix} x' \\ y' \end{Bmatrix} = \begin{bmatrix} \cos \beta & \sin \beta \\ -\sin \beta & \cos \beta \end{bmatrix} \begin{Bmatrix} x \\ y \end{Bmatrix} \quad (11.1.3)$$

where x' , y' are the coordinates of the point x , y in the principal direction coordinate system, and β is the angle between the Cartesian axes and the principal axes. The angle can be different for each element.

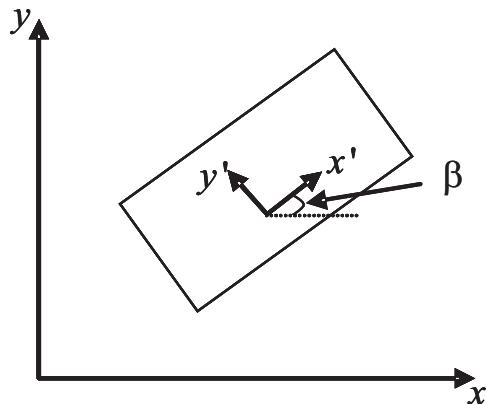


Figure 11.1.2: Rotation of axes

The same theory for anisotropy can be applied to any tensor material properties such as molecular diffusion coefficients.

11.2 Anisotropic permeability for pressure or hydraulic head

Knowing the theoretical background in 9.1, we formulate a simple flow problem to show the difference of three results obtained from isotropic, orthotropic, and anisotropic flow conditions.

Problem definition:

A unit square of the porous medium is created and discretized with triangle elements as in Figure 11.2.1. To generate flow in the model domain, two constant pressure boundary conditions are applied to the top left corner and the bottom right corner. The pressure difference between these two points is set to be unity.

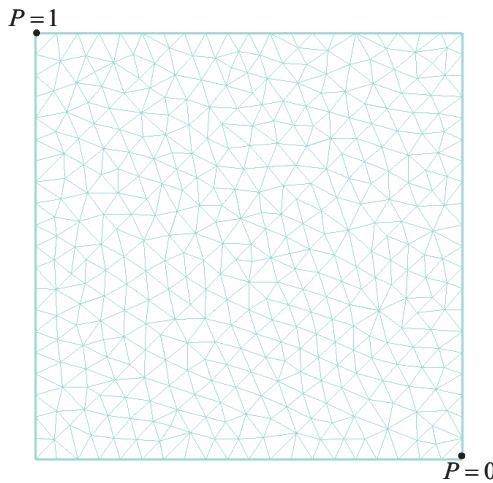


Figure 11.2.1: Boundary conditions and grid

As for material properties for flow system, permeability is set to have isotropic, orthotropic, and anisotropic over the whole model domain and provided in Table 11.2.

Material Types	Permeability(m^2)
Isotropic	$k_{xx} = k_{yy} = 10^{-14}$ and $k_{xy} = k_{yx} = 0$
Orthotropic	$k_{xx} = 10^{-14}$, $k_{yy} = 10^{-15}$, and $k_{xy} = k_{yx} = 0$
Anisotropic	$k_{xx} = 5.5 \times 10^{-15}$, $k_{xy} = 4.5 \times 10^{-15}$, $k_{yx} = 4.5 \times 10^{-15}$, $k_{yy} = 5.5 \times 10^{-15}$

Table 11.2.1: Various flow types set by material properties

Anisotropic ratio is set to be 10 to 1 for the x and y axes respectively for the orthotropic case while the anisotropic case uses the same ratio for the x' and y' axes rotated 45° counter-clock-wise from the x and y axes.

The resulting pressure distributions for the three different flow system are provided in Figure 11.2.2.

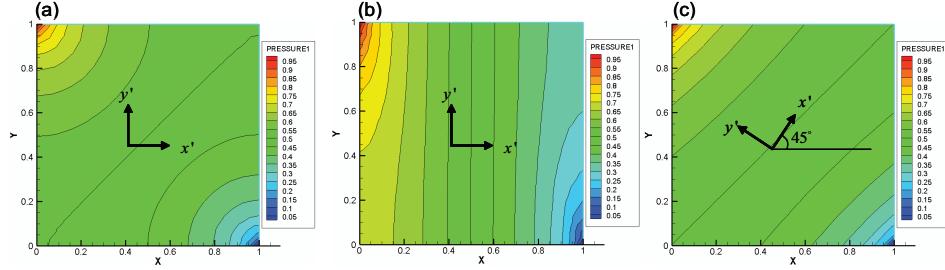


Figure 11.2.2: Pressure distributions for (a) isotropic, (b) orthotropic, and (c) anisotropic permeability

Note that there is no technical difference between the orthotropic and anisotropic cases when full values of permeability tensor are given and set into GeoSys/RockFlow. However, users have two options for orthotropic cases in setting up .mmp files using different keywords such as ORTHOTROPIC and ANISOTROPIC. In the case that diffusion coefficients are treated as tensor via tortuosity, ORTHOTROPIC keyword is no longer valid. Therefore, ANISOTROPIC keyword should be used for Case (b) in anisotropic diffusion via tortuosity.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>soil_layer</i>	Anisotropy	benchmarks\Anisotropy\permeability

11.3 Anisotropic tortuosity for molecular diffusion coefficients

As mentioned previously, the theory is exactly same with permeability. One thing to note before introducing another benchmark problem for anisotropic diffusion is that there is clear distinction between hydrodynamic dispersion and molecular diffusion. Since the hydrodynamic dispersion for mass transport in porous media is mainly a function of velocity and dispersivity, the hydrodynamic dispersion may be influenced more significantly by anisotropic hydraulic conductivity as well as pressure distributions than molecular diffusion. However, the hydrodynamic dispersion has also the molecular diffusion term. In this section, this molecular diffusion is treated as tensor via tortuosity that is a material property for instance clay.

The dispersion tensor can be written as (Bear, 1979)

$$\widehat{D} = \tau D_m \hat{\delta} + \alpha_T |v| \hat{\delta} + (\alpha_L - \alpha_T) \frac{\vec{v}_i \vec{v}_j}{|v|} \quad (11.3.1)$$

where τ is the tortuosity tensor ($-$), D_m is the coefficient of molecular diffusion (L^2T), δ is the Kronecker-delta (unit tensor) ($-$), α_T is the transverse dispersivity (L), v is the characteristic value of macroscopic velocity (LT^{-1}), α_L is the longitudinal dispersivity (L), and, \vec{v}_i and \vec{v}_j are the velocities in i and j directions respectively (LT^{-1}).

Problem definition:

On the unit square of the porous medium created for the previous flow system, as well as one constant concentration boundary condition is applied, a constant line source is introduced to study the difference of component diffusive transport in various types of media. The transport boundary and source condition are depicted in Figure 11.3.1.

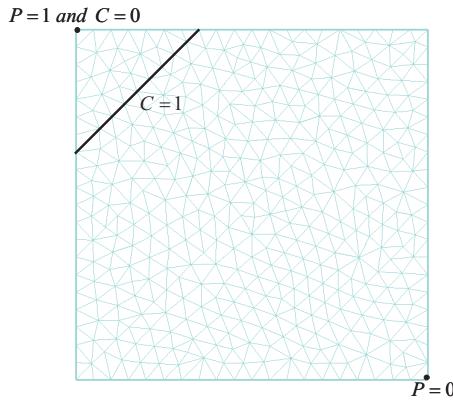


Figure 11.3.1: Boundary conditions and a line source for transport model

As for material properties for molecular diffusive transport, tortuosity is set to have isotropic and anisotropic over the whole model domain and provided in Table 11.3.

Material Types	Tortuosity
Isotropic	$\tau_{xx} = \tau_{yy} = 1$ and $\tau_{xy} = \tau_{yx} = 0$
Anisotropic	$\tau_{xx} = 0.55$, $\tau_{xy} = 0.45$, $\tau_{yx} = 0.45$, $\tau_{yy} = 0.55$: 45° CCW $\tau_{xx} = 0.55$, $\tau_{xy} = -0.45$, $\tau_{yx} = -0.45$, $\tau_{yy} = 0.55$: 135° CCW

Table 11.3.1: Isotropic and anisotropic tortuosity set for the componential molecular diffusive transport

An anisotropic ratio is set to be 10 to 1 for the x' and y' axes rotated 45° counter-clock-wise from the general directions. The equivalent tortuosity expression in the principal directions of anisotropic tortuosity in general coordinate system can be given as

$$\tau' (x', y') = \begin{bmatrix} 1 & 0 \\ 0 & 1.0 \end{bmatrix} \rightarrow \tau (x, y) = \begin{bmatrix} 0.55 & 0.45 \\ 0.45 & 0.55 \end{bmatrix} \quad (11.3.2)$$

The resulting concentration contours for the three different material systems are provided in Figure 11.3.2.

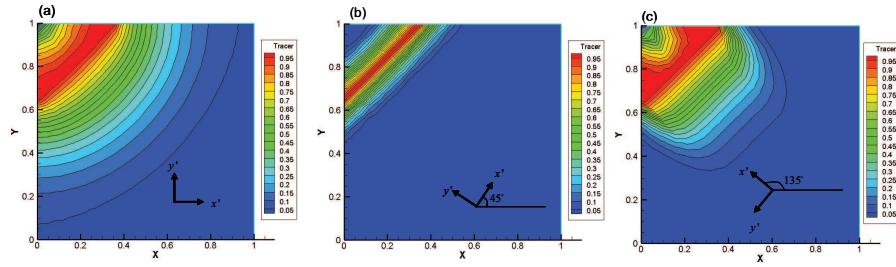


Figure 11.3.2: Concentration contours at $t = 1.0 \times 10^8$ seconds for (a) the isotropic, (b) anisotropic media (45 degrees rotated CCW), and (c) (135 degrees rotated CCW)

Finally, the medium is configured to have one bedding subject to anisotropic diffusive transport and all the rest model domain isotropic as depicted in Figure 11.3.3. The resulting concentration contours for this bedding problem is also provided in Figure 11.3.3.

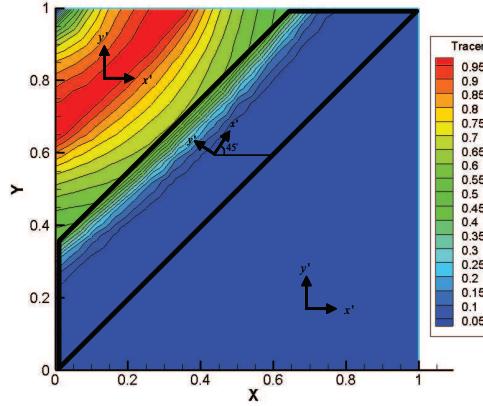


Figure 11.3.3: Concentration contours at $t = 1.0 \times 10^8$ seconds for the porous medium with an anisotropic bedding

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>soil_layer</i>	Anisotropy	benchmarks\Anisotropy\moleculardiffusion

11.4 Converting an angle of orientation to tensor

Currently, a universal function for converting an arbitrary angle to tensor is not written yet. In obtaining full tensor values from orthotropic tensor in the global coordinates, the direction of rotation and the magnitude of the angle should be handled carefully. The direction of rotation is counter-clock-wise and the reference tensor should be an identity matrix. Then, the converting function can be written such that

$$K = T^t K' T \quad (11.4.1)$$

Note that one anisotropic material rotated 180 degrees CCW becomes exactly same anisotropic material. This is obvious from Equation 11.4.1, because 180 degrees produce exactly same matrix K .

To clarify the conversion, one example is prepared and explained in Figure 11.4.1. Suppose that an anisotropic medium has the ratio of 10 (i.e., $10x' = y'$, to satisfy this ratio, we can make countless tensors. Thus, we set $\begin{bmatrix} 1 & 0 \\ 0 & 0.1 \end{bmatrix}$ for conversion). Note that we talk about anisotropy in principle coordinates thus the coordinate system is single quotation marked. Now we can arbitrarily select rotation angles. Figure 11.4.1 shows some geometrically meaningful angles together with transformed matrix of Equation 11.4.1.

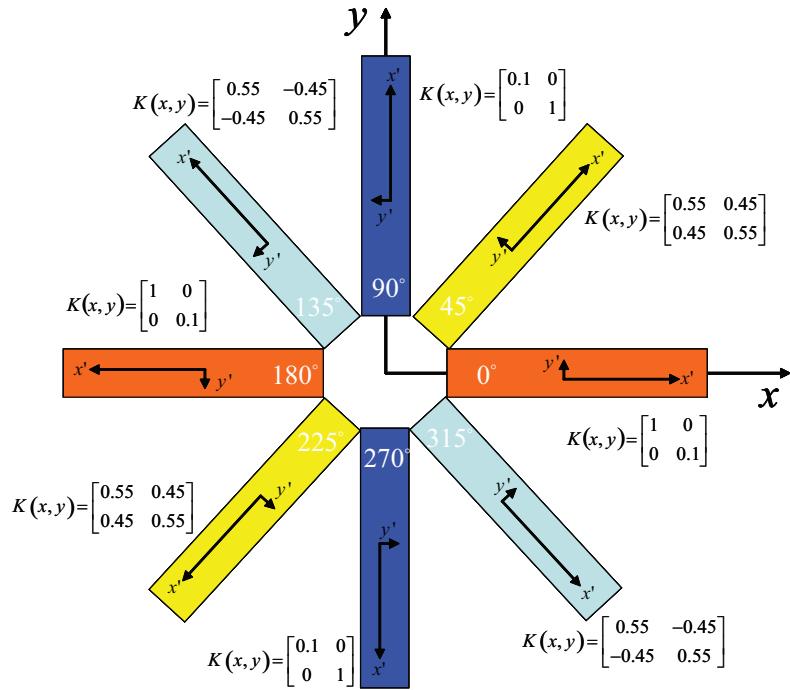


Figure 11.4.1: Transformed tensors referenced from $[1, 0][0, 1]$ in the principle coordinates

In extension to the second rank tensors in other words three dimensions, this direction of the rotation, the magnitude of the two angles, and the rotating axes should carefully be defined when the angles are used to compute the corresponding tensors internally. The transform matrix for three dimensions rotated along the y axis with α degrees CCW and the x axis with β degrees CCW can be written as

$$T = \begin{bmatrix} \cos \alpha & \sin \alpha \sin \beta & -\cos \alpha \sin \beta \\ 0 & \cos \beta & \sin \beta \\ \sin \alpha & -\cos \alpha \sin \beta & \cos \alpha \cos \beta \end{bmatrix} \quad (11.4.2)$$

Since the determinant of T is unity, we can use Equation 11.4.1 to compute full tensor values. This universal converting function will be provided in the future. Until then, full values of tensor should be used in GeoSys/RockFlow for simulating anisotropic problems.

Coupled Processes

Chapter 12

Surface/Subsurface flow coupling – H-Proceses

This chapter deals with the coupling of rivers and overland flow with the variably saturated zone and aquifers.

12.1 Theory

For the coupling of flow processes on separate but adjacent domains exchange fluxes are calculated at common interfaces. The exchange fluxes between overland and variably saturated flow read

$$q_{of}^{sf} = k_{a'} \Lambda (h^{of} - h^{sf}), \quad \Lambda = \frac{K^c}{a'}, \quad q_{sf}^{of} = -q_{of}^{sf} \quad (12.1.1)$$

where h^{of} is the overland flow water head, h^{sf} the matric head in the variably saturated zone, Λ is the leakance, a' the interface thickness, and the scaling factor $0 \leq k_{a'} \leq 1$, given by

$$k_{a'} = S^{2(1-S)} \quad (12.1.2)$$

$$S = \min \left(\max \left(\frac{H}{a'}, 0 \right), 1 \right), \quad (12.1.3)$$

where H is the surface flow water depth, ensures that infiltration does not exceed the available water on the surface. For the coupling conductivity K^c the saturated soil hydraulic conductivity is taken.

The exchange fluxes between overland and groundwater flow read

$$q_{of}^{gf} = \Lambda (h^{of} - h^{gf}), \quad q_{gf}^{of} = -q_{of}^{gf} \quad (12.1.4)$$

where h^{gf} is the groundwater flow head. The exchange fluxes between river and groundwater flow read

$$q_{of}^{gf} = \frac{P}{B} \Lambda (h^{of} - h^{sf}), \quad q_{gf}^{of} = -q_{of}^{gf} \quad (12.1.5)$$

where P is the wetted perimeter and B the channel width. For a channel with rectangular cross section $P = 2H_a + B$. Is the groundwater level below the river bed the exchange fluxes become

$$q_{of}^{gf} = \Lambda H, \quad q_{gf}^{of} = -q_{of}^{gf} \quad (12.1.6)$$

Figure 12.1.1: Exchange fluxes between (a) overland and variably saturated flow q_{of}^{sf} , (b) river and aquifer flow q_{of}^{gf} , calculated with an interface (conductivity K^c) between the surface flow compartment (friction coefficient C_r) and variably zone/aquifer compartment (conductivity K).

12.2 Benchmarks examples

12.2.1 Horton flow

Problem definition

This example is based on the experiments by Smith and Woolhiser, 1971 [64] for initially drained conditions. Infiltration excess overland (Hortonian) flow was generated by 15 minutes of artificial precipitation at a rate of 4.2 mm min^{-1} on a soil flume with a length of 12.2 m, a width of 5.1 cm, and a slope of 0.01. The experimental setup is shown in Figure 12.2.1 with the discretization meshes used in the simulations. Both overland and variably saturated flow are simulated one dimensionally with line elements.

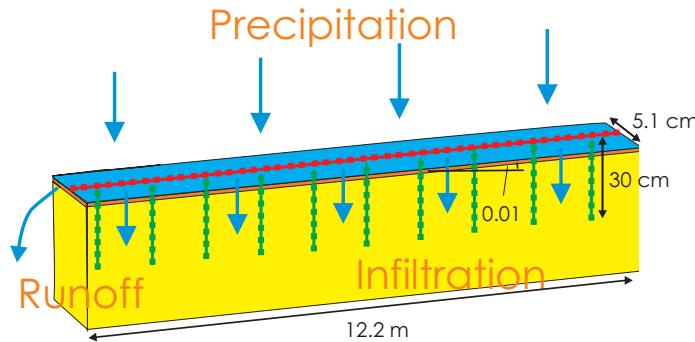


Figure 12.2.1: Setup and discretization meshes in the Smith and Woolhiser, 1971 [64] benchmark example.

Items	Symbol	Setting	Unit
Fluid			
Kinematic viscosity	ν	177	$\text{mm}^2 \text{min}^{-1}$
Density	ρ	0.756	g mm^{-3}
Overland flow			
Surface friction	C	80000	$\text{mm}^{-1} \text{min}^{-1}$
	j	1	—
	l	2	—
Unsaturated flow			
Porosity	ϕ	0.42	—
Residual saturation	S_r	0.05	—
Hydraulic conductivity	K	1.7	mm min^{-1}
Pore size	α	0.006	mm^{-1}
Grain size distribution	m	0.75	—
Interface			
Conductivity	K^c	1.7	mm min^{-1}
Thickness	a'	1	mm
Immobile depth	a	1	mm

Table 12.2.1: Hydraulic parameters in the simulations of the laboratory experiment by Smith and Woolhiser, 1971 [64].

Initial and boundary conditions

The overland flow compartment is initially dry ($H = 1 \times 10^{-6} \text{ m}$) and initial soil saturation is 0.2 uniformly. A critical depth boundary condition assigned at the overland flow outlet. At the residual boundaries no-flow is assigned

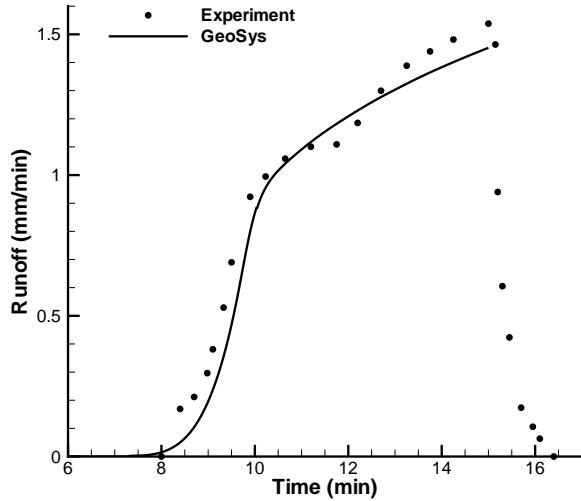


Figure 12.2.2: Simulated and measured outflow hydrographs in the Smith and Woolhiser, 1971 [64] benchmark example.

Material properties

A uniform soil representation is chosen. Light oil was used as a fluid. Surface friction is described by the laminar Chézy resistance to flow relationship. The soil-water-characteristic curves by VanGenuchten are used. Parameters are given in Table 12.2.2. Wool_little_lines_coup describes overland flow and soil flow one-dimensionally with line elements. Wool_little_hex_coup uses quadrants for overland flow which continue to three-dimensional soil flow hexahedra. Time steps are 2s. The material and fluid properties used for the simulations are given in Tab. 12.2.2. Soil heterogeneity is neglected and the fluid parameters correspond to light oil. Surface friction is described by the laminar Chézy resistance to flow relationship. The soil-water-characteristic curves by VanGenuchten are used for the Richards soil flow description.

Results

Runoff at the free-fall outlet is taken for comparison of experimental and simulation data (Figure 12.2.2). Time steps are 1 second. Line element sized for overland flow are $\Delta x = 12.2$ cm and for flow in the variably saturated zone $\Delta x = 1$ mm.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>Wool_lines_coup</i>	H	benchmarks\COUPLED_FLOW\

12.2.2 Dunne flow

Problem definition

This example is based on the experiments by Abdul and Gilham, 1984 [97] which were designed to examine the role of capillary fringe on runoff generation processes. Precipitation was applied for 20 min on a soil flume with a length of 1.4 m, a width of 8 cm, and a slope of 0.12 (Figure 12.2.3). The initial groundwater level is set at the height of the outlet such that immediately overland flow occurs. In the simulations the flume part above the initial groundwater level is simulated with Richards equation and below with Darcy groundwater equation.

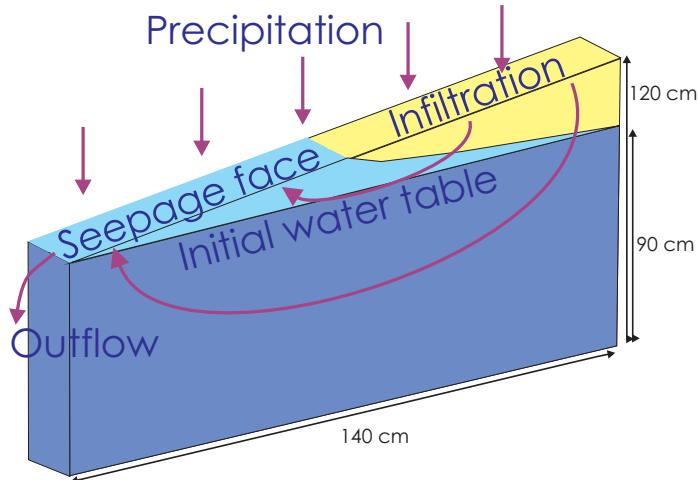


Figure 12.2.3: Setup of the Abdul and Gilham, 1984 [97] benchmark example.

Items	Symbol	Setting	Unit
Overland flow			
Surface friction	C	5.39	$\text{m}^{1/3}\text{s}^{-1}$
Immobile depth	a	0.5	mm
Variably saturated flow			
Porosity	ϕ	0.34	–
Residual saturation	S_r	0.0	–
Hydraulic conductivity	K	5×10^{-5}	m s^{-1}
Pore size	α	2.4	m^{-1}
Grain size distribution	m	0.8	–
Groundwater flow			
Porosity	ϕ	0.34	–
Specific storage	S	0.0	–
Overland/soil Interface			
Conductivity	K^c	5×10^{-5}	m s^{-1}
Thickness	a'	0.5	mm
Soil/aquifer Interface			
Leakance	Λ	5×10^{-4}	s^{-1}

Table 12.2.2: Hydraulic parameters in the simulations of the laboratory experiment by Abdul and Gilham, 1984 [97].

Initial and boundary conditions

Material properties

Results

Measured and simulated outflow are compared in Fig. 12.2.4.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>abdul_lab</i>	H	benchmarks\COUPLED_FLOW\

12.2.3 Aquifer recharge from channel

Problem definition

This example deals with a confined aquifer with inflow by a rectangular channel (Figure 12.2.5). An analytical solution is given by Glover, 1978 [37].

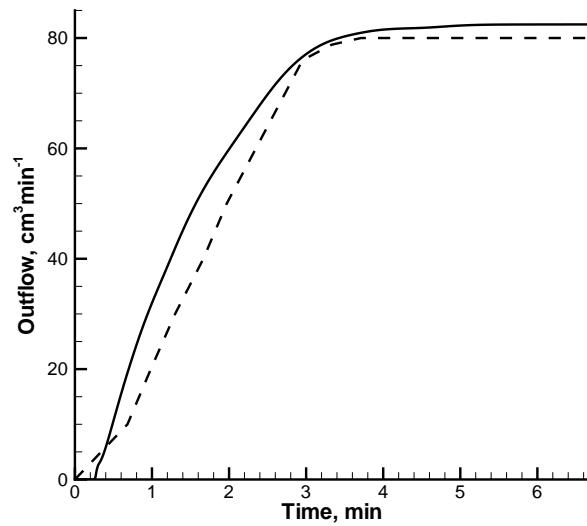


Figure 12.2.4: Simulated and measured outflow hydrographs in the Abdul and Gilham, 1984 [97] benchmark example.

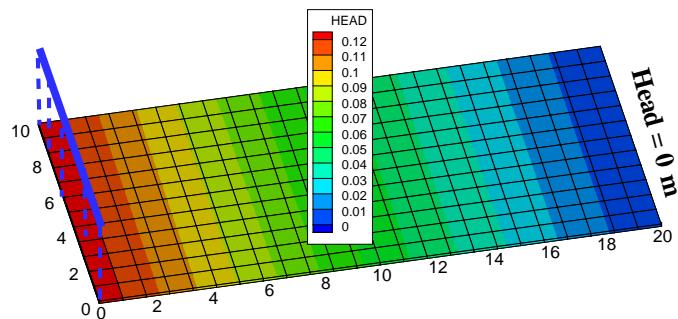


Figure 12.2.5: Setup of the Glover, 1978 [37] benchmark example.

Initial and boundary conditions

Channel initial and boundary conditions are 3m for water depth. Initial ground-water head is 0m. The head at the boundary opposite of the channel is 0. At

the remaining boundaries no-flow is imposed.

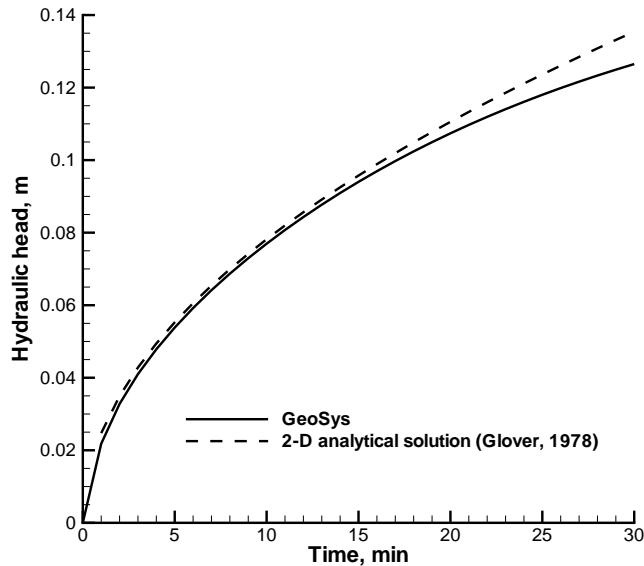


Figure 12.2.6: Comparison of Simulated groundwater depths below the river bed with the analytical solution by Glover, 1978 [37].

Material properties

The domain is discretized with 24×12 quadrants and the time step size is 60s. Simulation parameters are given in Tab. 12.2.4.

Table 12.2.3: Parameters for aquifer recharge example

Parameter	Symbol	Setting	Unit
Friction coefficient	C	333	ms
Corresponding Manning coefficient	n	3×10^{-3}	1/ms
Channel width	B	14	m
Leakance	3.33×10^{-6}	1/s	
Rill depth/ Interface layer thickness	a	0	m
Surface structure parameter	ϵ	0	m
Specific yield	S_y	0.2	1/m
Permeability	k	1×10^{-3}	m^2
Aquifer thickness	L	25	m

Results

Comparison of simulation results and analytical solution is shown in Fig. 12.2.6.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>riv1_quad_coup</i>	H	benchmarks\COUPLED_FLOW\

12.2.4 Flood at channel junction

Problem definition

Two uniform rectangular channels confluence symmetrically and form a larger rectangular channel which continues uniformly. The aquifer is unconfined, flat, homogeneous, and has a size of $10000m \times 4000m$ (Figure 12.2.7). A flood waves starts propagating at both upstream inlets and merge at the junction. Manning's roughness coefficient is constant throughout as well as the slope of about 0.0001. The total time is 5 days and comprises a part of the rising limb of the flood. Two scenarios are considered by varying the aquifer initial conditions such that flow occurs from the channels to the aquifer or vice versa. The total time is 30 days and comprises the rising and falling limb of the flood. These examples were proposed by [98]. Benchmarking is based on code comparison.

