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Implementation and testing of an improved methodology to simulate resaturation processes with DarcyTools

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Contents

1 Introduction

1.1 Background

DarcyTools, a numerical single-phase (water) flow code, includes an interface where the modeller can adapt the code to study specific, or unconventional, problems. /Svensson 2010a/ programmed the interface to simulate the resaturation process of initially partially saturated and backfilled drifts in a simplified manner. In short, during unsaturated conditions, i.e. when the pressure is negative, the value of the specific storage for saturated conditions is switched to a value representing unsaturated conditions incorporating the air filled pore space. The approach implies some major simplifications with respect to the processes involved in two-phase flow.

1.2 Objectives

In the work reported here, an elaborated approach is presented that incorporates a transient saturation dependent moisture capacity into the definition of the specific storage and hence includes the capillarity. Doing so, the saturation dependent capillarity of the backfilling, which may strongly affect the evolution of the resaturation process, is taken into account.

1.3 This report

Chapter 2 gives the theoretical background of the simplified and the elaborated approaches to simulate two-phase flow within the single-phase framework in DarcyTools and describes their implementations into DarcyTools.

In Chapter 3, calculation results of a generic test case with the elaborated approach are compared to calculations performed with the simplified approach by /Svensson 2010a/ as well as to results from TOUGH2.

Chapter 4 contains a test case that mimics the situation at the Forsmark site.

Finally, some conclusions and an assessment of the elaborated approach's applicability in the field of backfill resaturation processes are presented in Chapter 5.

2 Theoretical background

2.1 Unsaturated flow

Unsaturated flow conditions occur during the different stages in a repository for spent nuclear fuel (construction, operation, post-closure). Different processes and properties such as capillarity and relative permeability act upon the hydraulic behaviour of the system and may affect the duration of the resaturation.

The usual forms of the governing equations for flow in saturated and unsaturated porous or porous-fractured media are as follows:

Saturated transient water flow

The transient flow equation for water is based on Darcy's law and is usually written in the following form (sources and sink terms neglected):

$$S_s \frac{\partial h}{\partial t} = div\left[K \cdot \nabla h\right] \qquad (2\text{-}1)$$

With:

- S_s [1/m] as the specific storage of the porous medium, $S_s = \rho g(\alpha + \phi\beta)$, with ρ as the water density [kg/m^3], g as the gravitational acceleration [m/s^2], ϕ as the kinematic porosity [-], α as the compressibility [1/Pa] of the porous medium and β as the compressibility [1/Pa] of water.
- t [s] as the time,
- K [m/s] as the hydraulic conductivity,
- h [m] as the hydraulic head, $h = z + \frac{p}{\rho g}$, with z as the elevation [m] and p as the water pressure [Pa].

Unsaturated transient water flow

The unsaturated transient flow equation for water, usually referred to as the Richards equation, is based on Darcy's law for the unsaturated medium. It is written (see, e.g. /Freeze and Cherry 1979/) in the following form:

$$\frac{\partial \theta}{\partial t} = div\left[K(h) \cdot \nabla h\right] \qquad (2\text{-}2)$$

With:

- $\theta = \phi \cdot S_w$ [-] as the specific volumetric moisture content (product of kinematic porosity and water saturation S_w [-]). It is related to the water pressure using the retention curve of the unsaturated medium.
- $K(h)$ [m/s] as the pressure (or saturation) dependent hydraulic conductivity.

In unsaturated media, the term $\frac{\partial \theta}{\partial t}$ can be written as $C(S_w)\frac{\partial p}{\partial t}$ with $C(S_w) = \frac{\partial \theta}{\partial p_c}$ referred to as the specific moisture capacity [1/m in hydraulic units] in the literature and p_c as the capillary pressure [Pa]. This formulation is used in order to solve the unsaturated flow equation in terms of pressure.

The following table summarises the differences between the saturated and unsaturated isothermal (freshwater) flow equation parameters presented above:

Table 2-1. Saturated vs. unsaturated flow equation parameters.

Saturated flow	Unsaturated flow
Hydraulic conductivity K is a constant	Hydraulic conductivity K is a function of the water pressure or of the saturation
Specific storage S_s is a constant	Specific moisture capacity $C(S_w)$ is a function of the pressure or of the saturation

2.2 Simplified approach ("constant S_s")

The simplified approach used by /Svensson 2010a/ is recalled below. It is based on the following steps:

- The negative pressure corresponding to the capillary pressure level of the backfill material at the prescribed initial saturation is computed according to the capillary pressure (retention) curve of the material.
- The value for the specific storage S_s is set to a *constant* value for the unsaturated backfill material in the following manner: The specific storage S_s is considered as the ratio of the initially air filled volume in the backfill to the bulk volume of unsaturated material and the head difference:

$$S_s\big|_{backfill} = \frac{\phi(1-S_{w,ini})\,\rho g}{\Delta p} = \left.\frac{\phi\cdot(1-S_{w,ini})}{h_{ini}-h_{(p=p_{at})}}\right|_{backfill} \tag{2-3}$$

with $\phi(1 - S_{w,ini})$ as the difference between the initially air filled pore space in the backfill and fully saturated conditions and p_{at} as the reference atmospheric pressure (0 Pa).

In this way S_s represents the unsaturated pore space to be resaturated. As soon as the pressure is positive, the backfill is considered as saturated and the S_s is switched to the value for fully saturated conditions. It is important to note that with this definition (non-linear) capillary effects are not taken into account.

2.3 Elaborated approach ("dynamic S_s")

In order to account for the capillary effects, the specific storage S_s is derived from the specific moisture capacity in the following manner:

Equating equations 2-1 and 2-2 yields:

$$S_s \frac{\partial h}{dt} = \frac{\partial \theta}{\partial t} \tag{2-4}$$

or:

$$S_s \frac{\partial\left(z + \dfrac{p}{\rho g}\right)}{\partial t} = \frac{\partial(\phi S_w)}{\partial t}$$

with ϕ = constant and z = constant follows:

$$\frac{S_s}{\rho\cdot g}\frac{\partial p}{\partial t} = \phi\frac{\partial S_w}{\partial t}$$

Hence, the specific storage to be assigned in DarcyTools can be written as:

$$S_s = C(S_w) = \rho\cdot g\cdot\phi\cdot\frac{\partial S_w}{\partial p} \tag{2-5}$$

The differences between the simplified approach by /Svensson 2010a/ and the suggested approach in this chapter are exemplified for the backfill "30/70" (bentonite/crushed rock) material parameters provided in /Svensson 2010a/, cf. Figure 2-1.

