R-07-25

Modelling of SWIW tests with DarcyTools 3.0

Calle Hjerne, Geosigma AB

May 2007

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1402-3091
SKB Rapport R-07-25

Modelling of SWIW tests with DarcyTools 3.0

Calle Hjerne, Geosigma AB

May 2007

Keywords: DarcyTools, SWIW test, Tracer test, Hydrogeology.

Abstract

This report presents a model implemented with DarcyTools with the purpose of simulating SWIW tests. The model was used to evaluate two previously performed tests in KSH02 borehole sections 422.3–423.3 m and 576.8–579.8 m within the on-going site investigation in the Oskarshamn area. Homogeneous as well as heterogeneous hydraulic conductivity were used. The model uses a multi-rate exchange with immobile zones to simulate diffusion.

The results show that it was possible to obtain a good fits to the data from SWIW tests for both the homogeneous as well as for the heterogeneous case. However, when a good fit was obtained with homogeneous conditions, the penetration depth of the tracers into the formation was independent, or nearly independent, of the kinematic porosity in the model. The simulations using a heterogeneous conductivity did not display this behaviour regarding the penetration depth of uranine (non-sorbing) in the model. Hence, the heterogeneous hydraulic conductivity may represent a more realistic case than the homogeneous conditions.

A sensitivity analysis showed that it was possible to obtain a good fit within rather limited intervals regarding the fitting parameters (k and $\beta_{t,uranine}$) used for the non sorbing tracer, uranine. The fitting parameters used for the sorbing tracer, cesium (R_m and $\beta_{t,cesium}$), on the other hand, showed a strong correlation, making this evaluation more uncertain. Furthermore, the sensitivity analysis showed that the results are dependent on the maximum exchange rate, α_{max}.

Sammanfattning

Denna rapport presenterar en modell som byggts upp i DarcyTools med avsikt att simulera SWIW-tester. Modellen användes för att utvärdera två tester som tidigare utförts i KSH02 sektionerna 422,3–423,3 m och 576,8–579,8 m inom den pågående platsundersökningen i Oskarshamnsområdet. Både homogena förhållanden såväl som heterogen hydraulisk konduktivitet användes under simuleringarna. Modellen använder *multi-rate* utbyte med den immobila zonen för att simulera diffusion.

Resultatet visar att det är möjligt att erhålla en bra passning till data från SWIW tester med både homogen och heterogen hydraulisk konduktivitet i modellen. Emellertid blir inträngningsdjupet av spårämnena i formationen oberoende, eller näst intill oberoende, av den kinematiska porositeten i modellen om homogen konduktivitet används och bra passningar erhålls. Simuleringar med heterogen konduktivitet uppvisar inte denna effekt med avseende på inträngningsdjupet av det icke sorberande spårämnet, uranin. Det verkar alltså som om fallet med heterogen konduktivitet skulle kunna vara mer realistiskt än fallet med homogena förhållanden.

Känslighetsanalysen av simuleringarna visar att relativt avgränsande intervall av passningsparametrarna för uranin (k and $\beta_{t,uranine}$) kan erhållas med bibehållen bra passning. Däremot uppvisar passningsparametrarna för cesium (R_m and $\beta_{t,cesium}$) en stark korrelation varför denna utvärdering blir mer osäker än för uranin. Vidare visar känslighetsanalysen att resultaten är beroende av den maximala utbyteskoefficienten, α_{max}.

Contents

1 Introduction

The first objective of the project described in this report was to develop a general model with the purpose of simulating SWIW tests using the DarcyTools software. Secondly, the model was used to evaluate two specific SWIW tests previously performed in KSH02 within the on-going site investigations in the Oskarshamn area. Furthermore, another objective was to investigate the possibilities and limitations of DarcyTools as an instrument for evaluation of SWIW tests in general.

2 SWIW test

The principle for a SWIW test (Single Well Injection Withdrawal tracer test) is that one or several tracers are injected into the rock formation and then later being pumped back. Evaluation of the breakthrough curves may then provide information about the rock formation. A SWIW test consists of a number of phases:

1. Pre injection: only water is injected.
2. Tracer injection: water and tracers are injected.
3. Chaser phase: only water is injected in order to push the tracers further out into the rock formation.
4. Pumping phase: the water is pumped back and the tracer concentrations are measured.

In between these phases, there may be waiting periods when the water neither is injected nor pumped. In this report, simulations concerning SWIW tests in KSH02 422.3–423.3 m as well as 576.8–579.8 m is discussed. In the section 422.3–423.3 m there is one flowing fracture while there are three or four flowing fractures in 576.8–579.8 m. For more information about SWIW tests in general and these tests in particular, see Gustafsson and Nordqvist (2005) /1/.

3 General descprition of the SWIW test model

The model has been implemented in DarcyTools 3.0 (beta version 2005-10-03). In this report, only those details of DarcyTools that are important regarding parameter fitting and results are presented. For more information regarding DarcyTools, see Svensson et al. (2004) /2/.

3.1 Grid network

The model was two-dimensional with one layer in the z-direction. The domain in x- and y-direction was 75 m. The height of the model was set to the section length for each SWIW test, respectively. The maximum size of the grid cells was defined for different areas in the model. These areas were shaped as cylinders where cells inside or on the border of these cylinders was set to a certain maximum cell size. The radius of the cylinders may easily be changed so that the total number of cells easily can be changed. The borehole and its border consist of cells of various sizes inside and on the border of a cylinder with the radius 0.038 m.

3.2 Time steps

The model was constructed so that the length of the time steps was constant between given times, for example time steps of 10 s between 1,200 s and 1,400 s. The time steps may therefore be varied in order to reduce the total number of time steps needed for a simulation. Shorter time steps have been used when particles were introduced or when the flow rate in the model was altered.

