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DarcyTools, Version 2.1

Concepts, methods, equations and demo simulations

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March 2004

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This report concerns a study which was conducted in part for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

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Preface (by Urban Svensson)

As the first author of this report, I take the liberty to write a preface and explain a few things about the work leading to version 2.1 of DarcyTools. This is necessary as Hans-Olof and Michel have not been involved in the writing of the main part of the report, and they may not even share all the views expressed.

The contributions from Hans-Olof and Michel can be specified as follows:

Hans-Olof: Development of methods and writing of software for generation of fracture networks and their representation (in terms of properties) in the continuum model. Development of methods and writing of software for the particle tracking routine PARTRACK. Author of Appendices B, C and D.

Michel: Development and writing of the software for the solution of the continuum problem. Author and owner of the solver MIGAL. Author of Appendix A.

My contribution has been in the development of concepts and methods, real world applications and tests. I have also coordinated the efforts and done my best to ensure that we deliver the product our client, SKB, expects.

Abstract

DarcyTools is a computer code for simulation of flow and transport in porous and/or fractured media. The fractured media in mind is a fractured rock and the porous media the soil cover on the top of the rock; it is hence groundwater flows, which is the class of flows in mind.

DarcyTools is a general code for this class of problems, but the analysis of a repository for nuclear waste is the main intended application.

A number of novel features are introduced in DarcyTools. The most fundamental is perhaps the method to generate grid properties (DarcyTools is a continuum porous-media code); a fracture network, with properties given to each fracture, is represented “directly” in the computational grid. This method is believed to result in very accurate anisotropy and connectivity properties.

The report focuses on the concepts, assumptions, equations and key features of DarcyTools. The main part of the report is fairly short; a number of appendices give more detailed accounts of various aspects of the code.

Abstract (Swedish)

DarcyTools är ett datorprogram för simulering av flöde och transport i ett poröst och/eller sprickigt medium. Det sprickiga mediet är ett sprickigt berg och det porösa mediet jordlagret som täcker berget; det är således grundvattenströmning som är applikationsområdet.

DarcyTools är ett generellt program för grundvattenströmning, men tillämpningar som rör analyser av förvar för uttjänt kärnbränsle står i fokus.

Ett antal nya koncept och metoder utgör hörnpelare i DarcyTools. Den kanske mest fundamentala av dessa rör metoden för att representera hydrauliska egenskaper i beräkningsnätet (DarcyTools är en så kallad "porös kontinuum kod"). Metoden bygger på en direkt representation av ett spricknätverk, som kan innefatta upp till en miljon sprickor. Tanken är att denna metod skall ge en god beskrivning av bergets anisotropi och sprickors konnektivitet.

Rapporten beskriver koncept, antaganden, ekvationer och illustrerar nyckelegenskaper. Huvuddelen av rapporten är tämligen kort; ett antal appendix beskriver olika aspekter av programmet mer i detalj.

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1 Introduction

1.1 Background

DarcyTools is a computer code for simulation of flow and transport in porous and/or fractured media. The fractured media in mind is a fractured rock and the porous media the soil cover on the top of the rock; it is hence groundwater flows, which is the class of flows in mind.

DarcyTools is developed by a collaborative effort by SKB AB (The Swedish Nuclear Waste Management Company AB) and CFE AB (Computer-aided Fluid Engineering AB). It builds upon earlier development of groundwater models, carried out by CFE AB during the last ten years. The following reports, by the present writer, give a general account of this work and hence give a background to the work to be described in this report:

- Groundwater flow at Äspö and changes due to the excavation of the laboratory, Svensson (1991). This report gives predictions of the influence of the laboratory *prior* to its construction.
- A regional analysis of groundwater flow and salinity distribution in the Äspö area, Svensson (1997a). Results from this study have been useful for generating boundary conditions for smaller scale models.
- A site scale analysis of groundwater flow and salinity distribution in the Äspö area, Svensson (1997b). This model may be considered as representing a synthesis of the detailed information provided in Rhén et al. (1997).
- Representation of fracture networks as grid cell conductivities, Svensson (1999a). This report describes, for the first time, the principles used for generating property fields in DarcyTools.
- A laboratory scale analysis of groundwater flow and salinity distribution in the Äspö area, Svensson (1999b). In this study the new methods were applied and evaluated.
- PARTRACK –A particle tracking algorithm for transport and dispersion of solutes in a sparsely fractured rock, Svensson (2001a). This report describes the particle tracking techniques used in DarcyTools.
- Impact of the tunnel construction on the groundwater system at Äspö. Task 5, Äspö Task Force on Groundwater Flow and Transport of Solutes. Svensson, Laaksoharju and Gurban (2002).

These reports give a general overview of the developments that have lead to the present version of DarcyTools. It should also be pointed out that in the listed reports the CFD code PHOENICS (Spalding, 1981) was used as an equation solver. DarcyTools is based on a solver called MIGAL (Ferry, 2002). It has however been carefully evaluated that the two solvers produce very similar solutions and the reports listed are thus still valid as background reports for DarcyTools.

The present report will focus on the theoretical basis of DarcyTools. Two accompanying reports cover other aspects:

- Verification and Validation, Svensson (2004) (Hereafter Report 2).
- User's Guide, Svensson and Ferry (2004) (Hereafter Report 3).

“Real world applications” of DarcyTools can be found in Svensson (2001c) and in Follin and Svensson (2002).

Two basic approaches in groundwater modelling can be identified; in one we define grid cell conductivities (sometimes called the continuum porous-medium (CPM) approach, Jackson et al., 2000), in the other we calculate the flow through the fracture network directly (DFN approach). Both approaches have their merits and drawbacks, which however will not be discussed here (for a discussion, see Sahimi, 1995). Instead we will try to combine the approaches, meaning that we first generate a fracture network and then represent the network as grid cell properties.

The traditional way to calculate grid cell conductivities in continuum models is through an upscaling procedure (for reviews see: Wen and Gómez-Hernández (1996), Renard and de Marsily (1997) and Pozdniakov and Tsang (1999)). These methods are however of no direct use in the present work. Attempts have been made, see La Pointe et al. (1995), Niemi et al. (1999) and Jackson et al. (2000), to use a DFN-model to calculate grid cell conductivities. This method has similarities with the present approach as the cell conductivity will be based on the properties of a fracture network. We will however not use a DFN-model to estimate the grid cell conductivities; instead the fracture network is represented “directly” in the continuum model. Methods to include a limited number (say 10-20) of major fracture zones in a CPM-model have been presented, see for example Svensson (1997) and Gómez-Hernandez et al. (1999). The method in DarcyTools is different from these methods in that all fractures and fracture zones are considered, when the conductivity field is generated. This means that we may need to represent 10^5 to 10^6 fractures as grid cell conductivities. Further, if the properties (geometry, transmissivity, etc) of the major fracture zones are known, these zones are treated deterministically, while unknown, or background, fractures are generated from statistical distributions.

1.2 Objectives and scope

The objectives of this report can be summarised as:

- Provide the theoretical basis of DarcyTools
- Illustrate how DarcyTools works, through simple demo simulations
- Discuss and evaluate the present status of DarcyTools

It will not be possible to review applications of DarcyTools in this report.

1.3 The Äspö HRL

The present report will not describe real world applications. Several references to model studies and field data related to Äspö Hard Rock Laboratory (HRL) will however be made and a brief introduction to Äspö HRL will therefore be given.

The Äspö Hard Rock Laboratory is located near the Oskarshamn nuclear power plant on the east coast of Sweden, see Figure 1-1. The access tunnel starts on the mainland, continues under the Baltic and reaches the spiral part of the tunnel beneath the island of Äspö. The total length of the tunnel is 3600 metres and it reaches a depth of 450 metres below ground surface. A vertical elevator shaft connects the laboratory to the Äspö Research Village.

Mean precipitation minus evapotranspiration, P-E, has been estimated to be about 200 mm/year for the region, Rhén et al. (1997). For the island of Äspö one can expect that the groundwater recharge (i.e. P-E) is smaller as the distance to the sea is shorter (no storage of water in lakes and ponds during periods of heavy precipitation). A value of 100 mm/year was used in the site scale model.

Around the island of Äspö the Baltic Sea has a salinity of about 0.6%. It is known from boreholes on Äspö that the fresh water lens below Äspö has a thickness of 100 to 200 metres under natural conditions; below this level the salinity increases to reach a value of about 2% at a depth of 800 metres below ground. As the water density increases with salinity we have a density stratified water below the island of Äspö. This is an important feature of the groundwater flow system.

Three model domains are outlined in Figure 1-1; these will be referred to throughout the report.

The major fracture zones at Äspö are shown in Figure 1-2 and boreholes in Figure 1-3. These figures will be referenced to when field measurements are discussed.

1.4 Outline

The main part of the report is fairly short; this with the intention that the reader should be able to get a good overview of DarcyTools from a few hours of reading. The appendices will provide more detailed descriptions of various central topics.

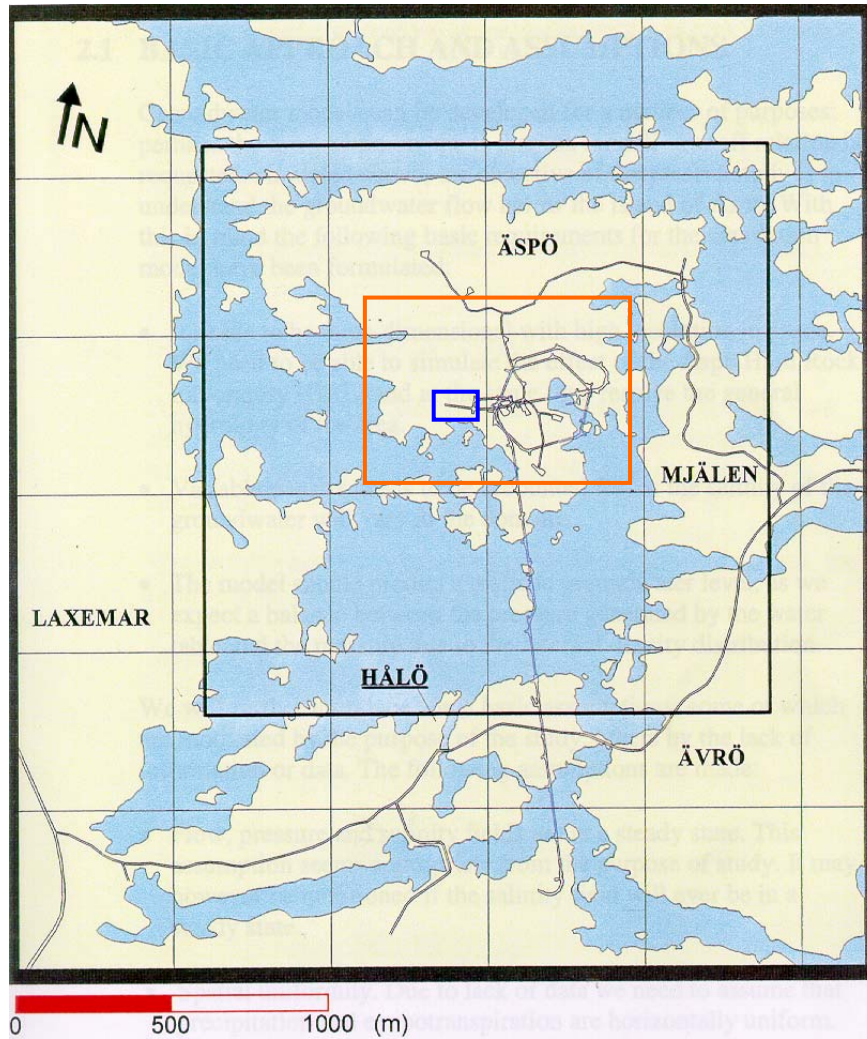
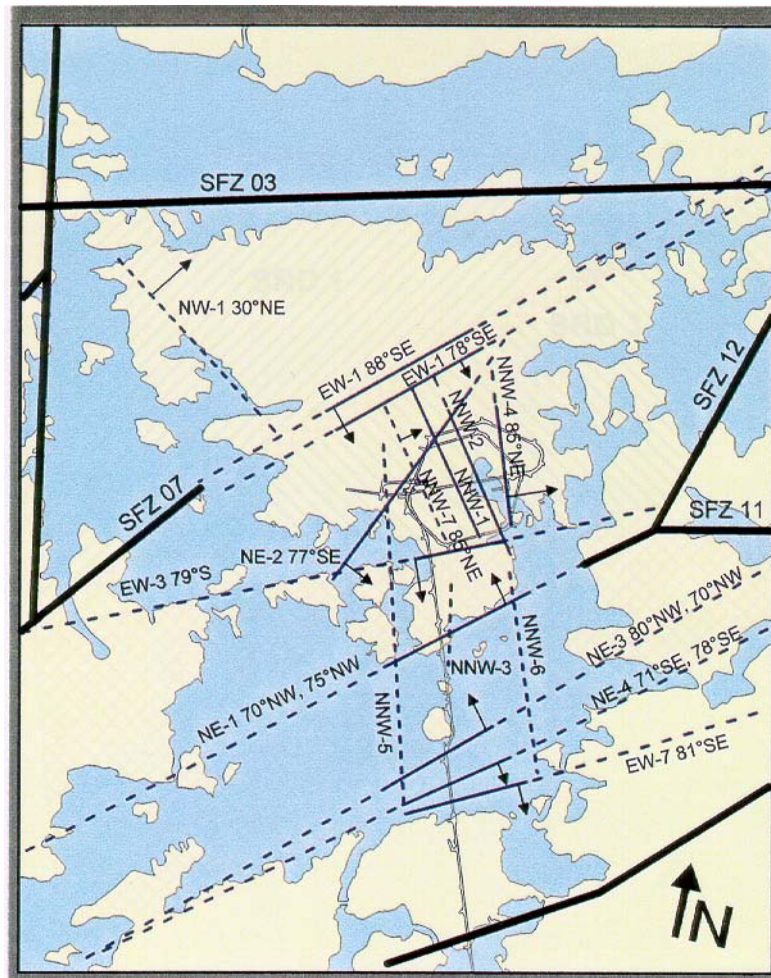


Figure 1-1. The island of Äspö and the Äspö Hard Rock Laboratory. The black rectangle shows the area of the Site scale model, Svensson (1997b). The red rectangle shows the Laboratory model (Svensson, 1999) and the blue rectangle indicates the domain for the Repository model (Svensson, 2001).