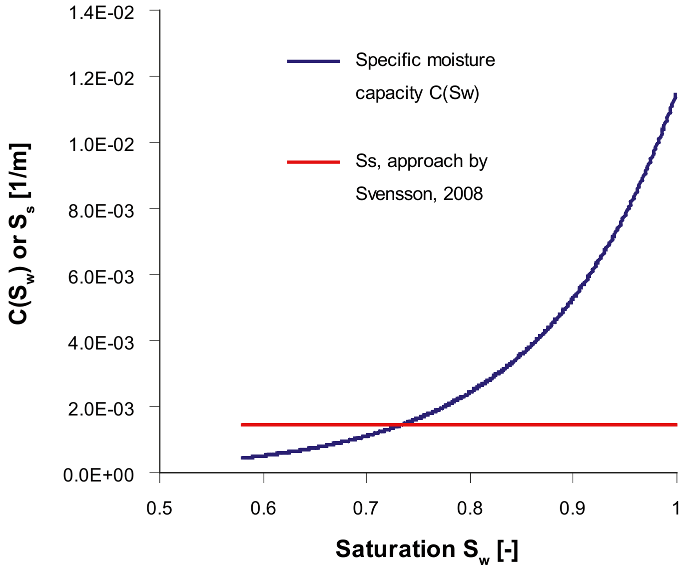

Figure 2-1. *Backfill 30/70 (bentonite/crushed rock) – Specific moisture capacity C(S_w) (equation 2-5) and equivalent specific storage S_s for unsaturated conditions based on /Svensson 2010a/.*

In the following, the simplified approach will be referred to as “constant S_s” and the elaborated approach as “dynamic S_s”; “dynamic” as the specific storage is handled as a variable parameter during unsaturated conditions according to equation 2-5.

2.4 Implementation in DarcyTools

As mentioned above, DarcyTools provides an interface (fif-file) that can be used to adapt (programme) the code to study specific, or unconventional, problems. The implementation of the “dynamic S_s” approach is as follows:

At the beginning of each new time step, the specific storage (equation 2-5) and the relative permeability[1] of each cell and cell-face in the resaturation area (backfill) are calculated based on the pressure field of the previous time step. The corresponding parameters in the host rock remain unchanged as no desaturation is considered to occur here during the resaturation process of the backfill.

An excerpt of the relevant coding in the interface fif-file is given in Appendix 1.

---

[1] According to the relative-permeability – saturation relation to be applied

3 Testing of the elaborated approach in DarcyTools and comparison with TOUGH2

3.1 Model setup and paramterisation

The testing is based on an axial symmetric 2-D model used by /Börgesson et al. 2006/ to investigate rock and backfill properties, considering the main specifications and processes involved in the resaturation of backfilled drifts and shafts in a deep repository (cf. /Börgesson et al. 2006/, Figure 5-1).

From the study by /Börgesson et al. 2006/, the three following test cases were selected for the evaluation of the suggested approach (cf. /Börgesson et al. 2006/, Chapter 5, Table 5-2):

- Friedland Clay backfilling and a fracture frequency of 1 m in the host rock (see /Börgesson et al. 2006/, case "aa5")
- 30/70 (bentonite/crushed rock) backfilling and a fracture frequency of 1 m in the host rock (see /Börgesson et al. 2006/, case "aa5")
- Friedland Clay backfilling and a fracture frequency of 24 m in the hostrock (see /Börgesson et al. 2006/, case "ac1")

The last two cases were expected to cover the minimum and maximum range of the resaturation times between 0.5 and about 200 years.

All DarcyTools calculations were performed with version 3.2 of DarcyTools /Svensson et al. 2010/[2]. The model domain is illustrated in Figure 3-1.

Comparative calculations for all three cases were performed with the simplified approach by /Svensson 2010a/ as well as with TOUGH2 (module EOS9[3]). The modelling mesh for the DarcyTools calculations is the same as in the calculations by /Svensson 2010a/. For the TOUGH2 calculations an axial-symmetric mesh with an identical discretisation in the radial dimension as in the DarcyTools mesh was used.

The parameterisation of the model setup, the host rock and backfill properties conforms to the corresponding cases in /Börgesson et al. 2006/ as well as /Svensson 2010a/ and are summarised in Table 3-1 and Table 3-2.

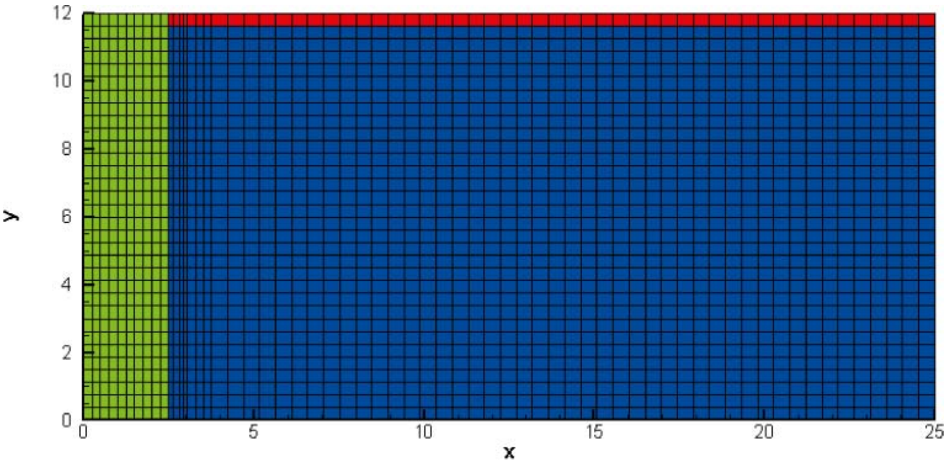

Figure 3-1. *Model domain of the axial-symmetric 2-D flow model, with backfill (green), host rock (blue) and fracture (red).*

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[2] It is noted that the current documentation of DarcyTools relates to version 3.4 /Svensson et al. 2010/, but that the differences are insignificant for the applications reported here.