3.3 Simulation of tracers

The model uses both methods available in DarcyTools to simulate tracers, particle tracking (PARTRACK) and the advection-diffusion equation. Diffusion into immobile zones was simulated, for both methods, in the model as a multi-rate exchange with immobile zones. Hence, the diffusion in the water phase in the advection-diffusion equation was set close to zero in order to compare the two methods. The volume of the mobile zone in each cell (V_m) was set by the kinematic porosity (Poros in DT30) multiplied with the total volume of the cell (V_{tot}). The relative size of the immobile zone was set by the parameter β_t (bettot in DT30). The parameter β_t may be read as the volume ratio of immobile and mobile zone ($\beta_t=V_{im}/V_m$). Hence, the volume of the immobile zone in each cell was the product of the connected porosity, total volume of the cell and β_t ($V_{im}=Poros \cdot V_{tot} \cdot \beta_t$). The distribution of β_t across the domain was defined by the variable FWS (flow wetted surface). If FWS is homogeneous across the domain so will also β_t be. In the borehole, no exchange with the immobile zone was desired, hence FWS in these cells was set to zero.

The immobile zone was regarded as a number of volumes with no significant conductive flow. Each volume may be regarded as a box with a side length of l. The exchange between the mobile zone and these boxes was defined using a mass exchange coefficient, α. The coefficient α depends on the molecular diffusion, D_{mol}, and the length l according to the Equation 3-1. In the model, α_{max} and α_{min} was defined, i.e. the highest and lowest allowed α, respectively. The coefficeint α_{max} relates to the smallest fracture thought to play a role in the exchange between immobile and mobile zones.

$$\alpha = \frac{D_{mol}}{l^2} \qquad \text{(Equation 3-1)}$$

The fitting parameter k may be interpreted as the late time slope of the breakthrough curve. The parameter k decides how the immobile volume is distributed over the spectrum of different α.

Sorption, both in mobile and immobile zone, may only be used with particle tracking in DarcyTools. The sorption is controlled by the retardation factors R_m and R_{im}, for the mobile and immobile zone respectively. The retardation factors in DarcyTools are actually magnifying factors of the volumes regarding the tracer since the sorption is simulated by enlarging the volumes in order to increase the transportation time. Only one set of particles may be used in a simulation. Hence, fitting to the breakthrough curves was done using one tracer at the time.

During the tracer injection a fully mixed section was assumed. The concentration of the tracers in the borehole section may therefore be calculated according to Equation 3-2 during the tracer injection.

$$C = (C_0 - C_{in})e^{-(\frac{Q}{V_{bh}+K_a A_{bh}})t} + C_{in} \qquad \text{(Equation 3-2)}$$

C = concentration of tracer in the borehole section t seconds after starting the tracer injection

C_0 = concentration of tracer in the borehole section at the start of the tracer injection

C_{in} = concentration of tracer in the injection water

V_{bh} = volume in the borehole section (m^3 water)

K_a = distribution coefficient (surface) (m)

Q = flow rate (m^3/s)

Equation 3-2 was also used to calculate the concentration during the chaser injection. However, C and C_0 are then in relation to chaser injection instead of the tracer injection. Introduction of both particles and concentration for the advection-diffusion equation was controlled by Equation 3-2.

During the pumping phase, the section was assumed to not be fully mixed. Hence, the concentration on the border of the borehole section was used for comparison with the measured concentrations from the SWIW tests.

Two ways of introducing particles in the model have been tested. The first way, which also has been used for the results in this report, was to introduce them in cells on the border of the borehole as described above. This method must be used if sorbing tracers are used and if it is desired to simulate sorption to the borehole wall. One advantage was also that it was possible to define an end location for the particles in the borehole without making a restart of the simulation. This will make the simulations less time consuming. One disadvantage was that the programming to make a start location file was far from simple. One row for each particle is required in such a file.

The other way to introduce the particles in the model was to place them continuously in all cells inside the borehole. The fraction of particles (of the total number of particles) which was put into each cell was related to the relative sizes of the cells. The advantage of this was that the programming to make the start location file was simple because only one row per cell is required in such a file. The disadvantage was that sorbing particles may not be simulated and an end location can be used only if the simulation includes a restart.

3.4 Model parameters

Several parameters have to be defined in the model. The transmissivity was assumed to be $2.3 \cdot 10^{-7}$ m^2/s for 422.3–423.3 m and $9.0 \cdot 10^{-8}$ m^2/s for 576.8–579.8 m. These assumptions coincides with the simulation performed by Gustafsson and Nordqvist (2005) /1/. The storativity was assumed to be $1 \cdot 10^{-5}$ for both sections.

Both sections were simulated with a homogenous fracture. In addition, simulations of 422.3–423.3 m were performed using a fracture with heterogeneous conductivity with a standard deviation of ln(K)=2.0 and an isotropic correlation length of 1.0 m.

Different kinematic porosities were tested in the simulations. Both of the sections were simulated with the porosity of 0.002 which also was used by Gustafsson and Nordqvist (2005) /1/. In addition, 0.0002 was used for 422.3–423.3 m and 0.00004 for 576.8–579.8 m. These porosities were assumed to be the aperture, based on Equation 3-3 as suggested by Svensson et al. (2004) /2/, divided by the section length.

$$e_T = 2.0T^{0.6} \qquad \text{(Equation 3-3)}$$

e_T = transport aperture (m)

T = transmissivity (m^2/s)

The limit for α_{min} and α_{max} was treated differently in the simulations. Different α_{max} was used while α_{min} was set to $1 \cdot 10^{-10}$.

4 Some implementation details for running the SWIW test model with DarcyTools

4.1 Files

The model consists of a number of files used in DarcyTools 3.0. The main files are cif.xml, fif.f and prpgen.f. In addition, a number of other files facilitate the processing of the results and the control of the model.

4.1.1 cif.xml

The file cif.xml contains the majority of the code that controls the SWIW model. It defines the grid, governing equation and most of the variables.