0 500 1000 (m)

- Regional structure
- Certain conductive structure
- - - Probable conductive structure
- Possible conductive structure

Figure 1-2. Major fracture zones in the area, after Rhén et al. (1997).

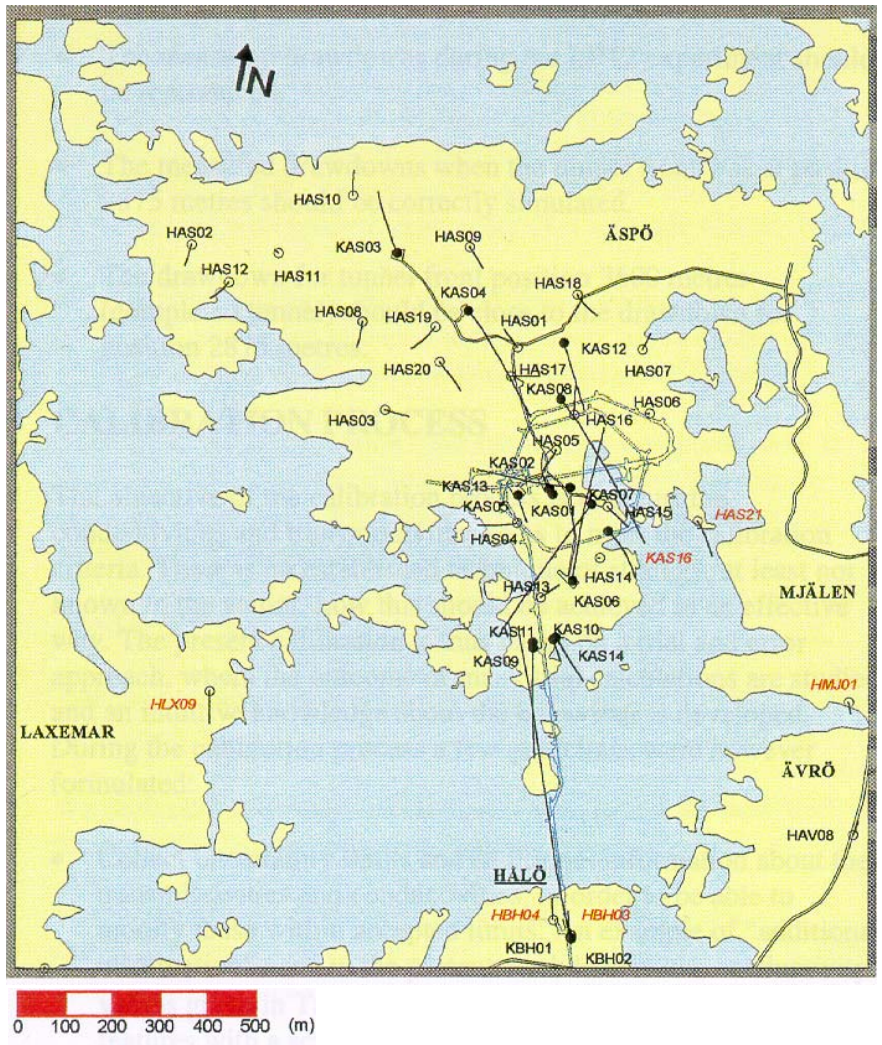


Figure 1-3. Boreholes in the Äspö area.

2 Situation considered

2.1 Introduction

As mentioned, it is flow and transport in fractured and/or porous media that is the application area for DarcyTools. In this section a general description of physical processes, scales, etc that need to be considered will be given. It is hoped that the picture painted is one that most geohydrologists can agree upon (concepts and assumptions built into DarcyTools are not discussed in this context). The description is generic, but inspired by the conditions at and experiences from the Äspö Hard Rock Laboratory (HRL). The fractured rock in mind is hence a sparsely fractured granite.

2.2 The 10 km scale view

The regional groundwater flows in unconfined aquifers introduces the concepts of recharge and discharge areas, see Figure 2-1. Recharge areas, i.e. where a net inflow is found, are usually found in topographically high places while the discharge areas are located in topographic lows. The discharge areas may take the form of a stream, river or a lake.

The general flow pattern is hence from high to low areas; a system of local flow cells is formed and the groundwater table follows the surface topography. However, this is an idealized picture which is based on the assumptions of a steady, constant density flow in a homogeneous aquifer. These assumptions are seldom fulfilled and care should hence be taken when interpreting field data, based on this view. In particular, most natural aquifers are anisotropic and heterogeneous.

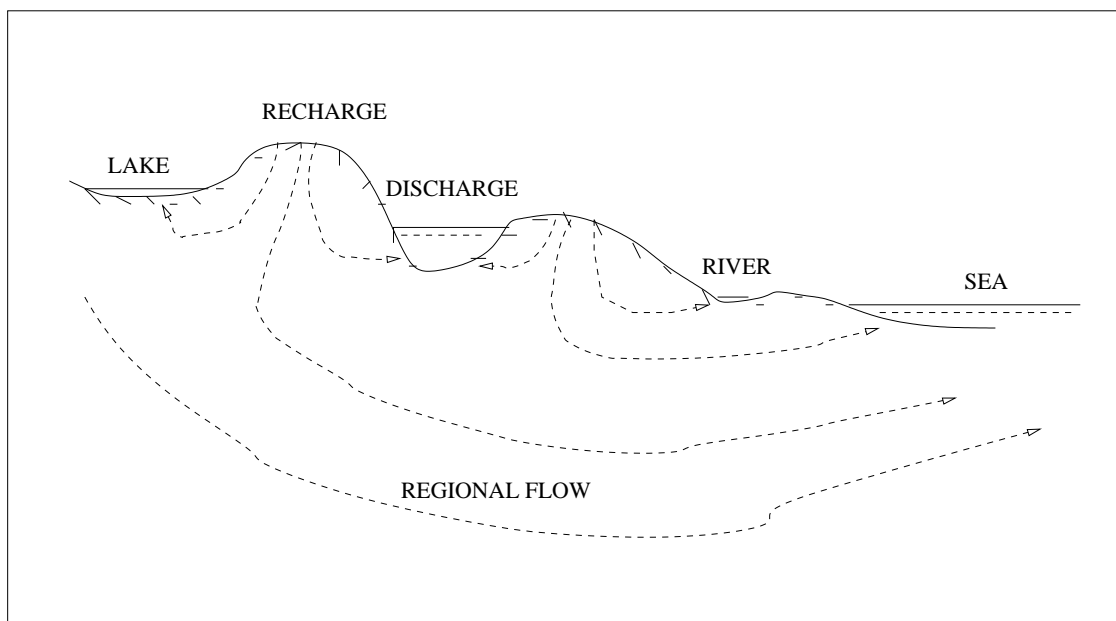


Figure 2-1. Situation considered – the 10 km scale view.

2.3 The km scale view

A km scale view is given in Figure 2-2. Let us assume that it is of interest to determine the origin of water leaking into the tunnel. Two main sources are precipitation and seawater (excluding brine water from below). To track the precipitation water one has to follow a water parcel through the unsaturated zone, down to the saturated soil cover and finally its way through the fracture network. It is essential to determine the position of the groundwater table, as it determines the pressure gradients in the porous media and may influence the conditions deep into the rock. The other source, the seawater, introduces density effects, as the seawater is heavier than fresh water. The heavier saltwater penetrates the coastal zone and modifies the pressure distribution (the Ghübern Herzberg relation). Due to this effect the inflow to the tunnel may be dominated by seawater *or* the precipitation water; all depending on the actual conditions (density difference, tunnel position, etc).

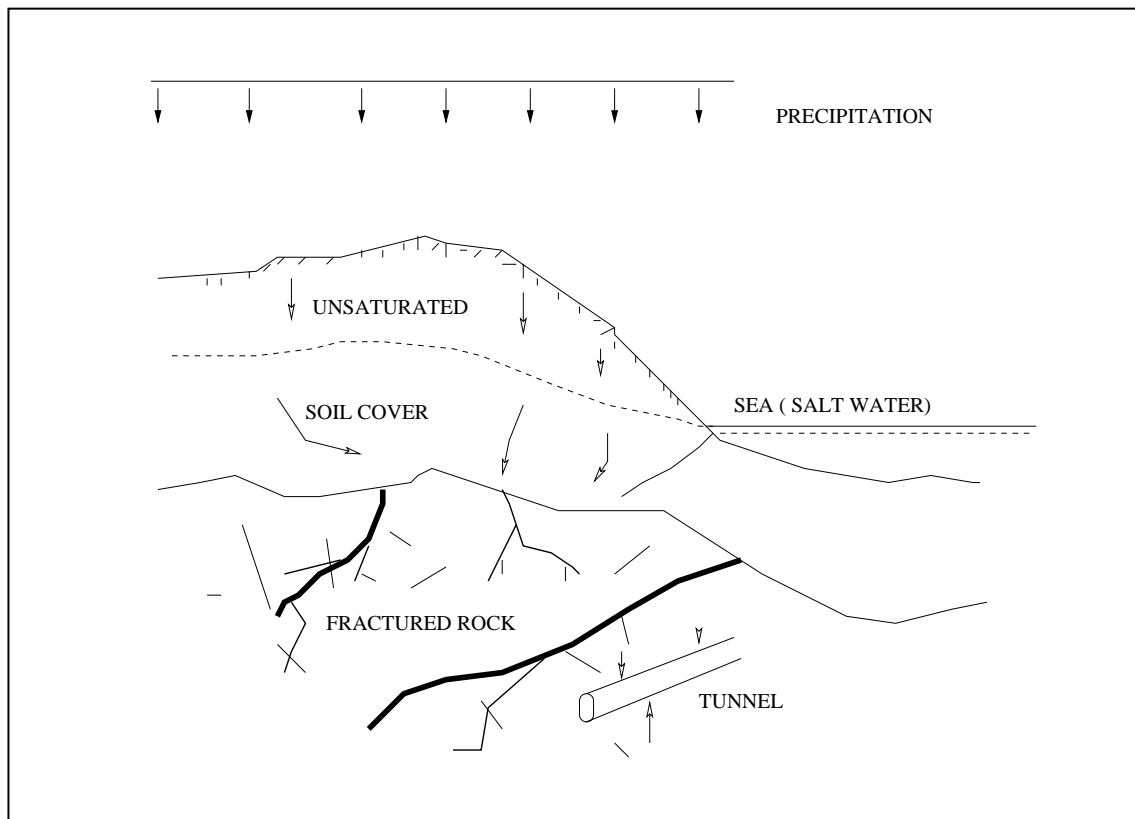


Figure 2-2. Situation considered – the km scale view.

2.4 The m scale view

The main novel features of DarcyTools are concerned with the fracture network and we will therefore focus on the description of fractures (giving the porous media less attention). In Figure 2-3 part of a fracture network is shown. Different parts of the network have been marked with letters; these parts will now be described:

A: Represents a fracture zone. The fracture zone is assumed to be composed of a number of smaller fractures through which the flow takes place. Most of the small fractures do however not contribute to the flow but are still important for transport and dispersion of a tracer. Fracture zones are often the main flow conductors due to their high transmissivity and size (length scale >100 metres). The thickness is typically > 1 metre.

B: Some fractures are best characterised as “a single opening”. Typically the thickness, or the aperture, is of the order of 10^{-3} metres. The fractures marked with **B** in Figure 2-3 have a through-flow and may hence contribute to the total flow rate. If the transport time through the **B** fractures is different from the transport time in the fracture zone a dispersion effect will also result from the parallel flow path.

C: Isolated fractures or groups of fractures can not contribute to the flow, transport or dispersion, as flow in the matrix is neglected. In the numerical model these are removed before the generation of grid data is performed.

D: Some fractures, or fracture zones, may form “dead end systems”. The exchange with fractures with a significant flow is then by molecular diffusion. When storage of water over long time periods, say longer than 100 years, is studied it is essential to represent the dead-end systems correctly.

E, F: There is always a lower limit on the fracture size that can be represented correctly in a numerical simulation. In the present study it will be assumed that fractures below a certain size, to be discussed, do not contribute significantly to the total flow. However, for transport and dispersion it is probably necessary to consider all scales, as a large fraction of the pore volume is expected to be due to the small scale features of the porosity field.

2.5 The mm scale view

It was mentioned above that the opening, or aperture, of a fracture is typically of the order of 1 mm or smaller. The aperture has however not a constant value, as is illustrated in Figure 2-4. On this scale it is useful to introduce the notions of the mobile zone, for the volume that has flowing water, and the immobile zone which represents all volumes with stagnant water. In Figure 2-4, the stagnant pools, the crossing fractures and the matrix may all contain stagnant water. The fracture may also contain material of various kinds, so called gouge material.

The geometrical complexity of a fracture opening is essential to consider when small scale dispersion processes are to be described. The exchange between the mobile and immobile zones is often assumed to be due to molecular diffusion only.

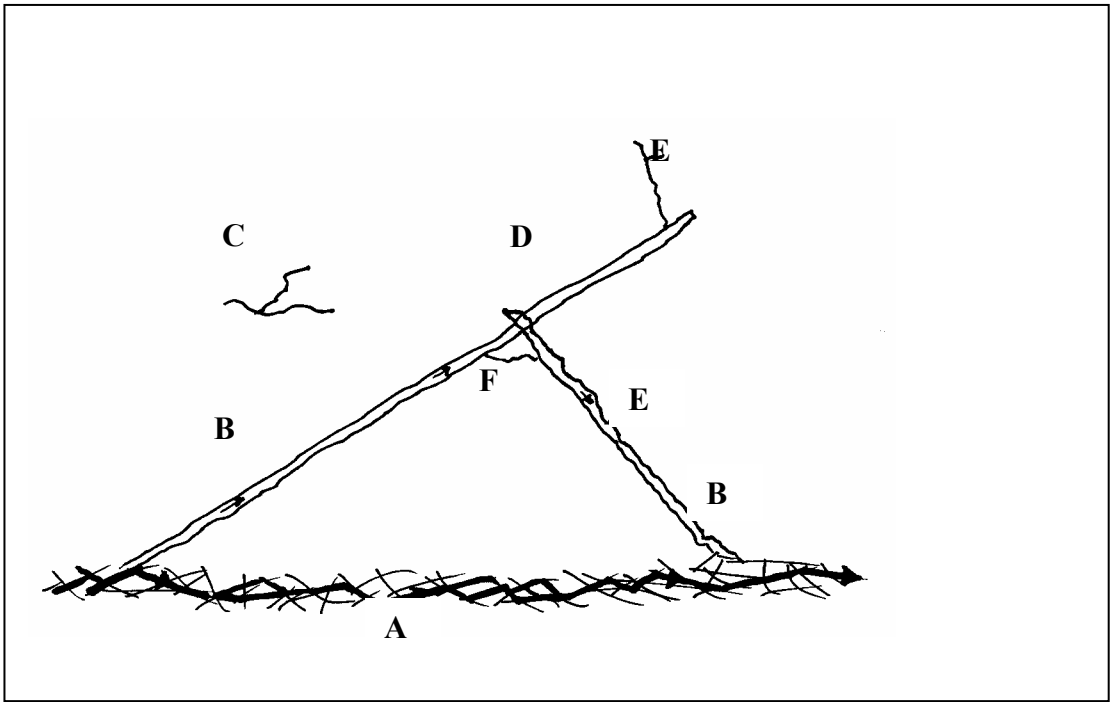


Figure 2-3. Situation considered – the m scale view.