[3] In module EOS9 liquid flow is described with a generalized formulation of the Richard's equation for unsaturated flow. The gas phase is treated as a passive bystander at constant pressure (cf. /Pruess et al. 1999/).

Table 3-1. Parameterisation of the hydraulic parameters of the host rock, the fractures, initial and boundary conditions.

Parameter	Unit	Value/Description
Hydraulic conductivity in fracture (frequency = 1 m); aa5	m/s	2.5×10^{-7}
Hydraulic conductivity in fracture (frequency = 24 m), ac1	m/s	2.5×10^{-9}
Hydraulic conductivity of the undisturbed host rock matrix	m/s	1.0×10^{-13}
Fracture width	m	0.02
Specific storage	Pa^{-1}	1.0×10^{-8}
Initial saturation	–	Fully saturated
Initial pressure	MPa	5.0
Outer boundary condition		Fixed at 5 MPa

Table 3-2. Parameterisation of the hydraulic parameters of the backfilling materials 30/70 (bentonite/crushed rock) and Friedland Clay (cf. /Börgesson et al. 2006/, TR-06-14 Chapter 5.3.3).

Parameter	Unit	30/70 (bentonite/crushed rock)	Friedland Clay
dry density	t/m^3	1.75	1.59
void ratio e	–	0.57	0.7
porosity n	–	0.36	0.41
density solid (grain)	t/m^3	2.74	2.703
w_m (water ratio at saturation)	–	0.207	0.259
Initial conditions			
e_0	–	= e	= e
Sr_0	–	0.58	0.3
Intrinsic permeability	m^2	5×10^{-18}	7×10^{-19}
Relative permeability law	–	$K_p = S_r^{\delta} K$ K_p… hydraulic cond. of partly saturated soil, S_r … degree of saturation, K…intrinsic hydraulic conductivity of soil, δ… exponent	
exponent δ in the permeability law	–	10	3
Storage coefficient (p>0, saturated)	1/m	1×10^{-5}	3×10^{-5}
retention curve		details – see below	details – see below

The retention curve for the two-phase characteristics of the backfilling materials is parameterised as follows:

$$S_w = a + \frac{b}{d}\cdot(c - \log(-p_c)) \tag{3-1}$$

with S_w as the saturation of the water phase, p_c as the capillary pressure and the fitting parameters a, b, c and d to 0.58, 0.29, 6.02 and 0.98 for 30/70 (bentonite/crushed rock) and to 0.3, 0.7, 7.633 and 2.46 for Friedland Clay (cf. /Svensson 2010a/).

For the TOUGH2 calculations the so called TRUST function /Narasimhan et al. 1978/ was fitted to the given retention curves in order to get equal conditions.

$$p_c = \begin{cases} -p_e - p_0\left[\dfrac{1-S_l}{S_l - S_{lr}}\right]^{1/\eta} & for \quad S_l < 1 \\ 0 & for \quad S_l = 1 \end{cases} \tag{3-2}$$

With the fitted parameters in Table 3-3:

Figure 3-2 shows a comparison of the applied capillary pressure saturation curves for backfill material 30/70 (bentonite/crushed rock) in DarcyTools and TOUGH2.

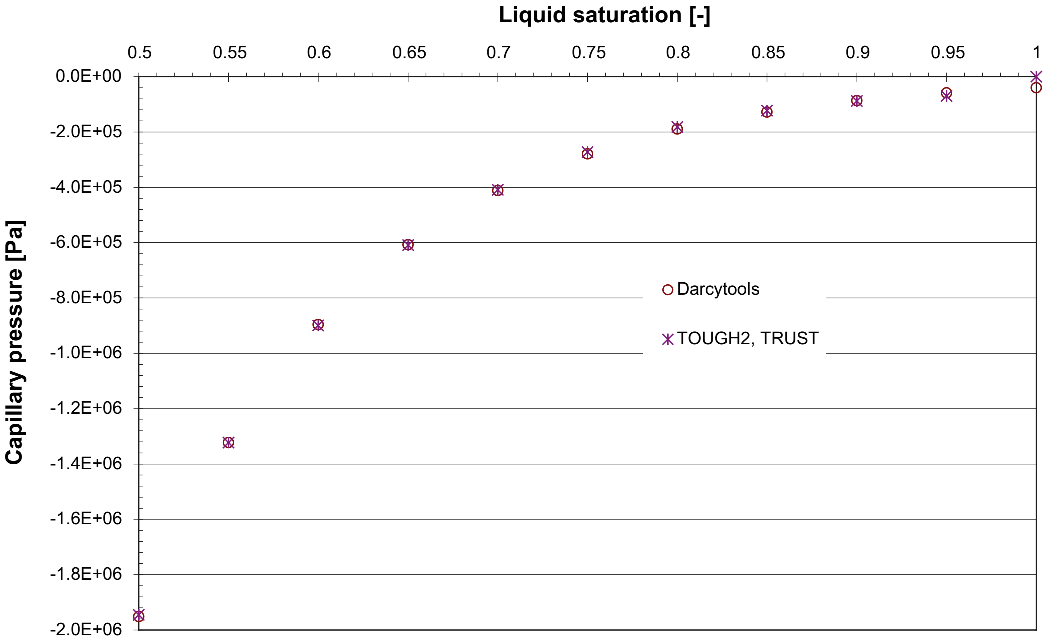

Figure 3-2. *Comparison of parameterised capillary pressure functions for 30/70 (bentonite/crushed rock) backfill used in DarcyTools and in TOUGH2.*