Initial and boundary conditions

Initial water depth in the rivers is $4.5m$ and the aquifer is set at $z = 0$. The initial head for the aquifer is $h = 32$ m for scenario I and $h = 35$ m for scenario II. At the aquifer boundaries constant head and no-flow conditions are imposed (Figure 12.2.7). At the river inlets the inflow rises linearly from $100m^3/s$ to $350m^3/s$ between $t = 3$ and $t = 10$ days and declines again linearly to the initial value between $t = 11$ and $t = 17$ days. At the channel outlet a normal depth boundary condition is assigned.

Material properties

The simulation parameters for the channels and aquifer are given in Tab. 12.2.4.

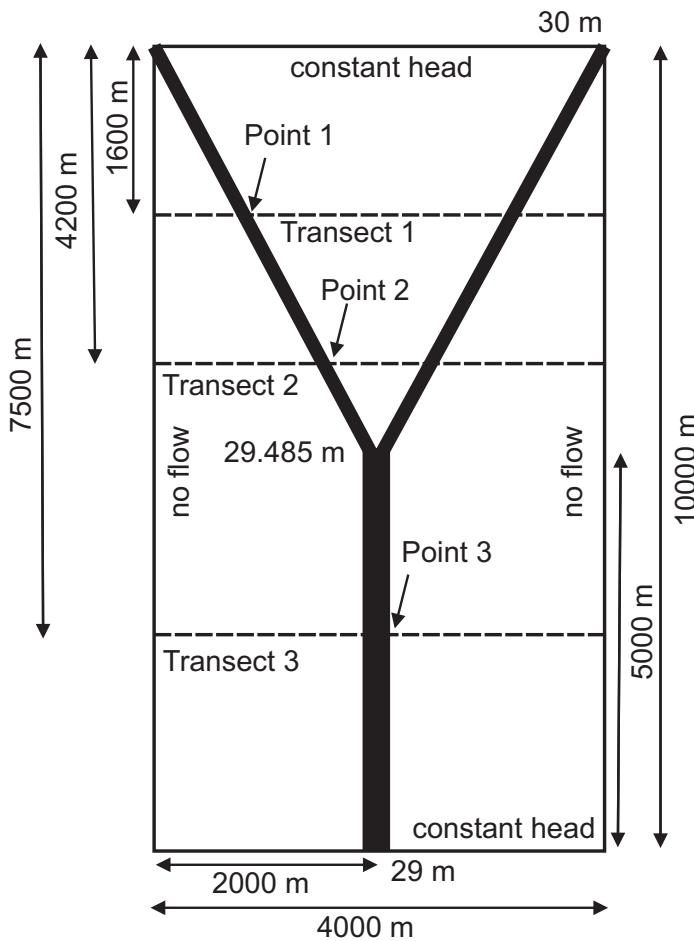


Figure 12.2.7: Setup of the Gunduz and Aral, 2005 [98] benchmark example.

Table 12.2.4: Parameters for channel junction examples

Items	Symbol	Setting	Unit
Friction coefficient	C	40	ms
Corresponding Manning coefficient	n	0.025	$1/ms$
Width of upstream channels	B	30	m
Width of downstream channel	B	45	m
Leakance	Λ	3.33×10^{-6}	$1/s$
Rill depth/ Interface layer thickness	a	0	m
Surface structure parameter	ϵ	0	m
Specific yield	S_y	0.2	$1/m$
Permeability	k	1×10^{-9}	m^2

Results

Figs. 12.2.8-12.2.11 show groundwater heads and river stages at Points 1-3 and groundwater heads at transect I for both scenario I and II.

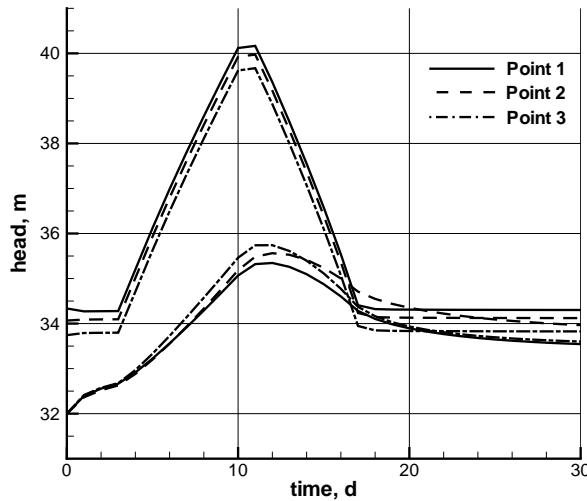


Figure 12.2.8: Groundwater heads and river stages of the Gunduz and Aral, 2005 [98] benchmark example for scenario I.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>biFork1_coup</i>	H	benchmarks\COUPLED_FLOW\
<i>biFork2_coup</i>	H	benchmarks\COUPLED_FLOW\

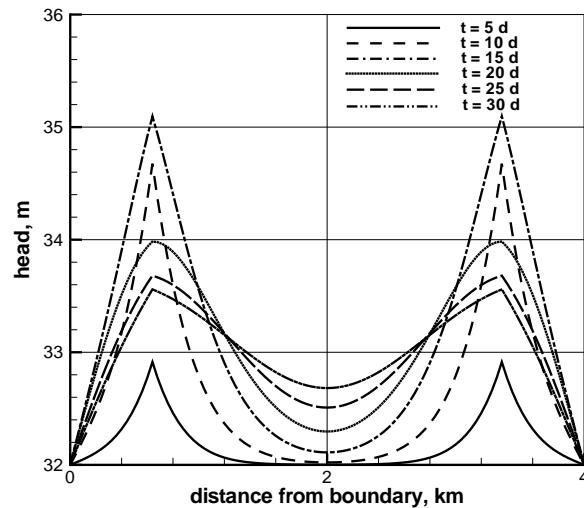


Figure 12.2.9: Groundwater heads at transect I of the Gunduz and Aral, 2005 [98] benchmark example for scenario I.

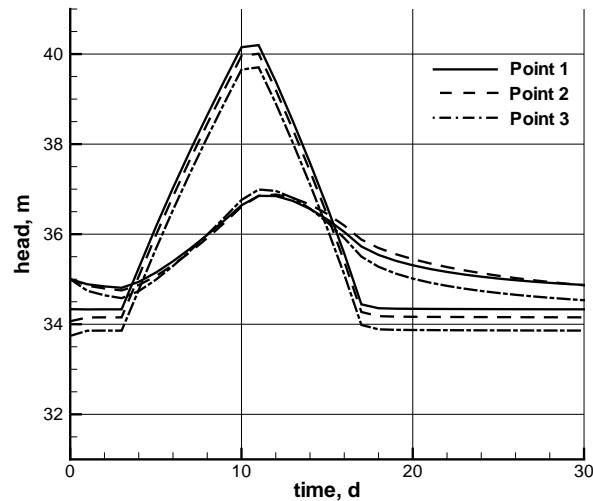


Figure 12.2.10: Groundwater heads and river stages of the Gunduz and Aral, 2005 [98] benchmark example for scenario II.

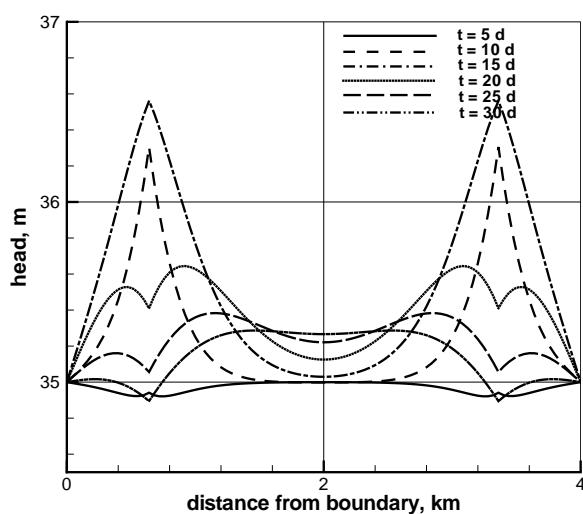


Figure 12.2.11: Groundwater heads at transect I of the Gunduz and Aral, 2005 [98] benchmark example for scenario II.

Chapter 13

Consolidation – H^nM -Processes

13.1 Theory

We consider flow of an incompressible fluid (liquid) in a deforming porous medium. The system consists of two phases (liquid and solid phase). The unknown field functions are liquid pressure p and solid displacement \mathbf{u} . For the determination of the unknown field functions we combine the mass balance equations and the momentum balance equation of fluid and solid phases ([99], [100]).

The deformation process is modelled by the system

$$\nabla \cdot (\boldsymbol{\sigma} - p\mathbf{I}) + \rho\mathbf{g} = \mathbf{0} \text{ in } \Omega , \quad (13.1.1)$$

$$\boldsymbol{\sigma} - \mathbf{C}\boldsymbol{\varepsilon}(\mathbf{u}) = \mathbf{0} \text{ in } \Omega , \quad (13.1.2)$$

where $\boldsymbol{\sigma}$ denotes the effective stress, and the momentum balance equation is modified such that it incorporates stresses and forces connected to the fluid pressure. Here, \mathbf{I} denotes the identity, \mathbf{g} denotes the gravity vector and \mathbf{C} is the elasticity tensor representing the dependence of strain and stress for a linear elastic material law.

Fluid flow in deformable porous media is described by the following mass and momentum balance equations,

$$\nabla \cdot \mathbf{w} + \nabla \cdot \frac{\partial \mathbf{u}}{\partial t} = 0 \text{ in } \Omega , \quad (13.1.3)$$

$$\mathbf{w} + \frac{\mathbf{k}}{\mu} (\nabla p - \rho\mathbf{g}) = \mathbf{0} \text{ in } \Omega . \quad (13.1.4)$$

In consolidation theory, the fluid mass balance equation (13.1.3) has an extra term due to the deformation process. The second equation (13.1.4) is denoted as the Darcy law. Here, \mathbf{w} denotes the volumetric flux of the fluid and p the liquid phase pressure. \mathbf{k} denotes the permeability tensor, μ is the liquid viscosity, and ρ is the density of the porous medium. Hereby we assume solid grains itself are incompressible, i.e. $d^s \rho / d^s t = 0$

After applying Galerkin finite element approach to eqns . (13.1.1) and (13.1.3) build a set of coupled linear equations to be solved for the primary variables liquid pressure p and solid deformation \mathbf{u} of the p/\mathbf{u} formulation of the consolidation problem. The resulting equation system can be compactly written in following form

$$\begin{bmatrix} \mathbf{K}_{pp}^* & \frac{1}{\Delta t} \mathbf{C}_u^* \\ \mathbf{K}_{up}^* & \mathbf{K}_{uu}^* \end{bmatrix} \begin{bmatrix} \hat{\mathbf{p}}^{i+1} \\ \hat{\mathbf{u}}^{i+1} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_p^* + \frac{1}{\Delta t} \mathbf{C}_u^* \hat{\mathbf{u}}^i \\ \mathbf{f}_u^* \end{bmatrix} \quad (13.1.5)$$

The above algebraic equation system (13.1.5) for determination of the primary variables of the p/\mathbf{u} formulation, i.e. nodal pressures and displacements.

13.2 Saturated consolidation

Equation system (13.1.5) is solved with a one-step monolithic algorithm. Moreover, the Newton-Raphson method is adopted to deal with the nonlinearity.

13.2.1 Poro-elastic column (1D)

Problem definition

The example is a simple one dimensional problem for which an analytical formula for its solution is known. We consider a porous column bounded by rigid and impermeable walls, except on its top where a mechanical pressure load σ_0 is prescribed and which is free to drain. Suppose that the length of the column is H . The boundary and initial conditions for the problem are depicted in Figure 13.2.1: The analytical solution for this problem can be found in [101] as

$$\begin{aligned} \sigma_D &= -1 + \sum_{n=0}^{\infty} \frac{2}{M} \sin(M x_D) e^{-M^2 t_D} \\ u_D &= 1 - x_D - \sum_{n=0}^{\infty} \frac{2}{M} \cos(M x_D) e^{-M^2 t_D} \\ p_D &= \sum_{n=0}^{\infty} \frac{2}{M} \sin(M x_D) e^{-M^2 t_D} \end{aligned} \quad (13.2.1)$$

where $x_D = x/H$, $t_D = (\lambda + 2\mu)kt/\eta H^2$, $M = 1/2\pi(2n+1)$ are non-dimensional quantities and $\sigma_D = \sigma/p_0$, $u_D = u(\lambda + 2\mu)/p_0 H$, $p_D = p/p_0$ are dimensionless effective stress, displacement and pore pressure, respectively.

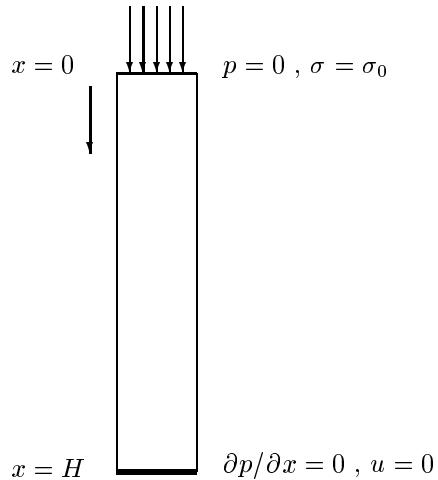


Figure 13.2.1: Column test problem

Material properties

The material parameters used in the computation are given in Table 13.2.1. The load put on the strip is -10^3 Pa , time step size is $\Delta t = 1.0 \text{ s}$ and the total simulation time is $t = 10 \text{ s}$.

Parameter	Unit	Value
Young's modulus	3×10^4	N/m^2
Poisson's ratio	0.2	–
Permeability	10^{-10}	m^2
Fluid viscosity	10^{-3}	Pa s

Table 13.2.1: Material parameters

Results

Time step size is proposed as 1s. Comparison of the results for fluid pressure and effective stress obtained by the LS-MFEM, GFEM and the analytical solution are shown in Figure 13.2.2

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
hm_tri	HM	benchmarks\HM\

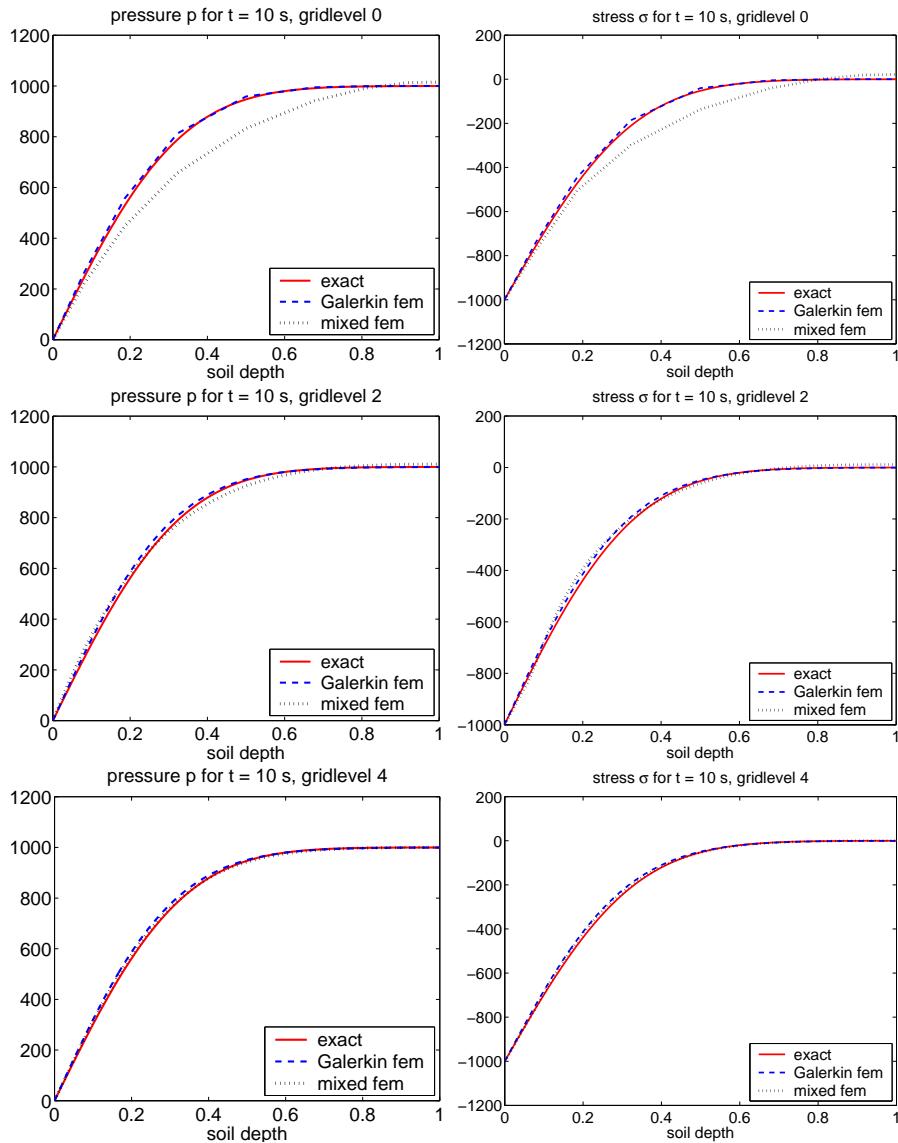


Figure 13.2.2: Simulated fluid pressures (left) and effective stress (right) at time $t=10\text{ s}$ by grids from the coarsest to finest one

13.2.2 Poro-elastic cube (3D)

Problem definition

We consider a vertical cross-section through a homogeneous soil. Due to symmetry we can limit the investigation to half of the domain. The model domain

is then extending 8 meters in length and 5 meters in height. The problem is solved in 2D and 3D space, respectively.

Initial and Boundary conditions

Boundary conditions are: strip loading ($\sigma_{yy} = \sigma_0$ in $x \in [0, 1]$), zero stresses ($\sigma_{yy} = \sigma_{xy} = 0$ in $x \in (1, 8]$) and zero pressure at the top; no horizontal flux, no horizontal displacements and zero shear stresses at left and right hand sides; no vertical flux and no displacements at bottom (Figure 13.2.3).

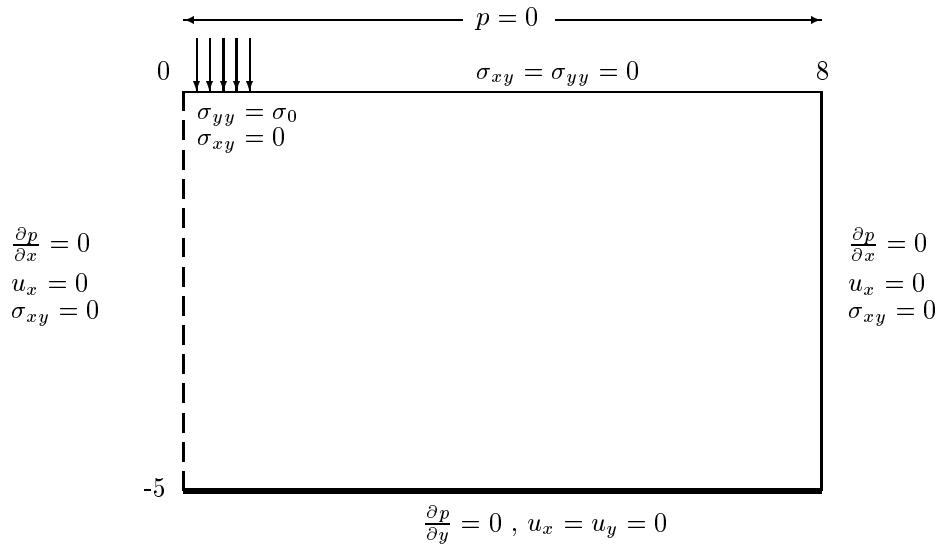


Figure 13.2.3: Footing problem

Material properties

The material properties of the porous medium for this case are given in Table 13.2.2.

Table 13.2.2: Material properties

Property	Value	Unit
Young's modulus	3×10^4	N/m ²
Poisson's ratio	0.2, 0.4	–
Permeability	10^{-10}	m ²
Fluid viscosity	10^{-3}	Pas

Results

The geometry is to expand the 2D domain by extruding the 2D shape of 1m in off-plane direction (13.2.4). Results at the critical step, i.e., the first step, are

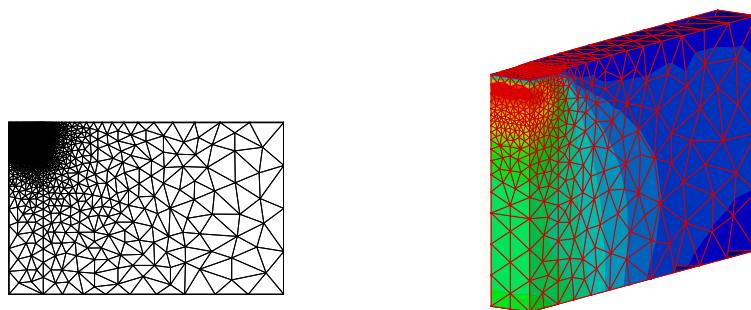


Figure 13.2.4: Analyzed models

shown in Fig. 13.2.5, 13.2.7 and 13.2.6

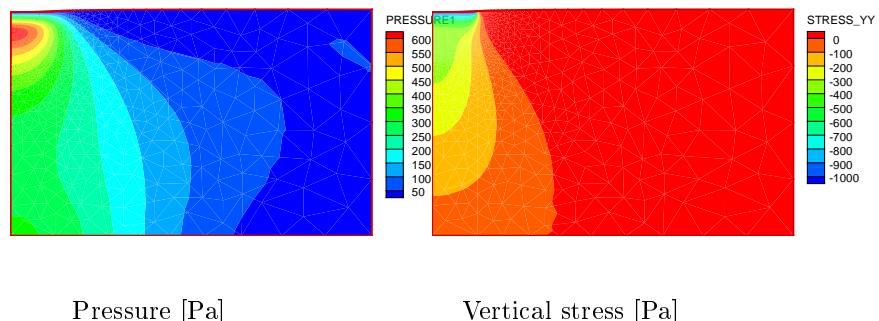


Figure 13.2.5: 2D: distribution

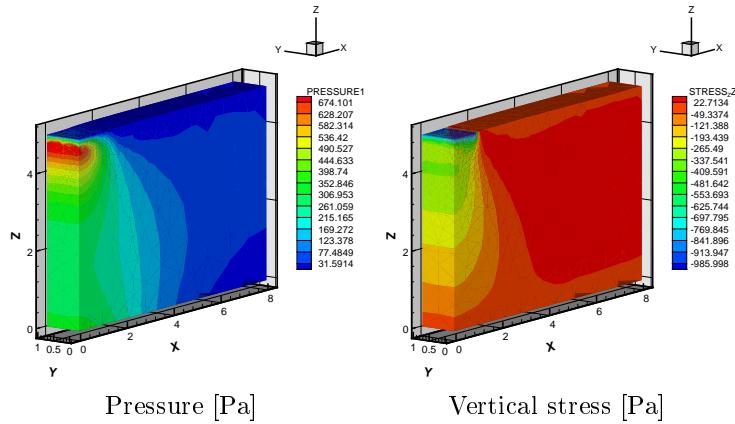


Figure 13.2.6: 3D: distribution

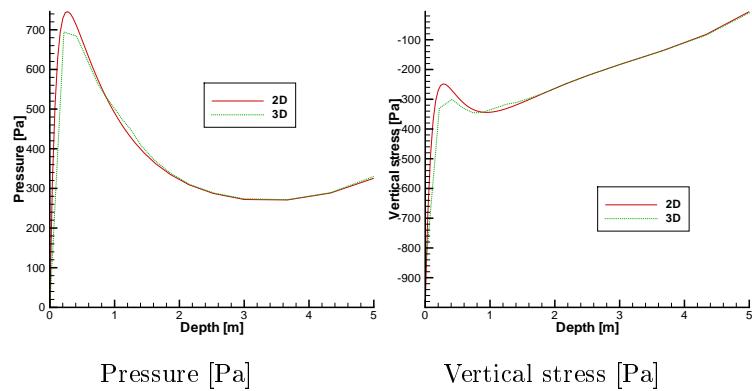


Figure 13.2.7: Comparison along symmetrical axis

The results produced by 2D model with triangle element and 3D model with tetrahedral element matches each other. This shows that all objects presented in this study work fine for TH coupling problem.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>hm_foot_tri& hm_foot_tet</i>	HM	benchmarks\HM\

13.2.3 Plastic consolidation

Problem definition

A quarter of the cylindrical sample of 5cm in diameter and 10cm in length under constant pressure. We assume that the plastic behavior the sample material can be represented by the Cam-Clay model and the problem is axisymmetrical.

Initial and Boundary conditions

The initial void ratio $e_0 = 1.5$ at such initial stress state

$$\sigma_r^0 = \sigma_\theta^0 = \sigma_z^0 = 50\text{kPa}$$

The top of sample is compressed down to 5cm. While the radial stress kept constant of 50kPa, i.e., the traction boundary condition at cylindrical surface must be zero. Both uncoupled and coupled cases are analyzed. For the coupled case, drainage is assigned on the bottom of the sample. The two case should give the same results. The displacement load is applied in 50 increments.

Material properties

Table 13.2.3 shows the material parameters.

Property	Value	Unit
Poisson's ratio	0.3	—
Slope of the critical line, M	1.2	—
Virgin compression index, λ	0.2	—
Swelling/recompression index κ	0.02	—
Initial pre-consolidation pressure	60	kPa
Permeability	10^{-11}	m^2
Fluid viscosity	10^{-3}	Pas

Table 13.2.3: Material properties

Results

The evolution of the deviatoric stress along with the axial strain are demonstrated in Fig. 13.2.8. Both uncoupled (see Section 8.3.3) and coupled cases give the same result as expected[79].

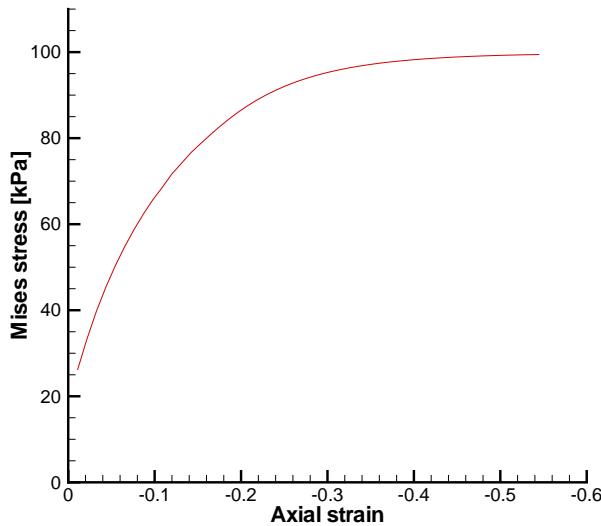


Figure 13.2.8: Mises stress vs axial strain: Cam-Clay consolidation

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>hm_cc_tri-s</i>	HM	benchmarks\HM\

13.2.4 Dynamic consolidation

Problem definition

This example is used just to demonstrate that the global assembly of matrices and vectors, the time stepping of dynamic problems are dealt with correctly. The example described below is modified from the footing example given in Section 13.2.2.

Initial and Boundary conditions

All stresses and pressure are zero at the beginning of deformation. Strip loading ($\sigma_{yy} = \sigma_0$ in $x \in [0, 1]$), zero stresses ($\sigma_{yy} = \sigma_{xy} = 0$ in $x \in (1, 8]$) and zero pressure at the top; no horizontal flux, no horizontal displacements and zero shear stresses at left and right hand sides; no vertical flux and no displacements at bottom (Figure 13.2.3).

Material properties

Material parameters are given in Table 13.2.4.

Property	Value	Unit
Young's modulus	3×10^4	N/m^2
Poisson's ratio	0.2, 0.4	—
Permeability	10^{-10}	m^2
Fluid viscosity	10^{-3}	$Pa\ s$

Table 13.2.4: Material properties of dynamic consolidation problem

Results

Constant time step size of 10s with time damping parameters:

$$\beta_1 = 0.51, \beta_2 = 0.515, \bar{\beta} = 0.51$$

Time duration is ten time steps.

The following figures, Fig. 13.2.9–13.2.12 show the distribution of state variables within the domain after 10 time steps. Such distribution is similar to the static case illustrated in Fig. 13.2.5.