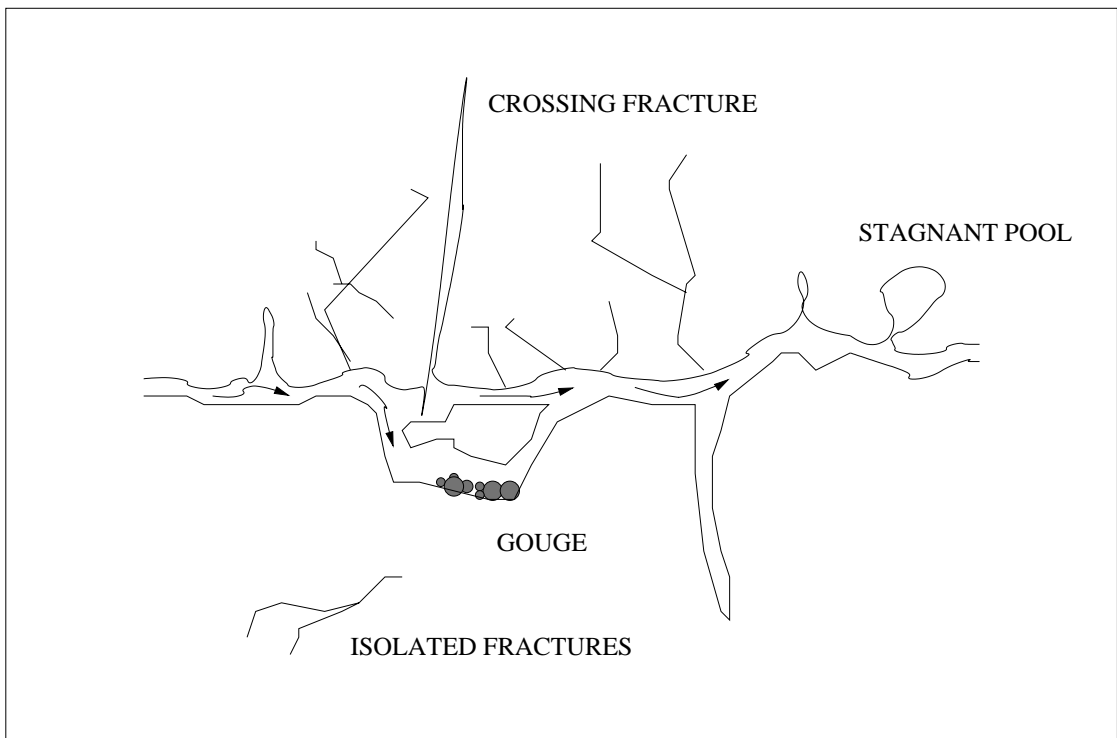


Figure 2-4. Situation considered – the mm scale.

2.6 The flow system

If only the flow field is of interest, we do not need to consider the detailed properties of a fracture (as outlined in Figure 2-4). The fracture transmissivity is normally what is needed. In addition the following topics may be of importance:

- A method to handle the unsaturated zone is required. Depending on the situation at hand the method may range from quite simple (only position of the groundwater table) to complex two-phase algorithms.
- Density stratification. If waters of different densities meet, it is essential to account for the effects.
- In addition to the fracture transmissivities one needs information about the conductivity of the soil cover, if present.

These are some of the key elements that govern the flow system. Note that we at this stage are not discussing the required input to a numerical model, which of course is more extensive (boundary conditions, properties, etc).

2.7 Transport and dispersion

When discussing transport and dispersion of solutes it is useful to distinguish between two different problems with respect to the time scale. The first kind of problem is the field experiment with a time scale from weeks to perhaps a year. A longer time scale, which may be thousands of years, needs to be considered when the water types present in the fracture network is to be analysed. At Äspö HRL, water from the last glaciation (about 11 000 years ago) has been found already at a depth of a few hundred metres. The relevant processes for the two problems will now be described, in turn.

Let us think of a typical field tracer experiment where a tracer is injected in one borehole and the arrival in another, pumped, borehole is studied. The curve describing the time distribution of the concentration in the pumped borehole is called the break through curve (BTC). Obviously the tracer is transported by advection between the two boreholes, and the flow field is hence an important element in the analysis. A number of dispersion processes will however affect the tracer as it travels through the fracture network. The most important of these are:

- **Intersections.** At a fracture intersection a tracer cloud may split up and enter pathways with different lengths and fluid velocities. This type of dispersion is often called macro-dispersion.
- **Channelling.** Spreading occurs within each fracture plane as the different streamlines have different path lengths and velocities. The flow channels may also merge or split up.
- **Taylor dispersion.** A velocity profile exists between the two bounding walls of the fracture. The resulting dispersion effect is called shear- or Taylor dispersion.

- **Matrix diffusion and sorption.** Interaction with the rock, stagnant pools and microfissures causes a number of processes that in effect lead to a delay and dispersion of a tracer pulse. These include: sorption on the fracture walls, diffusion into the rock matrix with sorption on inner surfaces and interaction with gouge.

As mentioned earlier, the diffusion into dead-end fractures of various sizes (see Figure 2-3 and 2-4) is by molecular diffusion. In order to illustrate the typical penetration depth for this process one may think of a substance with a certain molecular diffusion constant ($D_{mol} = 10^{-10} \text{ m}^2 / \text{s}$) and an experimental time scale of, say, one month ($t \approx 2.6 \times 10^6 \text{ s}$). The penetration length can then be estimated as $\sqrt{D_{mol} \times t} = 0.016$ metres. As the immobile zone is mainly made up of small fractures one can conclude that small scale dispersion is mainly governed by processes on the mm to cm scale.

For the transport problem on long time scales we may use the salinity field to illustrate some key features. First we can note the time scale for exchange in larger ($>$ metres) dead-end fracture systems. If we put $D_{mol} = 10^{-10} \text{ m}^2/\text{s}$ and $L = 10$ metres, we find that the time scale is 10^{12} seconds, or 30 000 years ($t = L^2 / D_{mol}$). It is thus not surprising to find water from the last glaciation, or the Litorina Sea (≈ 7 000 years BP), in the fracture system at Äspö HRL. Gravitational forces may further enhance the entrapment of water in dead-end zones. If, for example, Litorina water (which has higher salinity than the present Baltic water) is located in a dead-end fracture extending downwards from the mobile zone gravitational forces will enhance the entrapment. The same principle applies to glaciation water (which has a lower density than present Baltic water) in a dead-end fracture extending upwards from the mobile zone. If we further note that the volume of all immobile zones is larger than the volume of the mobile zone, one can draw the conclusion that the salinity field is “stiff” and requires very long time scales to reach a steady state. On a shorter time scale all processes listed above is of course also active for the dispersion of salt.

2.8 The transient nature of the problem

From the discussion of the salinity field one can conclude that the groundwater system is never in a steady state. Note that any change in the salinity field will modify the flow field as these are linked through the gravitational force.

In order to emphasise the transient nature of the problem the following list of processes have been compiled:

- Glaciations. Time scale of 10 000 to 100 000 years.
- Diffusion into dead-end fractures. Time scale from minutes to 100 000 years.
- Sea level variations. From daily variations to long time effects due to the land uplift.
- Precipitation. From daily, seasonal to yearly variations.
- Tidal effects. Time scale of one day.

The list can be made longer, but the message is probably clear “transient effects on a variety of scales need to be considered”.

2.9 Summing up

It was the intention of this section to describe the problem considered in a way that “most geohydrologists can agree upon”. Probably the reader will not accept that this has been achieved as one may put emphasis on different aspects of the problem (the important area of two-phase flows has for example not been mentioned, nor has the storativity and specific yield effects been described). Based on the qualitative descriptions given, it is however hoped that most readers will agree upon the following consensus statement:

- Flow, transport and dispersion in a sparsely fractured rock are governed by processes that have time scales ranging from minutes to thousands of years and space scales ranging from millimetres to several kilometres. The coupling between scales, in space and time, is strong and it is generally not possible to neglect these interactions.

3 Concepts, Assumptions and Methods

3.1 Introduction

The qualitative description of the previous section sets the scene for the concepts, assumptions and methods to be introduced in this section. If the previous section was general, the present section is very specific for DarcyTools. The descriptive presentation method will however be continued, leaving the mathematics to the section to follow. We will hence not try to “prove” the correctness of the concepts, assumptions and methods, as this will be the objective of a separate report (Report 2).

First a key assumption in DarcyTools will be presented, then the fracture network and its representation in the grid (including subgrid processes) is discussed. After this concepts related to transport are reviewed, then the groundwater table is discussed and finally some assumptions regarding properties are given.

3.2 The key assumption

The most fundamental assumption in DarcyTools is related to the structure of the fracture network, which is assumed to follow a power law distribution. More precisely it is assumed that the number of fractures per unit volume, n , in the length interval, dl , is given by:

$$n = I * \left[\left(\frac{l + dl}{l_{ref}} \right)^a - \left(\frac{l}{l_{ref}} \right)^a \right] / a \quad (3-1)$$

where I is the intensity, l_{ref} a reference length and a the power law exponent.

Depending on how I and a are chosen, networks with different characteristics can be generated. In DarcyTools it will be assumed that $a = -2.6$ (following La Pointe et al., 1999) and that I is given a value resulting in a “sparsely fractured rock” (details later). This is the situation at Äspö HRL (Rhén et al., 1997), where the major fracture zones have been thoroughly studied and it is believed that they provide the “first order” response in, for example, a pump test (Stanfors et al., 1999). The length scale of the major fracture zones is typically above, say, 300 metres and the transmissivity is of the order of $10^{-5} \text{ m}^2/\text{s}$. Fracture zones smaller than 300 metres have also been mapped at Äspö, and found to be hydraulically important, and should hence also be considered in the conductivity field. DarcyTools is developed for a fracture network of the kind found at Äspö HRL.

From this assumption it follows that the flow is distributed on relatively few flow channels, as it is the large scale fractures and zones that provide the connectivity in the network. In DarcyTools it will be assumed that all essential flow channels can be described in the computational grid. However, as discussed above, dispersion is often dominated by processes on the millimetre scale, which can not be described explicitly. This Separation Of Scales (SOS-concept) is a consequence of the sparsely fractured rock and will form the basis for the subgrid model to be described.

3.3 Concepts used for fracture descriptions

The real world fracture network will be represented as a system of conductive elements and storage volumes, see Figure 3-1 (which is based on Figure 2-3). As mentioned, not all fractures can be represented in the generated fracture network. The smallest fracture size, l_{\min} , is chosen to be comparable to cell size, Δ , in the computational grid. Fractures smaller than l_{\min} will be represented as storage volumes, which are defined as volumes that are in contact with the flow channels and exchange matter with these by molecular diffusion. Note that fracture **F** in Figure 3-1 will not be represented as a flow channel in the generated network, as it is supposed to illustrate a fracture smaller than l_{\min} .

Each of the conductive elements (A, B and D in Figure 3-1) is assumed to have a thickness, b_e , conductivity, K_e , kinematic porosity, θ_e , flow wetted surface, a_w and diffusion coefficient, D_e . The storage volumes (E and F in Figure 3-1) are described by their linear dimensions, volumes and diffusion coefficients. Below, it will be discussed how these parameters can be estimated.

If the open space in a fracture can be described as “the space between two parallel walls” it is easy to estimate the flow wetted surface (FWS); it will be $2 \text{ m}^2/(\text{m}^2 \text{ fracture})$. If the fracture is very irregular or have parallel flow channels it is harder to estimate a realistic value. In DarcyTools the FWS will be given as an input parameter for each major (or deterministic) fracture zone and each group of random fractures.

All properties (conductivity, porosity, diffusivity and FWS) are assumed to be uniformly distributed over the thickness of the conductive element.

Some nomenclature for fractures needs to be introduced. A fracture that has one single opening will in the following be called a single fracture, while a fracture zone consists of several crossing fractures. For a single fracture we call the width of the opening the aperture, which is typically less than 10^{-3} metres. For a major fracture zone, the thickness is typically 10 metres. In the present study, we will make no distinction between a single fracture and a fracture zone; both are idealised as an element with dimensions H (height), b (thickness) and L (length). If the transmissivity of the single fracture, or the fracture zone, is denoted T we can define the hydraulic conductivity of the element as $K = T/b$. In the following we will call the conductive element a fracture for short.

A few more things can be noted in Figure 3-1:

- Isolated fractures, **C**, are removed in the generated fracture network.
- The fracture zone, **A**, may have a varying thickness in the generated network. A method to generate conductive elements with varying thickness has recently been developed (described in Appendix C), but this method can presently only be used for major deterministic fracture zones (often 15-20 in number) as it is time-consuming on the computer.