3.2 Modelling results

3.2.1 Evolution of the resaturation

Figure 3-3 shows the calculation results of the temporal evolution of the water pressure in the last backfill element to become saturated for case "aa5" with Friedland Clay backfilling. In all three calculations – DarcyTools ("constant S_s" and "dynamic S_s" approach) and TOUGH2 – resaturation is completed after around 1,100 days or roughly 3 years. However, the characteristics of the pressure evolution during resaturation differ strongly between the DarcyTools calculation with the "dynamic S_s" approach and the simplified, "constant S_s" approach. Further, the pressure evolution in the TOUGH2 calculation shows a very similar behaviour in comparison to the "dynamic S_s" approach. They both reflect a characteristic incorporating the saturation dependent suction capacity of the Friedland Clay backfill. This leads to a resaturation of the backfill which propagates throughout the whole tunnel section and to a more even rise of the saturation. In case of a constant value for S_s, the saturation front is rather steep and does not show any saturation dependent acceleration or deceleration of the resaturation due to capillarity.

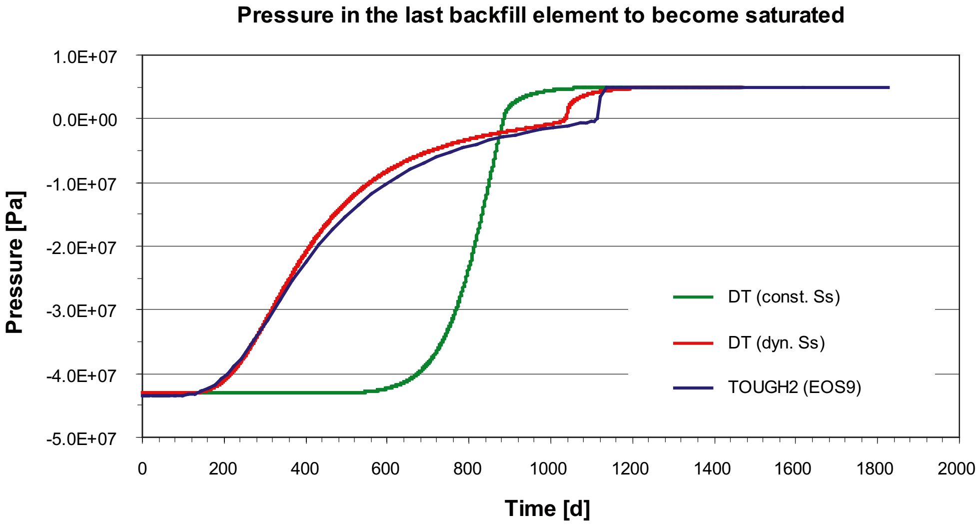

Figure 3-3. *Case "aa5" with Friedland Clay backfilling and a fracture frequency of 1 m – evolution of the pressure in the last backfill element to become saturated.*

3.2.2 Resaturation times

Table 3-4 to Table 3-6 list the results of all the performed calculations with respect to the resaturation time. For the DarcyTools calculations only time ranges can be stated, as no definite results were found. The reason for this lies in the significant influence of the time step. In case "aa5" with 30/70 backfilling for example, the resaturation times differ by a factor of 4 to 5 between the calculations with the biggest and the smallest time step chosen (10 respectively 0.25 days, cf. Table 3-5 and Figure 3-4.). In case "ac1" with Friedland Clay backfilling, the difference is less pronounced with a factor of 1 to 1.5 (time step of 10 resp. 0.5 years, cf. Table 3-6 and Figure 3-5). This correlation is found in either approach, "constant S_s" and "dynamic S_s". In both cases as well as with both approaches the resaturation time in general decreases with a decrease in the time step.

Table 3-4. Compilation of the calculated resaturation times for case "aa5" (backfill: Friedland Clay).

Case: aa5, Fr. Clay	t (p>0, S>99%)[4] [y]	t (p>0.9p₀) [y]	t (p>0.99p₀) [y]	t [y]
DT (constant S_s)	2.4–3.2	2.7–3.5	3.1–4.0	–
DT (dynamic S_s)	2.8–3.1	3.1–3.5	3.5–3.9	–
TOUGH2 (EOS9)	3.1	3.1	3.2	–
Börgesson[5]	–	–	–	4.3

Table 3-5. Compilation of the calculated resaturation times for case "aa5" (backfill: 30/70 (bentonite/crushed rock)).

Case: aa5, 30/70	t (p>0, S>99%) [y]	t (p>0.9p₀) [y]	t (p>0.99p₀) [y]	t [y]
DT (constant S_s)	0.4–1.8	0.5–2.0	0.5–2.0	–
DT (dynamic S_s)	0.2–1.1	0.3–1.2	0.3–1.3	–
TOUGH2 (EOS9)	0.4	0.4	0.4	–
Börgesson	–	–	–	0.5

Table 3-6. Compilation of the calculated resaturation times for case "ac1" (backfill: Friedland Clay).

Case: ac1, Fr. Clay	t (p>0, S>99%) [y]	t (p>0.9p₀) [y]	t (p>0.99p₀) [y]	t [y]
DT (constant S_s)	87–120	107–150	127–180	–
DT (dynamic S_s)	126–140	144–170	165–200	–
TOUGH2 (EOS9)	163	163	171	–
Börgesson	–	–	–	149–178

---

[4] p > 0 = considered state in DT, S > 99% = considered state in TOUGH2.

[5] Taken from /Börgesson et al. 2006, Table 5-2/. No information on the considered state of the resaturation is on hand.