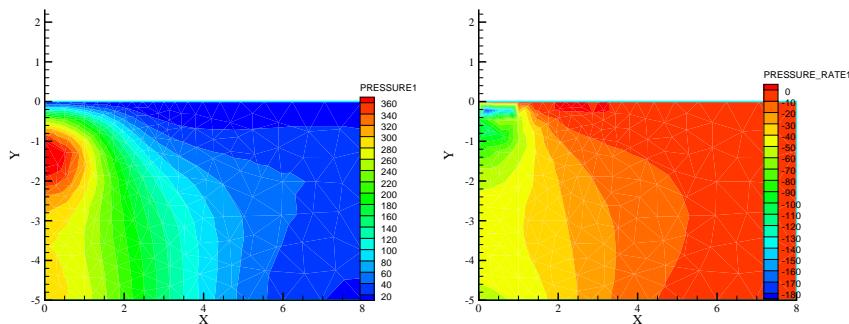


Figure 13.2.9: Fluid pressures p and rate of fluid pressure \dot{p}

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>hm-dyn-tri</i>	HM	benchmarks\HM\

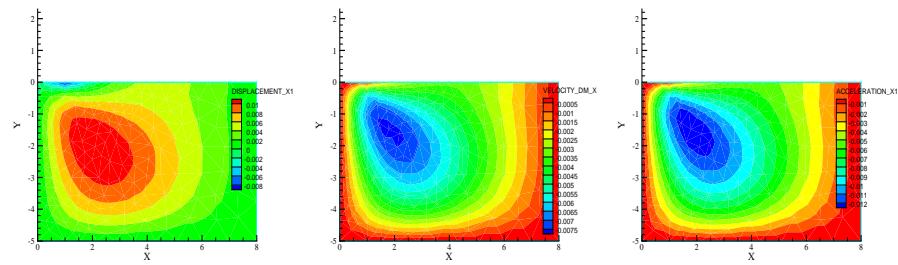


Figure 13.2.10: Displacement, its rate and acceleration: horizontal component

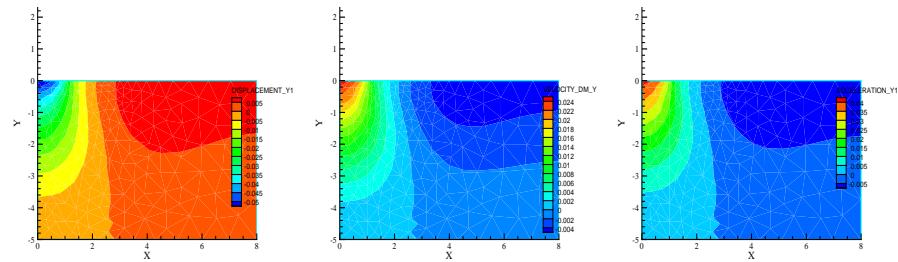


Figure 13.2.11: Displacement, its rate and acceleration: vertical component

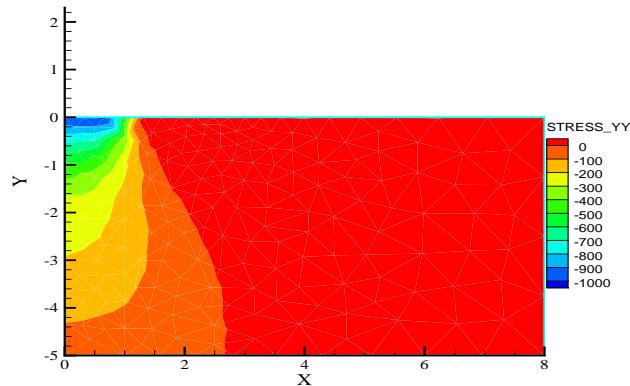


Figure 13.2.12: Vertical stress

13.3 Unsaturated consolidation

13.3.1 Theory

Fluid mass balance

The general fluid mass balance equation for unsaturated flow in a deformable porous medium is

$$\begin{aligned} nS^l \dot{\rho}^l + n\rho^l \dot{S}^l + nS^l \rho^l \mathbf{v}^{ls} + S^l \rho^l \nabla \cdot \mathbf{v}^s + S^l \rho^l \frac{1-n}{\rho^s} \dot{\rho}^s = \\ Q_\rho^l + S^l \frac{\rho^l}{\rho^s} Q_\rho^s \end{aligned} \quad (13.3.1)$$

Hereby, the basic assumption of Richards type models is that the gaseous phase is immobile, i.e. $\mathbf{v}^g = 0$. Assuming grain incompressibility for isothermal conditions (i.e. $\dot{\rho}^s = 0$) and no solid sources (e.g. resulting from chemical reactions) as well as applying the constitutive equations for fluid compressibility, capillary pressure, and Darcy flux, we obtain the following Richards equation for an unsaturated deformable porous medium.

$$nS^l \rho_0^l \beta_p \dot{p}^l - n\rho^l \frac{dS^l}{dp_c} \dot{p}^l - \nabla \left(\frac{k_{rel}^l \mathbf{k}}{\mu^l} (\nabla p^l - \rho \mathbf{g}) \right) + S^l \rho^l \nabla \cdot \dot{\mathbf{u}}^s = Q_\rho^l \quad (13.3.2)$$

Rearrangement with respect to the primary variables p^l, \mathbf{u}^s yields

$$\begin{aligned} \left(-n\rho^l \frac{dS^l}{dp_c} + nS^l \rho_0^l \beta_p \right) \dot{p}^l - \nabla \left(\frac{k_{rel}^l \mathbf{k}}{\mu^l} \nabla p^l \right) + S^l \rho^l \nabla \cdot \dot{\mathbf{u}}^s = \\ Q_\rho^l + \nabla \left(\frac{k_{rel}^l \mathbf{k}}{\mu^l} \rho \mathbf{g} \right) \end{aligned} \quad (13.3.3)$$

A constitutive equation, the water content function obtained by experiments, characterizes the relationship between p^l and S^l and therefore the derivative dS^l/dp_c .

Momentum balance

The deformation process is described by the momentum balance equation for the unsaturated porous medium in terms of stresses.

$$\nabla \cdot (\boldsymbol{\sigma} - \alpha_b S^l p^l \mathbf{I}) + \rho \mathbf{g} = \mathbf{0} \quad (13.3.4)$$

All symbols are denoted in chapter ??.

Numerical scheme

The standard Galerkin finite element approach is applied for the numerical solution of the PDEs (13.3.3) and (13.3.4) resulting into the following system of algebraic equations.

$$\underbrace{\begin{bmatrix} \mathbf{C}_{pp} & \mathbf{C}_{pu} \\ \mathbf{C}_{up} & \mathbf{C}_{uu} \end{bmatrix}}_{\mathbf{C}} \frac{d}{dt} \underbrace{\begin{Bmatrix} \hat{\mathbf{p}}^l \\ \hat{\mathbf{u}}^s \end{Bmatrix}}_{\mathbf{x}} + \underbrace{\begin{bmatrix} \mathbf{K}_{pp} & \mathbf{K}_{pu} \\ \mathbf{K}_{up} & \mathbf{K}_{uu} \end{bmatrix}}_{\mathbf{K}} \begin{Bmatrix} \hat{\mathbf{p}}^l \\ \hat{\mathbf{u}}^s \end{Bmatrix} = \underbrace{\begin{Bmatrix} \mathbf{r}_p \\ \mathbf{r}_u \end{Bmatrix}}_{\mathbf{r}} \quad (13.3.5)$$

where $\mathbf{C}_{up}, \mathbf{C}_{uu}, \mathbf{K}_{pu}$ are zero.

$$\begin{bmatrix} \mathbf{C}_{pp} & \mathbf{C}_{pu} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \frac{d}{dt} \begin{Bmatrix} \hat{\mathbf{p}}^l \\ \hat{\mathbf{u}}^s \end{Bmatrix} + \begin{bmatrix} \mathbf{K}_{pp} & \mathbf{0} \\ \mathbf{K}_{up} & \mathbf{K}_{uu} \end{bmatrix} \begin{Bmatrix} \hat{\mathbf{p}}^l \\ \hat{\mathbf{u}}^s \end{Bmatrix} = \begin{Bmatrix} \mathbf{r}_p \\ \mathbf{r}_u \end{Bmatrix} \quad (13.3.6)$$

Time discretization with explicit finite differences yields

$$\begin{aligned} & \left(\frac{1}{\Delta t} \mathbf{C}_{pp} + \theta \mathbf{K}_{pp} \right) \hat{\mathbf{p}}^l_{n+1} + \frac{1}{\Delta t} \mathbf{C}_{pu} \hat{\mathbf{u}}^s_{n+1} \\ &= \left(\frac{1}{\Delta t} \mathbf{C}_{pp} + (1 - \theta) \mathbf{K}_{pp} \right) \hat{\mathbf{p}}^l_n + \frac{1}{\Delta t} \mathbf{C}_{pu} \hat{\mathbf{u}}^s_n + \mathbf{r}_p \end{aligned} \quad (13.3.7)$$

$$\begin{aligned} & \theta \mathbf{K}_{up} \hat{\mathbf{p}}^l_{n+1} + \theta \mathbf{K}_{uu} \hat{\mathbf{u}}^s_{n+1} \\ &= (1 - \theta) \mathbf{K}_{up} \hat{\mathbf{p}}^l_{n+1} + (1 - \theta) \mathbf{K}_{pp} \hat{\mathbf{u}}^s_{n+1} + \mathbf{r}_u \end{aligned} \quad (13.3.8)$$

with following finite element matrices

$$\begin{aligned} \mathbf{C}_{pp}^e &= \int_{\Omega^e} \mathbf{N}_p^T \left[-n\rho^l \frac{dS^l}{dp_c} + nS^l \rho_0^l \beta_p \right] \mathbf{N}_p d\Omega^e \\ \mathbf{K}_{pp}^e &= \int_{\Omega^e} \nabla \mathbf{N}_p^T \left[-\frac{k_{rel}^l \mathbf{k}}{\mu^l} \right] \nabla \mathbf{N}_p d\Omega^e \\ \mathbf{C}_{pu}^e &= \int_{\Omega^e} \mathbf{N}_p^T [S^l \rho^l] \nabla \mathbf{N}_u d\Omega^e \\ \mathbf{r}_p^e &= \int_{\Omega^e} [Q_\rho^l] \mathbf{N}_p d\Omega^e + \int_{\Omega^e} \mathbf{N}_p^T \left[\frac{k_{rel}^l \mathbf{k}}{\mu^l} \rho^l \mathbf{g} \right] \nabla \mathbf{N}_p d\Omega^e \end{aligned} \quad (13.3.9)$$

$$\begin{aligned}
 \mathbf{K}_{up}^e &= \int_{\Omega^e} \mathbb{B}^T [\alpha_b S^l] \mathbf{m} \mathbf{N}_p d\Omega^e \\
 \mathbf{K}_{uu}^e &= \int_{\Omega^e} \mathbb{B}^T [\mathbb{C}] \mathbb{B} d\Omega^e \\
 \mathbf{r}_u^e &= \int_{\Omega^e} \mathbf{N}_u [\rho \mathbf{g}] d\Omega^e
 \end{aligned} \tag{13.3.10}$$

where \mathbf{m} is a mapping vector as

$$\mathbf{m} = [1 \ 1 \ 1 \ 0]^T$$

for plane strain problems and

$$\mathbf{m} = [1 \ 1 \ 1 \ 0 \ 0 \ 0]^T$$

for 3D problems

13.3.2 Liakopoulos Experiment

Problem definition

The first example is a drainage test based on an experiment by Liakopoulos (1965). Desaturation takes place due to gravitational effects. This example was studied previously by several authors, e.g. Liakopoulos (1965), Narasimhan & Witherspoon (1978), Zienkiewicz et al. (1990), Schrefler & Zhan (1993). Therefore, this example is well suited as benchmark, moreover, because of the lack of any analytical solutions for this type of coupled, non-linear problems. In this test example, multiphase flow in a deforming porous medium is studied. At first we employ the Richards approximation, i.e. air remains at atmospheric pressure.

The physical experiment of Liakopoulos was conducted in a column packed with so-called Del Monte sand. Moisture content and tension at several points along the column were measured with tensiometers (Fig. 13.3.1, Fig. 13.3.2).

In the simulation, the column is assumed has size of $0.1m \times 1m$ and discretized into 20 quadrilateral elements (Fig. 13.3.3).

Initial and boundary conditions

Based on the experiment, we assume that the initial pressure is zero everywhere in the domain. Boundary conditions for both fluid and displacement fields is depicted in Fig. 13.3.3. Such initial boundary conditions imply that the sample in fully saturated at the beginning, the water is allowed to flow out from the bottom boundary.

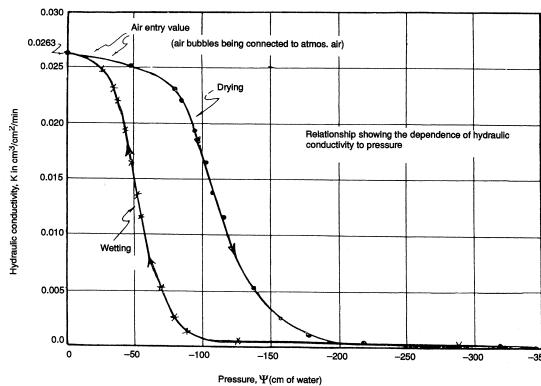


Figure 13.3.1: Hydraulic conductivity vs pressure, with $K = k\rho g / \mu$ and $\Psi = p / \rho g$ (Liakopoulos 1965)

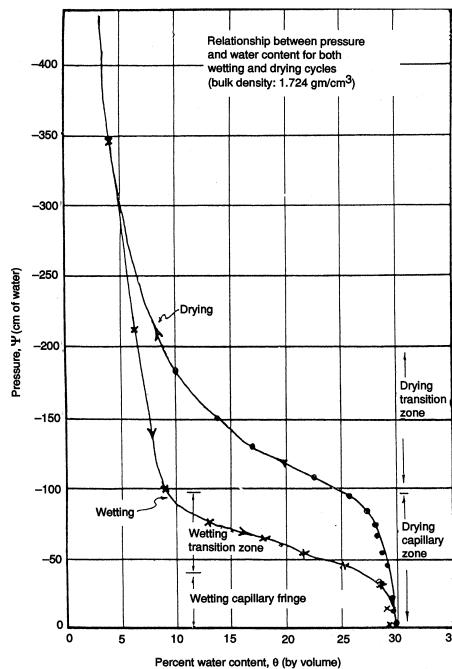


Figure 13.3.2: Hydraulic head vs water content, with $\Psi = p / \rho g$ and $\theta = nS$ (Liakopoulos 1965)

Material properties

The capillary pressure $p_c(S)$

$$p_c = \left(\frac{1-S}{1.9722} \times 10^{11} \right)^{\frac{1}{2.4279}} \quad (13.3.11)$$

$$\partial p / \partial \mathbf{n} = 0, \sigma_{yy} = 0, \sigma_{xy} = 0$$

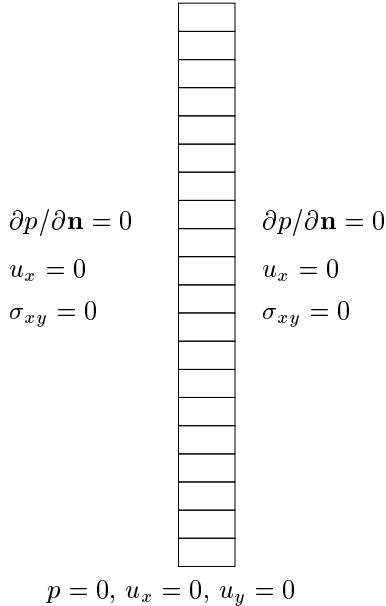


Figure 13.3.3: Boundary conditions

as well as the relative permeability relationships $k_{\text{rel}}(S)$

$$k_{\text{rel}} = 1 - 2.207(1 - S)^{1.0121} \quad (13.3.12)$$

fit the measured data for saturations larger than 0.84. The physical parameter are given in the table below.

Property	Value	Unit
Young's modulus, E	MPa	1.3
Poisson's ratio, ν	–	0.4
Solid grain density, ρ^s	kgm^{-3}	2000
Liquid density, ρ^l	kgm^{-3}	kgm^{-3}
Porosity, n	–	0.2975
Permeability, k	m^2	4.5×10^{-13}
Water viscosity, μ	Pas	10^{-3}
Gravity, g	ms^{-2}	9.806
capillary pressure $p_c(S)$	Pa	eqn. (13.3.11)
Relative permeability, $k_{\text{rel}}(S)$	–	eqn. (13.3.12)

Table 13.3.1: Material parameters

Results

We conduct two kinds of simulation such as: one is taking account of the gravity force as a load for displacement field, while the other ignore the the gravity force.

For the case of non-gravity force, Fig. 13.3.4 shows history profile of water pressure p , water saturation S , vertical solid displacement u_y and vertical stress σ_{yy} . Results of p , water saturation S , vertical solid displacement u_y agree with

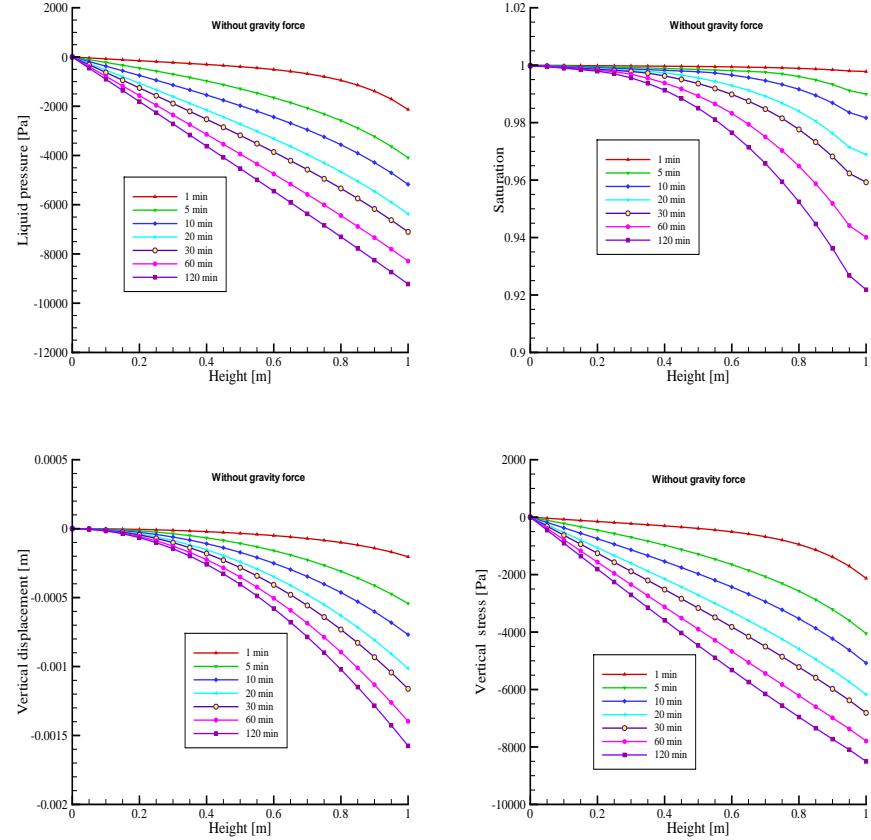


Figure 13.3.4: Simulated results (without gravity force), p , S , u_y , σ_{yy}

what given in [102] (see pages 167-172).

The vertical profile of results obtained by taking account of the gravity force are shown in Fig. 13.3.5. If compare the saturation result with that obtained by ignoring the gravity fore, one can easily find the desaturated procedure is enhanced apparently. This highlights the impact of displacement to water pressure

and the coupling effects.

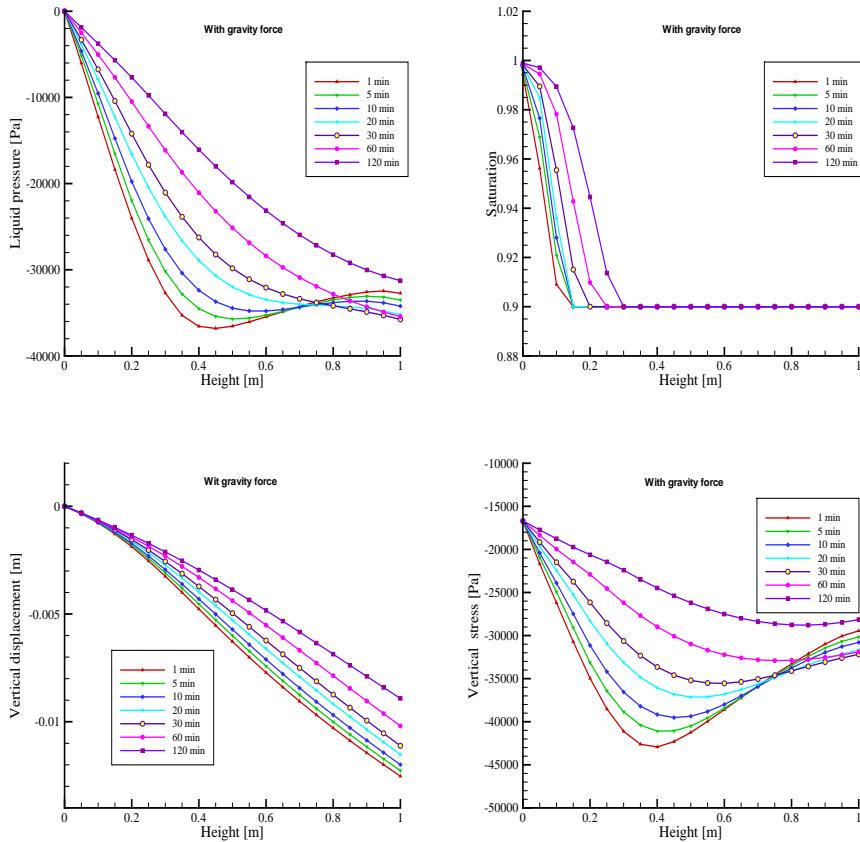


Figure 13.3.5: Simulated results (with gravity force), p , S , u_y , σ_{yy}

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>hm-unsat</i>	HM	benchmarksHM

13.3.3 DECOVALEX HM test case

DECOVALEX is an international code comparison project for the verification of thermo-hydro-mechanical (THM) and thermo-hydro-chemical (THC) numerical simulators [103] (see also sec. 17.2).

Definition

The original DECOVALEX-THM benchmark definition is a 2-D problem [103] (Fig. 13.3.6). For the comparison of different HM swelling models, we consider a simplified case representing a horizontal cross-section through the 2-D domain (Fig. 13.3.6, BME1H).

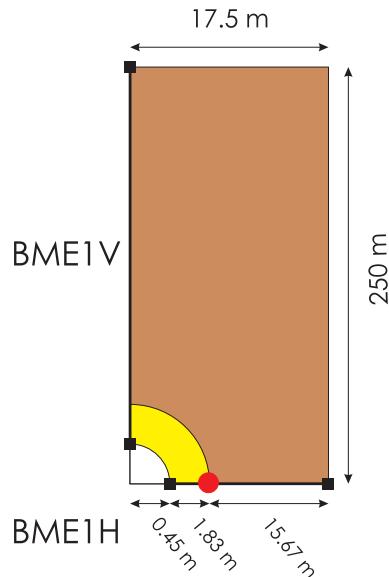


Figure 13.3.6: 2-D DECOVALEX THM definition and simplification for the benchmark exercise BME1H

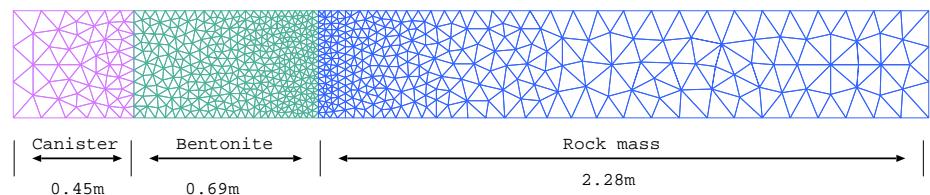


Figure 13.3.7: Mesh of the simplified BME1H model including canister, bentonite, and rock mass sections

The simplified model takes a rectangle shape. The mesh of the domain together with material types are shown in Fig. 13.3.7.

Fig. 13.3.8 illustrates the definition of initial and boundary conditions for the horizontal cross-section BME1H. Observation points are set at $x = 0.45\text{ m}$, $x = 1.10\text{ m}$ to record temporal breakthrough curves.

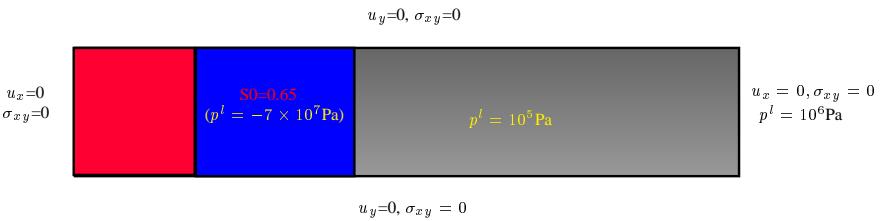


Figure 13.3.8: Simplified horizontal cross-section model

The material parameters for rock mass and bentonite are given in Table 13.3.2 and 13.3.3, respectively.

Parameter	Unit	Value
Density	kg/m^3	2700
Young's modulus	GPa	35
Poisson ratio	-	0.3
Porosity	-	0.01
Saturated permeability	m^2	1.0×10^{-17}

Table 13.3.2: Rock Mass

Parameter	Unit	Value
Density	kg/m^3	1600
Young's modulus	MPa	317
Poisson ratio	-	0.35
Saturated permeability	m^2	2.0×10^{-21}

Table 13.3.3: Bentonite

The dependency of capillary pressure as well as relative permeability on liquid saturation for both of rock and bentonite are depicted in Fig. 13.3.9.

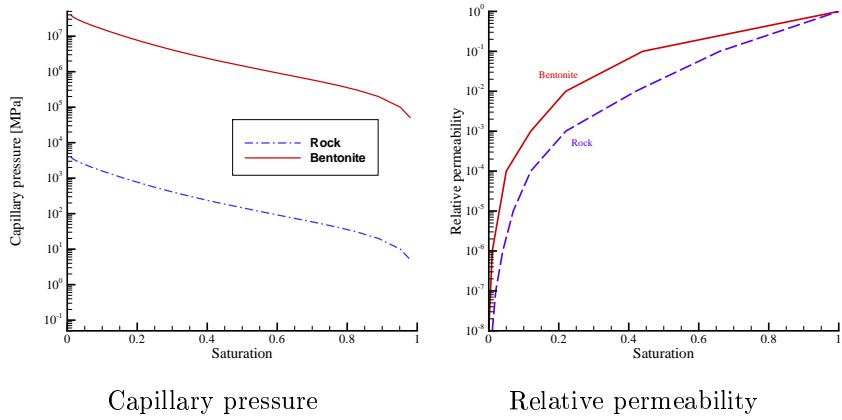


Figure 13.3.9: Capillary pressure - relative permeability - functions

Results

Fig. 13.3.10 displays a contour plot of saturation and vertical swelling stress in the domain. Apparently, the swelling stress in the bentonite is induced by change of water saturation.

Fig. 13.3.11 shows the simulated horizontal profiles (top) and temporal evolutions at observation point (bottom) of water saturation and swelling stress based on the linear swelling model (13.4.4) proposed by Rutqvist (2005) [104].