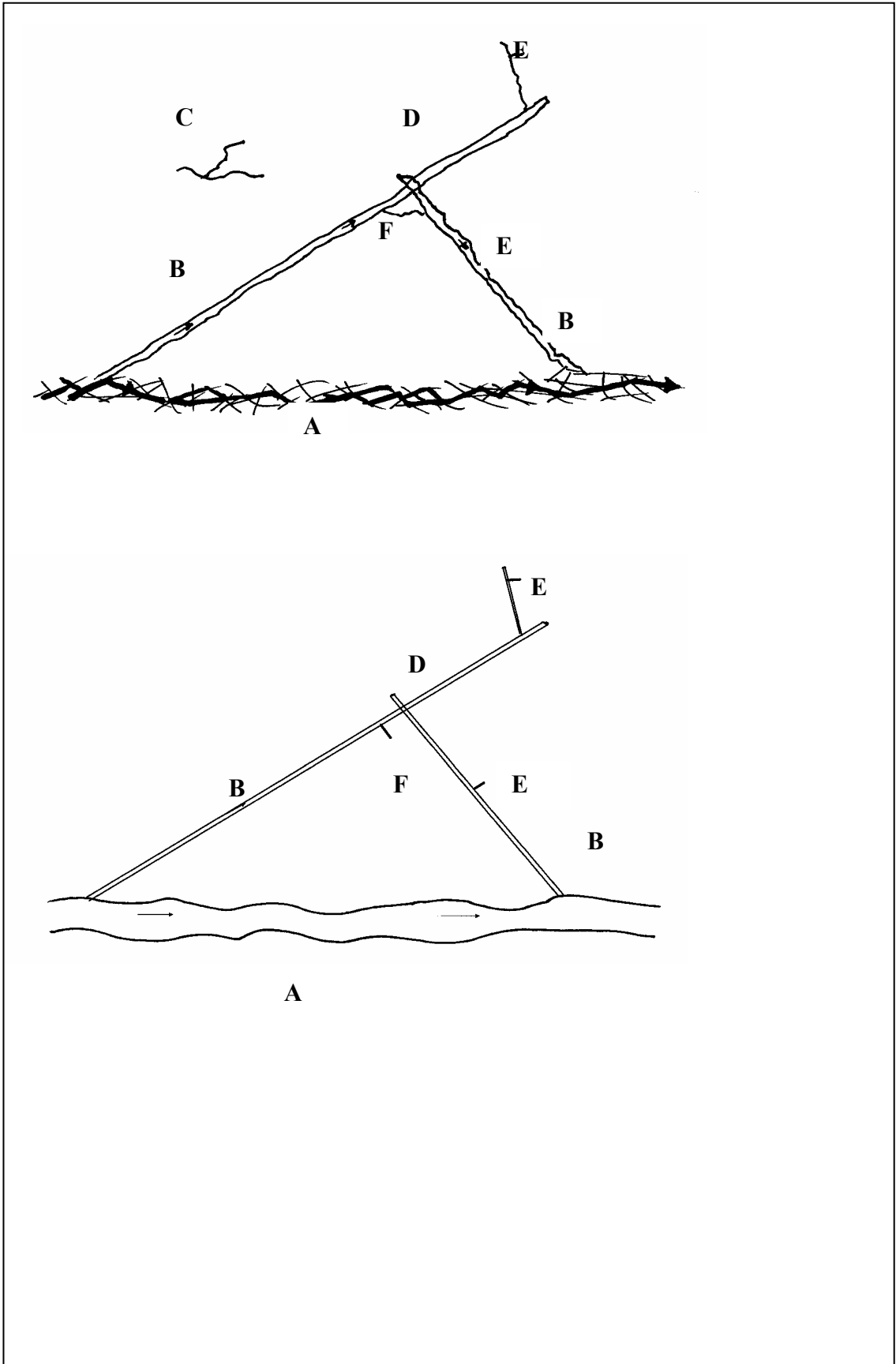


Figure 3-1. Representation of the real world fracture network (top) as conductive elements and storage volumes.

3.4 Representation of properties on a grid

Most numerical models of groundwater flow subdivide the studied domain into smaller volumes. If a computational grid is defined, we call these smaller volumes grid cells, and we apply the conservation laws and other constitutive relations to these. Also material properties, like hydraulic conductivity and porosity, need to be specified for the grid cells. These properties are often measured on a smaller scale (support scale) and a technique to express these on the scale of the grid cells is thus needed (upscaling). When material properties for all grid cells have been obtained, the flow simulation can be performed. In DarcyTools, we will however not follow this traditional route and the main argument for this can be stated as follows:

- In a sparsely fractured rock it is believed that most of the flow is due to a limited number of major fractures and fracture zones. The main task is thus to identify these and to represent them in the numerical model. If a refined modelling is required, the next size class of fractures or fracture zones should be considered. From this point of view it seems more logical to first consider large fractures, and then progressively smaller ones, than to upscale properties from a small scale.

It is not possible to represent all fractures in the grid, simply because there are too many. In DarcyTools the smallest fracture considered will often be of the same size as the grid size. Smaller fractures, $l < l_{\min}$, are however also of importance (for dispersion) and in DarcyTools represented as storage volumes (immobile zones), see Figure 3-2. In fact, storage volumes are defined as *all* immobile zones, with $l < l_{\min}$, that exchange matter with the flowing water by molecular diffusion only.

We have thus subdivided all fractures in contact (isolated fractures are not considered) into conductive elements and storage volumes. Storage volumes will be treated as subgrid effects and are represented in the subgrid model FRAME, to be described below. Conductive elements generate all grid properties by the GEHYCO-method which can now be formulated as:

- A conductive element contributes to the grid value of a variable by an amount which is equal to the intersecting volume times the value of the variable in question. Contributions from all elements that intersect the control volume are added and the sum is divided by the volume of the cell.

This basic principle will now be explained and illustrated, using Figure 3-3. A conductive element of thickness b is crossing a computational grid, which has a cell size of Δ . A staggered grid is to be used, which means that scalar quantities, like pressure and salinity, are stored at cell centres while velocity vectors are stored at cell wall centres, see Figure 3-3. This grid arrangement was first introduced by Harlow and Welch (1965) and is described in textbooks, see for example Patankar (1980). Each variable is assumed to be representative for a certain control volume, which is the volume the discretized equations are formulated for. For a velocity cell it is clear that the driving pressure force can be easily formulated. As we are going to apply the Darcy law to the velocity cell we also need a relevant cell conductivity to obtain the cell wall velocity. How to calculate this conductivity, and other properties, is the main subject of the GEHYCO-method.

To obtain the porosity, as an example, of the scalar cell marked in Figure 3-3 the following steps are performed.

- Calculate the intersecting volume between the conductive element and the cell; this volume is marked in the figure.
- If the porosity of the conducting element is θ_e , the contribution to the free volume is $\theta_e V_i$, where V_i is the intersecting volume.
- Calculate the contributions from all conductive elements that cross the cell.
- Obtain the cell porosity as the sum of all contributions divided by the cell volume.

In Figure 3-3 a control volume for a velocity cell is also marked. The procedure to obtain the conductivity for this control volume is analogue to the steps above.

By this procedure the porosity, flow wetted surface and storativity are determined for all scalar cells and the conductivities and diffusivities for all cell walls.

An assumption in the statement above is that "contributions from all elements that intersect a cell are added". If two, or more, fractures intersect a velocity cell, the cell conductivity should represent a fracture intersection (neglecting the case of parallel fractures of various orientation). Neretnieks (1993) discusses various concepts about channelling at intersections, but concludes that no firm information is available. He cites however a number of observations that support the idea that "fracture intersections form easy pathways". In lack of any firm information, it will therefore be assumed that contributions can be added. Fracture intersections will hence form "easy pathways".

The basic principle of the method is obviously very simple but, as will be demonstrated, still general enough to handle even complex fracture networks. A few properties of the method can already at this stage be identified:

- All cell wall conductivities will be different, as we generate three conductivity values (in a 3D case) for each scalar cell. A conductivity field that is anisotropic on the cell scale is hence always generated.
- A fracture smaller than the cell size can not generally contribute to the anisotropy or correlation of the conductivity field.

Some simple calculations that illustrate the GEHYCO method, and also demonstrates the accuracy that can be expected, can be found in Appendix G.

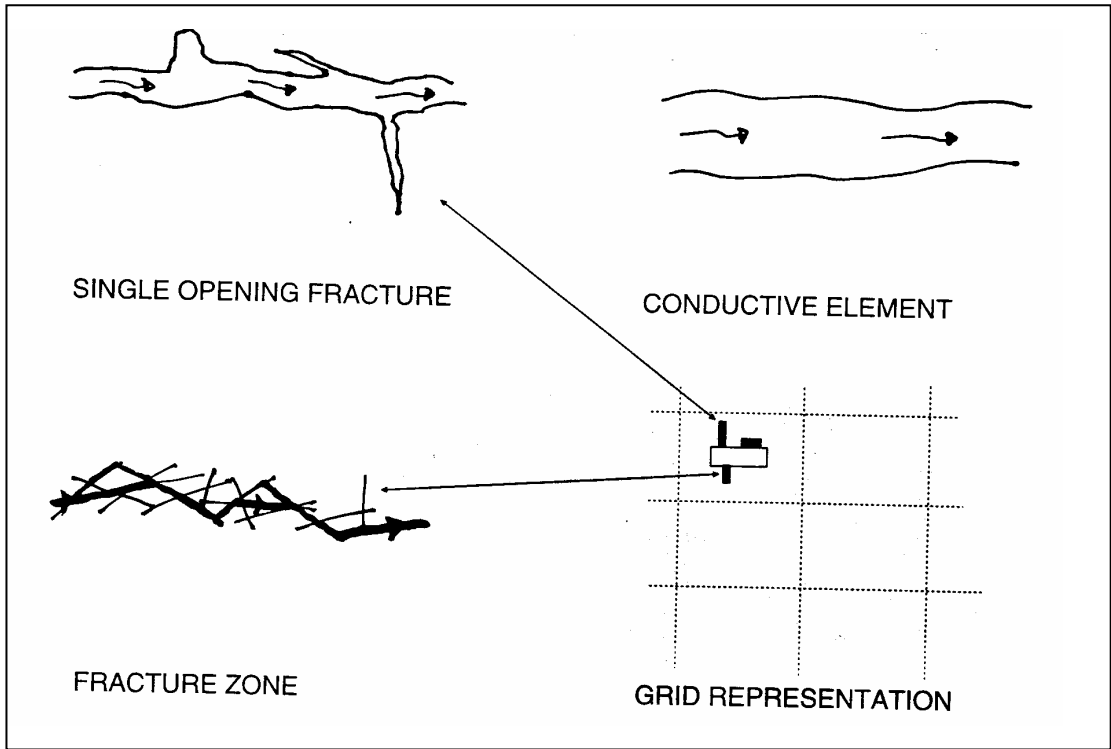


Figure 3-2. Representation of kinematic (or mobile) and storage (or immobile) volumes in the grid. The open rectangle in the grid represents a kinematic volume (generated by the conductive element), while filled rectangles represent storage volumes.

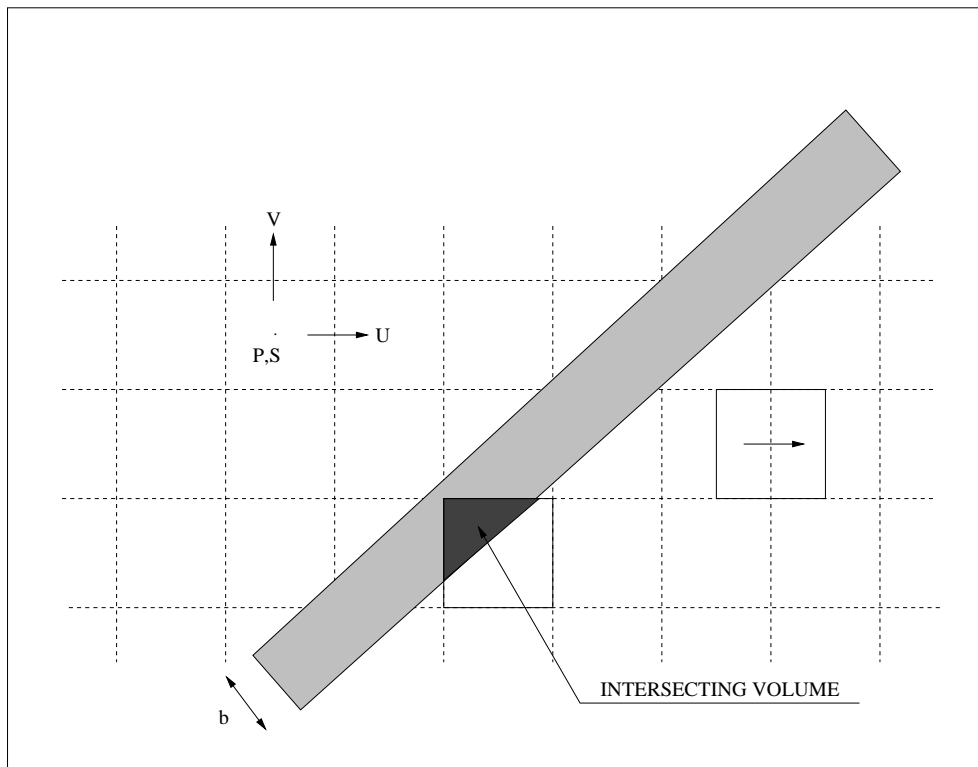


Figure 3-3. Illustration of concepts and methods for calculating grid properties.

3.5 Subgrid processes, FRAME

In Figure 3-4 some subgrid processes and concepts are introduced. Let us consider a computational cell with a through flow, i.e. a cell with a flow channel. The flow “sees” a certain surface area, the flow wetted surface (FWS), as it passes the cell. The FWS may bring the flowing water in contact with other fractures, gouge material, stagnant pools, etc. Most of these volumes can be expected to have stagnant water and mass exchange is hence due to molecular diffusion. For a stagnant pool the relevant diffusion coefficient may be that for pure water, while diffusion into crossing fractures and the rock matrix may proceed with a diffusion rate that is several orders of magnitude smaller. As above, we will call the volume with flowing water the mobile zone and the volumes with no advection the immobile zone. Fractures and volumes which are not in contact with the mobile zone are of course of no relevance and can be excluded from the discussion.

The situation outlined in Figure 3-4 is quite complicated and does not lend itself to direct descriptions of individual processes. In order to derive a simple model that can be employed in large (many grid cells) 3D models, the following basic assumption will be made:

- The immobile zones can be represented by a set of boxes, each with its own length scale, volume and effective diffusion coefficient.

The idealised problem is illustrated in Figure 3-5. The box with the smallest length-scale (dimension perpendicular to the mobile zone) will have the largest diffusion coefficient and normally also the largest contact area with the mobile zone. This volume will hence have a fast response. The actual response time can be estimated from the length scale, l , and the effective diffusion coefficient, D_e , as:

$$t \approx \frac{l^2}{D_e}$$

For $l = 10^{-3}$ m and $D_e = 10^{-10}$ m²/s the time is 10^4 s (\approx 3 hours). For $l = 1$ m and $D_e = 10^{-12}$ m²/s the time will be 10^{12} s (30 000 years), which illustrates that both short and long time scales may be treated within the same concept. In the following we will call these boxes storage volumes, which thus represent an idealised view of the immobile zones.