Figure 3-4. *Case "aa5" with 30/70 (bentonite/crushed rock) backfilling – resaturation time with respect to the chosen time step.*

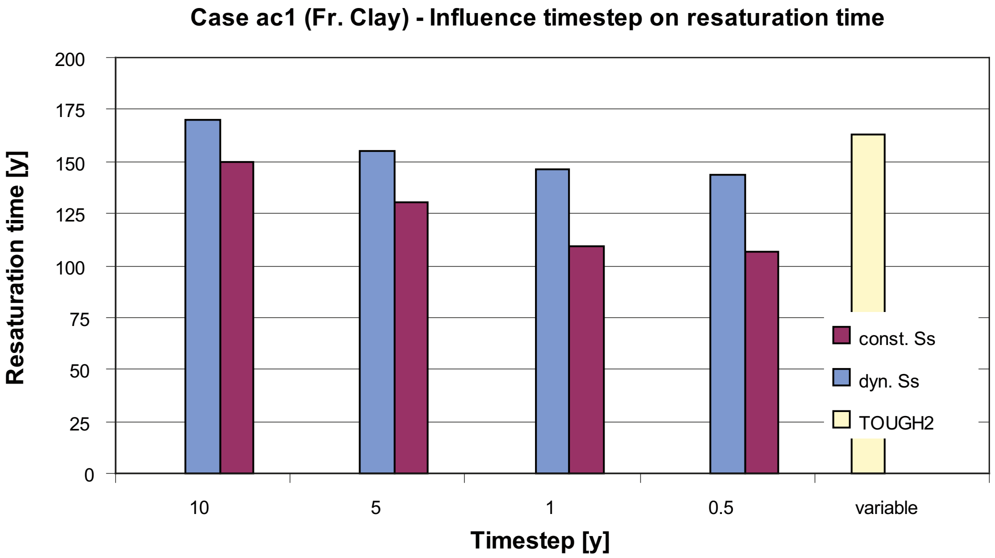

Figure 3-5. *Case "ac1" with Friedland Clay backfilling – resaturation time with respect to the chosen time step.*

3.3 Technical and numerical issues

The simulation results in the previous chapter show that the time step strongly influences the calculated duration of the resaturation. For the suggested approach of a "dynamic S_s" one can conclude that, the smaller the time step the more accurate the result will be (cf. Figure 3-4, Figure 3-5). However, this does not hold for all cases. Hence, the choice of the "right" time step is a key aspect in the light of accuracy. Unlike in TOUGH2 the time step is not evaluated automatically by the solver with respect to the convergence, but simply has to be defined by the user (cf. Figure 3-6). This calls for a thorough assessment of this issue by the user, e.g. by running multiple simulation runs with different time steps, by introducing a scheme for time step automation incorporating a sensitivity assessment of the time step or by running comparative calculations with different flow codes.

A general conclusion that the results are in better agreement with the TOUGH2 results when the time step size is reduced cannot be drawn. Moreover, further aspects possibly influencing convergence have not been assessed (e.g. capillarity of the backfill material). Further investigations based on a sophisticated numerical concept are needed if this issue is to be resolved.

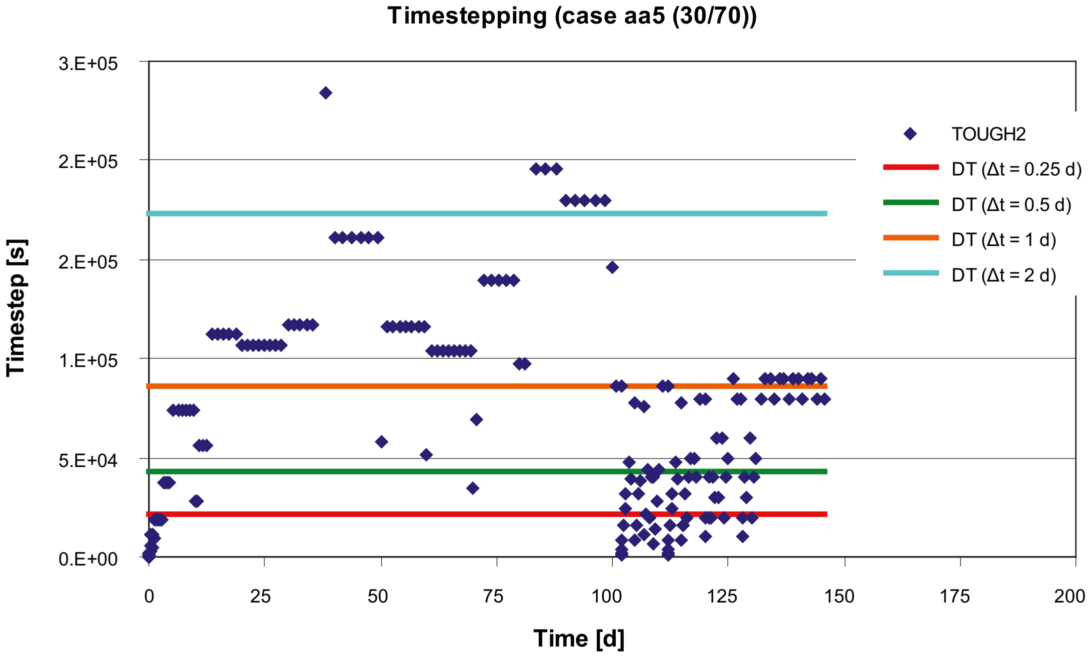

Figure 3-6. *Case "aa5" with 30/70 (bentonite/crushed rock) backfilling – illustration of the different static time steps applied in the different DarcyTools calculations and the automatic time step control in TOUGH2.*

4 Test case

4.1 Model setup and parameterisation

In this chapter, the results of the DarcyTools calculations of the generic test case "Forsmark" are presented. No comparative TOUGH2 calculations were performed.

The model setup and parameterisation are based on the run-files provided by /Svensson 2010b/.

Test case "Forsmark" represents a vertical section of the foreseen repository with one tunnel which is intersected by two deterministic fractures. The host rock, with a superimposed random fracture field, is represented by use of the so called cell removal feature. The deterministic fractures form the sole hydraulic connection between the host rock and the backfilled tunnel. Figure 4-1 shows the model-setup and the observation points at which the results are presented.