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>hm_swelling</i>	HM	HM/LinearSwelling

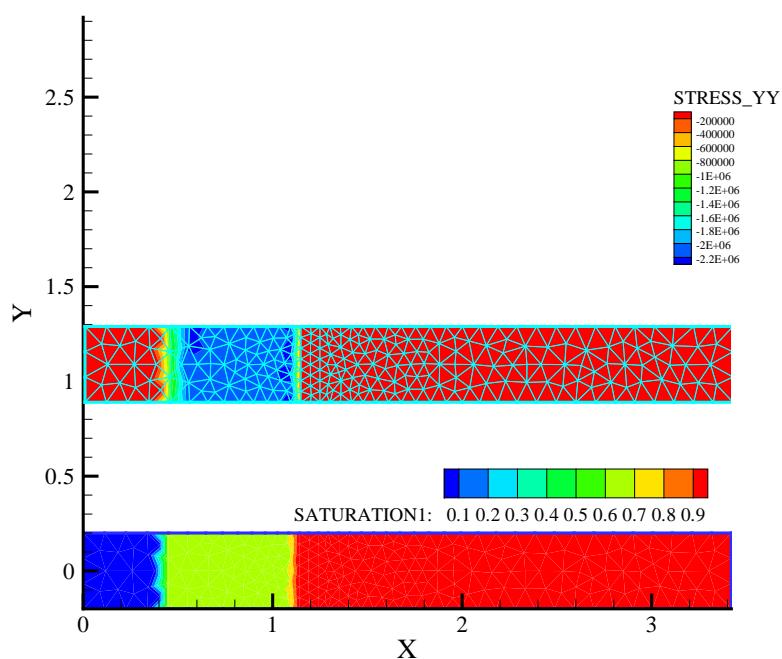


Figure 13.3.10: Distribution of saturation and vertical swelling stress

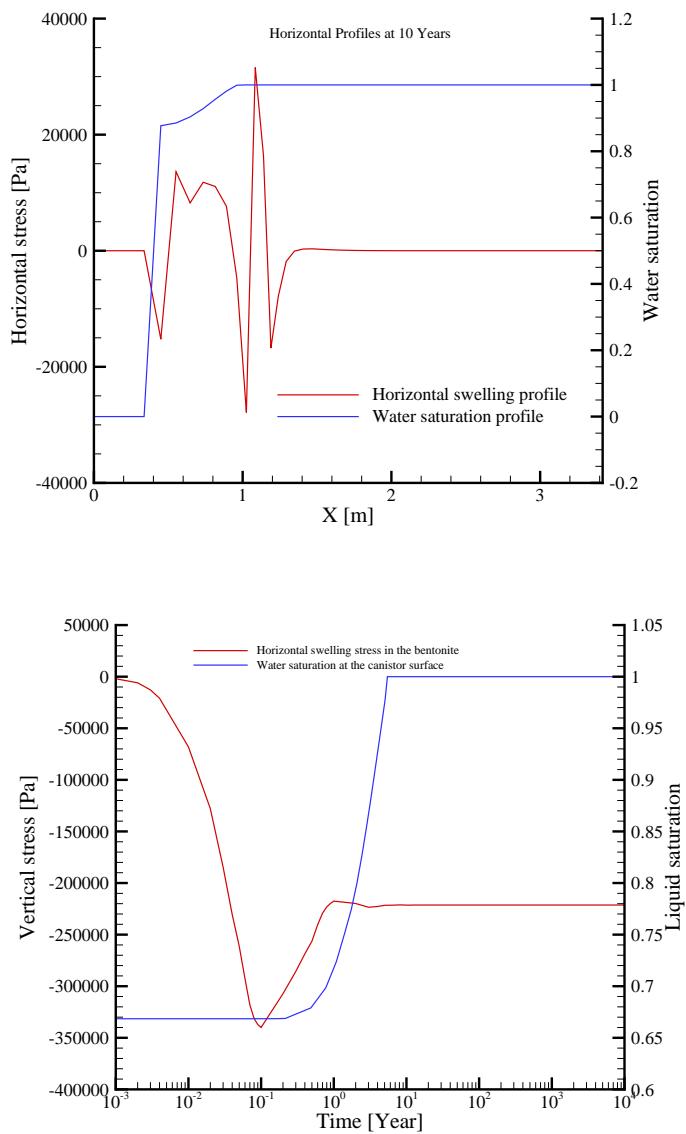


Figure 13.3.11: Horizontal profile (top) and temporal evolution at observation point (bottom) of water saturation and swelling stress

13.4 Two-phase flow consolidation - H²M Process

13.4.1 Theory

Balance equations

The fluid mass balance equations for two-phase flow in a deformable porous medium (H²M process) using capillary pressure p_c and gas pressure p^g as primary variables (pp model) is

$$n\rho^l \frac{\partial S^l}{\partial p_c} \dot{p}_c + \rho^l S^l \nabla \cdot \dot{\mathbf{u}} + \nabla \cdot \left[\rho^l \frac{\mathbf{k}k_{rel}^l}{\mu^l} (-\nabla p^g + \nabla p_c + \rho^l \mathbf{g}) \right] = Q^l \quad (13.4.1)$$

$$\begin{aligned} -n\rho^g \frac{\partial S^l}{\partial p_c} \dot{p}_c + n(1 - S^l) \left(\frac{\partial \rho^g}{\partial p^g} \dot{p}^g + \frac{\partial \rho^g}{\partial p_c} \dot{p}_c \right) + [\rho^l S^l + \rho^g (1 - S^l)] \nabla \cdot \dot{\mathbf{u}} \\ + \nabla \cdot \left[\rho^g \frac{\mathbf{k}k_{rel}^g}{\mu^g} (-\nabla p^g + \rho^g \mathbf{g}) \right] = Q^g \end{aligned} \quad (13.4.2)$$

momentum balance in terms of stress equilibrium

$$\nabla \cdot (\sigma - \alpha_b (S^g p^g + S^l p^l) + \rho g) \quad (13.4.3)$$

Swelling models

A simple model was proposed by Rutqvist (2005) [104], which defines the increment of swelling stress being proportional to the liquid (water) saturation increment

$$\Delta\sigma^{sw} = \alpha \Delta S^l \Delta\sigma^{sw} = \alpha (\Delta S^l)^2 \quad (13.4.4)$$

example in sec. 15

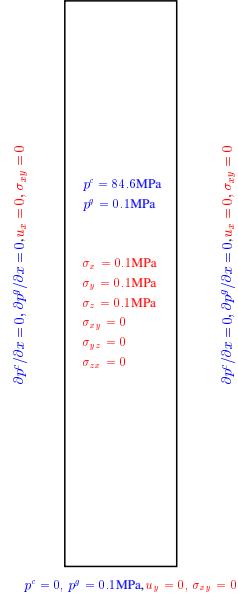
TEP model, for more details see [105], example in sec. 13.4.2

13.4.2 TEP test case

Definition

Fig. 13.4.1 shows the axi-symmetric model domain for the confined swelling test as well as the initial and boundary conditions for the two-phase flow consolidation problem.

$$\partial p^c / \partial y = 0, p^g = 0.1 \text{ MPa}, u_y = 0, \sigma_{xy} = 0$$



$$p^c = 0, p^g = 0.1 \text{ MPa}, u_y = 0, \sigma_{xy} = 0$$

Figure 13.4.1: Model set-up with initial and boundary conditions

The hydraulic and fluid properties are given in Table 13.4.1.

Meaning	Value	Unit
Liquid density, ρ^l	1000	kg/m^3
Liquid viscosity, μ^l	10^{-3}	$Pa\ s$
Gas density, ρ^g	Clapeyron equation (D7)	kg/m^3
Gas viscosity, , μ^g	1.8×10^{-5}	$Pa\ s$
Intrinsic permeability	0.6×10^{-20}	m^2
Porosity	0.4	m^3/m^3
Media properties for liquid:		
Relative permeability:	Power law $k_{rel}^l = S_e^3$	
Residual saturation	0	—
Maximum saturation	1	—
Water retention:	van Genuchten	
Exponential index, m	0.42	—
Air entry pressure, p_0	62	MPa
Relative permeability of gas, k_{rel}^g	$5.103 \times 10^{-12} [e(1 - S^l)]^{4.3}$	e , void ratio

Table 13.4.1: Hydraulic properties

The parameters of the thermo-elasto-plastic swelling model are given in Table 13.4.2. Cam-Clay plasticity.

Meaning	Value	Unit
Slope of the critical state line, M	1.5	—
Virgin compression index, λ_p	1.5	—
Swelling/recompression index, κ	0.1	—
Initial preconsolidation pressure, p_c	8.0	MPa
Initial void ratio, e	0.7	--
Poisson ratio	0.4	—
Initial ($s = 0$) elastic slope for $1 + e - p$, κ_{i0}	0.01	—
Initial ($\sigma = 0$) elastic slope for $1 + e - s$, κ_{s0}	0.25	—
Minimum bulk modulus, K_{min}	10	MPa
First parameter for κ_s , α_{ss}	-0.03	MPa ⁻¹
Second parameter for κ_s , α_{sp}	-0.1609	—
Parameter for κ_i , α_i	-0.003	MPa ⁻¹
Reference mean stress, p_{ref}	0.1	MPa

Table 13.4.2: Plasticity parameters

Results

Fig. 13.4.2 shows the temporal evolution of water saturation on the bottom of the sample.

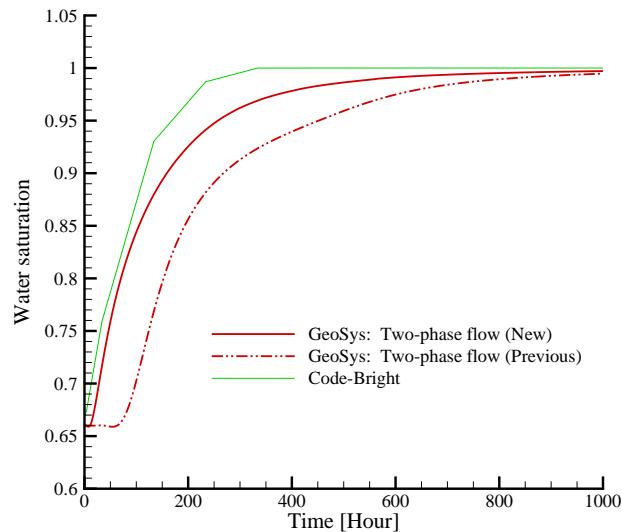


Figure 13.4.2: Vertical stress evolution at the sample bottom

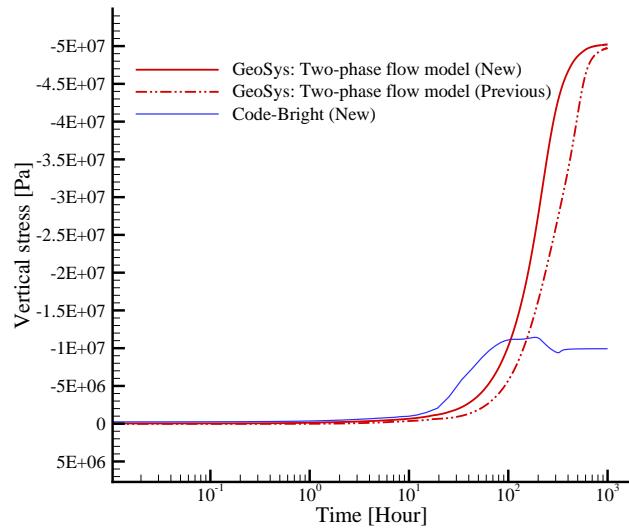


Figure 13.4.3: Water saturation evolution at the sample bottom

Fig. 13.4.3 shows the temporal evolution of the vertical effective stress on the bottom of the sample.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>h2m_tep</i>	H2M	H2M/TEP

Chapter 14

Thermo-Mechanics – TM-Processes

14.1 Theory

Heat transport in solids or porous media

For heat transport problem in any medium, the governing equation is given by

$$\rho C_p T' = -\nabla \mathbf{q}_T + Q_T(\mathbf{x}, t), \mathbf{x} \in \mathbb{R}^3 \quad (14.1.1)$$

where ρ is medium density, $C_p(T)$ is the specific heat capacity, Q_T is heat source and \mathbf{q}_T is the heat flux, which takes the forms

$$\mathbf{q}_T = -K_e \nabla T \quad (14.1.2)$$

for solid and

$$\mathbf{q}_T = -K_e \nabla T + n \sum_{\gamma}^{phase} (\rho^{\gamma} C_p^{\gamma}) T \mathbf{v}, \gamma = \text{liquid, gaseous} \quad (14.1.3)$$

for porous media considering of advective and diffusive fluxes with K_e the heat conductivity. For porous media, the specific heat capacity consists of portions of solid, liquid and gaseous phase as

$$\rho C_p = \sum_{\gamma}^{phase} (\rho^{\gamma} C_p^{\gamma}) \quad (14.1.4)$$

where γ specifies solid, liquid or gaseous phase. The boundary conditions are given by

$$\mathbf{q}_T \cdot \mathbf{n} = q_r^T, \text{ or } T = T_r, \forall \mathbf{x} \in \partial\Omega \quad (14.1.5)$$

and the initial condition reads

$$T(\mathbf{x}, t) = T_0(\mathbf{x}), \forall \mathbf{x} \in \Omega \quad (14.1.6)$$

with \mathbf{n} , the normal direction at $\mathbf{x} \in \partial\Omega$

Thermal stress

We consider the total strain rate $\Delta\epsilon$ can be admissible decomposed into components such as reversible (elastic), temperature deduced as

$$\Delta\epsilon = \mathbb{C}(\Delta\epsilon^e - \alpha \Delta T) \quad (14.1.7)$$

where α is the thermal expansion. With the generalized Hook's law, the total stress with the thermal effect can be expressed as

$$\Delta\sigma = \mathbb{C}(\Delta\epsilon - \alpha \Delta T) \quad (14.1.8)$$

with \mathbb{C} the constitutive tensor.

The volume of a solid is increasing or decreasing with temperature changes. Homogeneous bodies expand evenly in each direction by increasing temperatures. In this case no variation of the stresses occurs. If the deformation of the solid is prevented, the stresses are increasing or decreasing with temperature changes (Beitz et al., 1987). This phenomenon can be easily calculated by analytical solutions of the Hooke's linear elastic model. The equations of the mechanical behaviour base on the Hooke's law for linear elastic materials:

$$\varepsilon_x = \frac{1}{E} \cdot (\sigma_x - \nu \cdot (\sigma_y + \sigma_z)) + \alpha \cdot \Delta T \quad (14.1.9)$$

$$\varepsilon_y = \frac{1}{E} \cdot (\sigma_y - \nu \cdot (\sigma_x + \sigma_z)) + \alpha \cdot \Delta T \quad (14.1.10)$$

$$\varepsilon_z = \frac{1}{E} \cdot (\sigma_z - \nu \cdot (\sigma_x + \sigma_y)) + \alpha \cdot \Delta T \quad (14.1.11)$$

with

ε_i – strains

σ_i – stresses in Pa

E – Young's modulus in Pa

ν – Poisson's ratio

α – thermal expansion in K^{-1}

ΔT – temperature change in K

indices:

x, y, z - x, y, z -direction.

14.2 Thermo-Elasticity

14.2.1 Thermo-elastic plate (2D)

We first solve a plane strain TM coupling problem, then solve this problem again with 3D model.

All parameters are dimensionless. Time step size is 0.1 and the simulation runs 100 steps.

Benchmark name: *tm2D*.

Geometry and mesh : A rectangle domain with size of 10×10 . The domain is discretized into quadrilateral elements (Fig. 14.2.1).

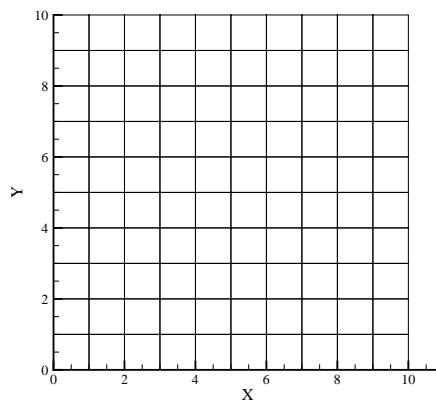


Figure 14.2.1: Mesh for TM coupling plane strain problem

Material: Table 14.2.1.

Table 14.2.1: Material properties for TM coupling plane strain problem

Property	Value	Unit
Young's modulus	3×10^3	--
Poisson's ratio	0.3	--
Density	1.0	--
Thermal expansion	1	--
Thermal capacity	1	--
Thermal conductivity	1	--

Initial and boundary conditions : Initial condition is given by

$$\sigma_0 = 0, T_0 = 198.15$$

Boundary condition is depicted in Fig. 14.2.2.

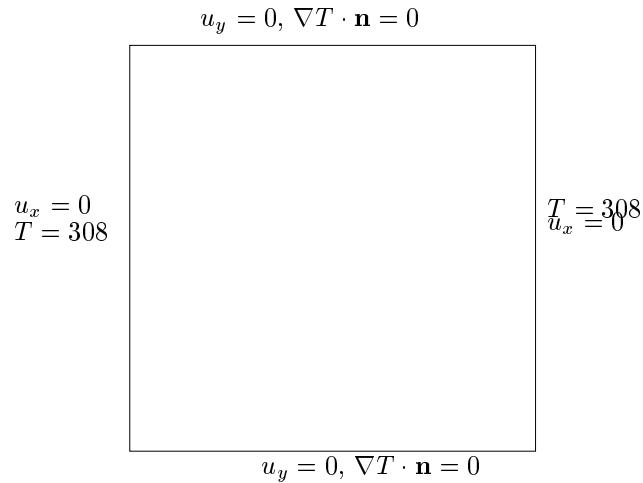


Figure 14.2.2: Boundary conditions for TM coupling plane strain problem

Results: Fig. 14.2.3 provides the distribution of temperature and vertical stress after 100 time steps. The vertical stress distribution shows the effect of gravity force.

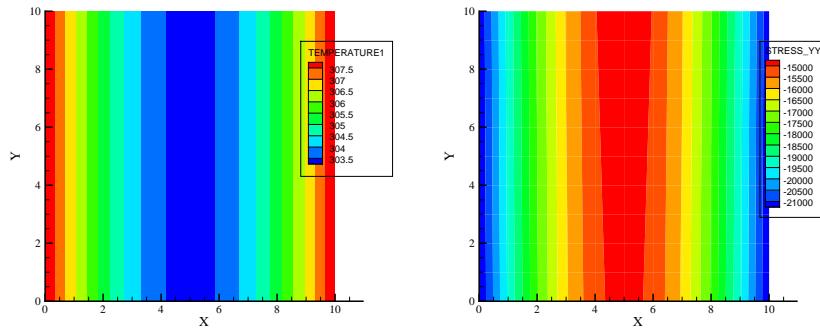


Figure 14.2.3: Distribution of temperature and vertical stress

14.2.2 Thermo-elastic cube (3D)

3D simulation of the problem given in Section 14.2.1.

Benchmark name: *tm3D*.

Geometry and mesh : Extrude the 2D model in off-plane direction for 1 unit. The domain is discretized into hexahedra (Fig. 14.2.4).

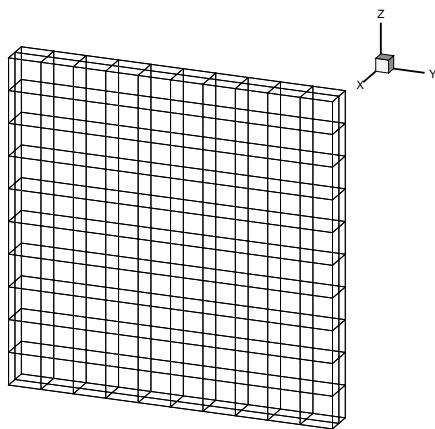


Figure 14.2.4: Mesh for TM coupling 3D problem

Material: Table 14.2.1.

Initial and boundary conditions : Similar to that described in Section 14.2.1 for plane strain problem.

Results: Fig. 14.2.5 provides the distribution of temperature and vertical stress after 100 time steps. The distribution is identical to that given in Fig. 14.2.3 for plane strain problem.

Fig. 14.2.6 gives a comparison about the variation of state variables at the gravity center of 2D and 3D model. The results agree well with each other.

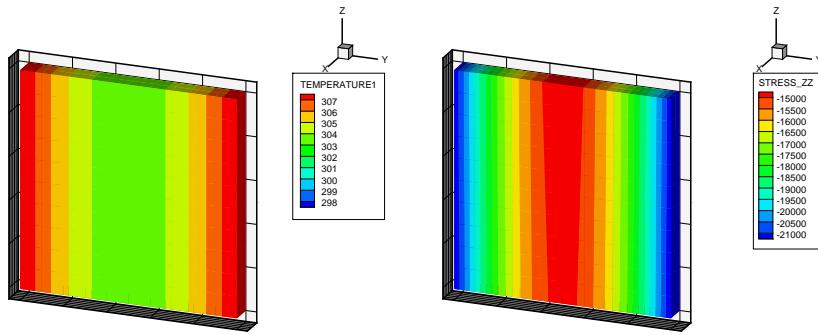


Figure 14.2.5: Distribution of temperature and vertical stress

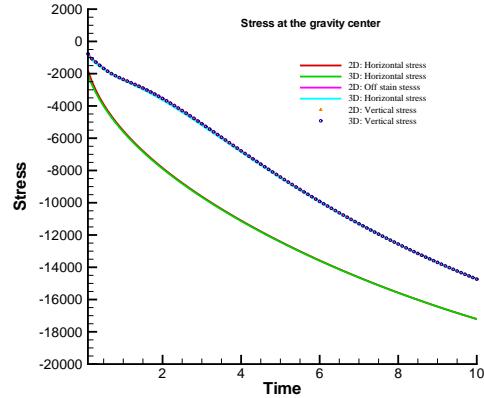


Figure 14.2.6: Comparison of 2D, 3D results

14.2.3 Homogeneous material (3 D)

Problem definition

The top and the bottom of a solid body that consists of one homogeneous material are heated. The xy -plane is the horizontal plane. The height of the body is in z -direction. The dimensions of this 3 D-model are 10 m in all directions. As deformations in x - and y -direction are suppressed, the increasing temperature evokes stresses within the solid. The aim of the calculation is to find out the isotropic state of stress that is reached after the whole solid is heated. Fig. 14.2.7 shows a sketch of the calculation area.

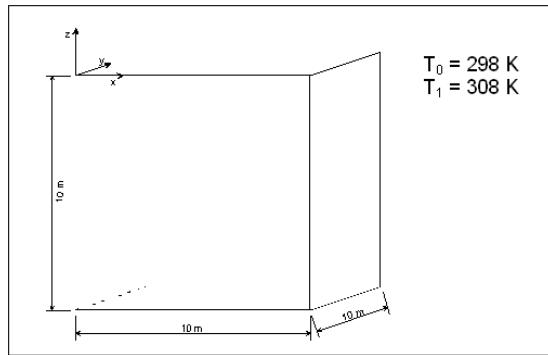


Figure 14.2.7: Calculation area with one material

Assumptions

Temperature: constant temperature in the whole body at the beginning, heating of the body about 10 K

Solid: homogeneous, anisotropic, finite dimensions, no deformation at the boundaries, linear elastic material behaviour, isotropic thermal expansion, different thermal expansion for the materials

Model set-up of the 3 D numerical model

The dimensions of this 3 D-model are 10 m in all directions. Deformations perpendicular to the outer surfaces are suppressed. The initial temperature in the whole area is 298 K. At the top and at the bottom of the model thermal boundary conditions are set with a temperature of 308 K. Thereby the heating of the solid about 10 K is simulated. The used parameters of the solid represent the material behaviour of concrete (Tab. 14.2.2). 1000 elements and 1331 nodes are used. The calculation is divided in 384 time steps with a constant time step length of 900 seconds. That means the heating of the solid within 4 days is simulated. The calculation model is sketched in Fig. 14.2.8.

Evaluation method

The analytical solution can be derived from the time independent Eqns. 14.1.9 to 14.1.11 with the assumptions of no deformation and an isotropic thermal expansion:

$$\begin{aligned} \varepsilon_i &\equiv 0 \\ \sigma_x &= \sigma_y = \sigma_z = -\frac{\alpha \cdot \Delta T \cdot E}{1 - 2 \cdot \nu} \end{aligned} \quad (14.2.1)$$

symbol	quantity	value
T_0	Initial temperature (before heating)	298 K
T_1	Temperature after heating	308 K
ρ	Density of the solid	2.2 t·m ⁻³
E	Young's modulus of the solid	25 GPa
ν	Poisson ratio	0.27
α	Thermal expansion	6.0·10 ⁻⁶ K ⁻¹
c	Thermal capacity	1.0 J·kg ⁻¹ ·K ⁻¹
κ	Thermal conductivity	1.0 W·m ⁻¹ ·K ⁻¹

Table 14.2.2: Used parameters

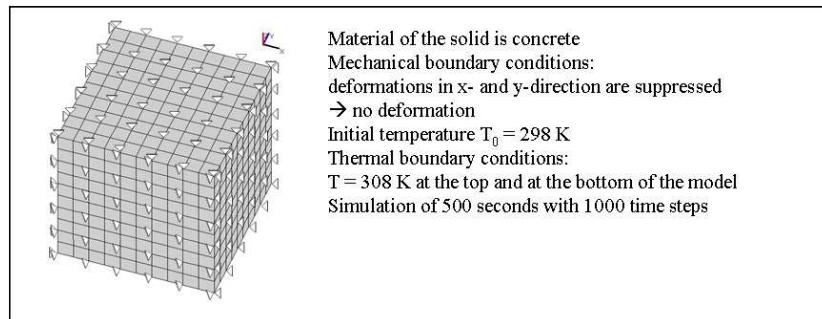


Figure 14.2.8: Calculation model (3 D)

Eqn. 14.2.1 provides the stresses after heating the solid and shows an isotropic state of stress.

Results

With the analytical solution in Eqn. 14.2.1 and the used parameters the stress values in the solid amount. This isotropic state of stress is reached after the whole solid is heated. The temporal development of the stresses in the centre of the model (at node 665) calculated is presented in Fig. 14.2.9. The results of the 3 D simulation show an exact agreement with the analytical solutions.

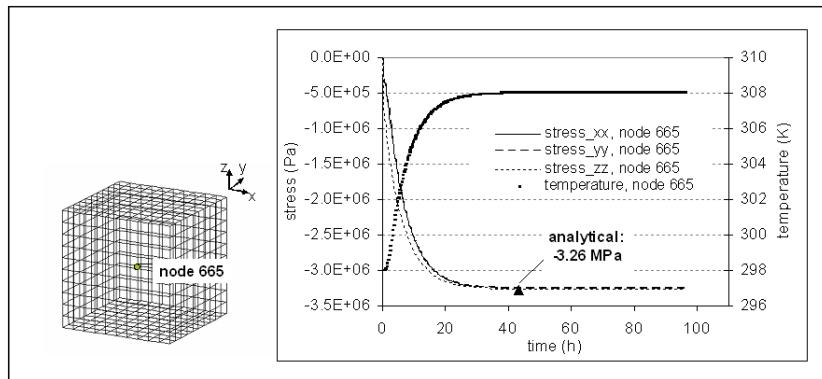


Figure 14.2.9: Temporal stress development in the centre of the calculation model (node 665)

Path in the benchmark deposit	Used code	Used version	Date of simulation run
TM\heating\cube\ tm_01_3Du	GeoSys/RockFlow	RockFlow 4, rf4 4.05.07	Dec. 2007

14.2.4 Composite materials (3 D)

Problem definition

If there are 2 materials with different thermal expansions the volume changes of the materials will be uncommon. The material with the higher thermal expansion expands more than the material with the low thermal expansion. If deformations at the outer boundaries are prevented, different states of stress will occur in these two materials. But the stresses perpendicular to the parting plane must be equal. The values of the stresses as a result of temperature changes can also easily be calculated by the Hooke's linear elastic model. The aim of this simulation is to specify the stresses at several areas in the solid. Fig. 14.2.10 shows a sketch of the calculation area.

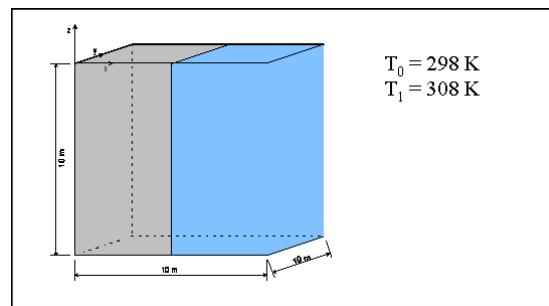


Figure 14.2.10: Calculation area with two different materials

Model set-up of the 3 D numerical model

The calculation was done with a 3 D model. The xy -plane is the horizontal plane. The height of the body is in z -direction. The dimensions of this 3 D model are 10 m in all directions. The model includes 1000 elements and 1331 nodes. Deformations perpendicular to the outer surfaces are suppressed. Deformations in x - and z -direction are suppressed. The initial temperature in the whole area is 298 K. At the top and at the bottom of the model thermal boundary conditions are set with a temperature of 308 K. Thereby the heating of the body about 10 K is simulated. The used parameters of the solids represent the material behaviour of concrete. The calculation is divided in 1000 time steps with a constant time step length of 0.5 seconds. A sketch of the calculation model is shown in Fig. 14.2.11.

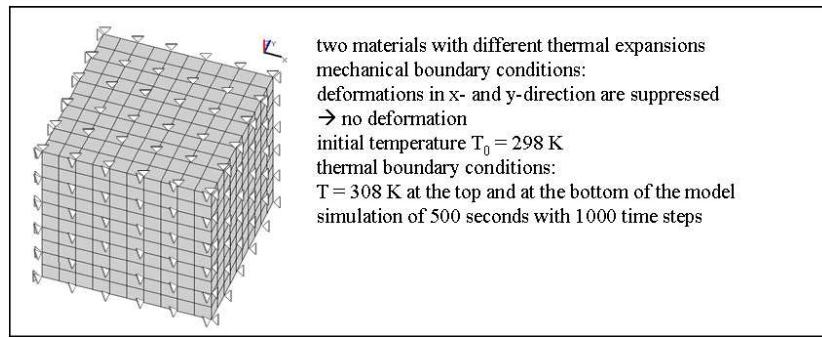


Figure 14.2.11: Calculation model (3D) with 2 materials

Evaluation method

The equations of the mechanical behaviour base on the HOOKE's law for linear elastic materials (see Eqns. 14.1.9 to 14.1.11). The analytical solution can be

symbol	quantity	value
T_0	Initial temperature (before heating)	298 K
T_1	Temperature after heating	308 K
ρ	Density of the solid	2.2 t·m ⁻³
E	Young's modulus of the solid	25 GPa
ν	Poisson ratio	0.27
α_1	Thermal expansion of material 1	6.0·10 ⁻⁶ K ⁻¹
α_2	Thermal expansion of material 2	1.2·10 ⁻⁵ K ⁻¹
c	Thermal capacity	1.0 J·kg ⁻¹ ·K ⁻¹
κ	Thermal conductivity	1.0 W·m ⁻¹ ·K ⁻¹

Table 14.2.3: Used parameters

derived from these time independent equations with the assumptions of suppressed deformations in y - and z -direction and an isotropic thermal expansion:

$$\varepsilon_x = \varepsilon_z \equiv 0$$

Additionally the stresses in x -direction (perpendicular to the parting plane between the two materials) must be equal:

$$\sigma_{x1} = \sigma_{x2}$$

Further the expansion of the one material leads to a compression of the other material with the same value in x -direction:

$$\varepsilon_{x1} = -\varepsilon_{x2}$$

With these limiting conditions the analytical solutions are:

$$\varepsilon_{x1} = \frac{\Delta T}{2} \cdot (\alpha_1 - \alpha_2) \cdot \left(\frac{1 + \nu}{1 - \nu} \right) \quad (14.2.2)$$

$$\varepsilon_{x2} = -\varepsilon_{x1} = -\frac{\Delta T}{2} \cdot (\alpha_1 - \alpha_2) \cdot \left(\frac{1 + \nu}{1 - \nu} \right) \quad (14.2.3)$$

$$\sigma_{x1} = \sigma_{x2} = E \cdot \frac{\varepsilon_{x2} \cdot (1 - \nu) - \alpha_2 \cdot \Delta T \cdot (1 + \nu)}{1 - \nu - 2\nu^2} \quad (14.2.4)$$

$$\sigma_{y1} = \sigma_{z1} = \frac{\nu \cdot \sigma_{x1} - \alpha_1 \cdot \Delta T \cdot E}{1 - \nu} \quad (14.2.5)$$

$$\sigma_{y2} = \sigma_{z2} = \frac{\nu \cdot \sigma_{x2} - \alpha_2 \cdot \Delta T \cdot E}{1 - \nu} \quad (14.2.6)$$

indices:

1 – material 1

2 – material 2

Eqns. 14.2.2 to 14.2.6 provide the strains and stresses after heating the body of two materials. The state of stress is anisotropic.