The next step is to devise methods to calculate the FWS, storage volumes, diffusion coefficients, etc. Fractal scaling laws will be used in this context and as we have adopted a multirate diffusion approach we call the subgrid model FRAME (a subgrid model based on FRActal scaling laws and Multirate Equations). Methods to derive the FWS are described in detail in Appendix E, and here we will focus on the properties of the storage volumes. The following steps will determine these:

- Divide the immobile volumes, illustrated in Figure 3-4, into a number of size groups with respect to the length-scale.
- Generate the number of fractures in each size group from a power-law with exponent a (fractal dimension). Note that the same power-law as used for the resolved fracture network is used also for the subgrid system. This will give the number of fractures per m³, for the size group in question.

- Only immobile zones in contact with the FWS can be in contact with the mobile zone. Modify the number of fractures in each size group with respect to this constraint.
- Assume that the aperture of a fracture is proportional to the length scale, i.e. $e_T \sim l^\gamma$. Note that for $l \gg l_{\min}$, it can be expected that the immobile zones are due to fractures. For $l \approx l_{\min}$ the volumes are perhaps due to stagnant pools and it may be questionable to speak about an aperture.
- The effective diffusion coefficient, D_e , is expected to be close to the molecular value for water, D_m , for the smallest volumes and then show a decreasing trend with the length scale of the immobile zone. The following relation is assumed:

$$D_e = D_m \left(\frac{l}{l_{\min}} \right)^\Psi$$

By these steps the volume, contact area and effective diffusion coefficient have been determined for each storage volume, as a function of a , γ and Ψ . However, these parameters will not be specified individually as they can be related to the “late time slope of the breakthrough curve”; this will be further discussed in Section 4 (see also Appendix B), where the details of the model implementation are described.

Regarding the size interval to be considered, it was shown above that a length scale of 10^{-3} m results in a storage volume that has a response of the order of a few hours. Smaller, or faster, boxes are probably not required, unless a very fast experiment is to be simulated. The upper limit should be the cell size, Δ , as larger fractures are normally treated explicitly in the resolved fracture network. However, Δ is often in the range 1-10 metres and the largest storage volume will hence be very slow. From a practical point of view (save computer time) the upper limit may hence be chosen with respect to the time scale of the problem considered. Note also that fractures in the resolved network may form dead-end systems that exchange matter with the flowing water by molecular diffusion only.

The concepts and assumptions introduced give a very simplified view of the expected subgrid processes. However, it should be remembered that the objective is to derive a subgrid model that can be employed in large 3D, transient models. It is hoped that FRAME strikes a good balance between complexity and efficiency.

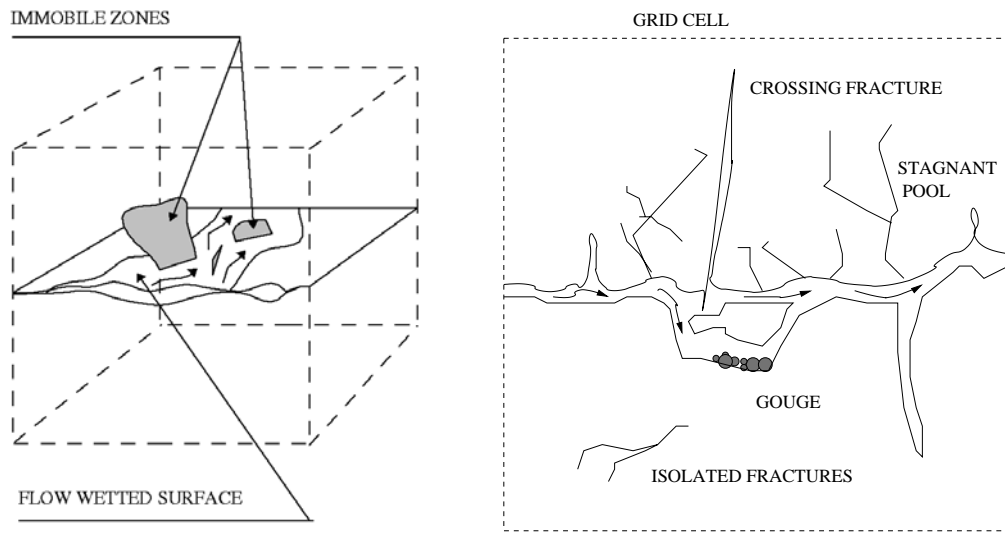


Figure 3-4. Illustration of subgrid processes and concepts.

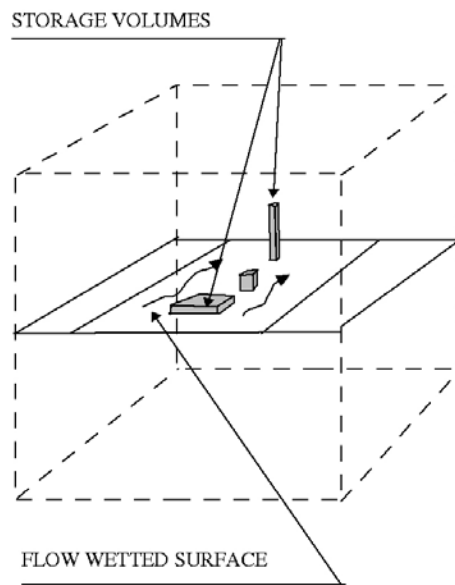


Figure 3-5. The assumed structure of subgrid volumes and areas.

3.6 Transport

DarcyTools has two built-in options for transport simulation; a particle tracking algorithm, PARTRACK, and advection/dispersion equations. The reasons why two methods are needed are based on the following assumptions:

- Salinity. The salinity field strongly influences the flow field through the density field. It is difficult to describe the salinity field by a set of particles and an advection/dispersion equation is therefore the best choice.
- Temperature. The main heat flux component is conduction and an advection/dispersion equation is hence the obvious choice for this variable. It will further be assumed that the water and rock is always in thermal equilibrium and only one temperature is thus solved for.
- Tracers. Simulation of tracer transport is best performed with a particle approach as this method is free from numerical dispersion effects. It is also possible to treat sorbing tracers (like radionuclides) with this technique.

These are the main scalars that need to be considered in applications. If additional scalar simulations are requested a decision about the most appropriate method has to be taken.

Transport of salt and tracers are assumed to be restricted to the water phase. Dispersion is hence due to mixing at fracture intersections (macro dispersion) and exchange with immobile zones (micro dispersion, as embodied in FRAME). FRAME is hence developed for both the advection/dispersion equation (as used for salt) and PARTRACK (as used for tracers).

3.7 Groundwater table

As was stated in Section 2, the groundwater table may determine the pressure field deep down into the rock. Unfortunately it is not straight forward to calculate the position of the groundwater table. From the literature two methods are available:

- The variably saturated approach, which means that the unsaturated zone is included in the simulation and that the so called Richards equation is solved.
- Free surface approach. The main assumption of the method is that the conditions in the unsaturated zone do not significantly affect the position of the groundwater table.

A novel method to determine the groundwater table, which is inbetween these two, is introduced in DarcyTools. The basic idea is as follows: If a simulation like the one in Figure 3-6 is performed without taking any notion of the groundwater table a certain pressure distribution results. A surface with atmospheric is calculated, but pressure gradients and hence a horizontal flow is calculated above this surface; this is obviously not correct. The key feature of the method is to prevent the horizontal flow above the surface of atmospheric pressure by simply reducing the horizontal conductivity. This is done in an iterative manner, meaning that the position of the atmospheric pressure is determined and horizontal conductivities are recalculated (note that if a rising surface is calculated, the horizontal conductivities below the surface should be restored to the

fully saturated values). It can be shown, see Report 2, that this method gives a steady state groundwater table that is in agreement with available analytical solutions.

The transient problem introduces a new feature; if the groundwater table is lowered a delayed drainage of the volumes above the water table will occur. A significant amount of water can be released and affect the position of the water table. In DarcyTools this *specific yield effect* is described by a source term in the mass balance equation:

$$Q_{sy} = k_{sy} V_{sy}(t) \quad [\text{m}^3/\text{s}]$$

$$\frac{dV_{sy}}{dt} = -Q_{sy}$$

where V_{sy} is the volume of drainable water at time t and k_{sy} a time constant for the drainage. We thus keep track of the drainable water in each cell above the water table and let this water be transported, by gravity, down to the water table. In the Verification and Validation report, it is shown that this approach gives results that are in fair agreement with available analytical solutions.

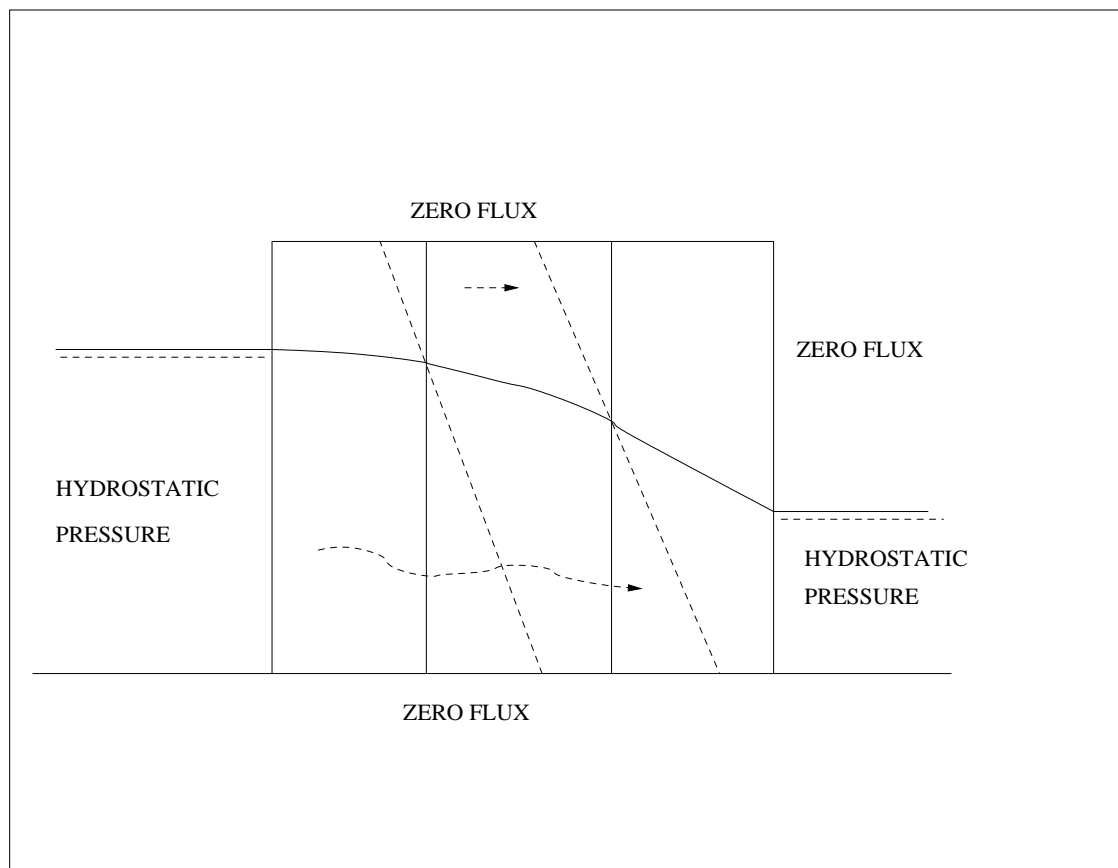


Figure 3-6. Illustration of concepts used for determination of the groundwater table.

3.8 Porosity and state laws

Finally, we will briefly review some assumptions related to the properties of the media and fluid.

The porosity field is based on the porosities ascribed to the conductive elements. In the analysis of the resulting porosity field it is however of interest to also characterise the porosity as based on the volume of the computational domain. For this reason the following definitions will be used:

- θ_a is the porosity based on all generated fractures, including isolated fractures or clusters of fractures.
- θ_c is the connected part of θ_a , i.e. isolated fractures and clusters have been removed.
- θ_f is the part of θ_c that has a significant flow, i.e. stagnant volumes have been removed.

θ_f requires a definition of what should be called "stagnant volumes". The definition to be adopted here is:

- If the stagnant parts of the kinematic porosity field are neglected, i.e. the porosity is put to zero, this should result in a reduction of the flow through the domain that is smaller than 1%. This should be fulfilled for pressure gradients in all three coordinate directions.

These porosity measures will be further analyzed in Section 7.3. Other media properties are flow wetted surface and storativity. Also these will be calculated as grid cell data, based on the ascribed values to the conductive elements. In the fracture network the conductivity of conductive elements is specified; this because input data are often given as a transmissivity, T , and a thickness, b , and the conductivity is then T/b . In the simulation model the permeability is however used as the influence of fluid properties needs to be taken into account.

State laws for water that take into account the effects of pressure, temperature and salinity are very complex indeed. For the present range of applications, it is expected that the following assumptions are adequate:

- Density is linearly and quadraticly (i.e. two terms) related to both salinity and temperature.
- Viscosity is linearly and quadraticly (i.e. two terms) related to temperature.
- Specific heat of mass is linearly and quadraticly (i.e. two terms) related to salinity.

As the user will have access to the coefficients of these relations, details in next section, it is expected that it will always be possible to tune the relations to a specific application, with a high degree of accuracy.

4 Mathematical formulation

4.1 Introduction

As all concepts and assumptions have been discussed, the equations can be presented without lengthy discussions.

First the conservation and state laws will be presented and then, as in the previous sections, various features will be dealt with; now with focus on the mathematical formulation.

4.2 Conservation and state laws

Conservation of mass:

$$\frac{\partial \rho \theta}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = Q \quad (4-1)$$

where ρ is fluid density, θ porosity, u , v and w Darcy velocities and Q a source/sink term. The coordinate system is denoted x , y , z (space) and t (time).

Mass fraction transport equation:

$$\begin{aligned} \frac{\partial \rho \theta C}{\partial t} + \frac{\partial}{\partial x} \left(\rho u C - \rho \gamma D_x \frac{\partial C}{\partial x} \right) \\ + \frac{\partial}{\partial y} \left(\rho v C - \rho \gamma D_y \frac{\partial C}{\partial y} \right) \\ + \frac{\partial}{\partial z} \left(\rho w C - \rho \gamma D_z \frac{\partial C}{\partial z} \right) = Q C + Q_c \end{aligned} \quad (4-2)$$

where C is transported mass fraction, D_x , D_y and D_z the normal terms of the diffusion-dispersion tensor and Q_c a source/sink term. When C is salinity, the source term represents the exchange with immobile zones and Q_c is determined by the subgrid model FRAME. Note that the diffusion coefficients are the effective coefficients that include the porosity, see further explanation in connection with Equation (4-11) below.