4.1.2 prpgen.f

This file is edited by the user in order to provide input for the model. Some of the changes worth mentioning are:

- The parameter FWS was set to zero for the cells inside and on the border of the borehole to prevent matrix diffusion in the borehole. This was necessary since β_t, the volume ratio between immobile and mobile zone, was defined by FWS. Since the mobile zone in the borehole was large, so will also the immobile zone be in this area. This was of course not adequate and was avoided by setting β_t to zero by setting FWS to zero in the borehole. Since the particles and the concentration was defined on the border of the borehole one might discuss if FWS should be zero or two, as in the rest of the model. However, this turned out to be of lesser importance, practically.
- The porosity in the borehole cells was set so that the volume of water in the section was the same as during the SWIW test. This was important since the volume of water controls the concentration of particles and boundary conditions for the AD-equation during the injection.
- Start and stop time as well as flow rates during the different phases of a SWIW test was defined in the prpgen.f file. The times were written to a file (prp_ursbss.dat) which was called upon from fif.f during the model run.
- The file that controls the introduction of particles (prp_startloc.dat) was also created in prpgen.f. The objective was to simulate a concentration just outside the borehole assuming a fully mixed borehole section. The code for this purpose was however rather difficult to penetrate. Therefore, another file was created (kontroll_startloc.dat) which easily was imported to Excel for checking that the particles were introduced as intended. In this section of prpgen.f, the variable Ka (distribution coefficient) and Abh (area of borehole wall) was defined since they affect the concentration of sorbing tracers in the borehole during the injection.

4.1.3 fif.f

Three subroutines, usrdt, usrbss and usrout, have been modified in fif.f compared with the file DarcyTools creates at the start of a new project.

The time step length used in the simulation was defined in usrdt. The simulation was divided into several time periods where each period has its own time step length. Each period was represented as a row in the code. The code may easily be changed by using an excel file

(Tidschema.xls). The code was automatically generated in this file if step length, start and stop time were defined. The total number of time steps was also calculated. It was obvious that large time steps during changes in flow rate, as for example at the transition from injection to pumping, might make the solution unstable. Therefore, smaller time steps have been used around such flow changes.

The subroutine usrbss was used in the model to set boundary condition for the mass equation and the AD equation. For this purpose, a file (prp_usrbss.dat) containing times and flow rates, created in prpgen.f, was called upon.

In usrout, a number of files containing results from the simulation were created. For chosen areas, in the formation and the borehole, the number of particles, the concentration and the pressure was written to a file. The particles in each area are summed up, while the concentration and the pressure were calculated as a weighted average based on the cell size. Another file that was created contained the number of particles in each cell at a specific time and the distance from the cell centre to the borehole centre. Time steps of particular interest include the time step before the withdrawal which enables a calculation of the average maximum tracer penetration depth into the formation.

4.1.4 Other files

In order to facilitate the use of the model some other files may be used:

- Conv_res.f90: This program reads the files which were created by fif.f, processes the data and produces a new file which was easy to use in Tecplot. The program transformed the number of particles to C/C0 incoming to the borehole.
- Calc_residual.f90: The program reads a file containing C/C0 from the SWIW test and a file produced by Conv_res.f90. The residuals (both relative and absolute) were calculated and summed. This may be helpful when fitting parameters.
- kontroll_startloc.dat: The best use of this file was to control the introduction time for each particle. It was easiest to open the file in Excel and paste it to the specified place in kontroll_startloc.xls. It was also possible to paste the file res_t_ad.dat which is created by Conv_res.f90 to control the concentration regarding the AD equation.

4.2 Running the model

The model has been used and fitted to data from SWIW tests in KSH02 422.3–423.3 m and 576.8–579.8 m. A fit was done according to the following steps:

1. Transmissivity, porosity, storativity, α_{min} and α_{max} were assumed to be known and were defined in the model.
2. Fitting was firstly executed with $\beta_{t,uranine}$ (bettot) and k to uranine.
3. When a good fit was obtained to uranine, the k and $\beta_{t,uranine}$ parameters were used in the fitting of cesium (sorbing). The fitting parameters for cesium are $\beta_{t,cesium}$ and R_m (retention factor mobile zone) which both are introduced and used separately in the model. The retention factor for the immobile zone, R_{im}, was calculated according to Equation 4-1.

$$R_{im} = R_m \frac{\beta_{t,cesiume}}{\beta_{t,uranine}} \qquad \text{(Equation 4-1)}$$

4. New values for α_{min} and α_{max} were put into the model since they are affected by R_{im} according to:

$$\alpha_{\min,cesium} = \alpha_{\min,uranin} / R_{im}$$
$$\alpha_{\max,cesium} = \alpha_{\max,uranin} / R_{im} \qquad \text{(Equation 4-2)}$$

5 Results

The simulations with the model were made with the purpose of fitting simulated breakthrough curves to measured concentrations from SWIW tests in KSH02, sections 422.3–423.3 m and 576.8–579.8 m. The model was first fitted to uranine data by using k and $\beta_{t,uranine}$. The values of k and $\beta_{t,uranine}$ were subsequently used when fitting the model to the breakthrough curve for cesium, which was the sorbing tracer. The parameters used for this fit were R_m and $\beta_{t,cesium}$.

In general, the behaviour and effects found during the simulations are similar for the two different sections, 422.3–423.3 m and 576.8–579.8 m in KSH02. Hence, the disposition in this part of the report is segmented by formation property (homogeneous/heterogeneous conductivity) and tracer substance and not by test section.

In most simulations PARTRACK and the advection-diffusion equation displayed breakthrough curves very similar to each other. However, sometimes they differ slightly from each other. In such cases, the breakthrough curve from PARTRACK was used since it also was possible to simulate cesium with that method in DarcyTools.

The breakthrough curve from the SWIW test in section KSH02 576.8–579.8 m was more scattered than the corresponding curve in 422.3–423.3 m. Hence, fitting the model to the breakthrough curve was somewhat more difficult and subjective in 576.8–579.8 m than in 422.3–423.3 m. The consequence of this may be a less reliable result for the section 576.8–579.8 m. The majority of the simulations were therefore made on 422.3–423.3 m, especially in the sensitivity analysis.