Results

With the analytical solution in Eqns. 14.2.2 to 14.2.6 and the used parameters the values of the strains in x -direction at the parting plane amount

$$\varepsilon_{x1} = -5.219178 \cdot 10^{-5}$$

$$\varepsilon_{x2} = 5.219178 \cdot 10^{-5}$$

The values of the stresses are

$$\sigma_{x1} = \sigma_{x2} = -4891304.34 \text{ Pa} = -4.8913 \text{ MPa}$$

$$\sigma_{y1} = \sigma_{z1} = -3863907.08 \text{ Pa} = -3.8639 \text{ MPa}$$

$$\sigma_{y2} = \sigma_{z2} = -5918701.60 \text{ Pa} = -5.9187 \text{ MPa}$$

This anisotropic state of stress is reached after the whole body is heated. The temporal stress developments in several nodes calculated with both RockFlow and

GeoSys/RockFlow are presented in Fig. 14.2.12 and Fig. 14.2.13.

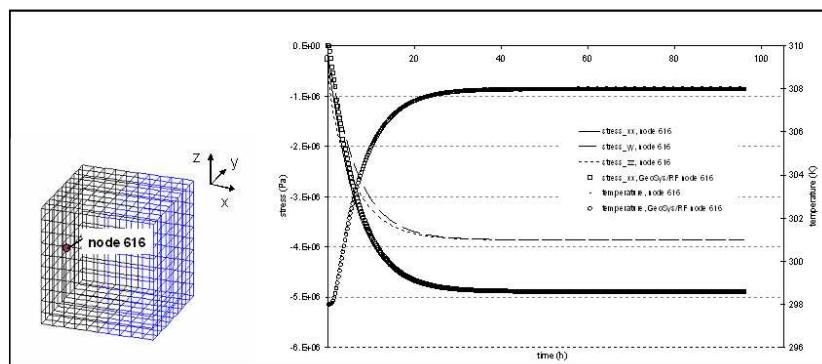


Figure 14.2.12: Temporal stress development in node 616

The results of the 3 D simulation show an exact agreement with the analytical solutions.

Path in the benchmark deposit	Used code	Used version	Date of simulation run
TM\heating\cube\2_mat\GeoSys/RockFlow\tm_02_3Du	GeoSys/RockFlow	RockFlow 4, rf4-507	Dec. 2007

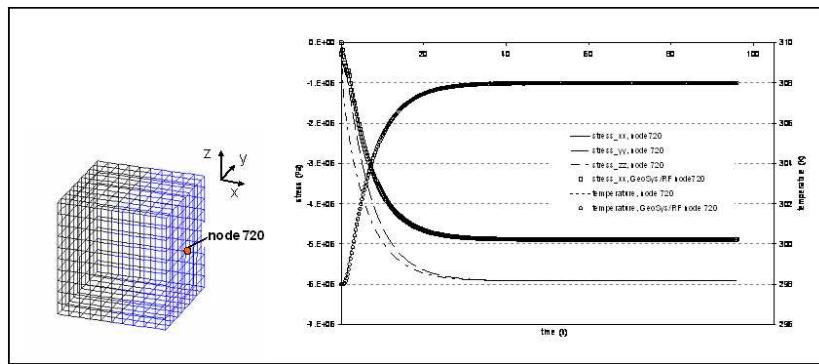


Figure 14.2.13: Temporal stress development in node 720

14.2.5 Temperature increase in a hollow cylinder

Problem definition

A hollow cylinder which consists of a solid of a constant temperature is exposed to a higher temperature at the surface of its hole. As a result of the increased temperature the cylinder is expanding. The aim of this calculation is to get out the radial displacement as well as the temperature distribution that are caused by the thermal expansion process by the use of an axisymmetric model. Fig. 14.2.14 shows a sketch of the calculation area.

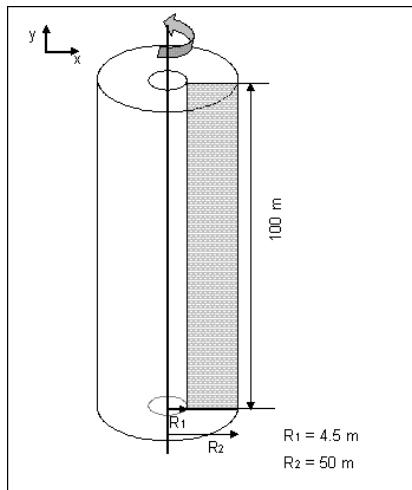


Figure 14.2.14: Calculation area (grey area)

Assumptions

Temperature: constant temperature in the whole body at the beginning, heating of the cylinder at the inner surface

Solid: homogeneous, finite dimensions, no deformation in y -direction at the bottom and the top, no deformation in x -direction at the right border, linear elastic material behaviour, isotropic thermal expansion

Model set-up of the 2 D numerical model

The axisymmetric model is in the xy -plane. The inner radius $R1$ of the cylindrical model is 4.5 m and the outer radius $R2$ 50 m. The cylinder is 100 m high. The initial temperature in the whole area is 25°C. As boundary condition deformations in y -direction at the bottom and the top are suppressed, as well as deformations in x -direction at the right border. At the right boundary of the model a thermal boundary condition is set with a constant value of 25°C. At the left boundary a source term for heat flux of $q = 30 \text{ W/m}^2$ is defined. Thereby the continuous heating of the solid is simulated. The used parameters of the solid are listed in Tab. 14.2.4. The simulation of only one time step is done. The numerical model consists of 766 elements and 426 nodes. It is sketched in Fig. 14.2.15.

symbol	quantity	value
T_0	Initial temperature (before heating)	25°C
q	Heat source	30 W/m ²
ρ	Density of the solid	2.0 t·m ⁻³
E	Young's modulus of the solid	2.5 GPa
ν	Poisson ratio	0.25
α	Thermal expansion	4.2·10 ⁻⁵ K ⁻¹
κ	Thermal conductivity	5.5 W·m ⁻¹ ·K ⁻¹

Table 14.2.4: Used parameters

Evaluation method

For the hollow cylinder with the inner radius $R1$ and the outer radius $R2$ the following analytical solution for radial displacement u_r , stress σ_r and temperature

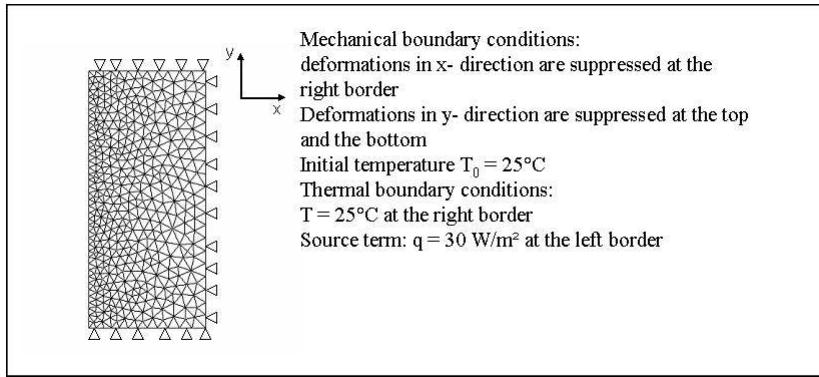


Figure 14.2.15: Calculation model (2 D, axisymmetric) of the hollow cylinder

in dependency on the radius was used (Wang II, 2007).

$$u_r = \frac{q R_1 \beta}{2 \psi \kappa} \cdot r \cdot \left(\ln r - \frac{1}{2} \right) + \frac{A_0}{2} r + \frac{A_1}{r} \quad (14.2.7)$$

$$\begin{aligned} \sigma_r = & \psi \left[-\frac{q R_1 \beta}{2 \psi \kappa} \cdot r \cdot \left(\ln r + \frac{1}{2} \right) + \frac{A_0}{2} - \frac{A_1}{r^2} \right] \\ & + \lambda \left[-\frac{q R_1 \beta}{2 \psi \kappa} \cdot r \cdot \left(\ln r - \frac{1}{2} \right) + \frac{A_0}{2} + \frac{A_1}{r^2} \right] \\ & - \beta \left[\frac{R_1 q}{\kappa} \ln \left(\frac{R_2}{r} \right) + T_0 \right] \end{aligned} \quad (14.2.8)$$

$$T(r) = \frac{R_1 q}{\kappa} \ln \left(\frac{R_2}{r} \right) + T_0 \quad (14.2.9)$$

where

$$\psi = \lambda + 2G \quad \text{and} \quad \beta = \alpha(3\lambda + 2G)$$

with

- λ – Lamé elastic constant
- G – shear modulus
- α – thermal expansion coefficient
- κ – thermal conductivity
- A_0, A_1 – integration constants

At the outer surface of the hollow cylinder (where $r = R_2$) there is no deformation, that means the displacement u_{R2} is zero. Therefore Eqn. 14.2.7 is set equal to zero for this boundary and adapted to A_0 .

$$A_0 = -\frac{2 A_1}{R_2^2} - 2 \cdot B \cdot \left(\ln R_2 - \frac{1}{2} \right) \quad (14.2.10)$$

where

$$B = \frac{q R_1 \beta}{2 \psi \kappa}$$

At the inner surface of the hollow cylinder (where $r = R_1$) no stress is effected by the expansion because this boundary is phreatic. Therefore Eqn. 14.2.8 is set equal to zero and A_1 is calculated by using Eqn. 14.2.11.

$$A_1 = \frac{\beta \left(\frac{R_1 q}{\kappa} \ln \left(\frac{R_2}{r} \right) + T_0 \right) + \lambda B \left(\ln R_1 - \frac{1}{2} \right) + \psi B \left(\ln R_1 + \frac{1}{2} \right) - \left(\frac{\lambda + \psi}{2} \right) 2 B \left(\ln R_2 - \frac{1}{2} \right)}{\frac{\lambda - \psi}{R_1^2} - \frac{\lambda + \psi}{2} \cdot \frac{2}{R_1^2}} \quad (14.2.11)$$

After having solved this equation, A_1 is used to calculate A_0 . The results are:

$$A_0 = 5.96 \cdot 10^{-3}$$

$$A_1 = -1.19 \cdot 10^{-1}$$

Results

The results of the analytical equations for stresses, displacements and temperatures are compared to those of the numerical simulation by GeoSys/RockFlow. Fig. 14.2.16 shows the temperature distribution over the radius of the hollow cylinder. In Fig. 14.2.17 displacements in radial direction that are caused by the thermal expansion are depicted. In addition you can find the induced stresses in Fig. 14.2.18. Obviously, with the axisymmetric model a GeoSys/RockFlow simulation generates comprehensible results that meet well the analytic solution.

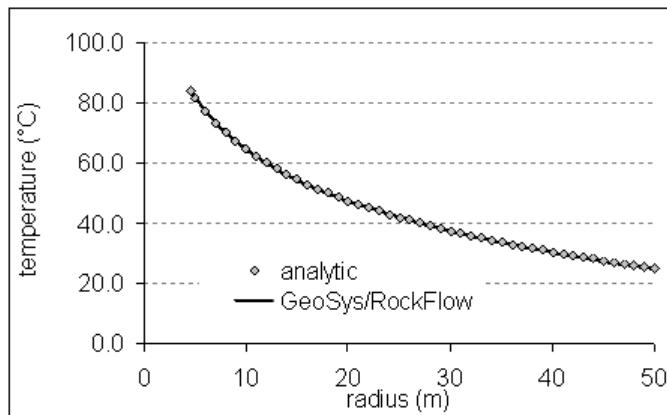


Figure 14.2.16: Temperature distribution over the radius

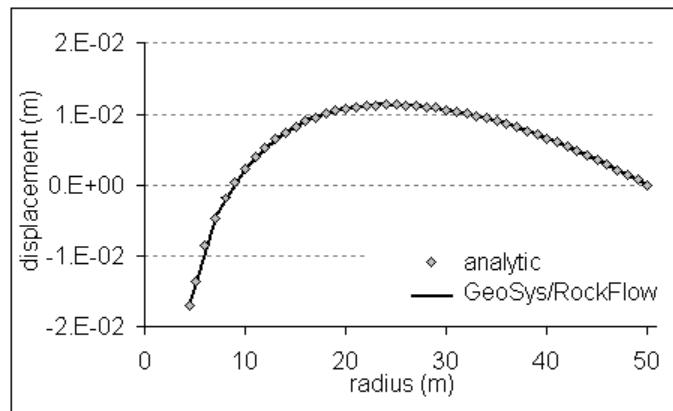


Figure 14.2.17: Displacements in radial direction

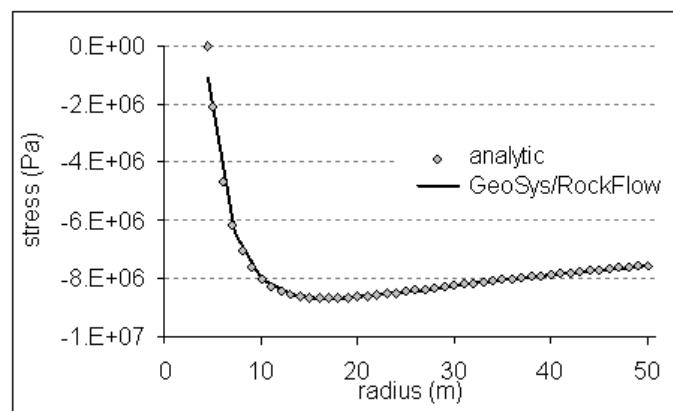


Figure 14.2.18: Stresses in radial direction

Path in the benchmark deposit	Used code	Used version	Date of simu- lation run
\TM\heating\hollowcylinder\ TM_axi	GeoSys/RockFlow	RockFlow 4, rf4-502.exe	July 2007

Chapter 15

Thermo-mechanical consolidation – THM-Processes

15.1 Theory

For thermo-mechanical consolidation, the vapor diffusion is considered. The governing equations, which are essential for the analysis, are detailed hereafter.

15.1.1 Non isothermal flow in porous media

Consider a general case of a flow problem in deformable porous media under the Richard's approximation. With the classical Darcy's law, the large scale water flow \mathbf{q}_w is defined as

$$\mathbf{q}_w = -nS \left(\rho_w \frac{k_{rel}\mathbf{k}}{\mu} (\nabla p - \rho\mathbf{g}) \right) \quad (15.1.1)$$

where S is water saturation, p is the water pressure, ρ is density, n is effective porosity of the media, μ is viscosity of flow, k_{rel} is the relative permeability tensor, \mathbf{g} is the gravity force by density and \mathbf{k} denotes permeability. Meanwhile, we consider vapor flow filled pores due to molecular diffusion, which is coupled with temperature. Similar to what is defined in [?], the vapor flow is given by

$$\mathbf{q}_v = -D_{pv} \nabla P - f_{Tv} D_{Tv} \nabla T \quad (15.1.2)$$

where $f_T v$ is a thermal diffusion enhancement factor takes value of 1.0 in the present simulation, D_{pv} and D_{Tv} are diffusion coefficients takes form as

$$\begin{aligned} D_{pv} &= \frac{D_v \rho_v}{\rho_w R T_{abs}} \\ D_{Tv} &= D_v \left(h \frac{\partial \rho_{vs}}{\partial T} - \frac{\rho_v P}{\rho_w R T_{abs}^2} \right) \end{aligned} \quad (15.1.3)$$

with h , the relative humidity according to

$$h = e^{P/\rho_w R T_{abs}} \quad (15.1.4)$$

$R = 461.6 \text{ J/kgK}$, the specific gas constant for water vapour, ρ_{vs} , the saturated vapour density given by

$$\rho_{vs} = 10^{-3} e^{19.891 - 4975/T_{abs}} \quad (15.1.5)$$

and vapour density $\rho_v = h \rho_{vs}$.

The expressions of flow defined in (15.1.1) and (15.1.2) lead the governing equation of flow field in the terms of mass balance equation given by

$$\begin{aligned} n \left[\frac{\rho_w - \rho_v}{\rho_w} \frac{\partial S}{\partial p} + S \beta_p + (1 - S) \frac{\rho_v}{\rho_w^2 R T_{abs}} \right] \frac{\partial p}{\partial t} \\ + \nabla \cdot (\mathbf{q}_w + \mathbf{q}_v) / \rho_w + S \frac{\partial}{\partial t} (\nabla \cdot \mathbf{u}) \\ n \frac{1 - S}{\rho_w} \left(h \frac{\partial \rho_{vs}}{\partial T} + \frac{\rho_v p}{R T_{abs}^2} \right) \frac{\partial T}{\partial t} = 0 \end{aligned} \quad (15.1.6)$$

for any point $\mathbf{x} \in \Omega \subset \mathbb{R}^n$ with n the dimension of the real space. In eqn. 15.1.6, β_p is the storativity. The unknown of eqn. (15.1.6) to be solved are saturation of the phase S , fluid pressure p and the coupling term, i.e. temperature and displacement \mathbf{u} , deduced by solid deformation. The boundary conditions for this problem can be simplified for this Richard's flow model

$$\mathbf{q}_w \cdot \mathbf{n} = q_r, \forall \mathbf{x} \in \partial\Omega \quad (15.1.7)$$

or Dirchlet type as

$$p = p_r, \quad S = S_r, \forall \mathbf{x} \in \partial\Omega \quad (15.1.8)$$

This initial-boundary-value-problem can be solved with the corresponding initial condition of unknowns.

15.1.2 Deformation

Assuming solid grains itself are incompressible, i.e. $d^s \mathbf{u} / d^s t = 0$, deformations in porous media can be described by the momentum balance equation in the terms of stress as

$$\nabla \cdot (\boldsymbol{\sigma} - Sp \mathbf{I} - \alpha \mathbf{I} \Delta T) + \rho g = 0 \quad (15.1.9)$$

and for bentonite material

$$\nabla \cdot (\boldsymbol{\sigma} - \alpha \mathbf{I} \Delta T) + \rho \mathbf{g} = 0 \quad (15.1.10)$$

and for rock, where $\boldsymbol{\sigma}$ is the effective stress of the porous medium, α is the thermal expansion coefficient, \mathbf{I} is the identity. Density of porous media consists of the portion contributed by liquid l and by the portion contributed of solid as $\rho = n\rho^l + (1 - n)\rho^s$.

The swelling pressure in bentonite is calculated by

$$\boldsymbol{\sigma}_{sw} = S^2 \sigma_{sw}^{max} \mathbf{I}$$

15.1.3 Heat transport

For heat transport problem, we consider the convective transport, i.e. the transport of heat by flow. There are two basic kinds of convection recognized such as *forced convection* and *free convection*. In the former, the velocity of convective motion does not have any impact on the temperature on the fluids and the heat energy transport is forced by the flow movement. In the latter, flow velocities are driven solely by buoyancy effects in the fluid, and these are related to temperature change through the coefficient of thermal expansion. In real ground water systems, there is a mixture of both types of convection. The simple expression of heat flux in forced convection is given by

$$\mathbf{q}_T = -K_e \nabla T + n \sum_{\gamma}^{phase} (\rho^{\gamma} C_p^{\gamma}) T \mathbf{v} \quad (15.1.11)$$

where K_e is the heat conductivity, $\sum_{\gamma}^{phase} (\rho^{\gamma} C_p^{\gamma}) T \mathbf{v}$ is the flux of heat transported by velocity \mathbf{v} per unit area, and across the entire rock face this flux is reduced by the effective porosity, n . With the definition of heat flux (15.1.11), the governing equation of the convective heat transport can be derived for any point $\mathbf{x} \in \Omega \in \mathbb{R}^n$ as

$$\sum_{\gamma}^{phase} (\rho^{\gamma} C_p^{\gamma}) \frac{\partial T}{\partial t} - \nabla \mathbf{q}_T + Q_T = 0 \quad (15.1.12)$$

with boundary condition

$$\mathbf{q}_T \cdot \mathbf{n} = q_T|_r, \text{ or } T = T_r, \forall \mathbf{x} \in \partial\Omega \quad (15.1.13)$$

and initial condition

$$T(\mathbf{x}) = T_0(\mathbf{x}), \forall \mathbf{x} \in \Omega \quad (15.1.14)$$

15.1.4 Repository in crystalline rock with unsaturated bentonite buffer: DECOVALEX Task IV - THM1

Problem definition

This example is dealing with fully coupled thermo-hydraulic-mechanical (THM) processes in geotechnical applications. This model is developed in the framework of Task D of DECOVALEX III project (www.decovalex.com). This DECOVALEX test case was designed by [106] for modeling THM coupling processed in FEBEX type nuclear waste repository. Fig. 15.1.1 illustrates the set-up of the model, in which, V_1, \dots, V_6 indicate the observation points.

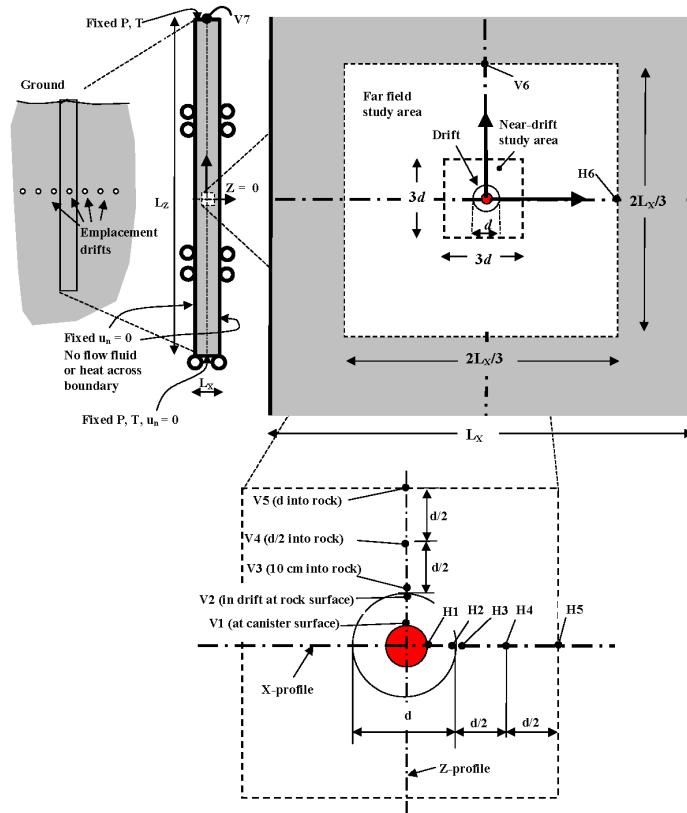


Figure 15.1.1: Model step-up ([106])

A full scale simulation of this problem is given in [107]. The results are compared with that obtained by other research teams[108]. In order to save benchmark running time and keep the original physics of the problem, this benchmark takes a patch cut from the full domain and the results of the full scale simulation at

the edge of the patch as boundary condition. The initial stress is obtained by excavation simulation. The simulation gives results of THM processes till 1000 years. The domain contains that occupied by the waste canister, bentonite buffer and surrounding rock. A triangular mesh of the domain is shown in Fig. 15.1.2.

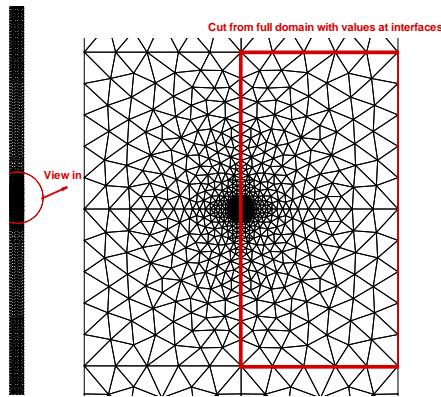


Figure 15.1.2: Near field of DECOVALEX THM1 model

The simulation is split in two phases. In the first phase, an initial state of stress, water pressure and temperature are established by excavation simulation. The operation simulation, that means the THM simulation after having installed the canister and bentonite, is done in a second phase.

The simulation of the excavation phase was done within 4 steps (Wang et al., 2007). At first the initial stress of the whole domain was calculated. Then the released force on the surface of the excavation tunnel was obtained. In a third step the domain with the excavation was analysed with the released force as unique boundary condition. The last step is the combination of step 1 and 3: the stress after excavation. After this the initial conditions of water pressure and temperature were calculated by simulating one time step of the TH coupled process. In the second phase the THM coupled processes in the bentonite and the near field rock mass on the base of the described initial condition set-up are modelled for a period of 1 million years under the assumption that the permeability of the rock mass and bentonite is constant. The initial and boundary conditions that are indicated in Fig. ?? are relevant for the simulation run. To avoid flow within the canister domain the method of activating and deactivating elements was applied. Thus during the flow process the elements of the canister are devoid with a zero Neumann boundary condition on the surface of the canister. The heat power function which represents the source term of heat (due to radioactive decay, Fig. ??) in the canister was given in a graphical form to

the simulation teams (Birkholzer et al., 2007).

Initial and Boundary conditions

Values of variables at the cut interfaces of the full scale domain are taken as boundary condition directly (see Fig. 15.1.2 and cf. [107] and [108]).

Material properties

The material parameters for rock mass and bentonite are given in Table 15.1.1 and 15.1.4, respectively.

Parameter	Unit	Value
Density	kg/m^3	2700
Young's modulus	GPa	35
Poisson ratio	-	0.3
Biot's constant	-	1
Thermal expansion coefficient	-	1.0×10^{-5}
Thermal conductivity	W/mK	3
Thermal capacity	J/kgK	900
Porosity	-	0.01
Saturated permeability	m^2	1.0×10^{-17}

Table 15.1.1: Rock Mass

Density	kg/m^3	1600
Young's modulus	MPa	317
Poisson ratio	-	0.35
Biot's constant	-	1
Tortuosity	-	0.8
Porosity	-	0.41
Thermal expansion coefficient	-	1.0×10^{-5}
Thermal conductivity	W/mK	$c_s = 1.38T + 732.5$
Thermal capacity	J/kgK	$\kappa_m = 1.28 - \frac{0.71}{1+e^{10(S_w - 0.65)}}$
Saturated permeability	m^2	2.0×10^{-21}

Table 15.1.2: Bentonite

A time-depending heat power function is given in order to describe the heat source condition of the containment. Measured soil-water-characteristic curves

are used in order to describe the thermo-hydraulic behaviour. The dependency of capillary pressure as well as relative permeability on liquid saturation for both of rock and bentonite are depicted in Fig. 15.1.3.

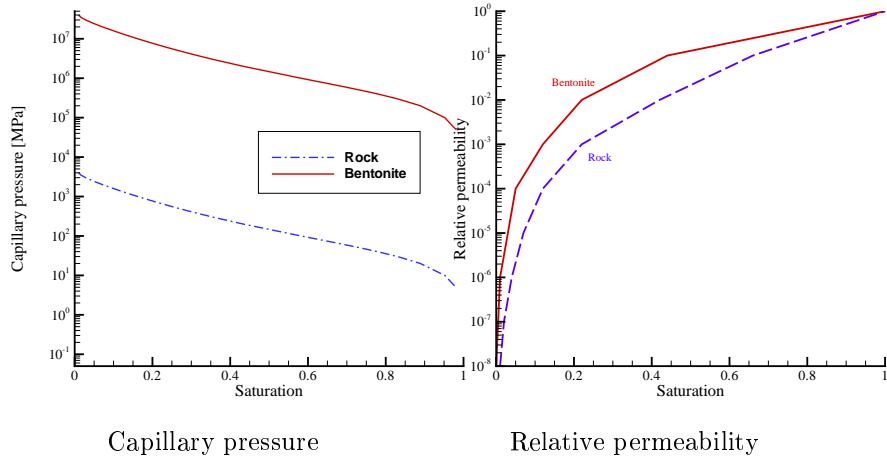


Figure 15.1.3: Capillary pressure - relative permeability - functions

Results

Evaluation method: The numerical results are compared to those of the simulation programmes TOUGH-FLAC (TH processes coupled in TOUGH; M-processes with FLAC) and ROCMAS (THM processes coupled) (Birkholzer et al., 2007).

Fig. 15.1.4 provides the distribution of temperature and saturation after 1 year.

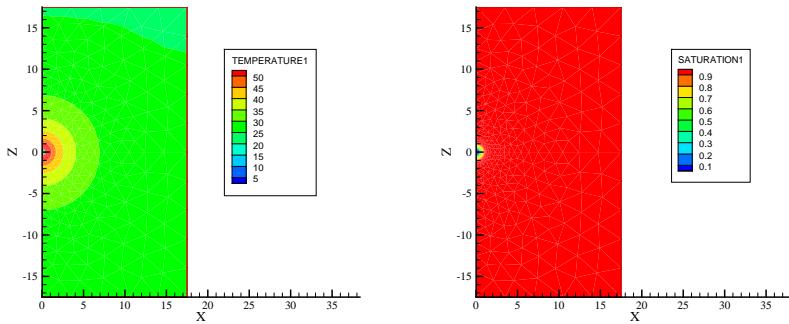


Figure 15.1.4: Distribution of temperature and saturation

Fig. 15.1.5 provides the distribution of vertical stress and fluid velocity after 1 year.

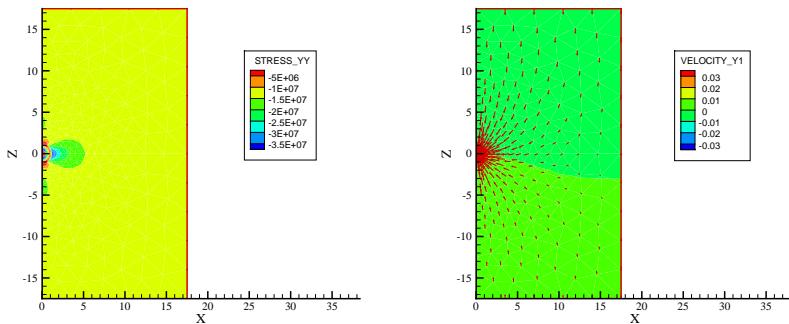


Figure 15.1.5: Distribution of vertical stress and fluid velocity

Fig. 15.1.6 shows the evolution of temperature and saturation at observation points.