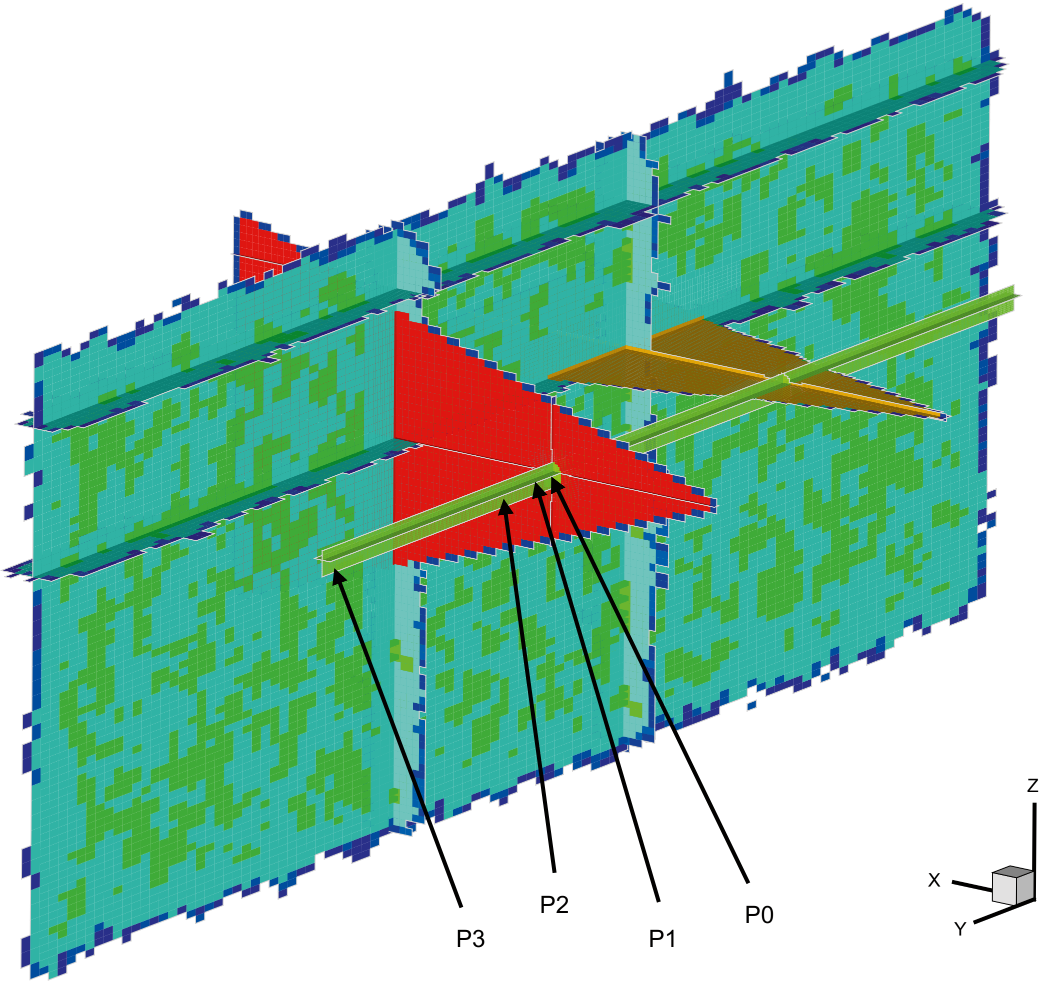

Figure 4-1. Model "Forsmark", with observation points P0, P1, P2 and P3.

4.2 Results test case "Forsmark"

For the purpose of comparison testcase "Forsmark" was performed with both approaches, "dynamic S_s" and "constant S_s" (here referred as cases F05d and F02c). The evolution of the pressure and the saturation at the observation points P0 to P3 are presented in Figure 4-2 and Figure 4-3. The evolution of the resaturation of the whole tunnel is shown in Figure 4-4.

The findings are as follows:

- Resaturation is finished after around 9,000 years with the "dynamic S_s" approach and after around 11,000 years with a constant value of the specific storage (see Figure 4-4),
- the characteristics of the pressure buildup is less steep in the case with a variable value for the specific storage.

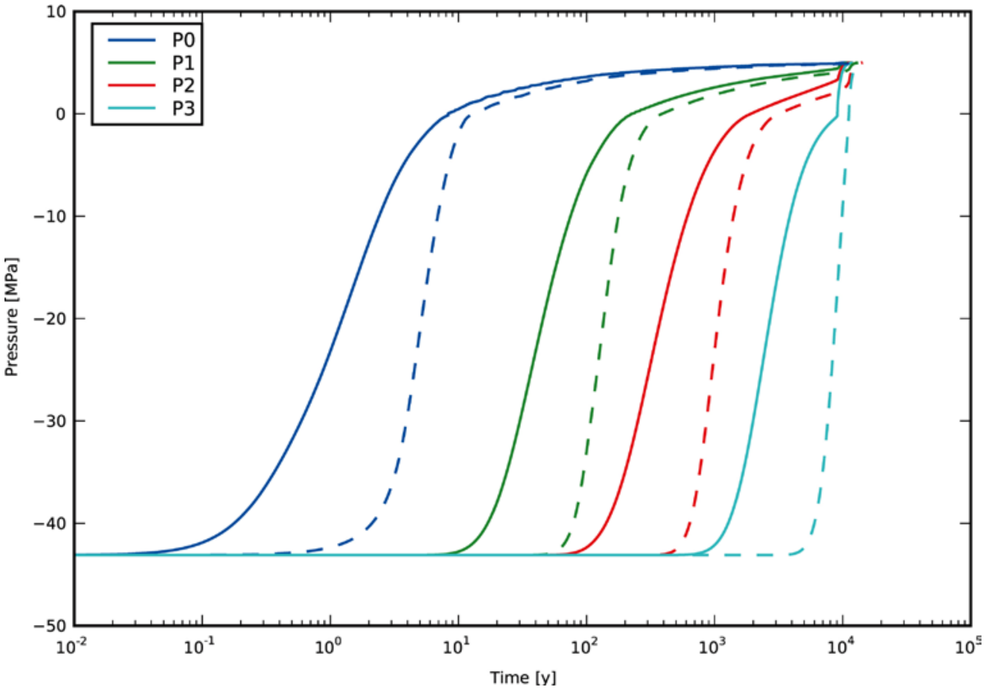

Figure 4-2. *Pressure evolution at observation points P0 to P3 with "dynamic S_s" (solid lines) and "constant S_s" (dashed lines).*