The parameter α_{max} was, during the first simulations, set to $1 \cdot 10^{-3}$ in accordance to recommendation by Svensson /4/. However, it was obvious that an increase of α_{max} resulted in a different fit to the curve. Hence, different α_{max} values were used during the simulations in order to determine where a further increase of α_{max} had no or little effect on the fit.

The quality of the fit has been judged visually. Hence, a degree of subjectivity is unavoidable. However, some help using residual analysis has been used during the fitting process. Since each run of the model took about 10 min, obtaining optimal parameters was still time consuming.

5.1 Homogeneous conductivity

5.1.1 Uranine

The first approach in the simulations was to set α_{max} to $1 \cdot 10^{-3}$. It was possible to achieve a good fit to the breakthrough curve for both SWIW tests with the assumed porosities. When α_{max} was increased it was obvious that k had to be lowered while $\beta_{t,uranine}$ could more or less be the same in order to still have a good fit. For α_{max} higher than 0.1, further increase had some but rather small effect on the simulations. An example of a simulated breakthrough curve is shown in Figure 5-1, where both PARTRACK and the advection-diffusion equation fit relatively well to the uranine data.

Tables 5-1 and 5-2 show different sets of fitting parameters that resulted in a good fit to the breakthrough curve for uranine using the specified parameters. The average penetration depth is also displayed in the table. It may be compared with the average penetration depth, assuming only advective transport and no exchange with immobile zones, i.e. $\beta_{t,uranine}$ was set to zero, which is also displayed in the tables. Obviously, these simulations, with $\beta_{t,uranine}$ set to zero, did not result in any good fit to the breakthrough curve and are only displayed in Tables 5-1 and 5-2 for illustration of penetration depth if no exchange with the immobile zone occur. According to the simulation results displayed in Tables 5-1 and 5-2 it seems like the porosity had no or little effect on the penetration depth for uranine. As for example, when α_{max} was set to 0.1 in Table 5-1, the penetration depth was 0.33 m regardless if the porosity was 0.002 or 0.0002. Furthermore, the penetration depth is significantly less than the depth assuming no exchange with immobile zones.

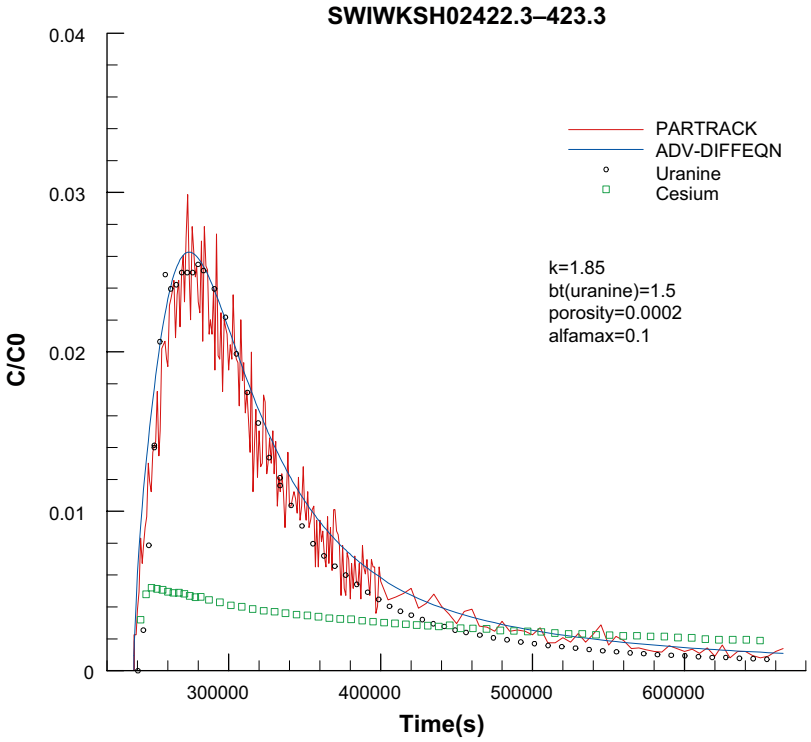

Figure 5-1. *Example of a breakthrough curve from simulation of uranine in KSH02 422.3–423.3 m.*

Table 5-1. Results from uranine simulations of KSH02 422.3–423.3 m using a homogeneous conductivity.

Fixed parameters		Fitting parameters		Average penetration depth (m)
Kinematic porosity	α_{max}	k	$\beta_{t,uranine}$	
0.002	0.001	2.1	0.1	0.17
0.002	0.1	1.85	0.15	0.33
0.002	–	–	0	5.82
0.0002	0.001	2.1	1.0	0.18
0.0002	0.1	1.85	1.5	0.33
0.0002	–	–	0	19.67

Table 5-2. Results from uranine simulations of KSH02 576.8–579.8 m using a homogeneous conductivity.

Fixed parameters		Fitting parameters		Average penetration depth (m)
Kinematic porosity	α_{max}	k	$\beta_{t,uranine}$	
0.002	0.001	2.0	0.1	0.07
0.002	0.1	1.75	0.15	0.26
0.00004	–	–	0	2.94
0.00004	0.001	2.0	5.0	0.07
0.00004	0.1	1.75	7.5	0.26
0.00004	–	–	0	26.04

Another interesting observation was that the relative size of the immobile zone, i.e. $\beta_{t,uranine}$ multiplied with the kinematic porosity, seemed to be constant regardless of the size of the mobile zone.

5.1.2 Cesium

During the simulations of cesium in the two test sections it was found that the correlation between the fitting parameters, R_m and $\beta_{t,cesium}$, was rather large. Hence, many combinations of these two parameters resulted in similar fits to the measured breakthrough curve. In Tables 5-3 and 5-4, selected sets of parameters are presented.