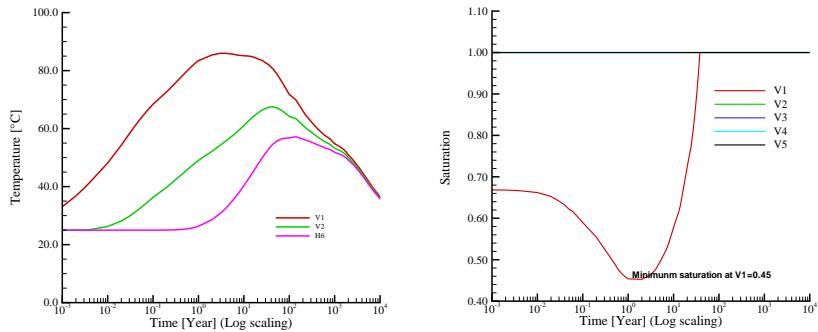


Figure 15.1.6: Evolution of temperature and saturation

Fig. 15.1.7 shows the evolution of horizontal stress and vertical displacement at observation points.

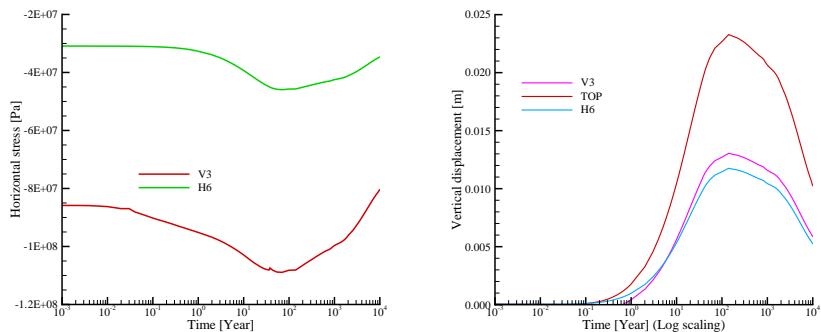


Figure 15.1.7: Evolution of horizontal stress and vertical displacement

Fig. 15.1.8 gives vertical velocity profile along horizontal line cross the canister center.

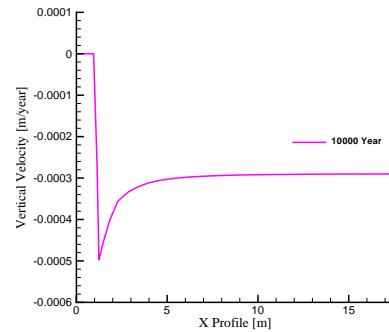


Figure 15.1.8: Vertical velocity profile

The above results agree with that obtain by using a full domain.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>thm-decov</i>	THM	benchmarks\THM\

Chapter 16

Non-isothermal two-phase flow consolidation

16.1 Balance equations

In section 15 we considered non-isothermal flow in an unsaturated deformable porous medium using the Richards model. In this section we treat the partially saturated porous media as multi-phase system composed of constituents with the voids of the solid skeleton filled with water and gas. Similar to what presented in [109], we assume that capillary pressure p_c , gas pressure p^g , temperature T , and solid displacement \mathbf{u} are primary variables to describe the state of the porous media. The general notation for the multi-phase, multi-componental formulation is

$$\rho_k^\gamma \quad (16.1.1)$$

where k is component and γ is phase identification. The governing equations are given hereafter.

16.1.1 Non-isothermal two-phase flow

For liquid water ρ^l , vapor ρ_w^g and the solid skeleton ρ^s , the mass balance is governed by the following equation:

$$\begin{aligned} n(\rho^l - \rho_w^g)(\frac{\partial S^l}{\partial T}\dot{T} + \frac{\partial S^l}{\partial p_c}\dot{p}_c) + n(1 - S^l)(\frac{\partial \rho_w^g}{\partial T}\dot{T} + \frac{\partial \rho_w^g}{\partial p_c}\dot{p}_c) \\ + [\rho^l S^l + (1 - S^l)\rho_w^g]\nabla \dot{\mathbf{u}} - \nabla \left[\rho^g \frac{M_a M_w}{M_g^2} \mathbb{D}_w^g \nabla \left(\frac{p_w^g}{p^g} \right) \right] \\ + \nabla \left[\rho^l \frac{\mathbf{k} k_{rel}^l}{\mu^l} (-\nabla p^g + \nabla p_c + \rho^l \mathbf{g}) \right] \\ + \nabla \left[\rho_w^g \frac{\mathbf{k} k_{rel}^g}{\mu^l} (-\nabla p^g + \rho^g \mathbf{g}) \right] - \beta_T \dot{T} = 0 \end{aligned} \quad (16.1.2)$$

While, for dry air and the solid skeleton, the mass balance equation is given by

$$\begin{aligned} -n\rho_a^g(\frac{\partial S^l}{\partial T}\dot{T} + \frac{\partial S^l}{\partial p_c}\dot{p}_c) + (1 - n)(1 - S^l)\beta^s \rho_a^g \dot{T} \\ n(1 - S^l)(\frac{\partial \rho_a^g}{\partial T}\dot{T} + \frac{\partial \rho_a^g}{\partial p_c}\dot{p}_c + \frac{\partial \rho_a^g}{\partial p^g}\dot{p}^g) \\ + [\rho^l S^l + (1 - S^l)\rho_a^g]\nabla \dot{\mathbf{u}} \\ - \nabla \left[\rho^g \frac{M_a M_w}{M_g^2} \mathbb{D}_a^g \nabla \left(\frac{\partial p_a^g}{\partial p^g} \right) \right] \\ + \nabla \left[\rho_a^g \frac{\mathbf{k} k_{rel}^g}{\mu^l} (-\nabla p^g + \rho^g \mathbf{g}) \right] = 0 \end{aligned} \quad (16.1.3)$$

where ρ^l , ρ_w^g , ρ_a^g are liquid, vapor, air density, respectively; μ^l , μ^g are liquid and gas viscosities, respectively; $S^l = 1 - S^g$ is liquid saturation; M_w , M_a , M_g are water, air, and gas molar masses, respectively; \mathbb{D}_w^g is vapor diffusion coefficient; \mathbf{k} , k_{rel}^l , k_{rel}^g are saturated and relative permeabilities for liquid and gas phases, respectively; \mathbf{g} is gravity acceleration vector and $\beta_T = nS^l\beta^l + nS^g\beta^g + (1 - n)\beta^s$ is thermal expansion coefficient of the porous medium.

16.1.2 Deformation

The thermo-poro-elastic deformation process in the porous medium is described by the momentum balance in terms of stress equilibrium:

$$\nabla \cdot (\sigma - \alpha_b \max(p^g - S^l p_c, 0) - \beta_T (T - T_0) \mathbf{I}) + \rho \mathbf{g} = 0 \quad (16.1.4)$$

where σ is effective stress; α_b is Biot coefficient; T_0 is reference temperature and \mathbf{I} is identity tensor.

16.1.3 Heat transport

Heat transport in two-phase flow including storage, advection, diffusion processes in porous medium consisting of liquid, gas, and solid phases is described by following equation

$$c\rho \frac{\mathbf{p}T}{\mathbf{p}t} + (c\rho\mathbf{v})^f \cdot \nabla T - \nabla(\kappa\nabla T) = Q_T \quad (16.1.5)$$

where

$$\begin{aligned} c\rho &= nS^l c^l \rho^l + nS^g c^g \rho^g + (1-n)c^s \rho^s \\ (c\rho\mathbf{v})^f &= nS^l c^l \rho^l \mathbf{v}^l + nS^g c^g \rho^g \mathbf{v}^g \\ \kappa &= nS^l \kappa^l + nS^g \kappa^g + (1-n)\kappa^s \end{aligned} \quad (16.1.6)$$

are heat capacity, fluid phase part for heat advection, and thermal heat conductivity of the porous medium, respectively

16.2 Constitutive equations

16.2.1 Density

Liquid density is affected by thermal expansion effects

$$\rho^l(T) = \rho_0^l (1 - \beta_T^l (T - T_0)) \quad (16.2.1)$$

For the gaseous mixture, the ideal gas law is adopted for dry air and water vapour. Applying the Clapeyron equation and Dalton's law to describe the state of dry air, water vapour and moist air yields

$$p^g = p_a^g + p_w^g, \quad \rho^g = \rho_a^g + \rho_w^g, \quad (16.2.2)$$

with

$$\rho_a^g = \frac{M_a p_a^g}{RT}, \quad \rho_w^g = \frac{M_w p_w^g}{RT} \quad (16.2.3)$$

with R , the specific gas constant. The water vapour pressure p_w^g is given by the Kelvin-Laplace equation

$$p_w^g = p^{gw_s}(T) \exp \left(\frac{p_c^c M_w}{\rho^l R T} \right) \quad (16.2.4)$$

where p^{gw_s} is the water vapour saturation pressure. In the current version of GeoSys/Rockflow, we use an empiric formula for p^{gw_s}

$$p^{gw_s}(T) = \frac{RT}{M_w} [10^{-3} \exp(19.89 - 4975.9/T)] \quad (16.2.5)$$

16.2.2 Flux of gaseous mixture

Based on the Fick's law, the relative flux of the gaseous mixture can be obtained as

$$\mathbf{v}_a^g = -\frac{M_a M_w}{M_g^2} \mathbb{D}_a^g \nabla \left(\frac{p_a^g}{p^g} \right) \quad (16.2.6)$$

$$= \frac{M_a M_w}{M_g^2} \mathbb{D}_a^g \nabla \left(\frac{p_w^g}{p^g} \right) = -\mathbf{v}_w^g \quad (16.2.7)$$

where molar mass of the gaseous mixture is given by

$$\frac{1}{M_g} = \frac{\rho_a^g}{\rho^g} \frac{1}{M_a} + \frac{\rho_w^g}{\rho^g} \frac{1}{M_w} \quad (16.2.8)$$

16.2.3 Latent heat effects

The amount of latent heat required to vaporize the liquid pore water is given by

$$\Delta(\rho c) = \frac{n \rho^l S^l h_v}{\Delta T} \quad (16.2.9)$$

16.3 Test example

Problem definition

Hereby, we use a simple plane strain biaxial test to verify the implemented scheme. The sample of the test is homogeneous soil with size of 34cm height and 10 cm width. The set-up of the biaxial compression problem as proposed by [109] is shown in Fig. 16.3.1.

Boundary conditions

The bottom of the specimen is placed in a solid foundation. While the top of it is prescribed a vertical displacement 0.12cm. All boundaries are impervious for fluid flow and heat. The simulation starts with initial conditions of $p^c = 10^5$ Pa and $T = 30^\circ\text{C}$ in the whole domain.

Material properties

We assume that the deformation is plastic and the Drucker-Prager model is adopted. All material parameters are given in Table (16.3.1)

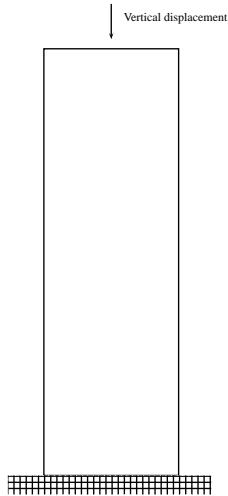


Figure 16.3.1: Plane strain biaxial test

Parameter	Unit	Value
Young's modulus	kPa	3×10^4
Poisson ratio	-	0.4
Parameter α	-	0.326599 (30° friction angle)
Parameter β	-	0.210128 (20° dilatancy angle)
Initial stress σ_0	kPa	29.69 (20 of initial cohesion)
Hardening modulus H	kPa	1000
Permeability	m^2	5×10^{-14}
Solid density	kg/m^3	2000

Table 16.3.1: Material parameters of the plane strain biaxial test

The water content curve, or the capillary-saturation function is depicted in Fig. 16.3.2. The relative permeability of water and gas is shown in Fig. 16.3.3.

Results

Fig. 16.3.4 and Fig. 16.3.5 show the distribution of several state variables in the domain after 12 time steps, when the top displacement reaches 0.12cm. Since there is not any other boundary conditions for flow process, the changes of gas/water pressure and water saturation are induced by the mechanical load solely.

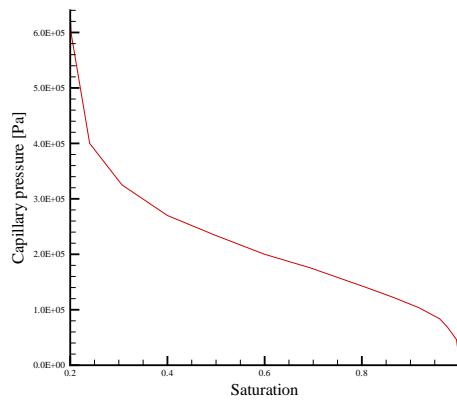


Figure 16.3.2: Capillary saturation function

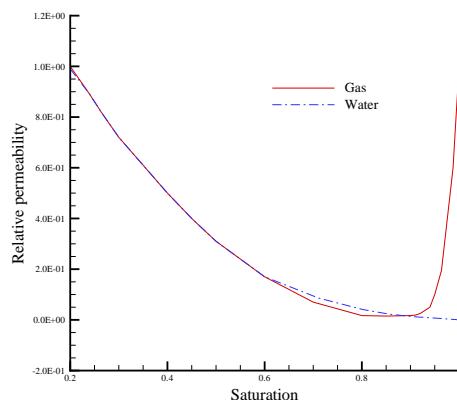


Figure 16.3.3: Vertical reaction of the top

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>th2m_quad</i>	TH2M	benchmarks\TH2M\

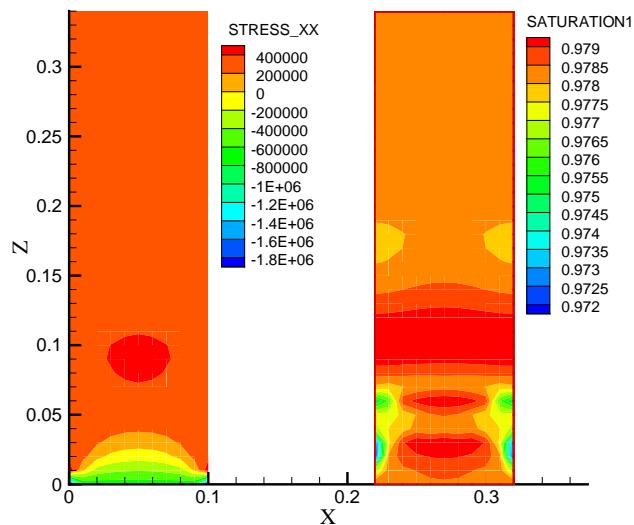


Figure 16.3.4: Distribution of horizontal stress and water saturation.

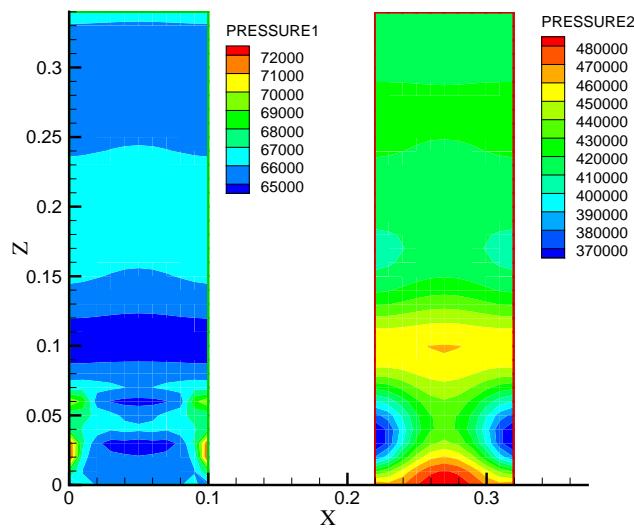


Figure 16.3.5: Distribution of capillary and gas pressure.

Chapter 17

THC-Process

17.1 Theory

The coupling between the simulation of mass transport by GeoSys/RockFlow and the calculation of chemical reactions under equilibrium conditions works by a coupling to the external equilibrium chemical solver PHREEQC. Once the hydraulic and thermal transport has been calculated, the mass transport is solved, the velocity vector being taken from the solution of the hydraulic equations. The concentrations of the species transported and the minerals present are given by the solution of the mass transport equations. The temperature is known from the solution of the heat transport equations. Temperature and concentration of the individual species are passed to PHREEQC (Parkhurst and Appelo 1999). PHREEQC calculates the equilibrium conditions and returns the concentrations of the various phases after reaction (McDermott et al., 2007).

17.2 Repository in crystalline rock with unsaturated bentonite buffer (THC1)

Problem definition

This calculation example, called Task D-THC 1, is done in the framework of the international DECOVALEX project. The model, which is described in the following, is a simplified 1 D benchmark test, which reproduces the processes in a generic repository in saturated crystalline rock where horizontal emplacement tunnels are backfilled with bentonite buffer material (Fig. ??, see chapter 8.1). The horizontal model begins at the left end with the heat source and includes bentonite and granite to the right of this source (Fig. 17.2.1). The model includes simulation of unsaturated flow, heat and mass transport coupled with a consideration of the reactions occurring (McDermott et al., 2007).

Model set-up of the 2 D numerical model

The material parameters for granite and bentonite buffer are given in Tab. ??, but the thermal conductivity of bentonite is set constant with a value of 1.3 W/(m·K) and the heat capacity of bentonite is defined by the following function:

$$c = (1600 \cdot (1.38 \cdot T + 732.5) + 1000 \cdot \Phi \cdot S \cdot 4162) / p.$$

The relationship between capillary pressure and saturation for both of granite and bentonite are depicted in Fig. ???. The relationship between relative permeability and saturation is described in Fig. ???. The model set-up including initial and boundary conditions is given in Fig. 17.2.1. The 1 D model begins from left end ($x = 0.45$ m) to right end ($x = 17.5$ m). It includes bentonite and granite and is discretised into 46 elements. The total simulation time is $1 \cdot 10^6$ years.

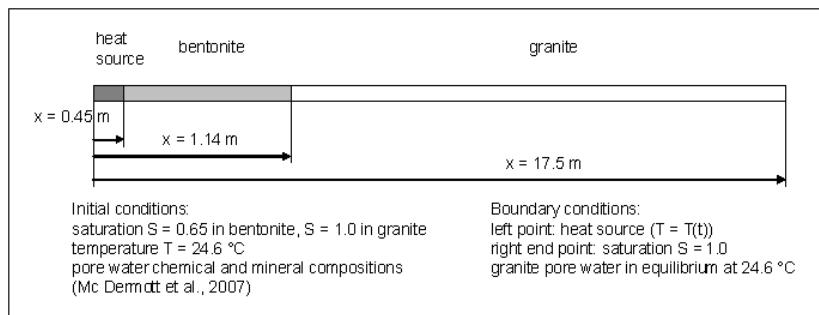


Figure 17.2.1: Calculation model (1 D)

The mineral compositions of granite, bentonite and the related initial as well as equilibrated aqueous chemical compositions of porewater in granite and bentonite are given in McDermott et al. (2007). In granite the minerals Quartz, K-Feldspat, Plagioclase, Annite and Phlogopite are present. In bentonite also Quartz and K-Feldspat can be found, but also the minerals Na-Montmorillonite, Calcite, Dolomite and Pyrite. For mass transport, mass diffusion is included and the coefficients of mass diffusion for all ions and anions are assumed to be the same $1 \cdot 10^{-9}$ m²/s. The minerals are immobile. The geochemically balanced fluid and element concentrations (C, Ca, K, Na, Mg, Cl, Si, Al, S, Fe) are given in McDermott et al. (2007). The geochemical reactions considered in the simulation are aqueous and mineral-solution interactions. The chemical reactions in porewater are taken from the PHREEQC database. The temperature dependence of the reactions was regarded.

Evaluation method

The numerical results of the THC benchmark investigation are compared to those of TOUGH-REACT.

Results

The comparison of the results is presented in Fig. 17.2.2 and Fig. 17.2.3 for the 1000 year simulation case. Significant dissolution and precipitation is predicted at the contact between the different material groups of bentonite and granite. Both models predicted similar mineralogical alterations at the same location and to the same degree (McDermott et al., 2007)

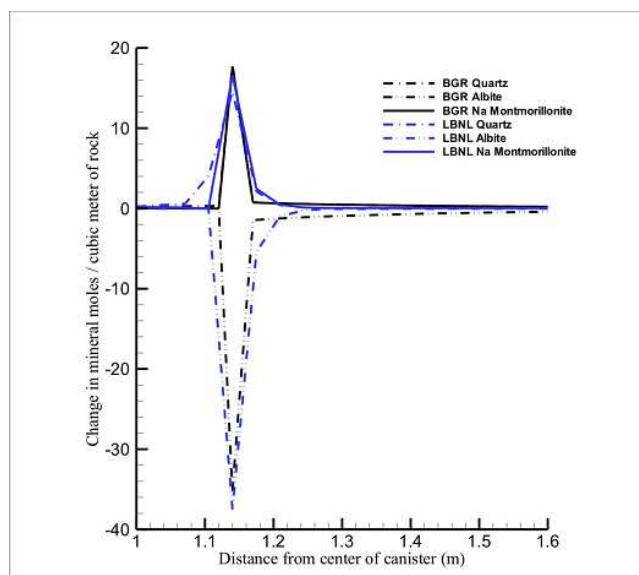


Figure 17.2.2: Deposition of Quartz, Albite and Na-Montmorillonite after 1000 years of emplacement

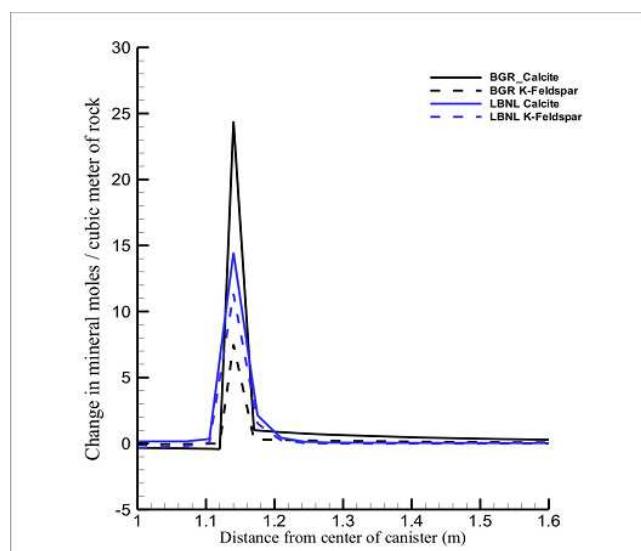


Figure 17.2.3: Deposition of Calcite and K-Feldspat after 1000 years of emplacement

Chapter 18

Density-dependent Flow – HC or THC

18.1 Theory

18.1.1 Governing Equation

The governing equations used for variable density flow consist of three fundamental conservation equations: (i) continuity equation of flow, (ii) momentum equation, and (iii) contaminant transport equation. In addition, these three equations are linked to the equations of the bulk fluid density and the hydrodynamic dispersion equations.

Equation of the Bulk Fluid Density

The linearized equation of the bulk fluid density under an isothermal state was formulated in terms of hydraulic head as,

$$\rho = \rho_0 (1 + \lambda_h (h - h_0) + \lambda_c C) \quad (18.1.1)$$

where h is the hydraulic head, λ is the reference hydraulic head, ρ is the density of fluid, ρ_0 is the reference density of the fluid, λ_h represents the coefficient of compressibility of the fluid associated with the change of the hydraulic head at constant mass fraction of the solute, λ_c is the coefficient of expansivity resulting from the change of the mass concentration of the solute at constant hydraulic head, and C is the relative concentration.

The relationship between density and concentration can also be approximated using other representations such as an exponential function as given by Kolditz

et al. [1998]. The equations describing the relationship between density and other relevant parameters are formulated based on experiments and are approximate relationships.

Another equation for describing the relationship between density and concentration (or mass fraction) is provided by Herbert et al. [1988] and used by Oldenburg and Pruess [1995]. This equation was derived from the assumption that when two liquids are well mixed, the masses or the volumes of respective components are additive. In this study, among these equations which describe the relationship between density and concentration, the linear equation obtained from the experiments is chosen to describe the relation between the bulk fluid density and concentration.

Continuity Equation of Flow

The macroscopic mass balance equation of the fluid averaged over a representative elementary volume (REV) in a porous medium is

$$\frac{\partial (S\phi\rho)}{\partial t} + \nabla \cdot (\phi\rho\vec{v}) = \rho Q_\rho \quad (18.1.2)$$

where S is the saturation ratio, ϕ is the porosity, t is the time, \vec{v} is the fluid velocity vector, and ρQ_ρ is the source term of the fluid mass in an aquifer. Based on Equation 18.1.2, the flow equation for a variably saturated porous medium can be written in terms of hydraulic head and mass concentration,

$$\phi \frac{\partial S}{\partial t} + SS_0^h \frac{\partial h}{\partial t} + S\phi\lambda_C \frac{\partial C}{\partial t} + \nabla \cdot \vec{q} + \lambda_c \vec{q} \cdot \nabla C = Q_\rho \quad (18.1.3)$$

where S_0^h is the specific storativity of a porous medium with respect to hydraulic head change and \vec{q} is the Darcy velocity vector. The head-based flow equation, Equation 18.1.3, has the advantage over pressure-based flow equations because numerically large static pressures may dominate the dynamic pressure differences that cause motion. The resulting pressure-based numerical scheme may therefore operate at less than optimum numerical efficiency. A more efficient way is to write the flow equation in terms of a quantity that can be directly related to the driving forces. Such a quantity is the equivalent freshwater hydraulic head, defined as $h = \frac{p}{\rho_0 g} + z$ [Frind, 1982].

Momentum Equation of Flow (the Darcy Equation) and Dispersive Flux

The momentum balance equation for variable-density fluid flow in a porous medium in terms of hydraulic head can be given as

$$\vec{q} = \phi \vec{v} = -\frac{\hat{k} \rho_0 \vec{g}}{\mu} \left(\nabla h + \left(\frac{\rho - \rho_0}{\rho_0} \right) \vec{e} \right) \quad (18.1.4)$$

where \hat{k} is the tensor of permeability of a porous medium and \vec{e} is the unit vector in the gravitational direction. The dispersion tensor can be written as Bear [1979]

$$\hat{D} = \gamma D_m \hat{\delta} + \alpha_T |v| \hat{\delta} + (\alpha_L - \alpha_T) \frac{\vec{v}_i \vec{v}_j}{|v|} \quad (18.1.5)$$

where γ is the tortuosity, D_m is the coefficient of molecular diffusion, $\hat{\delta}$ is the Kronecker-delta (unit tensor), α_T is the transverse dispersivity, v is the characteristic value of macroscopic velocity, α_L is the longitudinal dispersivity, and i and j are the velocities in and directions respectively.

Contaminant Transport Equation

The solute transport with a source is governed by the following advection-dispersion equation

$$\frac{\partial(\phi C)}{\partial t} + \nabla \cdot (\phi \vec{v} C) - \nabla \cdot (\phi \hat{D} \cdot \nabla C) = Q_C \quad (18.1.6)$$

where Q_C is the source term of the solute in terms of mass concentration. Ignoring the expansivity resulting from the change of mass concentration λ_C , Equation 18.1.6 can be written as follows

$$\phi \frac{\partial C}{\partial t} + (1 - \phi) \lambda_h C \frac{\partial h}{\partial t} + \phi \vec{v} \cdot \nabla C - \nabla \cdot (\phi \hat{D} \cdot \nabla C) + C Q_\rho = Q_C \quad (18.1.7)$$

Kolditz et al. [1998] defined approximation level of density variations in the mass equations when Equation 18.1.2 and 18.1.6 are expanded.

18.2 The Elder Problem

Benchmark name: *elder*.

Purpose: To verify density-dependent flow such as free convection, seawater intrusion, and possibly enhanced gas recovery with CO₂.

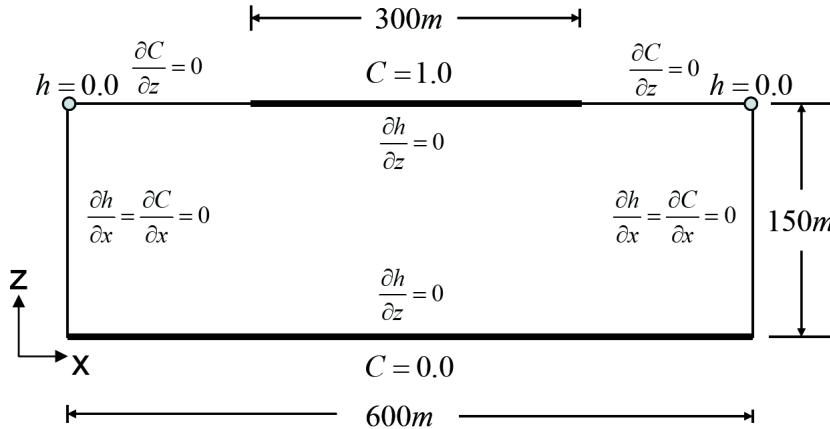


Figure 18.2.1: Boundary conditions of the Elder problem

Model description: The elder problem is a good example of free convection phenomena, where the fluid flow is driven purely by the density differences of the fluids. Figure 18.2.1 illustrates the boundary conditions of the Elder problem. Table 18.2.1 presents the specific parameters for the Elder problem used in this application.