Conservation of heat:

$$\begin{aligned}
\rho\theta\frac{\partial c_p T}{\partial t} + \frac{\partial (1-\theta)cT}{\partial t} \\
+ \frac{\partial}{\partial x}\left(\rho u c_p T - \lambda_x \frac{\partial T}{\partial x}\right) \\
+ \frac{\partial}{\partial y}\left(\rho v c_p T - \lambda_y \frac{\partial T}{\partial y}\right) \\
+ \frac{\partial}{\partial z}\left(\rho w c_p T - \lambda_z \frac{\partial T}{\partial z}\right) = \left(\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z}\right) c_p T + Q_T
\end{aligned} \tag{4-3}$$

where λ_x , λ_y and λ_z are the normal terms of the equivalent (i.e. rock with fluid) thermal conductivity tensor, c is the rock thermal capacity and c_p the specific heat of the fluid and Q_T a source/sink term. We are hence only solving for one temperature, assuming thermal equilibrium between the rock and the water.

The mass conservation equation is turned into a pressure equation under the well known Darcy's assumption:

$$\begin{aligned}
\rho u &= -\frac{K_x}{g} \frac{\partial P}{\partial x} \\
\rho v &= -\frac{K_y}{g} \frac{\partial P}{\partial y} \\
\rho w &= -\frac{K_z}{g} \frac{\partial P}{\partial z} - K_z(\rho - \rho_0)
\end{aligned} \tag{4-4}$$

where K_x , K_y and K_z are the local hydraulic conductivities in x , y and z direction, g the gravity acceleration, ρ_0 a reference fluid density and P the dynamic fluid pressure relative to the reference hydrostatic pressure.

$$P = p + \rho_0 g z \tag{4-5}$$

where p is the total pressure. The hydraulic conductivity, K , is related to the permeability, k , by the relation.

$$K = \frac{\rho g k}{\mu} \tag{4-6}$$

where μ is dynamic viscosity.

The fluid properties like the dynamic viscosity, μ , the density, ρ , and the specific heat, c_p , are given by state laws:

$$\mu = \mu_0 \left[1 + a_1 (T - T_\mu) + a_2 (T - T_\mu)^2 \right]^{n_\mu} \tag{4-7}$$

$$\rho = \rho_0 \left[1 + \alpha_1 S + \alpha_2 S^2 - \beta_1 (T - T_\rho) - \beta_2 (T - T_\rho)^2 \right] \quad (4-8)$$

$$c_p = c_{p0} (1 + b_1 S + b_2 S^2) \quad (4-9)$$

while the porosity θ and the compaction, γ , of the matrix are given the following dependencies:

$$\theta = \theta_0 \gamma \quad (4-10)$$

$$\gamma = 1 + (\sigma/\theta_0) (P - P_0) / \rho g \quad (4-11)$$

In the above formulas S represents the salinity (salt mass fraction), θ_0 a reference porosity field given for a reference pressure field P_0 and σ the specific storativity field. n_μ , a_i , b_i , α_i , β_i , μ_0 , ρ_0 , $C_{\rho 0}$, T_μ and T_ρ are constants.

In the advection/diffusion equation (4-2), it is common to write the diffusion coefficient as θD_{mol} , where D_{mol} is the molecular diffusion coefficient. In DarcyTools we choose to write the term as $\theta D_{mol} = \theta_0 \gamma D_{mol} = \gamma D$, where D is now the effective diffusion coefficient. The reason is that it is the effective diffusion coefficient that is specified for a conductive element and the GEHYCO-algorithm will hence deliver effective diffusion coefficients for cell walls. When a porous media case is simulated and the diffusion coefficients are specified, one thus needs to remember that it is the effective coefficients that should be given.

4.3 Fractures and fracture network

The relations to be discussed below are not an integral part of DarcyTools as they can be altered based on site specific information. It is hence more an illustration of the input data required. The relations given are largely based on data from Äspö HRL.

Fracture properties. The relations used to determine fracture properties, like transmissivity and porosity, are taken from a recent evaluation/ compilation (Appendix F). This compilation is far from exhaustive or complete, but is what is presently available. The following summarises the main relations:

- Transmissivity-fracture size:

$$T = \begin{cases} 10^{-5} (l/100)^2 & [m^2 / s] \text{ for } l \leq 100 \text{ metres} \\ 10^{-5} & [m^2 / s] \text{ for } l > 100 \text{ metres} \end{cases} \quad (4-12)$$

where T is transmissivity and l fracture size. The coefficients of this relation are accessible to the user and it is also possible to include a random term in the relation, see Report 3 for details.

- Transmissivity-transport aperture: Based on empirical relations and the cubic law it was found that the transport aperture, e_T , can be estimated as:

$$e_T = 2.0T^{0.6} \quad (4-13)$$

- Fracture size-thickness: Field data from Äspö HRL indicate that a fracture thickness, b , of 1% of the fracture length is a good choice. The fracture thickness is defined to include the flow channel, the gauge material, parallel flow paths, etc. It is hence often one or two orders of magnitude larger than the aperture. The kinematic porosity, n , is calculated from e_T and b ($n = e_T / b$).
- Diffusion coefficients: Molecular diffusion in a conductive element should be proportional to the product of the transport porosity and the diffusivity value in the pore water (Neretnieks, 1993). The proportionality constant is related to the properties of the pore space (constrictivity and tortuosity). In the simulations carried out in this report, we will simply assume that the diffusion coefficient for a conductive element is equal to the product of the kinematic porosity and the diffusion value in pure water.

Fracture orientation. Several projects have been carried out with the objective to characterise the fracture orientation at Äspö. In DarcyTools fracture sets of different orientations can be generated and the spread around these orientations is governed by a Fisher distribution (see Appendix D).

Fracture intensity. The fracture intensity is specified from a power law distribution. For a length interval, dl , we then get:

$$n = I * \left[\left(\frac{l + dl}{l_{ref}} \right)^a - \left(\frac{l}{l_{ref}} \right)^a \right] / a \quad (4-14)$$

where n is the number of fractures per unit volume, I the intensity, l_{ref} a reference length (=500 m) and a , the power law exponent, put to -2.6 (see LaPointe et al., 1999). At Äspö the intensity was determined to 10^{-8} by generating fractures in the interval 320 to 1 000 metres and compare the number with the number of deterministic fracture zones in the Laboratory domain. The intensity chosen gives 10 to 15 (different realisations) fracture zones in the length interval which can be compared to 12 deterministic fracture zones.

Fracture shape: The fractures are assumed to be squares, with length, L , and have a thickness, b . DarcyTools can apply a varying thickness, and hence properties, for a limited number of major fracture zones. A correlation structure can be specified for each of these zones by a method described in Appendix C.

4.4 FRAME

We will now return to the subgrid model FRAME described in Section 3. The influence from the immobile zones on the mobile concentration of a tracer is given by the source/sink term Q_c in Equation (4-2). Before Q_c can be specified some further developments of the ideas introduced in Section 3 are needed.

The starting point is the representation of the immobile water in storage volumes, as outlined in Figure 4-1. To simulate the mass transfer within a storage volume one needs to solve a 1D diffusion equation. However, as has been shown by Haggerty and Gorelick (1995), it is possible to simulate the transport within the storage volume by a series of boxes that exchange matter with the kinematic volume; see Figure 4-1. Using

this approach the term Q_c (in Equation 4-2) and the equations for the boxes will take the following form:

$$Q_c = -\sum_{j=1}^N \beta_j \frac{\partial (C_{im})_j}{\partial t} \quad (4-15)$$

$$\frac{\partial (C_{im})_j}{\partial t} = \alpha_j (C - (C_{im})_j), \quad j = 1, 2, \dots, N \quad (4-16)$$

where β_j represents the capacity ratios, α_j the first order mass transfer coefficient and $(C_{im})_j$, the tracer concentration in the immobile water represented by box j . The

total capacity $\beta_t \left(= \sum_{j=1}^N \beta_j \right)$ is equal to the volume ratio between the immobile and

mobile zones (for a non sorbing tracer). For "layered diffusion", which is the situation when a storage volume is in contact with a kinematic volume, Haggerty and Gorelick (1995) give the following expressions:

$$\alpha_j = \frac{(2j-1)^2 \pi^2 D_a}{4 a^2} \quad (4-17)$$

$$\beta_j = \frac{8}{(2j-1)^2 \pi^2} \beta_t \quad (4-18)$$

where D_a is the apparent pore diffusion coefficient and a the linear dimension of the storage volume. For further details about this "multi-rate model of diffusion", see Haggerty and Gorelick (1995).

As discussed in Section 3, FRAME is based on a power-law formulation. The main argument for this is that the fractal properties of the subgrid fracture network should be the same as for the resolved network. The use of a power-law formulation does however also support a further development of the model.

- As mentioned, all storage volumes are represented by a series of first order capacity boxes. When all storage volumes have been represented, the continuous distribution of capacities is also a power-law. This can be shown both numerically and analytically.
- It can further be shown that the slope of this distribution is related to the late time slope of the breakthrough curve, k .

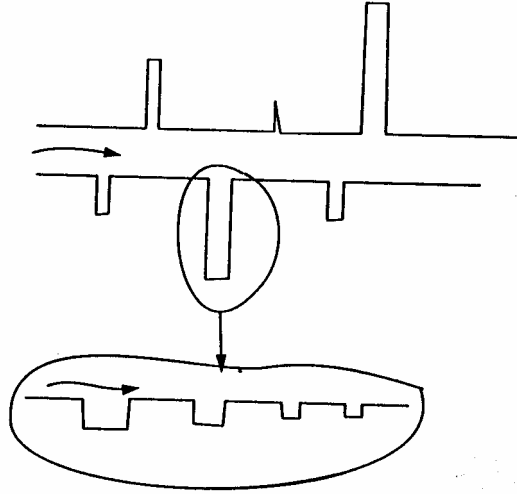


Figure 4-1. Illustration of how a storage volume is simulated as a series of first order boxes.

- In Section 3 the properties of the storage volumes were stated to be a function of three parameters: a , γ and Ψ . It can be shown, see Appendix B, that these are related to k as follows:

$$k = \frac{a - \gamma - 2\Psi + 1}{2 - \Psi} \quad (4-19)$$

These developments form the basis for the implementation of FRAME.

We will now return to the source term Q_c (Equation 4-15) and see how FRAME is specified for an advection/diffusion equation like (4-2). Let us further assume that C is salinity in this equation. The parameters that specify the model are:

- β_i , the volume ratio between the immobile and mobile zones.
- α_{\min} and α_{\max} , the minimum and maximum mass transfer coefficients. Note that these specify the length interval of the storage volumes considered as $\alpha_{\min} = D_{mol} / l_{\max}^2$ and $\alpha_{\max} = D_{mol} / l_{\min}^2$, where D_{mol} is the molecular diffusion coefficient and l_{\max} and l_{\min} the maximum and minimum lengths of storage volumes.
- k , the late time slope of the break-through curve. k determines how β_i is distributed over the spectrum of mass transfer coefficients.

In the numerical implementation a few more parameters need to be considered:

- n_α , the number of α -intervals that the total spectrum should be divided into.
- The FWS is also needed to consider in applications where a cell to cell variation of FWS is taken into account. The method employed is to calculate a β_i that varies from cell to cell. This is done by using FWS/vol_m (where vol_m is the volume of

the mobile zone) as a weighting factor and then ensure that the global mean of β_i has the prescribed value.

Thus:

$$\beta_{t,cell} = \overline{\beta}_{t,cell} \left(\frac{FWS}{vol_m} \right)_{cell} / \overline{\left(\frac{FWS}{vol_m} \right)}_{cell} \quad (4-20)$$

where overbars indicate a global average.

4.5 PARTRACK

The particle tracking routine in DarcyTools is called PARTRACK.

PARTRACK has two basic modes of operation; the first is the traditional way of moving the particle along the local velocity vector, while the second method uses the so called “cell-jump” approach. The second approach is believed to be more appropriate for transport in a fracture media and is therefore described in some more detail:

- A particle entering a scalar cell will, if no dispersion effects are activated, travel through the cell in a time which is equal to the free volume of the cell divided by the flow rate through the cell (a so called plug-flow). If dispersion effects are active the travel time will however be different and will also be different for different particles.
- When the particle is ready to leave the cell, it will leave through one of the cell walls that have an outgoing flow direction. The choice between cell walls with an outgoing flow is made with a likelihood that is proportional to the outflows. If several particles are traced, the cloud will thus split up in proportion to the flow rates. Complete mixing in a cell is hence assumed.

It should be noted that no time is spent when moving from one cell to the neighbour. Next we will discuss some details about the two points above.

When the particles are travelling through the cell, the retardation due to matrix diffusion, sorption and Taylor dispersion need to be accounted for. The concept of particle states is used to simulate these processes. As an illustration let's outline how Taylor dispersion can be simulated. If the velocity profile is described as a number of layers, each with a certain velocity, we identify these layers as the different states a particle can be in. If correct frequencies can be ascribed for moving to a neighbouring layer, it is realised that particles will experience different velocities when travelling through the cell and a Taylor dispersion effect will result. If we further should like to account for sorption on the fracture walls a particle state is also needed for this process. We also need to find out the frequency by which a particle will leave the velocity layer close to the wall and enter the "sorbed state" and also the frequency by which it will go back.

PARTRACK uses FRAME to account for matrix diffusion and sorption processes. The parameters introduced for FRAME applies also to PARTRACK. However, as PARTRACK can also handle sorbing tracers we need to introduce the retardation

factors for the mobile, R_m , and immobile zone, R_{im} . These will affect the FRAME parameters as follows:

- $\beta_t = \beta_n \frac{R_{im}}{R_m}$, where β_n is the volume ratio for a non-sorbing tracer.
- $\alpha_{\min} = D_{mol} / (l_{\max}^2 R_{im})$
- $\alpha_{\max} = D_{mol} / (l_{\min}^2 R_{im})$

If Taylor dispersion is simulated by PARTRACK a “cross diffusion coefficient”, $fxdift$, needs to be specified. A parabolic velocity profile is assumed and $fxdift$ is then equal to the diffusion coefficient divided by the square of the aperture.

4.6 Finite volume equations and solver

CFD (Computational Fluid Dynamics) methods transform the differential equations into algebraic ones, which can be solved by a computer and a computer program. DarcyTools uses the so-called finite volume method, which can be thought of as having three well-defined stages:

- 1) Discretize the computational domain into a number of cells, which fill entirely the domain.
- 2) Integrate each differential equation for each cell, to yield an algebraic equation.
- 3) Solve the resulting set of algebraic equations.