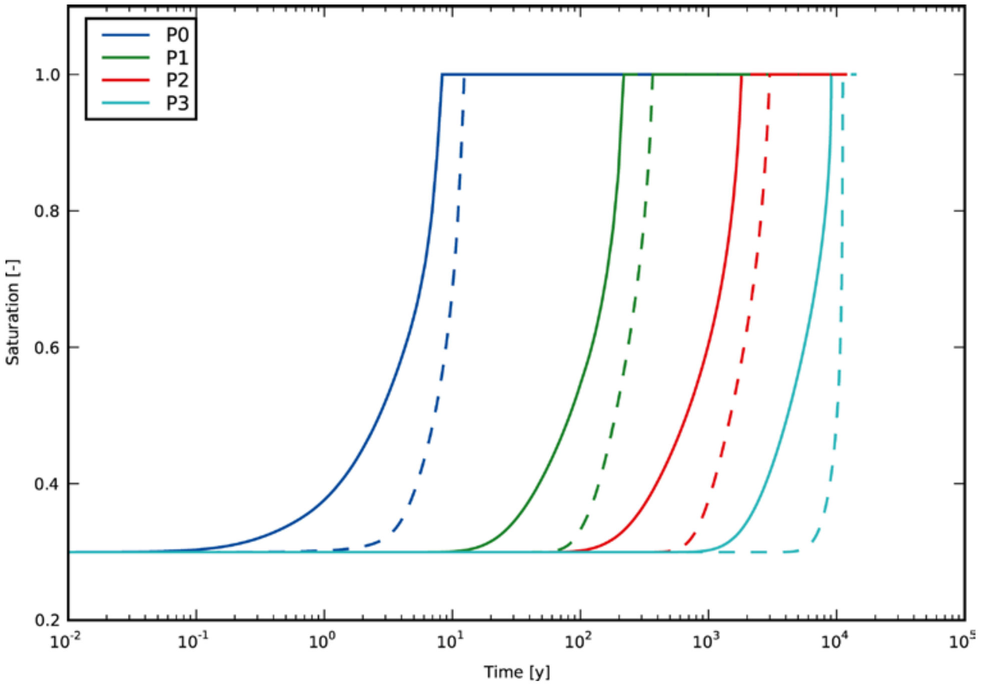

Figure 4-3. *Saturation evolution at observation points P0 to P3 with "dynamic S_s" (solid lines) and "constant S_s" (dashed lines).*

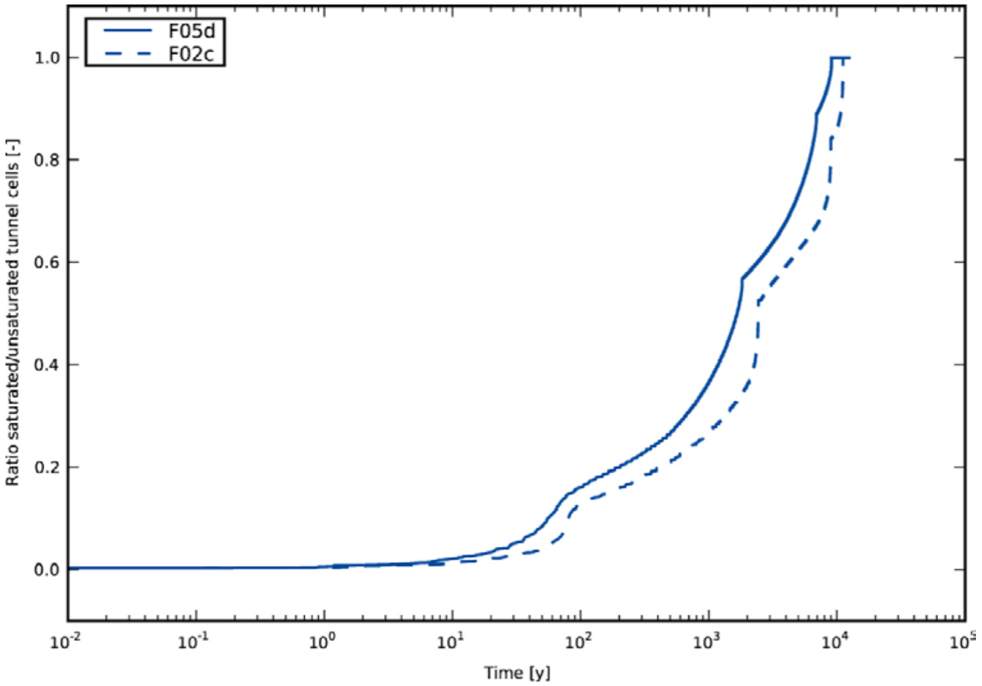

Figure 4-4. *Progress of the resaturation in the tunnel with "dynamic S_s" (solid line) and "constant S_s" (dashed line).*

5 Summary and conclusions

During the resaturation period of backfilled repository structures like drifts and shafts, two-phase flow processes strongly influence properties like relative permeability and capillarity, and hence the speed of resaturation. By architecture, DarcyTools, which is a single-phase flow code, is not designed for the representation of non-linear processes. In order to yet utilise DarcyTools for such applications, a simplified approach using a binary definition of the specific storage was suggested by /Svensson 2010a/. In this approach, two different values of the specific storage are applied depending on the algebraic sign of the pressure representing either unsaturated (negative pressure) or saturated conditions (positive pressure). In the work reported here, an elaborated approach is applied that incorporates a saturation dependent moisture capacity into the definition of the specific storage and hence includes the capillarity.

The elaborated approach is implemented into DarcyTools and a series of calculations have been performed on a generic and on a more realistic test model.

Comparative calculations for the same test cases have also been performed with the simplified approach of a constant value for the specific storage during unsaturated conditions as well as with TOUGH2 (module EOS9).