Symbol	Quantity	Value	Unit
D_m	Molecular diffusion coefficient	3.565e-6	$m^2 s^{-1}$
k	Permeability	4.845e-13	m^2
μ	Dynamic viscosity	10e-6	$kg m^{-1} s^{-1}$
g	Gravitational coefficient	9.81	ms^{-2}
α_L, α_T	Longitudinal and transverse dispersivity	0, 0	m
ϕ	porosity	0.1	—
ρ_0, ρ_s	Density of water and saltwater	(1,1.2)e3	$kg m^{-3}$

Table 18.2.1: Parameters for the Elder problem

Results: The mesh was created with hexahedral elements for further expansion to 3D applications. The grid density level is defined as the l th level that consists of 2^{2l+1} identical square elements. Based on the definition of the grid density, the number of the hexahedral elements is 8192. The isochlor is defined as a ratio of a density difference to the maximum density difference. Figure 18.2.2 shows the numerical results obtained from GeoSys/RockFlow as the solution of the Elder problem

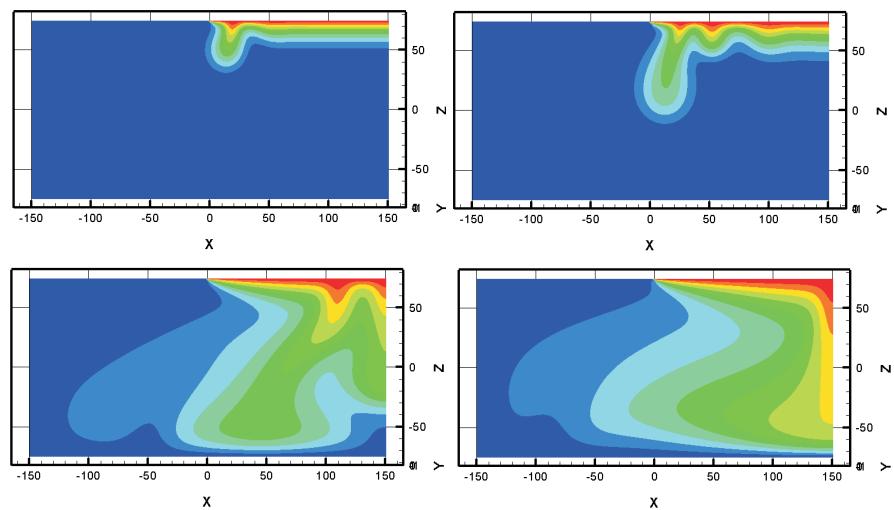


Figure 18.2.2: Isochlors of the Elder problem for 1, 2, 10, and 20 year at regular grid of level 6

Chapter 19

Isothermal two-phase flow – HH-Process

We consider isothermal two-phase flow processes in (sec.19.1). There are several formulations for simulating isothermal two-phase flow systems for instance isothermal two-phase flow system with respect to primary variables: (1) pressure-pressure, (2) pressure-saturation, and (3) saturation-saturation formulation.

19.1 Isothermal two-phase flow

Here we just ignored temperature effect and treated partially saturated sample as isothermal two-phase system composed of constituents with the voids of the solid skeleton filled with two immiscible fluid of two different phase, compressible gas with single component as air and incompressible liquid with single component as water. In the pressure-pressure formulation primary variables are gas pressure p^g , and capillary pressure p^c , whereas in pressure-saturation formulation primary variables are non-wetting phase saturation S_{nw} , and wetting phase pressure p_w .

19.1.1 Mass balance equation

Consider two-phase flow in porous media, e.g liquid (denoted by l) and gas (denoted by g). For each phase in two-phase fluid flow, the mass conservation is given by the following equation:

$$\frac{\partial}{\partial t} (nS^g \rho_k^g + nS^l \rho_k^l) + \nabla \cdot (\mathbf{J}_k^g + \mathbf{J}_k^l) = Q_k \quad (19.1.1)$$

where S is saturation, ρ stands for phase density, n is the porosity, \mathbf{J} is total flux. The subscript k in equation (19.1.1) denotes the components of phase, e.g

air ($k = a$) and water ($k = w$). For any phase $\gamma = (g, l)$, an advection vector $\mathbf{J}_{A_k}^\gamma$ and a diffusion vector $\mathbf{J}_{D_k}^\gamma$ makes up a total flux, i.e

$$\mathbf{J}_k^\gamma = \mathbf{J}_{A_k}^\gamma + \mathbf{J}_{D_k}^\gamma \quad (19.1.2)$$

According to the Darcy's equation, the advective part of the total flux be written as

$$\mathbf{J}_{A_k}^\gamma = -\rho_k^\gamma \frac{\mathbf{k} k_{rel}^\gamma}{\mu^\gamma} (\nabla p^\gamma - \rho^\gamma \mathbf{g}) \quad (19.1.3)$$

where \mathbf{k} is the intrinsic permeability, k_{rel}^γ is the relative permeability of the phase, and μ^γ is the viscosity.

The diffusion part of the total flux is given by Fick's law as

$$\mathbf{J}_{D_k}^\gamma = -n S^\gamma \rho^\gamma \mathbb{D}_k^\gamma \nabla \left(\frac{\rho_k^\gamma}{\rho^\gamma} \right) \quad (19.1.4)$$

where \mathbb{D} is a diffusion parameters in the terms of tensor. Since $\rho^\gamma = \rho_a^\gamma + \rho_w^\gamma$, we have

$$\mathbf{J}_{D_w}^\gamma + \mathbf{J}_{D_a}^\gamma = \mathbf{0} \quad (19.1.5)$$

under the assumption of $\mathbb{D}_a^\gamma = \mathbb{D}_w^\gamma$

Consider water-air mixture. We expand the mass balance equation (19.1.1) with the flux defined in equations (19.1.2) based upon the above equations (19.1.2, 19.1.3, 19.1.4). For water component, the diffusion part of the total flux take the form

$$\mathbf{J}_{D_w}^l = -n S^l \rho^l \mathbb{D}_w^l \nabla \left(\frac{\rho_w^l}{\rho^l} \right), \quad \mathbf{J}_{D_w}^g = -n S^g \rho^g \mathbb{D}_w^g \nabla \left(\frac{\rho_w^g}{\rho^g} \right) \quad (19.1.6)$$

Obviously, $\mathbb{D}_w^l = \mathbf{0}$. Therefore, the mass balance equation for water component can be written as follows

$$\begin{aligned} & \frac{\partial}{\partial t} (n S^g \rho_w^g + n S^l \rho_w^l) - \nabla \cdot \left[\rho_w^l \frac{\mathbf{k} k_{rel}^l}{\mu^l} (\nabla p^l - \rho^l \mathbf{g}) \right] \\ & - \nabla \cdot \left[\rho_w^g \frac{\mathbf{k} k_{rel}^g}{\mu^g} (\nabla p^g - \rho^g \mathbf{g}) \right] - \nabla \cdot \left[n S^g \rho^g \mathbb{D}_w^g \nabla \left(\frac{\rho_w^g}{\rho^g} \right) \right] = Q_w \end{aligned} \quad (19.1.7)$$

Since the capillary pressure p^c is chosen as one of the two unknowns of equation (19.1.1) and $S^g = 1 - S^l$, equation (19.1.7) becomes

$$\begin{aligned} & n(\rho_w^l - \rho_w^g) \frac{\partial S^l}{\partial t} + (1 - S^l)n \frac{\partial \rho_w^g}{\partial t} - \nabla \cdot \left[\rho_w^l \frac{\mathbf{k} k_{rel}^l}{\mu^l} (\nabla(p^g - p^c) - \rho^l \mathbf{g}) \right] \\ & - \nabla \cdot \left[\rho_w^g \frac{\mathbf{k} k_{rel}^g}{\mu^g} (\nabla p^g - \rho^g \mathbf{g}) \right] - \nabla \cdot \left[n S^g \rho^g \mathbb{D}_w^g \nabla \left(\frac{\rho_w^g}{\rho^g} \right) \right] = Q_w \end{aligned} \quad (19.1.8)$$

Similar to the previous procedure, the diffusion part of the total flux of air component can be written as

$$\mathbf{J}_{D_a}^l = -nS^l \rho^l \mathbb{D}_a^l \nabla \left(\frac{\rho_a^l}{\rho^l} \right), \quad \mathbf{J}_{D_a}^a = -nS^g \rho^g \mathbb{D}_a^g \nabla \left(\frac{\rho_a^g}{\rho^g} \right) \quad (19.1.9)$$

The density shift from air component to liquid ρ_a^l is very small and can be omitted. Therefore, we can assume $\mathbf{J}_{D_a}^l \approx 0$. As a consequence, the mass balance equation for air component is derived as:

$$\begin{aligned} & \frac{\partial}{\partial t} (nS^g \rho_a^g) - \\ & \nabla \cdot \left[\rho_a^g \frac{\mathbf{k}k_{rel}^g}{\mu^g} (\nabla p^g - \rho^g \mathbf{g}) \right] - \nabla \cdot \left[nS^g \rho^g \mathbb{D}_a^g \nabla \left(\frac{\rho_a^g}{\rho^g} \right) \right] = Q_a \end{aligned} \quad (19.1.10)$$

Expanding the temporary derivative term of equation (19.1.10) yields

$$\begin{aligned} & -n\rho_a^g \frac{\partial S^l}{\partial t} + (1 - S^l)n \frac{\partial \rho_a^g}{\partial t} - \\ & \nabla \cdot \left[\rho_a^g \frac{\mathbf{k}k_{rel}^g}{\mu^g} (\nabla p^g - \rho^g \mathbf{g}) \right] - \nabla \cdot \left[nS^g \rho^g \mathbb{D}_a^g \nabla \left(\frac{\rho_a^g}{\rho^g} \right) \right] = Q_a \end{aligned} \quad (19.1.11)$$

Mass balance equations (19.1.8) and (19.1.11) are exactly the same as that described in [109].

19.1.2 Pressure-pressure (pp) scheme

Based on the description of the isothermal two-phase flow in (sec.19.1); (19.1.8) and (19.1.11) can be modified in order to get governing equation for isothermal two-phase flow in a porous medium. In this formulation primary variables are gas pressure p^g , and capillary pressure p^c .

Basic equations of the isothermal two-phase flow system:

$$n\rho_w \frac{\partial S_w}{\partial p_c} \dot{p}_c + \nabla \cdot \left[\rho_w \frac{\mathbf{k}k_{relw}}{\mu_w} (-\nabla p^g + \nabla p^c + \rho_w \mathbf{g}) \right] = Q_w \quad (19.1.12)$$

$$\begin{aligned} & -n\rho_a \frac{\partial S_w}{\partial p_c} \dot{p}_c + n(1 - S_w) \left(\frac{\partial \rho_a}{\partial p^g} \dot{p}^g + \frac{\partial \rho_a}{\partial p_c} \dot{p}_c \right) + \\ & \nabla \cdot \left[\rho_a \frac{\mathbf{k}k_{rela}}{\mu_a} (-\nabla p^g + \rho_a \mathbf{g}) \right] = Q_a \end{aligned} \quad (19.1.13)$$

19.1.3 Pressure-saturation (pS) scheme

Based on the description of the isothermal two-phase flow in (sec.19.1); (19.1.8) and (19.1.11) can be modified in order to get governing equation for isothermal two-phase system. This formulation is based on total pressure. Primary variables of this formulation are wetting phase pressure p_w , and non-wetting phase saturation S_{nw} .

In addition, governing equations of the isothermal two-phase system is also based on following assumptions:

- Assumption: Immiscible (fractional) flow
- Macroscopic mass balance equation
 1. Pressure: p_w
 2. Saturation: S_{nw}
- Darcy law: Momentum equation
 1. Mobility by the relation between saturation and relative permeability
- Equation of the state
 1. Density is same for both wetting and non-wetting phase with a constant value

19.1.4 Liakopoulos experiment

Problem definition

This benchmark is based on an experiment by Liakopoulos [110] and is proposed by Lewis and Schrefler [102](pp 167–174). The Liakopoulos test case is already described and used for unsaturated consolidation in section 13.3.2. There you can find the complete problem definition.

The benchmark is simulated with different element types using the pressure-pressure scheme. The grids used in such simulations are illustrated in Fig. 19.1.1.

Results

The temporal evolution of vertical profiles of primary variables capillary and gas pressures are given in Fig. 19.1.2. Fig. 19.1.3 shows the vertical profiles for water saturation as a secondary variable. The results agree well with the findings by Lewis and Schrefler [102].

The results of the element test are depicted in Fig. 19.1.4 for capillary pressure. A comparison if the results between the two-phase flow model and the Richards model used in section 13.3.2 can be seen in Fig. 13.3.4.

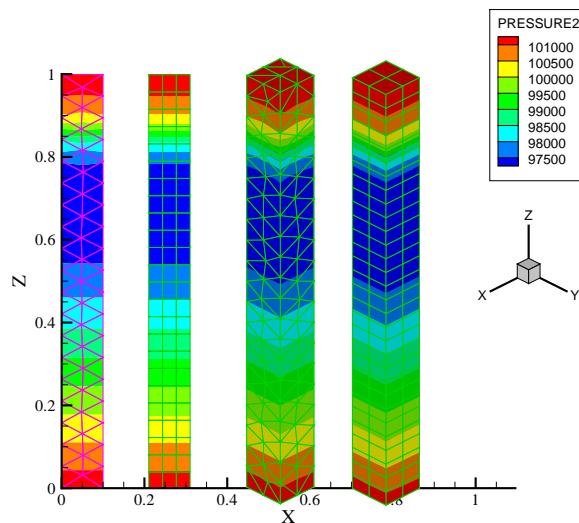


Figure 19.1.1: Grids with different element types for the Liakopoulos benchmark

Property	Symbol	Value	Unit
Porosity	n	—	2.975×10^{-1}
Permeability	κ	m^2	4.5000×10^{-13}
Liquid dynamic viscosity	μ_w	$Pa.s$	1.0000×10^{-3}
Gas dynamic viscosity	μ_a	$Pa.s$	1.8×10^{-5}
Liquid density	ρ_w	$kg.m^{-3}$	1.0000×10^3
Gas density	ρ_a	$kg.m^{-3}$	Ideal Gas Law's
Capillary pressure	p^c	Pa	Experimental Curve
Relative permeability	κ_{relw}	—	Experimental Curve
Relative permeability	κ_{rela}	—	Brook-Corey functions

Table 19.1.1: Material parameters for the Liakopoulos problem.

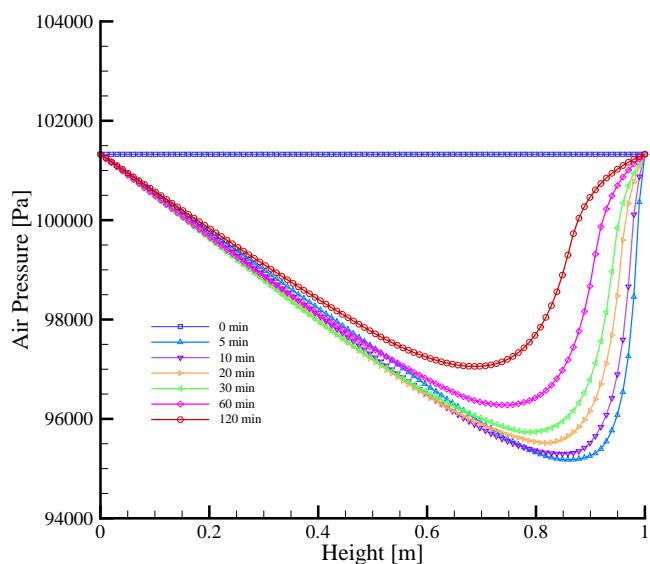
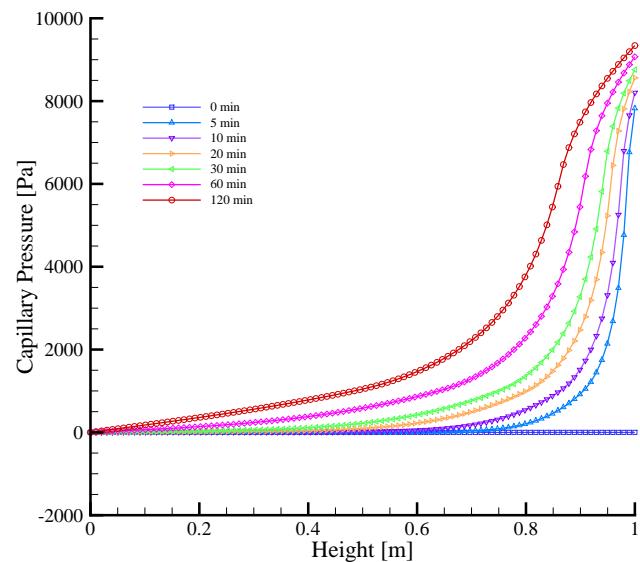


Figure 19.1.2: Vertical profiles of capillary (top) and gas pressures (bottom)

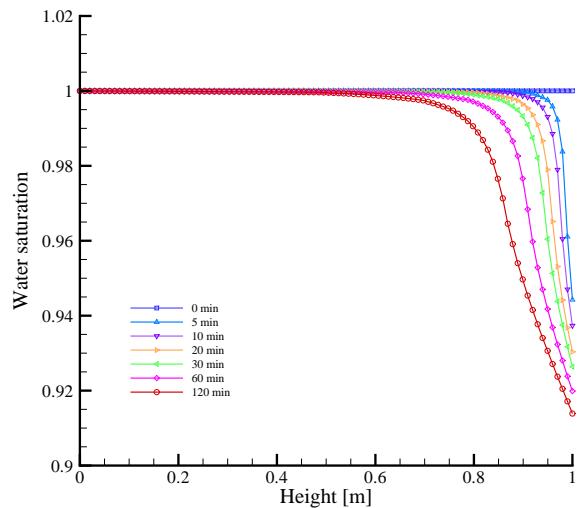


Figure 19.1.3: Water profile of water saturation

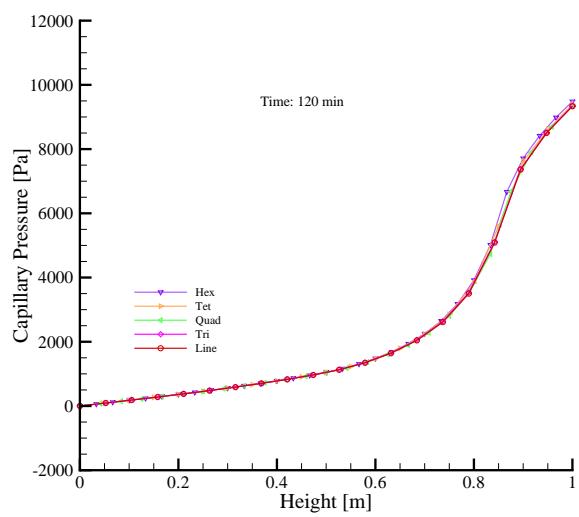


Figure 19.1.4: Results of element test

19.1.5 Buckley-Leverett problem

Theory

Buckley and Leverett [93] developed semi-analytical solution for the displacement of two immiscible fluids in porous media. Assuming constant fluid density (i.e. liquid flow), porosity, and no source/sink terms the fluid mass balance equation can be simplified.

$$n \frac{\partial S^\gamma}{\partial t} = -\nabla \cdot \mathbf{q}^\gamma \quad (19.1.14)$$

Buckley and Leverett derived the following expression

$$\frac{\partial S^l}{\partial f^l} = \frac{q_{tot}}{n} \frac{\Delta t}{\Delta x} \quad (19.1.15)$$

with the fractional flow function $f^\gamma = q^\gamma / q_{tot}$

$$f^1 = \left(1 + \frac{\mu_1}{k_1} \frac{k_2}{\mu_2} \right)^{-1} \quad (19.1.16)$$

1 and 2 are the fluid phase numbers. The position of the shock front separating the two fluid phases can be calculated from the following expression.

$$\Delta x = -\frac{q_{tot}}{n} \frac{\partial f^l}{\partial S^l} \quad (19.1.17)$$

Buckley and Leverett suggested that the capillary pressure is a function of the saturation only. Note that the original Buckley-Leverett considered the water and oil phase flow. Moreover, they assumed that the condition that the derivative of the capillary pressure with respect to the saturation is zero ($dp_{cwo}/dp_{cwo} = 0$) is a sufficient approximation that both gradients of water and oil are equal each other.

$$\frac{\partial p_w}{\partial x} = \frac{\partial p_o}{\partial x} + \frac{\partial p_{cwo}}{\partial x} = \frac{\partial p_o}{\partial x} + \frac{dp_{cwo}}{dS^w} \frac{\partial S^w}{\partial x} = \frac{\partial p_o}{\partial x} \quad (19.1.18)$$

Problem definition

The Buckley Leverett problem is frequently used to test numerical models for the functional relation between relative permeability and saturation. In comparison to the analytical solution, the problem is simplified to describe one fluid displacing the other residing fluid in aquifers or reservoirs. In the derivation of the analytical solution, the effect caused by capillary forces between two fluids is not considered.

A non-wetting phase displaces a wetting phase from left to right. The initial total velocity of the two-phase system is 1.0 m/s . The ratio of the dynamic viscosities is one, residual saturations are zero and the Brooks-Corey function ($\lambda = 2$) is used for the relative permeabilities. A space-time discretization of delta x = 0.025 m and delta t = 0.005 . The total simulation time is 0.4 s .

PS-Global

Saturation equation, the mass conservation equation is converted to the volumetric one by dividing with fluids density.

$$n \frac{\partial S_w}{\partial t} - \nabla \cdot \left(\frac{\mathbf{k} k_{relw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g}) \right) = q_w \quad (19.1.19)$$

$$n \frac{\partial S_{nw}}{\partial t} - \nabla \cdot \left(\frac{\mathbf{k} k_{relnw}}{\mu_{nw}} (\nabla p_{nw} - \rho_{nw} \mathbf{g}) \right) = q_{nw} \quad (19.1.20)$$

A new BL result is obtained by GeoSys multiphase module that solves in a global-implicit scheme. As shown in the figure, the global-implicit scheme produces more accurate result compared to that obtained by the sequential-coupling scheme. The result has little oscillation and is closer to the analytical solution particularly in the location of the sharp front of the intruding fluid.

One thing important to note is that the global scheme is sensitive to matrix solvers. LIS solver (BiCG with Jacobi preconditioner) works on Windows. However, this iterative solver for this benchmark takes much more time than the PARDISO (a parallel direct solver) that works only on Unix with GeoSys.

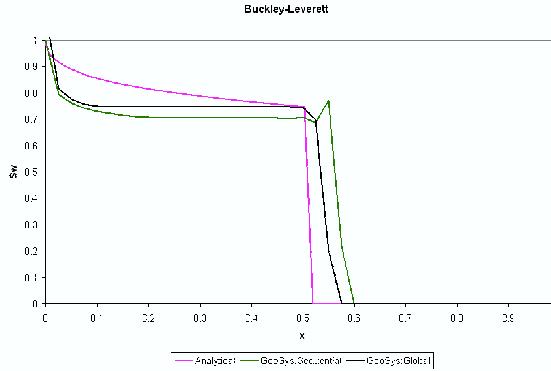


Figure 19.1.5

PS-Sequential

Adding (19.1.19) and (19.1.20) with using the relation $S_{nw} + S_w = 1$ and $p^c(S_w) = p_{nw} - p_w$, we get equation for wetting phase pressure, p_w and non-wetting phase saturation, S_{nw} .

$$-n \frac{\partial S_{nw}}{\partial t} - \nabla \cdot \left(\frac{\mathbf{k} k_{relw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g}) \right) = q_w \quad (19.1.21)$$

$$\nabla \cdot \left(\frac{\mathbf{k}k_{relw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g}) \right) + \nabla \cdot \left(\frac{\mathbf{k}k_{relnw}}{\mu_{nw}} (\nabla p_w + p_c - \rho_{nw} \mathbf{g}) \right) + q_w + q_{nw} = 0 \quad (19.1.22)$$

In (19.1.21), non-wetting phase saturation, S_{nw} can be easily solved explicitly with the known pressure obtained from (19.1.22).

The analytical solution for the frontal location of the infiltrating fluid is derived and found there is the discrepancy with previous results (Helmig and Huber 1998, Figure 9). In contrast to the previous results, the standard Galerkin-type method does tend to produce overestimated frontal infiltrating locations compared against the analytical solution. This can be explained by the diffusion term of the saturation originally omitted in the BL equation that makes purely advective transport. Handling this purely advective transport in general by the numerical models does introduce the numerical dispersion term naturally, and this added numerical dispersion can be interpreted by the saturation diffusion term.

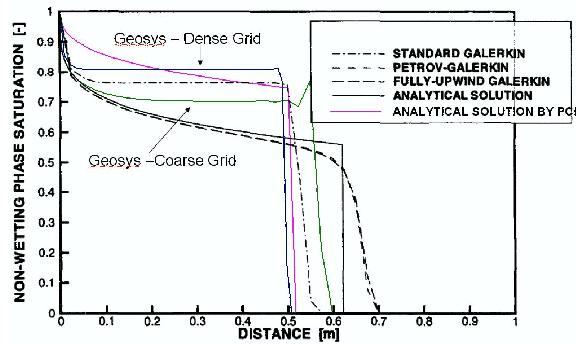


Figure 19.1.6

Problem definition

Buckley and Leverett developed semi-analytical solution for the displacement of two immiscible fluid in porous media. Assume saturated CO_2 displacing H_2O with constant fluid properties.

Results

Here, we show the saturation profile, S_w in Fig. 18.1.7 along 1 m column calculated with line element with space-time discretization of $\delta x = 0.025$ m and $\delta t = 0.005$ s. The total simulation time is 0.4 s; using the total-pressure-based pS-GLOBAL. Based on linear relation between saturation and relative permeability, saturation profile, S_w is shown in Fig. 18.1.8.

Property	Symbol	Value	Unit
Column length	L	m	1.0
Porosity	n	—	2.0×10^{-1}
Permeability	κ	m^2	1.0×10^{-10}
Water dynamic viscosity	μ_w	$Pa.s$	1.0×10^{-3}
Gas dynamic viscosity	μ_{nw}	$Pa.s$	7.0343×10^{-4}
Water density	ρ_w	$kg.m^{-3}$	1.0×10^3
Gas density	ρ_{nw}	$kg.m^{-3}$	7.73×10^2
Capillary pressure	$p^c(S)$	Pa	0
Relative permeability	$\kappa_{rel}(S)$	—	Brook-Corey functions

Table 19.1.2: Material parameters for the BL problem.

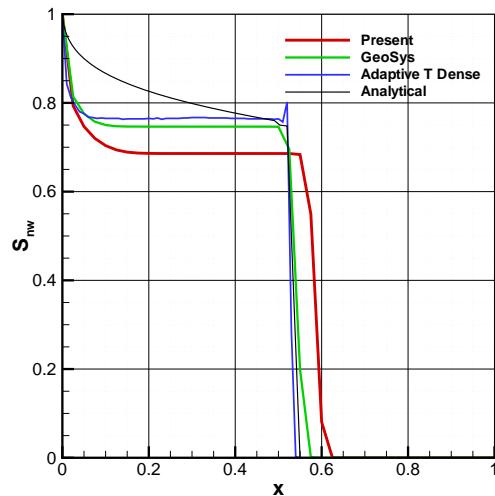


Figure 19.1.7: Saturation profile obtained with present analysis along with others.

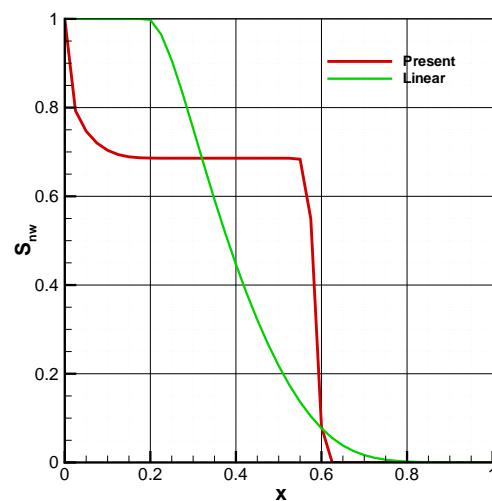


Figure 19.1.8: Saturation profile obtained with present analysis along with linear permeability and saturation relation.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>hm_unsat</i>	HH	MULTIPHASE

19.1.6 McWhorter problem

Theory

It is assumed that the flow of both wetting and non-wetting phases can be adequately described by the Dary's law if the phases are immiscible and incompressible.

$$n \frac{\partial S^\gamma}{\partial t} + \nabla \cdot \mathbf{q}^\gamma = 0, \gamma = w, nw \quad (19.1.23)$$

$$\mathbf{q}^\gamma = -\mathbf{K} \lambda^\gamma \nabla p^\gamma \quad (19.1.24)$$

where λ_w and λ_{nw} are mobility of wetting and non-wetting fluid. Both phase are linked by the state equation $S_w + S_{nw} = 1$ and $p_c = p_g - p_w$. Here total flux, $\mathbf{q}_t = \mathbf{q}_w + \mathbf{q}_{nw}$ once p_c is function of the S_w .