The differential equations were given in the previous sections. After the integration, step 2 above, an algebraic equation of the following type results:

$$a_P \Phi_P = a_W \Phi_W + a_E \Phi_E + a_S \Phi_S + a_N \Phi_N + a_B \Phi_B + a_T \Phi_T + S_\phi \quad (4-21)$$

where Φ denotes the variable in question, a coefficients and S_ϕ source terms. For further details see Appendix A.

It is equations of type (4-21) that are solved by the solver MIGAL (see Appendix A); in fact MIGAL can solve linked systems of this kind of equations, a feature that is used for the pressure-salinity coupling in the present set of equations.

5 Confidence building

5.1 Some definitions

During the last twenty years CFD (Computational Fluid Dynamics) has become a standard simulation tool in most engineering problems, dealing with groundwater flow and transport. This development has been driven by readily available software packages and the significant increase in affordable computer speed and memory capacity. CFD is however not a simple technique to use; generally speaking a basic understanding of several subjects like fluid mechanics, numerical analysis and computer software programming is required. For groundwater modelling an understanding of geohydrology is of course also needed. In an ongoing project, ERCOFTAC (Casey and Wintergerste, 2000), guidelines for CFD simulations are discussed and summarised. Partly based on this report, the following main sources of errors and uncertainties in groundwater simulations can be identified:

- **Mathematical model.** The mathematical model does not describe the real flow exactly. For example, in textbooks the approximations inherent in the Darcy equation are often analysed and listed. Another often used approximation is that the water is incompressible.
- **Discretisation.** Numerical solutions are performed on a grid in space and time. The difference between the solution on this grid and the exact solution of the modelled equations is called the discretisation error.
- **Convergence and round-off errors.** Typically a CFD simulation involves iterative procedures. Convergence errors occur because these iterations are stopped by a certain criteria before they are completed. Round-off errors are due to the limited number of digits when a number is stored in the computer memory.
- **Application uncertainties.** This includes uncertainties about the geometry of the domain (for example a fracture network), boundary conditions, fluid properties, etc.
- **Code errors.** It is difficult to get software “bug-free”.
- **User errors.** These are the errors that result from mistakes or carelessness by the user.

More points could have been listed (errors in postprocessing, interpretation of results, etc) but the list given probably gives the most important ones. In this context it may be of interest to refer to the following definitions (from ERCOFTAC):

Error: A recognisable deficiency that is not due to lack of knowledge.


Uncertainty: A potential deficiency that is due to lack of knowledge.

As the present report will deal with flow and transport in a fractured rock, one should view the points given from this perspective. The significance of the different points may still vary depending on the modelling approach chosen and the problem studied. Here we concern ourselves with a fracture network, as represented in a continuum model. All of the above discussed errors and uncertainties may still be relevant to consider and it is not easy, in the author's view, to neglect (or set priority to) any of the points. For the modelling approach chosen it is however expected that the "quality" of a simulation is strongly dependent on how well the fracture network is represented in the continuum model. The fracture network is however only partly known (geometry, properties, etc) and we therefore need to consider the uncertainty introduced.

The question whether a computer code is credible or not and methods to answer this question are given in a recent issue of the AIAA journal (AIAA, 1998). Based on the papers presented, Table 5-1 has been created. The table is an attempt to illustrate the actions involved in the confidence building process. A few comments to the table:

- The order (from top to bottom) is essential. It is not possible to achieve certification without having demonstrated verification and validation.
- There is a consensus in the literature about the definitions of verification and validation. Additional steps and actions in the confidence building are still open to discussion.
- Some authors emphasise that it is important to distinguish between confidence building in a computer code and in a specific application. Related to this issue is the concept "fitness for purpose". It is for example of little value to have a very accurate numerical solution if the algorithm is so slow that the code is impractical for its intended use.

Table 5-1. Processes and actions involved in confidence building.

C O N F I D E N C E B U I L D I N G 	Process	Definition	Action
	Verification	Demonstrate that the equations are solved correctly.	Comparison with analytical solutions and other models.
	Validation	Demonstrate that the right equations are solved.	Comparison with measurements (laboratory and field data).
	Certification	Assess whether the right things are done and whether they are done right.	Evaluate software construction and working procedures.
	More (QA-systems, wide range of applications, publications in international journals, etc)		

5.2 Verification of DarcyTools

The verification cases performed can be found in Report 2 and are summarised in Table 5-2.

All cases tested show “good result”, i.e. the comparison with the corresponding analytical solution, or another model study, is satisfactory; the reader is referred to the report to study the details.

A few words may however be needed to explain the objectives when selecting the test cases and the way the comparisons have been carried out.

- The test cases should include one, two and three dimensional, steady and transient cases.
- A wide range of relevant physical processes should be included, i.e. density stratification, unsaturated zones, storativity effects, etc.
- The representation of fractures in a continuum model is a key feature of DarcyTools and should be well covered by the test cases.

Some verification studies described in the literature are focused on grid refinement studies. Here the listed objectives have however been considered to be more important with the “fitness for purpose” argument in mind.

Table 5-2. Compilation of verification cases.

Group	Case	Comment
A. Numerical methods	A1. One dimensional transient diffusion A2. One dimensional steady advection/diffusion A3. Flow through a complex channel A4. Tests of grids A5. Test of pressure-salinity coupling	This group of cases intends to show that the numerical methods work as expected
B. Porous media	B1. Regional groundwater circulation B2. Steady ground-water table B3. Theis problem B4. Transient pressure in a borehole B5. Specific yield, Neuman (1975) B6. Horizontal well problem	This group considers some classical geohydrological testcases
C. Fractured media	C1. Three fractures in a two dimensional domain C2. Intersecting fracture zones C3. Single fracture in a box C4. Many fractures in a box C5. Percolation theory C6. Diffusion in a dead-end fracture C7. Matrix-fracture temperature problem	This group of cases deals with the representation of fractures in a continuum model
D. Transport and dispersion	D1. Taylor dispersion D2. Break-through-curve, PARTRACK D3. Break-through-curve, adv/diff eqn D4. Seven fractures in a 2D domain, PARTRACK D5. Three fractures in a 2D domain, PARTRACK D6. Single fracture in a box, PARTRACK	This group considers transport, retention, dispersion and particle tracking cases.
E. Buoyancy effects	E1. Henry's problem E2. The salt dome E3. Coupled temperature-salinity fields E4. Upconing E5. The floating island E6. Two fluid problem	This group considers comparisons where density stratification, due to salinity and temperature gradients, is a key factor.

5.3 Validation of DarcyTools

As validation should be concerned with comparisons with measurements and this report describes version 2.1 of DarcyTools, it is not surprising that very few such comparisons can be reported at this stage. However, as discussed in Section 1, it is relevant to include cases that were carried out with PHOENICS as the equation solver, as it has been carefully evaluated that the two solvers give very similar solutions. Note that the descriptions of the fracture network (GEHYCO) and other descriptions of physical processes are in most respects the same in the PHOENICS cases to be discussed, as in the present version of DarcyTools.

For simulations of flow and transport in a fractured rock, it is difficult to separate the steps “validation” and “calibration”. To discuss this we first need to define “calibration” (following AIAA, 1998):

- **Calibration** is the process of tuning a code, in order to improve its prediction of global quantities, for realistic geometries, of design interest.

If we require that validation studies should be concerned with comparisons with field measurements, we also need to accept that these measurements are obtained in conditions that are to a large extent unknown. We do not know the fracture network (its geometry, fracture properties, boundary conditions, etc). In the author’s view, we therefore have to accept the following tentative definition of validation:

- For the flow and transport in a fractured rock, validation of a simulation can be claimed if calibration can be performed with all adjustable parameters within realistic limits.

This definition immediately raises the question “what is realistic limits?”. For major fracture zones we may be able to define bounds for properties (thickness, transmissivity, porosity, etc) and these bounds then define the “realistic limits”. However, for most applications properties and boundary conditions can not be given with error bounds and we have to accept the admittedly weak definition given.

Validation cases are described in Report 2 and summarised in Table 5-3. As can be seen the validation cases are taken from calibration studies in various projects. We thus follow the definition of validation given above.

Table 5-3. Compilation of validation cases.

Case	Project (Reference)	Comments
A site scale validation (Case V1)	Impact of the tunnel construction on the groundwater system at Äspö. Task #5 Svensson et al. (2002).	Calibration focuses on: <ul style="list-style-type: none"> - Groundwater table - Pressure in boreholes - Kinematic porosity - Water composition Code: PHOENICS
A laboratory scale validation (Case V2)	A laboratory scale analysis of flow and salinity distribution in the Äspö area, Svensson (1999).	Calibration focuses on: <ul style="list-style-type: none"> - Fracture transmissivities - Pressure in boreholes - Conductivity distributions Code: PHOENICS
A repository scale validation (Case V3)	Prototype Repository Groundwater flow, pressure and salinity distributions around the Prototype Repository. Continuum model No1, Svensson (2001).	Calibration focuses on: <ul style="list-style-type: none"> - Tunnel inflows (skin) - Pressure in boreholes - Conductivity distributions Code: DarcyTools
An experimental scale validation (Case V4)	Simulation of tracer transport considering both experimental and natural, i.e. long, time scales, Svensson (2003).	Calibration focuses on: <ul style="list-style-type: none"> - PARTRACK - Sorbing and non-sorbing tracer retention. Code: DarcyTools

5.4 Concluding remarks

It is clear from this section that the process of confidence building is complex and involves many aspects. The bottom line is if a particular simulation is credible or not. The computer code, and its verification and validation, is of course a key factor when credibility is judged, but the user of the code is also important. CFD simulations are still far from routine calculations and the modeller normally takes a number of decisions when formulating the problem conceptually and mathematically. The “credibility of the modeller” is hence also factor to consider.

6 A SITE-LABORATORY-EXPERIMENTAL SCALE DEMO

6.1 Introduction

In the section on Confidence Building it was noted that DarcyTools, for obvious reasons, has not been widely tested in real world applications. The application to be discussed in this section has similarities with the conditions at Äspö HRL, but is generic in nature; it will hence not add to the validation studies reported. Instead the objective is to show some of the features and capabilities of DarcyTools in a realistic, but generic, application. The reason for keeping the demo generic is that the description of input data and results can be brief, as we can not discuss these in relation to field data.

The situation studied is outlined in Figure 6-1. It is a coastal site, with seawater of a brackish nature (salinity of 1%). We assume a certain precipitation on land and we hence have a density stratification to take into account. Two hills give a certain topography on land. A tunnel, with a certain inflow, will be placed below the small island in the laboratory volume shown in the figure. The focus of the analysis will be on the effects of the tunnel. The situation has a clear resemblance with the Äspö region. The fracture system will however be much simpler in this demo, as compared to the detailed information available for Äspö HRL. Four major fracture zones, shown in Figure 6-1, are assumed to represent the deterministic system. Random fractures will be generated to build a working fracture network.

It should be mentioned that the set-up of this demo in DarcyTools will be used as a worked example in the User's Guide (Report 3).

6.2 Problem specification

A summary of the problem specification is given in Table 6-1. It is not the intention to give a complete account of the input data; this is considered to be outside the scope (the specification of the fracture network would be lengthy, for example). A few comments may be needed as a complement to the key features in the table (see also Figure 6-1):

- **Domains.** The site model covers the whole domain, while the laboratory model is located below the island. The first of these two grids are of the BFC:s type (follows the topography), while the second grid is a cartesian one. The experimental model is placed in the laboratory model, but outside the tunnel area.
- **Properties.** Porosity is specified for each fracture and fracture zone. The diffusion coefficient is given a value of ten times the value for molecular diffusion for salt; this process is hence insignificant. Transmissivities, orientations, etc for the random fractures are set according to the values found appropriate for Äspö HRL.
- **Random fractures.** When the fracture network for the site domain is generated, random fracture in the interval 20 → 1000 metres are generated. Those random fractures that intersect the laboratory volume are imported as deterministic

fractures to this domain. Random fractures in the interval 10 - 20 metres are then added. The same procedure is repeated for the experimental volume; now with all fractures larger than 10 metres as deterministic and random fractures in the interval 2 – 10 metres.

6.3 Results

Some sample results will be presented for the situation with the tunnel present.

In Figure 6-2 a vertical section showing the salinity field can be found. The salinity fields show the typical fresh water lenses below land and the island. The upconing of salt water below the tunnel is also worth noting.

Next we study the flow field around the tunnel, see Figure 6-3. Two horizontal planes, roughly 100 metres above and below the tunnel, are shown. The lines formed by the vectors indicate fracture zones that supply the water flowing into the tunnel.

Finally the pressure field on the boundaries of the experimental volume is illustrated, see Figure 6-4. The blue colour indicates low pressure, which is generated by the tunnel.

6.4 Concluding remarks

The most important feature demonstrated in this application is probably the three fully coupled grids. The site domain covers a volume of $2 \times 2 \times 1 \text{ km}^3$, while the resolution in the experimental domain is 2 metres. The demo also demonstrates some important DarcyTools features like sections with prescribed inflow or skin, etc.