The following conclusions can be stated:

- The suggested approach of a “dynamic S_s“ does in fact show a saturation dependent evolution of the resaturation which results from capillary suction effects of the backfilling material,
- The calculation results for the performed generic test cases are in very well agreement with the comparative results obtained by TOUGH2,
- The simplified approach of a constant value for the specific storage does not show the characteristics of the saturation dependent capillarity,
- Independently of the applied approach (“constant S_s” or “dynamic S_s”), the performed tests revealed that in DarcyTools the time step, which has to be defined by the user, has a big influence on the calculated resaturation times. Therefore it is crucial always to assess the sensitivity of this parameter, e.g. by running multiple runs of the same test case with different time steps or to run comparative calculations with different flow codes.

Provided that the numerical issues are considered duly, it is advisable to apply the suggested approach of a “dynamic S_s” in future resaturation calculations with DarcyTools.

6 References

SKB's (Svensk Kärnbränslehantering AB) publications can be found at www.skb.se/publications.

Börgesson L, Fälth B, Hernelind J, 2006. Water saturation phase of the buffer and backfill in the KBS-3V concept – Special emphasis given to the influence of the backfill on the wetting of the buffer. SKB TR-06-14. Svensk Kärnbränslehantering AB.

Freeze R A, Cherry J A, 1979. Groundwater. Prentice-Hall, Inc. Eaglewood Cliffs, N.J.

Narasimhan T N, Witherspoon P A, and Edwards E L, 1978. Numerical model for saturated-unsaturated flow in deformable porous media, Part. 2: The algorithm. Water Res. Res. 14(2), 255–261.

Pruess K, Oldenburg C, Moridis G, 1999. TOUGH2 User's Guide, Version 2.0. Earth Sciences Division, Ernest Orlando Lawrence Berkeley National Laboratory, California, U.S.A.

Svensson U, 2010a. Evaluation of a new method to estimate the hydration time of the tunnel backfill. SKB R-10-06. Svensk Kärnbränslehantering AB.

Svensson U, 2010b. DarcyTools Version 3.4. Verification, validation and demonstration. SKB R-10-71, Svensk Kärnbränslehantering AB.

Svensson U, Ferry M, Kuylenstierna H-O, 2010. DarcyTools Version 3.4. Concepts, methods, and equations. SKB R-07-38. Svensk Kärnbränslehantering AB.

Appendix 1

Example for assignment of the two-phase parameters via the fif-file

```
!==============================================================================*
!===========                          FIF                         ============*
!===========                                                      ============*
!===========                   FORTRAN INPUT FILE                 ============*
!===========          Author: C.P. Enssle, AF-Colenco Ltd.        ============*
!===========        Description: dynamic modification of Ss       ============*
!==============================================================================*

 subroutine usrprop(eqname)

 use M_UTIL
 use M_GET
 implicit none

 character(len=*), intent(in) :: eqname

 real, dimension(:), pointer :: pressure, stora, permx, permy
 real, dimension(:), pointer :: permz, sat, time
 real :: grenzdruck, a, b, c, d, delta, mean_sat, mean_p, sat1, t,sat_forSs, dn
 real :: sat_i, pres_up, pres_low
 integer :: nbcells, i, mkc, nbx, nby, nbz, ih, il, mkh, mkl
 integer :: mktun, mdelta, mk, ilm, ihm
 real :: facmin, cnvrt, cndtun, ploc, plocl, ploch, satur, factor
 real :: xf0, yf0, zf0, x1, y1, z1
 real :: ss_hr, ss_tun_unsat, ss_tun_sat
 real :: p_hr_ini, p_tun_ini, sat_hr_ini, sat_tun_ini, n_hr, n_tun

 nbcells = GET_NBCELLS()
 nbx = GET_NBXFACES()
 nby = GET_NBYFACES()
 nbz = GET_NBZFACES()

 pressure => GET_VAR_VAL(‘pressure’)
 stora => GET_VAR_VAL(‘stora’)
 permx => GET_VAR_VAL(‘permx’)
 permy => GET_VAR_VAL(‘permy’)
 permz => GET_VAR_VAL(‘permz’)

! ==== paramter defintion =====================================================

 p_thresh = -150146.0 ! threshold pressure for saturation of 0.99(Friedland Clay)
 a=0.3 ! parameter in retention curve
 b=0.7
 c=7.633
 d=2.46
 delta=3. ! exponent in rel. permeability law
 facmin=0.0
 cnvrt=1.0E-7
 mktun=2
 mdelta=3
 cndtun=7.E-12
 ss_hr = 1.0E-8
 ss_tun_sat = 3.0E-5
 p_hr_ini = 5.0E+6
 p_tun_ini = -43.1E+6
 sat_hr_ini = 1.0
```

```
 sat_tun_ini = 0.3
 n_hr = 1.0E-3
 n_tun = 0.412

! ==== Storativity =============================================================

! ==== “dynamic” ==== (storativity coefficient according to derivation of dS/dp)

 DO i = 1, nbcells
    mk = GET_CELL_MK(i)
    ploc=pressure(i)
    stora(i)=ss_hr

    if(mk.eq.mktun)stora(i)=ss_tun_sat

    IF(mk.eq.mktun.and.ploc.lt.p_thresh)THEN
       stora(i)=9810.*n_tun*abs(b/d/log(10.)/(ploc))

    END IF

 END DO

! ==== relative permeability ===================================================

!   permx

 DO i=1,nbx

    call GET_XFACE(i,xf0,yf0,zf0,ih,il,y1,z1)
    ilm=0
    if(il.gt.0) ilm= GET_CELL_MK(il)
    ihm=0
    if(ih.gt.0) ihm= GET_CELL_MK(ih)

    if (ilm == mktun .and. ihm == mktun) then
       plocl = pressure(il)
       ploch = pressure(ih)
       ploc = max(plocl, ploch)
       satur = 1.0
       if(ploc.lt.0.)satur=a+b*(c-alog10(-ploc))/d
       if(satur.gt.1.)satur=1.0
       factor = satur**delta
       if(factor.lt.facmin) factor=facmin
       permx(i)=cnvrt*cndtun*factor
    endif

 END DO

…

 end subroutine

! ============================================================================
```