An example of a rather good fit is displayed in Figure 5-2. As seen in Figure 5-2 the simulated curve (PARTRACK) was rather noisy, especially during the early part of the curve. This was a common behaviour for the simulations of cesium. During simulation with an α_{max} of 0.1, it was not possible to achieve a good fit using k and $\beta_{t,uranine}$ from earlier simulations of uranine. One example of such a simulation is seen in Figure 5-3. The early part of the curve was clearly too low while the tail fits the measured data rather well. No clear reason for this effect was found except that it was related to the change in α_{max}.

5.2 Heterogenous conductivity

In some of the simulations, a heterogeneous conductivity field was used for section 422.3–423.4 m. The conductivity field was isotropic with a standard deviation of ln(K) at 2.0 and correlation length 1.0 m. The average conductivity was the same as in earlier simulations. Figure 5-4 displays the hydraulic conductivity in the central part of the model. The borehole centre is at (0,0).

Table 5-3. Results from cesium simulations of KSH02 422.3–423.3 m using homogeneous conductivity.

Fixed parameters				Fitting parameters		Resulting	
Kinematic porosity	α_{max}	k	$\beta_{t,uranine}$	Rm	βt,cesium	Rim	Average penetration depth (m)
0.002	0.001	2.1	0.1	1.5	15	165	0.01
0.0002	0.001	2.1	1.0	6	28	168	0.01
0.0002	0.1 [a)]	1.85	1.5	6	600	2,400	0.01

[a)] The fit was to low in the early part.

Table 5-4. Results from cesium simulations of KSH02 576.8–579.8 m using homogeneous conductivity.

Fixed parameters				Fitting parameters		Resulting	
Kinematic porosity	α_{max}	k	$\beta_{t,uranine}$	R_m	$\beta_{t,cesium}$	R_{im}	Average penetration depth (m)
0.002	0.001	2.0	0.1	1.5	6	90	0.01

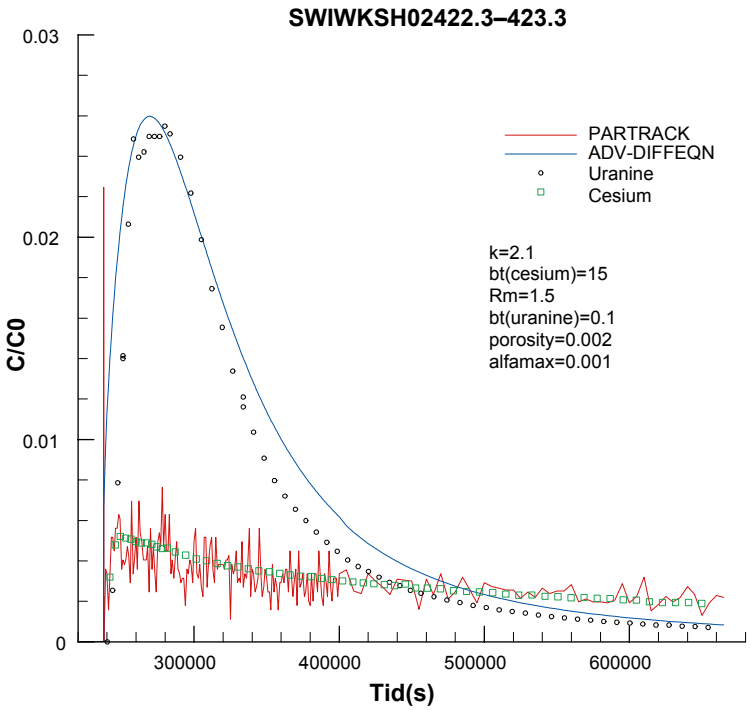

Figure 5-2. *Example of a breakthrough curve from simulation of cesium in KSH02 422.3–423.3 m using* α_{max}*=0.001.*

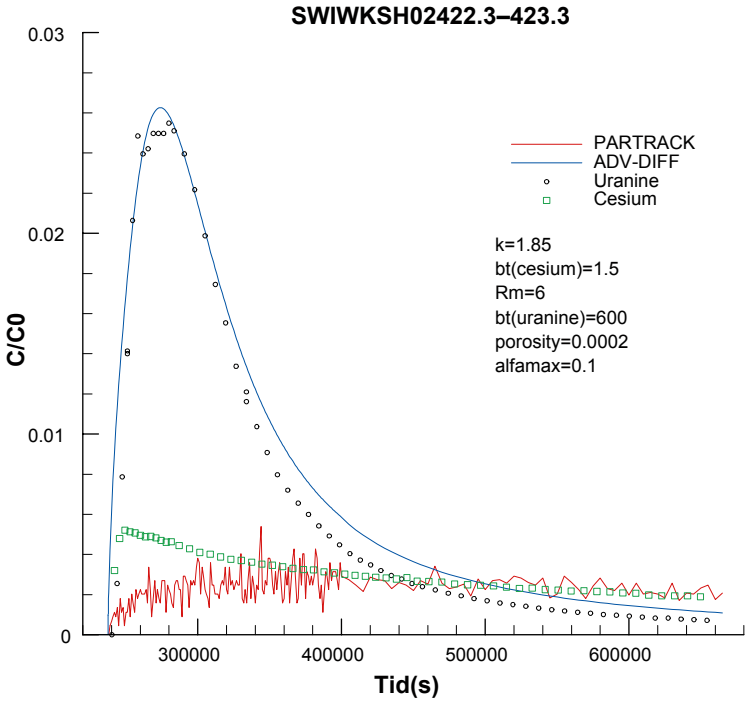

Figure 5-3. *Example of a breakthrough curve from simulation of cesium in KSH02 422.3–423.3 m using* α_{max}*=0.1.*