A formulation that is often used for two phase flow problem is so called fractional flow model. One of the attractive of this formulation is that the model become more accesible to analysis. Substracting equation (18.1.24) for both phases we have.

$$\mathbf{q}_w = f \mathbf{q}_t - D \frac{\partial S_w}{\partial x} \quad (19.1.25)$$

where

$$f = \frac{1}{1 + \frac{\lambda_{nw}}{\lambda_w}}, \quad D = -\lambda_{nw} f \frac{\partial p_c}{\partial S_w}$$

First term on the right of equation (19.1.25) is dictated by rate at which flux is injected on the boundary and second term represent the addition impelling force due to gradient of capillary pressure. Put equation (19.1.25) in equation (18.1.23) for wetting phase and assume that total flux, \mathbf{q}_t is space invariant.

$$\frac{\partial}{\partial x} \left(D \frac{\partial S_w}{\partial x} \right) - \mathbf{q}_t \frac{\partial f}{\partial S_w} \frac{\partial S_w}{\partial x} = n \frac{\partial S_w}{\partial t} \quad (19.1.26)$$

In the last benchmark (Buckley and Leveret) it is assume that force due to gradient of capillary pressure is very small as consequence of total flux, \mathbf{q}_t is large hence suressed the second order term in the equation.

Knowing the capilarity effect, model verification need a comparision with an analytical solution based on one by McWhorter and Sunada (1990). They developed an exact quasi-analytical solution of equation (19.1.26) for unidirectional displacement where non-wetting phase by wetting phase using the concept of a fractional flow function.

The fractional flow function is defined as ratio of wetting phase flux, \mathbf{q}_w to the total flux, \mathbf{q}_t . It has shown that this ratio is function of S_w only, when \mathbf{q}_t is inverselly prposanal to square root of the time.

Problem definition

The test benchmark problem for capillary effects is formulated as if the instantaneous displacement occurs in one-dimensional horizontal reservoir initially occupied by oil. Solution has been obtained through solving the governing equations (18.1.12) and (18.1.13) by pressure-pressure scheme described in sec (sec.19.1.2). Different from the Buckley-Leverett problem, here flow is governed by capillary force when water saturation at the left end of the horizontal column is kept to be one, while the right end is kept to be no flux at all. So for no source term is accounted.

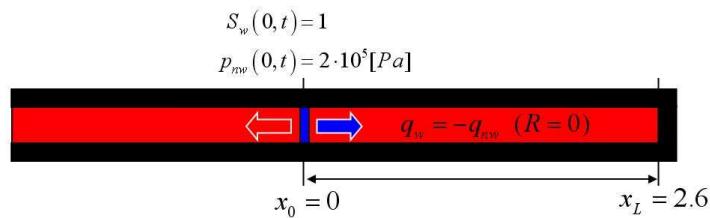


Figure 19.1.9: Schematic of the benchmark formulated to test McWhorter and Sunada's analytical solution.

Results

Based on the above discussion GeoSys produces agreeable solution. Fig. 18.1.10 shows water saturation profile, S_w with a fine grid along with 2.6m long horizontal column for different time steps. Line elements have been used with time and space discretization $\delta t = 0.5\text{s}$ and $\delta x = 0.05\text{m}$ respectively.

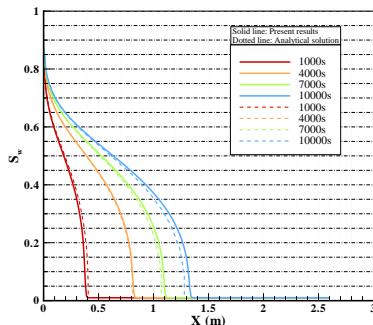


Figure 19.1.10: Water saturation, S_w profile of the present result along with analytical solution based on one by McWhorter.

Here, we have solved exactly same problem using the total-pressure-based saturation model in sequential iterative coupling scheme.

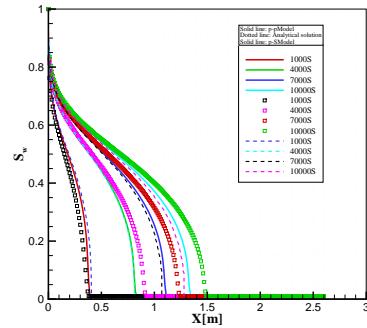


Figure 19.1.11: Water saturation, S_w profile in sequential iterative coupling scheme.

Unlike the pressure-pressure model, one downside for the total-pressure-based saturation model is less accurate for the problems dominated by capillarity (see Fig. 18.1.11). Since the pressure-pressure model directly solves for capillary pressure as a primary variable, the model has an advantage for the capillary related problems. On the other hand, the total-pressure-based saturation model is limited to the problems when dP_c/dS_w is close to zero. The condition for dP_c/dS_w close to zero caused physically in the cases of fractures, shear zones and transitions between heterogeneities.

Property	Symbol	Value	Unit
Column length	L	m	2.6
wetting dynamic viscosity	μ_w	$Pa.s$	1.0×10^{-3}
non-wetting dynamic viscosity	μ_{nw}	$Pa.s$	1.0×10^{-3}
wetting phase density	ρ_w	$kg.m^{-3}$	1.0×10^3
Non-wetting phase density	ρ_{nw}	$kg.m^{-3}$	1.0×10^3
Permeability	K	m^2	1.0×10^{-10}
Porosity	n	--	3.0×10^{-1}
Residual saturation of water	S_{rw}	--	0
Residual saturation of oil	S_{nrw}	--	0
Entry pressure	p_d	Pa	5.0×10^3
Soil distribution index	λ	--	2.0
Capillary pressure	$p^c(S_{eff})$	Pa	Brooks-Corey model
Relative permeability	$\kappa_{rel}(S_{eff})$	--	Brooks-Corey model

Table 19.1.3: Material parameters for the McWhorter problem.

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>mcut</i>	H2	McWhorter

19.1.7 Kueper problem

Theory

The former two benchmarks (Buckley-Leverett and McWorter) used for verification, both schemes are further tested for model validation with the benchmark chosen to test two-phase flow in heterogeneous media. Kueper and Frind (1991) developed the model to simulate their experiment for DNAPL penetration (Kueper et al., 1989). The simultaneous movement of a dense nonwetting phase (DNAPL) through an initially wetting phase (water) saturated heterogeneous porous media may be represented mathematically as a case of two-phase flow. A distinctive feature of the solution is that the primary variables solved for, wetting phase pressure and wetting phase saturation, are both existent throughout the solution domain regardless of whether the nonwetting phase is present.

The continuity equation of each phase (γ) can be defined by

$$\frac{\partial(n\rho^\gamma S^\gamma)}{\partial t} + \nabla \cdot (\rho^\gamma \mathbf{q}^\gamma) = \mathbf{Q}^\gamma, \gamma = w, nw \quad (19.1.27)$$

where n is porosity, S^γ is saturation, ρ^γ is density, \mathbf{Q}^γ is a source or sink term, and \mathbf{q}^γ is the Darcy velocity for phase γ defined by

$$\mathbf{q}^\gamma = -\mathbf{K} \frac{\kappa_r^\gamma}{\mu^\gamma} (\nabla p^\gamma - \rho^\gamma \mathbf{g}), \gamma = w, nw \quad (19.1.28)$$

where κ_r^γ is relative permeability, μ^γ is viscosity, p^γ is pressure for phase γ , \mathbf{K} is intrinsic permeability tensor and \mathbf{g} is the gravitational vector.

Inherently for saturation, the sum of all saturation in pore space is

$$\sum S^\gamma = 1 \quad (19.1.29)$$

Assuming relative preference (i.e., wettability) of the fluid to media exists and it is not negligible, the capillary pressures relation for a two-phase system is defined over representative elementary volume (REV) by

$$p_c = p_{nw} - p_w \quad (19.1.30)$$

where p_c is capillary pressure, p_{nw} is pressure for the non-wetting phase fluid and p_w is the wetting phase fluid.

Problem definition

A $60\text{cm} \times 80\text{cm} \times 0.6\text{cm}$ parallel-plate glass-lined cell was packed with four types of sands and initially fully saturated with water. The configuration of the assembled sand lenses and the two sets of the boundary conditions for the $p_w - S_{nw}$ and $p_c - p_{nw}$ schemes are illustrated in Figure 18.1.12. Concerning to the constitutive relation between relative permeability and saturation and capillary pressure and saturation, they have used the Brooks-Corey model.

Properties of Sands for the Brooks-Corey model are measured experimentally and summarized in table. The numerical solutions obtained from the $p_w - S_{nw}$ scheme and the $p_c - p_{nw}$ scheme for the benchmark Kueper and Frind (1991) are compared against each other in Figure 18.1.13.

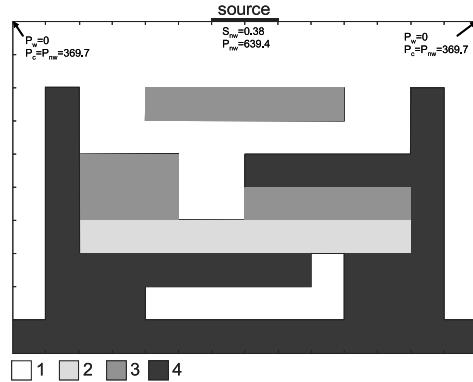


Figure 19.1.12: Configuration of heterogeneous media in parallel-plate cell.

Fluid and medium properties with numerical space and time discretization.

Fluid properties	Unit	Wetting fluid	Non-wetting fluid
Density	$kg.m^{-3}$	1.0×10^3	1.0×10^3
Viscosity	$Pa \cdot s$	1.0×10^{-3}	1.0×10^{-3}
Residual saturation	-	0.0	0.0
Maximum saturation	-	1.0	1.0

Medium properties	Unit	Medium
Δx	m	0.01
Δt	s	100
Porosity	-	0.3
Intrinsic permeability	m^2	1×10^{-10}
Brook-Corey's index	-	2
Entry pressure	Pa	5×10^3

Hydraulic properties of sands for the Brooks-Corey model.

Property	P_d (Pa)	λ (-)	S_{wr} (-)	$k(m^2)$	n (-)
1	369.73	3.86	0.078	5.04×10^{-10}	0.40
2	434.45	3.51	0.069	2.05×10^{-10}	0.39
3	1323.95	2.49	0.098	5.26×10^{-11}	0.39
4	3246.15	3.30	0.189	8.19×10^{-12}	0.41

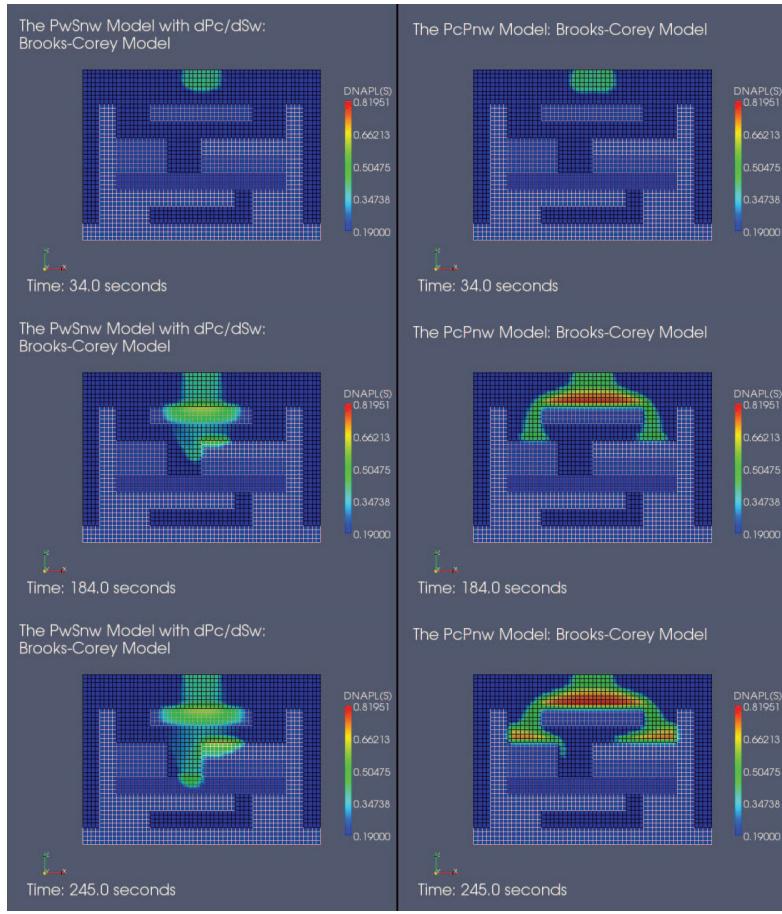


Figure 19.1.13: Comparison of the results obtained from the $p_w - S_{nw}$ and $p_c - p_{nw}$ schemes. The second column shows good agreement with observed distribution of DNAPL of the experiment (Kueper and Frind 1991).

Both schemes produce DNAPL plume propagation physically until the plume reaches to the less pervious media under the top medium in the model domain. The striking difference occurs at the interface between these two media. While the $p_w - S_{nw}$ scheme simulates the plume to infiltrate into the less pervious medium, the $p_c - p_{nw}$ scheme does the plume to bypass the less pervious medium. A similar experiment and simulation comparison against experimental observation are also conducted by Helmig and Huber (1998). They have reported unphysical fluid behavior captured by the $p_w - S_{nw}$ scheme, and this phenomenon can be avoided with fully upwind technique (Helmig and Huber, 1998).

Benchmark deposit

Benchmark	Problem type	Path in benchmark deposit
<i>Kueper</i>	H2	MULTIPHASE

Appendix A

Density of carbon dioxide

A fast way to estimate densities of fluids relating to thermodynamic boundary conditions is to read them out of a matrix. The following tables present the density of carbon dioxide at different temperatures and pressures. All density values are calculated from Equation ?? in section ??.

temperature C	pressure [MPa]					
	0.050	0.100	0.1013	0.200	0.300	0.500
190	1.40890	-	-	-	-	-
200	1.33590	2.69800	2.7345	-	-	-
210	1.27040	2.56170	2.5963	5.2116	7.9594	-
220	1.21120	2.43940	2.4722	4.9495	7.5367	12.974
230	1.15750	2.32880	2.3601	4.7152	7.1633	12.265
240	1.10840	2.22820	2.2581	4.5039	6.8298	11.646
250	1.06340	2.13630	2.1649	4.312	6.5292	11.097
260	1.02190	2.05190	2.0793	4.1369	6.2564	10.606
270	0.98360	1.97410	2.0001	3.9761	6.0072	10.161
280	0.94810	1.90210	1.9274	3.828	5.7785	9.7568
290	0.91510	1.83520	1.8597	3.6909	5.5675	9.3864
300	0.88434	1.77300	1.7966	3.5636	5.3723	9.0456
325	0.81585	1.63480	1.6565	3.2819	4.9416	8.2996
350	0.75726	1.51670	1.5369	3.0423	4.577	7.6736
375	0.70656	1.41470	1.4335	2.836	4.2638	7.1393
400	0.66224	1.32570	1.3433	2.6562	3.9916	6.677
425	0.62317	1.24720	1.2638	2.4981	3.7526	6.2725
450	0.58847	1.17760	1.1932	2.358	3.541	5.9154
475	0.55743	1.11540	1.1302	2.2328	3.3523	5.5975
500	0.52951	1.05940	1.0735	2.1204	3.1829	5.3126
525	0.50426	1.00880	1.0222	2.0188	3.0299	5.0558
550	0.48130	0.96283	0.97559	1.9265	2.8911	4.8229
575	0.46035	0.92087	0.93308	1.8424	2.7646	4.6108
600	0.44115	0.88242	0.89412	1.7653	2.6487	4.4168
700	0.37809	0.75619	0.76621	1.5124	2.2687	3.7814
800	0.33081	0.66158	0.67035	1.323	1.9844	3.3067
900	0.29404	0.58803	0.59582	1.1759	1.7635	2.9383
1000	0.26463	0.52921	0.53622	1.0582	1.587	2.6439
1100	0.24057	0.48109	0.48746	0.96197	1.4426	2.4033

temperature C	pressure [MPa]					
	0.750	1.000	2.000	3.000	4.000	5.000
220	1166.48	1167.03	1169.23	1171.4	1173.53	1175.62
225	1147.71	1148.32	1150.73	1153.1	1155.43	1157.72
230	19.095	1128.97	1131.64	1134.25	1136.8	1139.31
235	18.535	25.665	1111.85	1114.74	1117.56	1120.32
240	18.018	24.857	1091.24	1094.46	1097.6	1100.66
245	17.536	24.117	1069.65	1073.29	1076.81	1080.22
250	17.087	23.435	1046.88	1051.02	1055.01	1058.86
255	16.665	22.803	51.941	1027.42	1032	1036.39
260	16.269	22.215	49.914	1002.13	1007.49	1012.57
265	15.894	21.664	48.129	974.65	981.06	987.07
270	15.54	21.147	46.533	79.807	952.1	959.39
275	15.204	20.66	45.09	76.011	919.56	928.78
280	14.884	20.199	43.772	72.805	113.08	893.9
285	14.58	19.763	42.56	70.025	106.02	852.04
290	14.29	19.349	41.438	67.568	100.47	148.41
295	14.013	18.955	40.395	65.368	95.884	136.86
300	13.747	18.579	39.42	63.376	91.965	128.4
305	13.493	18.221	38.506	61.556	88.543	121.69
310	13.249	17.878	37.645	59.881	85.508	116.13
315	13.015	17.549	36.832	58.332	82.781	111.37
320	12.789	17.234	36.063	56.89	80.306	107.22
325	12.572	16.932	35.333	55.544	78.043	103.53
330	12.363	16.641	34.639	54.281	75.958	100.22
335	12.162	16.351	33.977	53.092	74.028	97.221
340	11.967	16.092	33.346	51.97	72.231	94.478
345	11.779	15.832	32.743	50.908	70.552	91.955
350	11.597	15.581	32.165	49.901	68.976	89.619
360	11.251	15.105	31.078	48.031	66.092	85.418
370	10.927	14.659	30.075	46.327	63.3509	81.726
380	10.621	14.241	29.143	44.765	61.173	78.44
390	10.333	13.848	28.276	43.326	59.045	75.484
400	10.062	13.477	27.464	41.992	57.094	72.804
410	9.8042	13.127	26.704	40.752	55.294	70.355
420	9.5603	12.796	25.989	39.594	53.627	68.104
430	9.3287	12.482	25.314	38.509	52.076	66.024
440	9.1085	12.183	24.678	37.491	50.628	64.094
450	8.8987	11.899	24.075	36.531	49.27	62.295
460	8.6988	11.629	23.504	35.625	47.995	60.613
470	8.5079	11.371	22.961	34.768	46.794	59.035
480	8.3254	11.125	22.444	33.956	45.659	57.55
490	8.1508	10.889	21.952	33.185	44.585	56.15
500	7.9835	10.664	21.482	32.451	43.566	54.826
525	7.5946	10.141	20.396	30.761	41.233	51.807
550	7.2425	9.6675	19.419	29.252	39.16	49.14
575	6.9222	9.2375	18.536	27.893	37.302	46.761
600	6.6294	8.8449	17.733	26.661	35.625	44.621
625	6.3608	8.4849	16.999	25.54	34.103	42.685
650	6.1133	8.1535	16.325	24.513	32.712	40.921
675	5.8846	7.8474	15.705	23.569	31.437	39.307
700	5.6725	7.5638	15.13	22.697	30.262	37.823
800	4.9589	6.6102	13.207	19.789	26.355	32.904
900	4.4056	5.8718	11.724	17.556	23.367	29.156
1000	3.9639	5.2826	10.544	15.783	21.001	26.196
1100	3.603	4.8014	9.5815	14.34	19.077	23.793

temperature C	pressure [MPa]					
	6.000	7.000	7.500	8.000	10.00	15.00
220	1177.69	1179.72	1180.72	1181.72	1185.63	1194.96
225	1159.97	1162.17	1163.26	1164.35	1168.59	1178.64
230	1141.77	1144.18	1145.37	1146.54	1151.15	1162.02
235	1123.02	1125.67	1126.97	1128.26	1133.28	1145.06
240	1103.65	1106.56	1107.99	1109.41	1114.92	1127.73
245	1083.55	1086.78	1088.36	1089.93	1095.99	1109.98
250	1062.59	1066.2	1067.96	1069.7	1076.42	1091.77
255	1040.62	1044.69	1046.67	1048.62	1056.11	1073.03
260	1017.43	1022.07	1024.32	1026.53	1034.95	1053.71
265	992.74	998.11	1000.7	1003.23	1012.8	1033.73
270	966.16	972.5	975.52	978.46	989.46	1013.01
275	937.12	944.77	948.38	951.86	964.71	991.45
280	904.68	914.25	918.68	922.92	938.22	968.93
285	867.13	879.8	885.48	890.82	909.56	945.3
290	820.77	839.25	847.07	854.2	878.06	920.4
295	753.39	787.63	799.88	810.4	842.67	894
300	182.31	706.06	733.9	753.17	801.62	865.82
305	166.26	243.08	389.85	656.77	751.67	835.48
310	154.99	210.63	253.36	327.71	685.77	802.54
315	146.25	191.97	222.11	261.29	586.02	766.51
320	139.11	178.74	203.04	231.91	448.28	726.83
325	133.08	168.48	189.27	212.9	358.04	683.09
330	127.87	160.11	178.52	198.87	310.25	635.51
335	123.27	153.05	169.7	187.79	280.11	585.4
340	119.18	146.95	162.24	178.65	258.62	535.55
345	115.48	141.59	155.8	170.89	242.11	489.42
350	112.12	136.82	150.13	164.16	228.8	449.2
360	106.19	128.61	140.52	152.93	208.25	387.08
370	101.1	121.75	132.6	143.82	192.74	343.43
380	96.643	115.86	125.88	136.18	180.38	311.48
390	92.694	110.73	120.06	129.63	170.18	286.97
400	89.155	106.18	114.95	123.9	161.53	267.42
410	85.954	102.11	110.4	118.84	154.05	251.33
420	83.036	98.436	106.31	114.31	147.48	237.78
430	80.36	95.09	102.6	110.21	141.63	226.14
440	77.892	92.024	99.215	106.49	136.39	215.98
450	75.605	89.2	96.102	103.07	131.63	207.01
460	73.477	86.584	93.227	99.928	127.3	199
470	71.488	84.151	90.558	97.016	123.32	191.79
480	69.625	81.88	88.072	94.307	119.65	185.24
490	67.874	79.752	85.747	91.778	116.24	179.26
500	66.223	77.753	83.566	89.41	113.07	173.76
525	62.477	73.239	78.652	84.085	106.01	161.74
550	59.186	69.294	74.369	79.458	99.93	151.63
575	56.264	65.807	70.592	75.385	94.626	142.97
600	53.645	62.694	67.225	71.762	89.941	135.43
625	51.282	59.892	64.201	68.511	85.761	128.78
650	49.136	57.354	61.464	65.573	81.999	122.86
675	47.176	55.041	58.972	62.901	78.592	117.54
700	45.377	52.922	56.691	60.457	75.486	112.72
800	39.435	45.945	49.193	52.435	65.349	97.199
900	34.924	40.668	43.532	46.389	57.759	85.74
1000	31.368	36.517	39.083	41.644	51.825	76.856
1100	28.486	33.158	35.485	37.807	47.04	69.73

Table A.0.1: 465

temperature C	pressure [MPa]					
	20.00	25.00	30.00	40.00	50.00	75.00
220	1188	1196.78	1205.06	1220.33	-	-
225	1172.07	1181.45	1190.25	1206.41	1229.78	-
230	1155.89	1165.92	1175.29	1192.39	1207.74	1240.63
235	1139.41	1150.17	1160.15	1178.27	1194.42	1228.76
240	1122.62	1134.16	1144.83	1164.03	1181.04	1216.9
245	1105.47	1117.9	1129.3	1149.68	1167.59	1205.04
250	1087.95	1101.35	1113.55	1135.19	1154.07	1193.18
255	1070.01	1084.49	1097.57	1120.58	1140.47	1181.32
260	1051.6	1067.29	1081.34	1105.83	1126.8	1169.46
265	1032.69	1049.74	1064.86	1090.93	1113.05	1157.6
270	1013.23	1031.8	1048.09	1075.88	1099.22	1145.74
275	993.16	1013.45	1031.04	1060.68	1085.32	1133.89
280	972.43	994.67	1013.68	1045.33	1071.33	1122.04
285	950.97	975.42	996.01	1029.82	1057.27	1110.2
290	928.71	955.68	978.02	1014.16	1043.14	1098.37
295	905.57	935.42	959.7	998.35	1028.94	1086.56
300	881.46	914.62	941.04	982.39	1014.67	1074.76
305	856.27	893.25	922.04	966.29	1000.35	1062.97
310	829.92	871.29	902.69	950.05	985.97	1051.22
315	802.33	848.72	883	933.68	971.55	1039.49
320	773.46	825.55	862.99	917.21	957.1	1027.79
325	743.3	801.8	842.66	900.63	942.63	1016.13
330	711.96	777.5	822.06	883.97	928.14	1004.51
335	679.68	752.73	801.21	867.25	913.66	992.95
340	646.9	727.58	780.17	850.5	899.19	981.43
345	614.18	702.22	758.98	833.72	884.76	969.98
350	551.54	651.72	716.55	800.23	856.03	947.28
360	496.14	603.1	674.75	767.03	827.61	924.9
370	449.68	557.99	634.51	734.39	799.62	902.87
380	411.63	517.36	596.59	702.64	772.18	881.23
390	380.5	481.55	561.5	672.08	745.45	860.03
400	354.77	450.35	529.46	642.96	719.54	839.31
410	333.19	423.27	500.5	615.44	694.59	819.07
420	314.83	399.72	474.48	589.59	670.67	799.37
430	298.99	379.13	451.16	565.45	647.87	780.21
440	285.14	361.01	430.25	542.98	626.2	761.62
450	272.92	344.95	411.46	522.12	605.67	743.6
460	262.02	330.61	394.52	502.79	586.26	726.18
470	252.21	317.72	379.18	484.89	567.95	709.36
480	243.34	306.07	365.24	468.31	550.68	693.14
490	235.24	295.46	352.51	452.94	534.42	677.52
500	217.77	272.64	325.03	419.1	497.78	641.03
525	203.3	253.87	302.37	390.67	466.18	608.02
550	191.06	238.08	283.31	366.46	438.78	578.19
575	180.5	224.54	266.99	345.6	414.84	551.22
600	171.28	212.77	252.82	327.4	393.77	526.81
625	163.12	202.4	240.36	311.36	375.06	504.66
650	155.83	193.18	229.3	297.09	358.33	484.49
675	149.27	184.9	219.39	284.29	343.27	466.06
700	128.34	158.65	188.05	243.83	295.34	405.95
800	113.04	139.62	165.44	214.66	260.55	361.14
900	101.27	125.04	148.15	192.37	233.89	326.23
1000	91.857	113.42	134.4	174.67	212.66	298.11

Table A.0.2: 465

temperature °C	pressure [MPa]				
	100.0	200.0	400.0	600.0	800.0
240	1257.21	-	-	-	-
245	1246.37	-	-	-	-
250	1235.57	-	-	-	-
255	1224.8	1314.84	-	-	-
260	1214.06	1306.44	-	-	-
265	1203.36	1298.11	-	-	-
270	1192.69	1289.84	-	-	-
275	1182.06	1281.64	-	-	-
280	1171.46	1273.5	-	-	-
285	1160.9	1265.43	1388.17	-	-
290	1150.37	1257.43	1382.04	-	-
295	1139.89	1249.48	1375.97	-	-
300	1129.45	1241.61	1369.95	-	-
305	1119.04	1233.79	1364	-	-
310	1108.69	1226.04	1358.11	1444.64	-
315	1098.38	1218.35	1352.28	1439.67	-
320	1088.12	1210.72	1346.5	1434.75	-
325	1077.91	1203.16	1340.78	1428.88	-
330	1067.76	1195.66	1335.11	1425.06	1493.71
335	1057.66	1188.22	1329.5	1420.28	1489.46
340	1047.62	1180.84	1323.95	1415.56	1485.25
345	1037.64	1173.53	1318.44	1410.88	1487.08
350	1027.73	1166.27	1312.99	1406.25	1476.96
360	1008.12	1151.94	1302.24	1397.12	1468.83
370	988.8	1137.86	1291.69	1388.16	1460.85
380	969.8	1124.01	1281.33	1379.38	1453.03
390	951.13	1110.41	1271.16	1370.75	1445.35
400	932.81	1097.04	1261.17	1362.28	1437.82
410	914.87	1083.91	1251.35	1353.97	1430.42
420	897.31	1071.02	1241.7	1345.79	1423.15
430	880.14	1058.36	1232.22	1337.76	1416
440	863.37	1045.94	1222.89	1329.87	1408.98
450	847	1033.74	1213.72	1322.1	1402.08
460	831.05	1021.78	1204.7	1314.46	1395.29
470	815.51	1010.04	1195.83	1306.94	1388.6
480	800.39	998.53	1187.1	1299.54	1382.03
490	785.67	987.24	1178.51	1292.26	1375.55
500	771.37	976.16	1170.05	1285.08	1369.17
525	737.38	949.42	1149.47	1267.6	1353.64
550	705.86	923.96	1129.67	1250.74	1338.65
575	676.71	899.74	1110.59	1234.45	1324.16
600	649.77	876.69	1092.21	1218.69	1310.14
625	624.9	854.75	1074.47	1203.43	1296.54
650	601.91	833.75	1057.35	1188.63	1283.34
675	580.64	813.97	1040.82	1174.27	1270.52
700	560.93	795	1024.84	1160.32	1258.04
800	494.96	727.46	966.02	1108.23	1211.18
900	444.32	671.1	914.22	1061.27	1168.47
1000	404.15	623.57	868.27	1018.66	1129.16
1100	371.36	583	827.2	979.76	1092.77

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