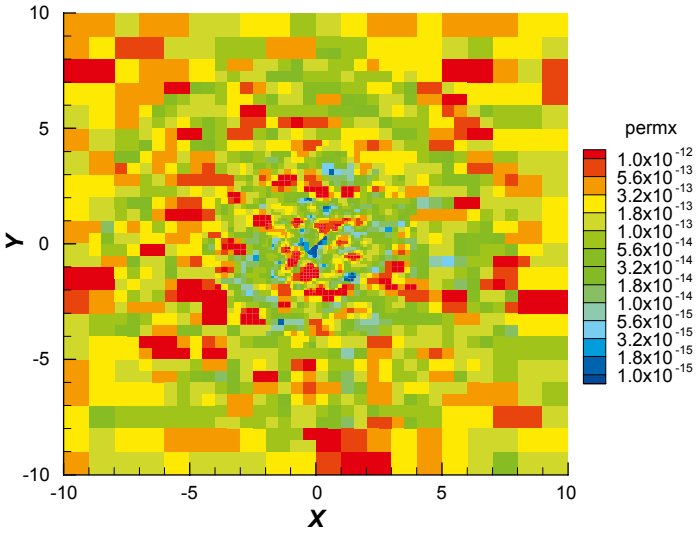

Figure 5-4. *Heterogeneous hydraulic conductivity (x-direction). The borehole centre is at (0,0).*

5.2.1 Uranine

Model fitting during heterogeneous hydraulic condition resulted in a lower $\beta_{t,uranine}$ than in the homogeneous case as shown in Table 5-4. Hence, the heterogeneous conductivity appears to contribute to the distribution of the transport times. Another interesting observation is that the average penetration depth, assuming a constant α_{max}, also depends on the porosity. This was not the case when homogeneous conductivity was used.

5.2.2 Cesium

Simulation of cesium with heterogeneous conductivity was also performed. It was possible to achieve a good fit, much like the fit displayed in Figure 5-2, when using the values given in Table 5-3. Despite that the parameters were close to the parameters in Figure 5-3 this fit did not display any low C/C0 in the early part. Hence, the heterogeneous conductivity plays an important role also in the simulation of cesium even though the tracer penetrates only a very short distance into the formation.

Table 5-5. Results from uranine simulations of KSH02 422.3–423.3 m using heterogeneous conductivity.

Fixed parameters		Fitting parameters		Average penetration depth (m)
Kinematic porosity	α_{max}	k	$\beta_{t,uranine}$	
0.002	0.1	1.85	0.12	1.40
0.002	–	–	0	5.54
0.0002	0.1	1.85	1.0	3.07
0.0002	–	–	0	17.59

Table 5-6. Results from cesium simulations of KSH02 422.3–423.3 m using a heterogeneous conductivity.

Fixed parameters				Fitting parameters		Resulting	
Kinematic porosity	α_{max}	k	$\beta_{t,uranine}$	Rm	$\beta_{t,cesium}$	R_{im}	Average penetration depth (m)
0.0002	0.1	1.85	1.0	6	350	2,100	0.01

5.3 Sensititivity analysis

Relatively good fits were possible to obtain with different sets of parameters. Often some sets fit better to the top of the breakthrough curve while other sets fit better to the tail. A simple sensitivity analysis was therefore performed. Observe that the fits have been judged by visual inspection and, thus, the results may be considered somewhat subjective.

The sensitivity analysis was mainly focused on the fitting parameters k and $\beta_{t,uranine}$ for uranine and R_m and $\beta_{t,cesium}$ for cesium. The effect of α_{max}, which has been discussed earlier, was also included in the analysis.

Since the sensitivity analysis requires a large amount of simulations, which was rather time consuming, it was focused on the SWIW test in KSH02 422.3–423.3 m. However, no behaviour of the simulations in section 576.8–579.8 m was found that contradicts the results of the sensitivity analysis of 422.3–423.3 m. Hence, these results could be more general than just the presented section.

5.3.1 Uranine

As discussed earlier in this report, the value of α_{max} has an effect on the simulation results. Figure 5-5 shows different α_{max} values and the corresponding k value that were judged to give the best fit to the data from the SWIW test in KSH02 422.3–423.3 m. The parameter k was in this analysis not divided into smaller steps than 0.5. The parameter $\beta_{t,uranine}$ was in all cases shown in Figure 5-5 between 0.1 and 0.15 and did not seemed to be affected by different α_{max} values. This effect is also visible in Figure 5-6 where the marginal of error regarding $\beta_{t,uranine}$ is shown for different sets of k and α_{max}.

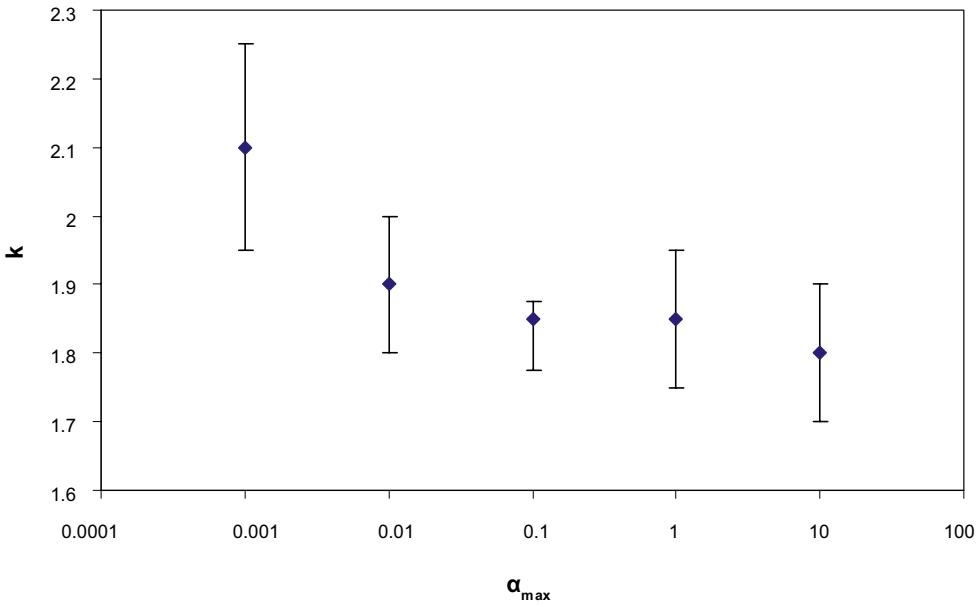

Figure 5-5. *k as a function of α_{max} which results in good fits for SWIW test in KSH02 422.3–423.3 m.*

Figure 5-5 also shows intervals of k for each α_{max}. The intervals represent values of k that were found the give a relatively good fit to the breakthrough curve. In the analysis, most of the simulations were performed with α_{max} set to 0.001 and 0.1. This explains the relatively small interval for α_{max} set to 0.1 compared to the surrounding α_{max}. When α_{max} was set to 0.001, the solution proved to be less sensitive regarding the parameter k. This is visible in Figure 5-5 as a rather large interval and in Figure 5-6.

5.3.2 Cesium

As mentioned earlier, several combinations of $\beta_{t,cesium}$ and R_m could be used and still obtain a good fit to the SWIW test data. Hence, the correlation between the two parameters was high, at least within certain intervals. In Figure 5-7 examples of such combinations of $\beta_{t,cesium}$ and R_m are displayed which all resulted in a good fit to the cesium data. In this case, $\beta_{t,uranine}$ was set to 1.0, k to 2.1 and the porosity to 0.0002.

An interesting observation regarding the sensitivity of the cesium simulation was that the product of $\beta_{t,cesium}$ and R_m that gave a good fit was more or less constant for a given porosity and α_{max}. This implies that R_{im}, as well as $\alpha_{max,cesium}$ and $\alpha_{min,cesium}$, according to Equations 4-1 and 4-2 was more or less constant. This was the case for simulations assuming homogeneous as well as heterogeneous conductivity.

5.3.3 Cell size

Since the penetration depth into the formation, especially regarding cesium, was rather short in the simulations, it was suspected that the cell size closest to the borehole was too large. Hence, different cell sizes were tested in the model. A reduced cell size close to the borehole appeared to have an effect on the cesium simulation. The most significant effect was that the spikes early in the breakthrough curve, as seen in Figure 5-2, were reduced. The effect of the reduced cell size on the tail of the breakthrough curve was rather small. This effect may further increase the uncertainty regarding the simulation of the sorption effect.

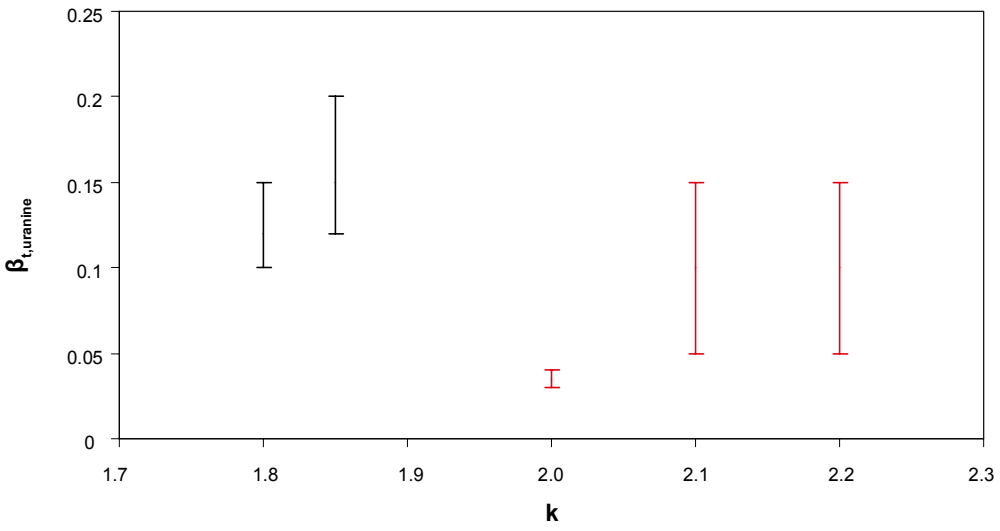

Figure 5-6. *Intervals of $\beta_{t,uranine}$ as a function of k which results in good fits for SWIW test in KSH02 422.3–423.3 m. α_{max} was set to 0.1 for the black intervals and set to 0.001 for the red intervals.*

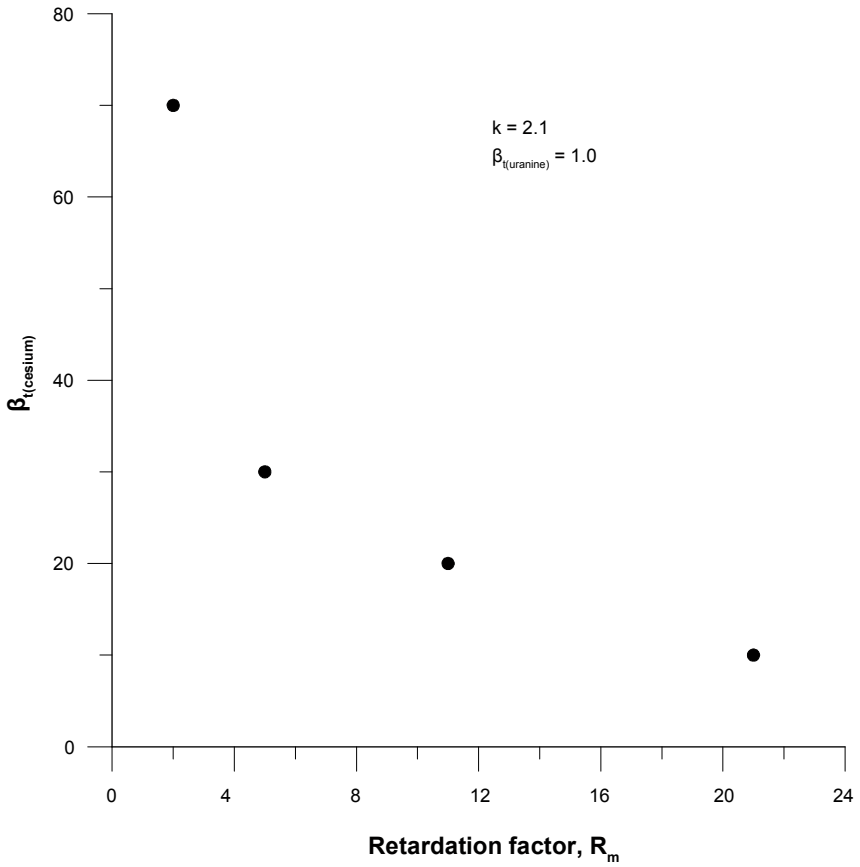

Figure 5-7. *Combinations of R_m and $\beta_{t,cesium}$ which results in good fits to cesium data from SWIW test in KSH02 422.3–423.3 m. k and $\beta_{t,uranine}$ are 2.1 and 0.1, respectively. The porosity is 0.0002.*

5.3.4 Other parameters

Regarding other parameters than those discussed above, as for example conductivity and the domain size, no sensitivity analysis has been performed.

No strict sensitivity analysis has been performed regarding the time resolution. However, during the development of the model the time step length was often modified. It did not appear to affect the solution in any major way except in one case. If long time steps were used during periods of variations in flow rates, as for example at the transition from chaser phase to withdrawal phase, the solution regarding the pressure became unstable. This was avoided by defining the time steps in the fif.f file so they may be altered during the simulation.

6 Discussion

The overall impression of DarcyTools was that it may be possible to use as a tool for evaluation of SWIW tests. However, some questions and possible improvements remains which is discussed below.

It was in general possible to achieve a very good fit of the model to data from the SWIW tests. Especially the fit of the tail of the breakthrough curve for uranine was much better than the evaluation, using the advection-dispersion equation, presented in SKB P-05-28 /1/. The SWIW tests used in this report have also been simulated using the advection-dispersion equation together with single rate matrix diffusion by Nordqvist /3/. The single-rate diffusion in those simulations appeared to improve the fit to the uranine data, especially to the tail. However, it seems, by visual inspection, like the multi rate approach used in DarcyTools improves the fit even further.

The parameters used in this report may be compared to other studies using DarcyTools by Svensson /4/ and /5/. In general, $\beta_{t,uranine}$ values obtained in this study are rather small. However, it was obvious that it was closely related to the assumed kinematic porosity. Hence, an even lower porosity would result in higher $\beta_{t,uranine}$. The parameter k obtained in these simulations coincides well with the value used by Svensson in /4/ and /5/ where k is set to 2.0. On the contrary, the parameter α_{max} was in Svensson /4/ set to $1 \cdot 10^{-3}$. In this study, it had to be set much higher in order to get results that were rather insensitive to a further change of α_{max}. However, one should keep in mind when comparing parameters from SWIW tests with other types of simulation that these tests are rather limited in time and space which may affect the resulting values. For example, the tested formation may be dominated by the fracture that was explicitly allocated in the model and not intercepted by many other smaller non-conductive fractures within the short distance that the tracer was transported. This could be a rather reasonable explanation of a relatively low $\beta_{t,uranine}$ value.

As indicated by the results in this report, the best fits, assuming a homogeneous conductivity, resulted in a rather short penetration depth of the tracers into the formation compared with pure advective transport. In addition, these fits resulted in a penetration depth that was independent, or close to independent, of the conductive porosity. This effect was not realistic and would indicate that the some other effect than advective transport was dominating the model, probably the exchange with the immobile zone.

If a heterogeneous conductivity field was employed, the relative size of the immobile zone had to be reduced in order to achieve a good fit to the data since the heterogeneity appears to contribute to the distribution of transport times. In this case, the relationship between the porosity and the penetration depth of the tracer was much more realistic than in the homogeneous case.

Since there are uncertainties about the penetration depth for the tracers it would be rather interesting to use this model for evaluation of multiple well tracer tests.

The sensitivity analysis shows that it was possible to obtain rather limited intervals for the parameters k and $\beta_{t,uranine}$ that results in a good fit. However, the intervals regarding k appeared to be dependent of α_{max}. The correlation between $\beta_{t,cesium}$ and R_m was rather high which made it hard to achieve reliable and conclusive results. On the other hand, the combinations of the two parameters that resulted in a good fit, assuming a fixed porosity and α_{max}, gave a R_{im} that was more or less constant. This may imply that the sorption in the immobile zone was more important for the model results than the sorption in the mobile zone.

The greatest limitation of using this model for the evaluation of SWIW tests is time, since each run takes about 10 minutes. Unfortunately, it takes rather many runs to obtain a reliable result. Therefore, it is desirable to shorten the time for a run or to implement an automatic parameter estimation tool in order to reduce the total time necessary for evaluation.

According to the results from the simulations, the tracers did not penetrate far into the formation. This is especially true for the sorbing cesium. The cell size close to the borehole may be of importance in the model and should therefore be small. An increase of the number of cells in the model makes the simulations more time consuming. If this model should be used for further evaluation of SWIW tests, it would probably be worthwhile to optimize the cell structure.

7 References

/1/ **Gustafsson E, Nordqvist R, 2005.** Oskarshamn site investigation. Groundwater flow measurements and SWIW tests in boreholes KLX02 and KSH02. SKB P-05-28, Svensk Kärnbränslehantering AB.

/2/ **Svensson U, Kuylenstierna H-O, Ferry M, 2004.** DarcyTools, Version 2.1 Concepts, methods, equations and demo simulations. SKB R-04-19, Svensk Kärnbränslehantering AB.

/3/ **Nordqvist R, 2005.** Extended evaluation of SWIW tests in KSH02. In prep.

/4/ **Svensson U, 2004.** Modelling flow, transport and retention in a sparsely fractured granite. Äspö Task Force: Tasks 6D, 6E, 6F and 6F2 (Draft).

/5/ **Svensson U, Follin S, 2004.** Simulation of tracer transport. Considering both experimental and natural, long, time scales. Äspö Task Force: Task 6A, 6B and 6B2. International Progress Report IPR-04-42. Svensk Kärnbränslehantering AB.