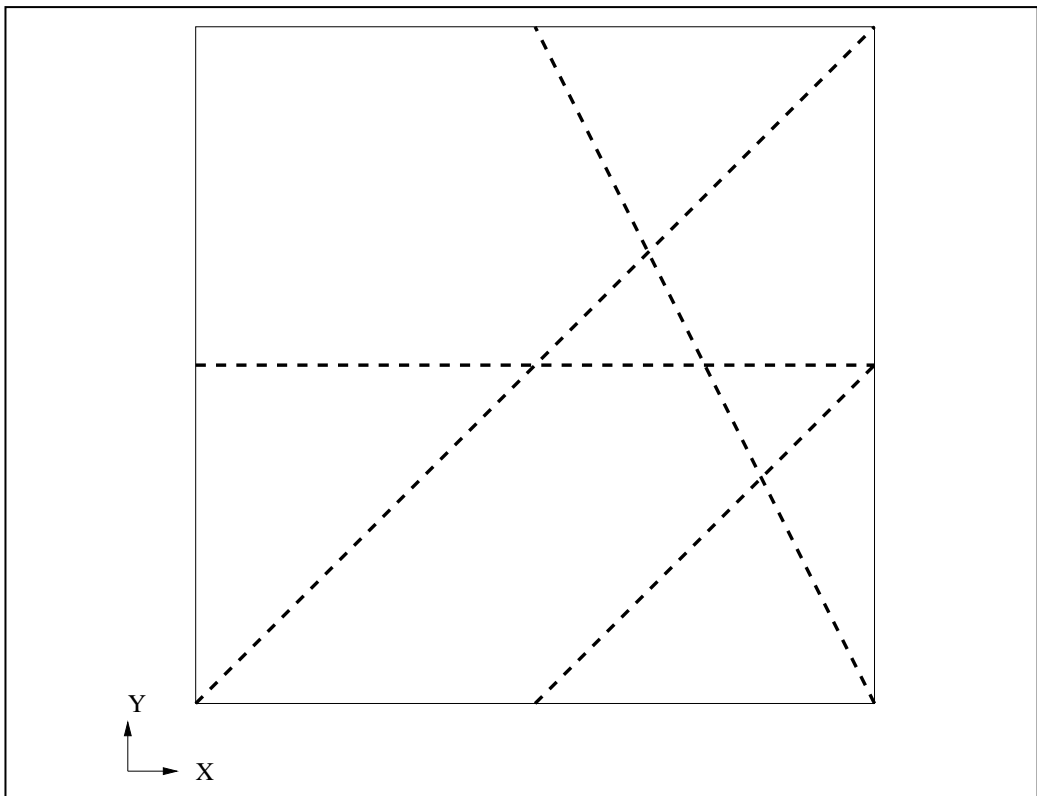
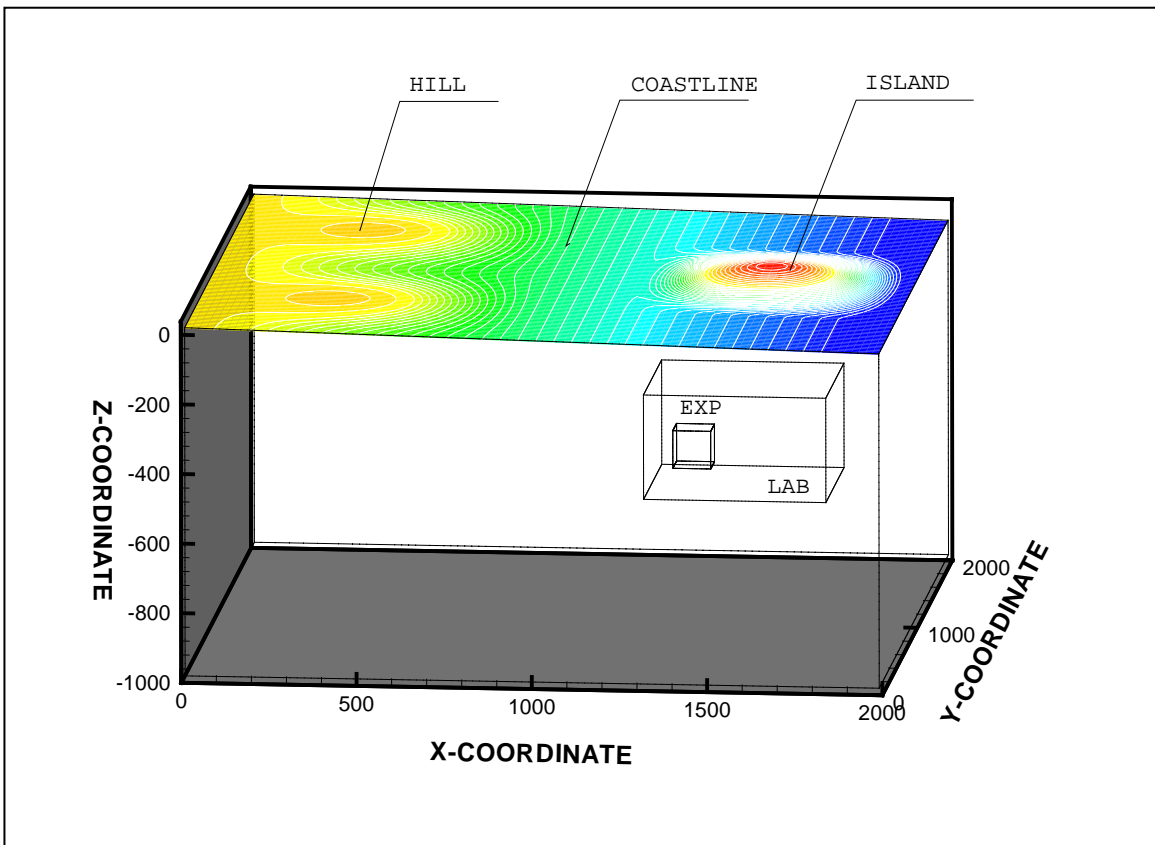


Figure 6-1. Situation considered (top) and deterministic fracture zones.

Table 6-1. Summary of problem specification.

<p>Domains and grids</p>	<p>Site: 2 x 2 x 1 km³ NX = 100, NY = 100, NZ = 50, Δ = 20</p> <p>Laboratory: 500 x 500 x 300 m³ NX = 50, NY = 50, NZ = 30, Δ = 10</p> <p>Experimental: 100 x 100 x 100 m³ NX = 50, NY = 50, NZ = 50 Δ = 2</p>
<p>Properties</p>	<ul style="list-style-type: none"> - Deterministic zones according to Figure 6-1, Transmissivity = 10⁻⁵ m²/s - Random fractures Site: $l = 20 \rightarrow 1000$ m Laboratory: $l = 10 \rightarrow 20$ m Experimental: $l = 2 \rightarrow 10$ m - Diffusion coefficients: 10⁻⁸ m²/s, constant - Porosity: 10⁻³, constant
<p>Boundary conditions</p>	<p>Top: Precipitation on land, 50 mm/year Pressure and salinity fixed below sea</p> <p>Vertical boundaries: Zero flux when boundary on land, prescribed pressure and salinity when below sea. Fixed salinity at bottom boundary.</p> <p>Tunnel : Three tunnel sections are defined; two with a prescribed skin (= 0.01) and one with a prescribed inflow (= 1 l/s).</p> <p>Groundwater table: As part of the simulation the groundwater table is calculated. The specific yield feature is not activated as we are only considering the steady state.</p>

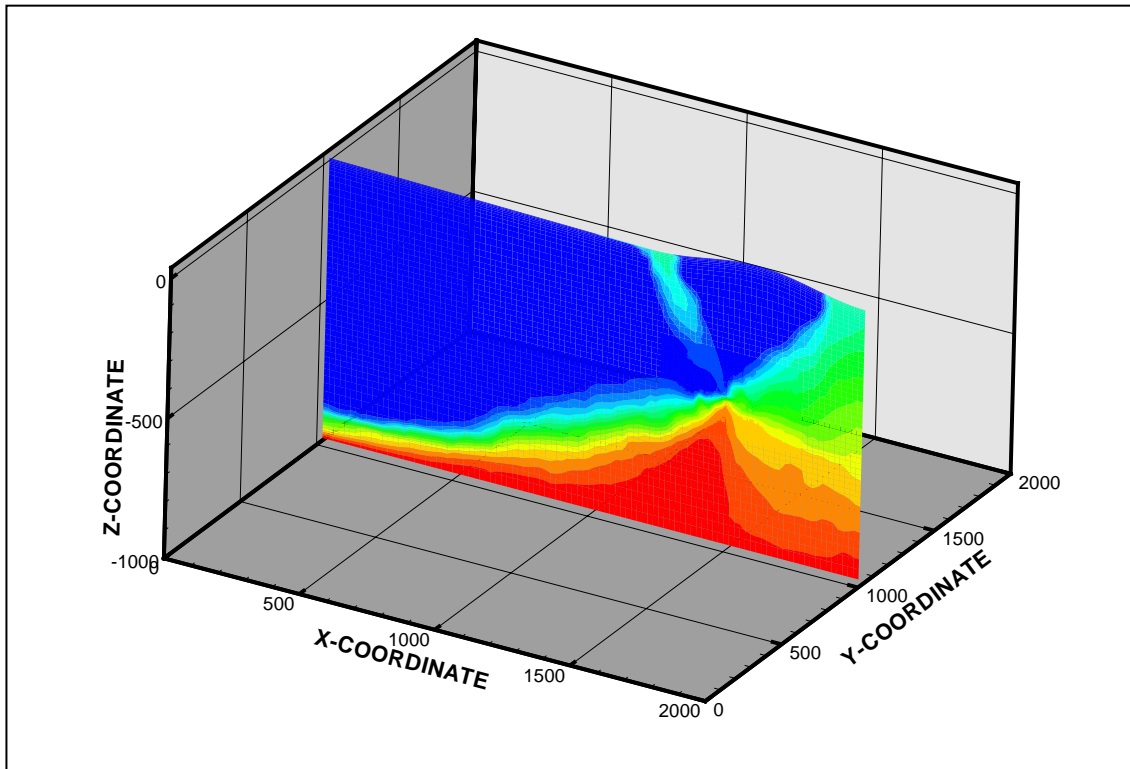


Figure 6-2. Vertical section through the island. Salinity field with upconing due to the tunnel. Blue colour indicates fresh water.

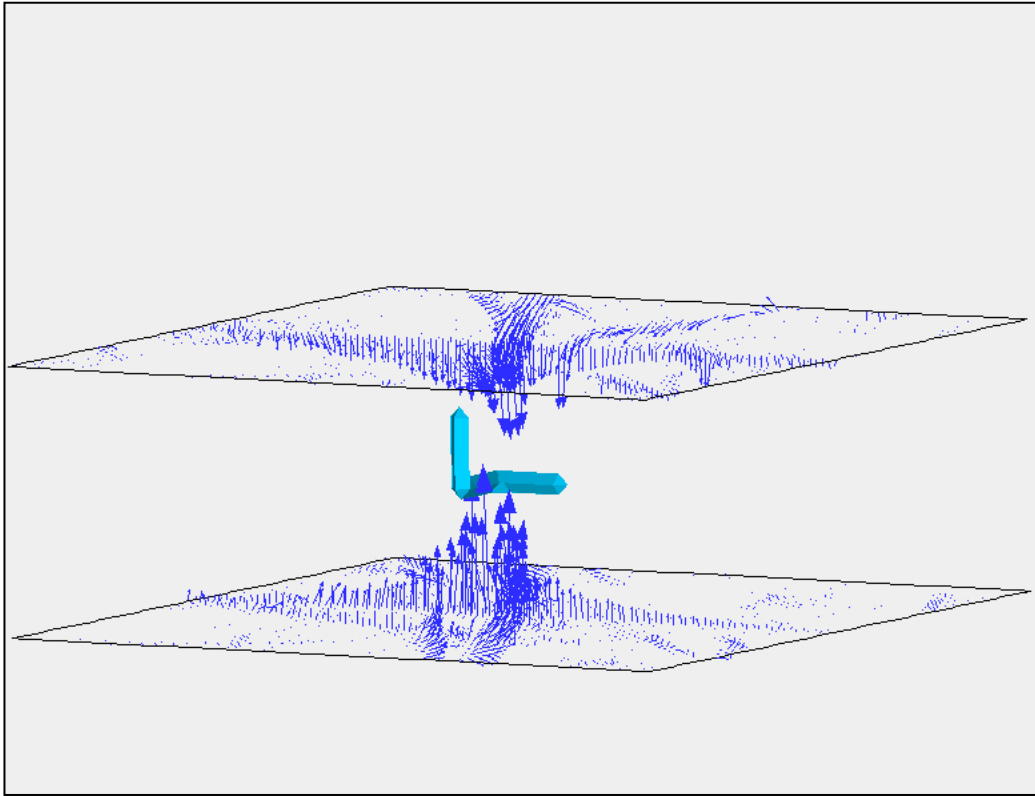


Figure 6-3. Velocity field above and below the tunnel, laboratory volume.

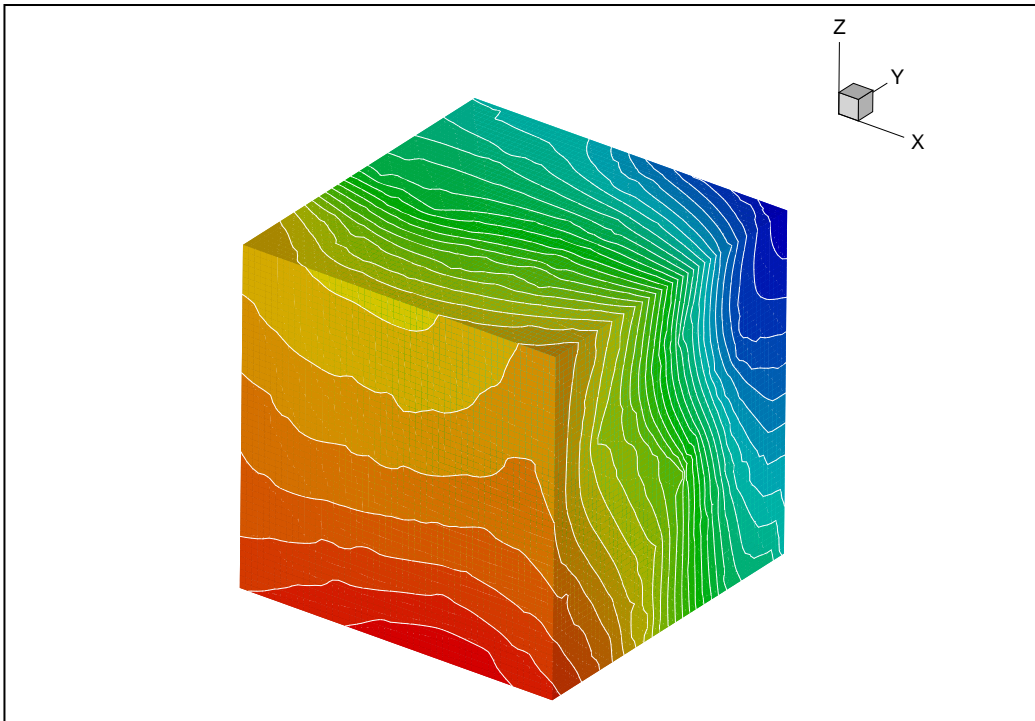


Figure 6-4. Pressure field on the boundaries of the experimental volume. Blue colour indicates low pressure.

7 Illustration of some key concepts

7.1 Introduction

Several development projects preceded the present report on DarcyTools. A number of fundamental issues dealing both with flow and transport in fractured rocks and numerical modelling techniques were addressed. It is not possible to include these studies in the present report, but a brief review of some key results is within scope. The reason for reviewing these related studies is that they illustrate the concepts used and highlight some aspects of DarcyTools that are believed to be essential for a groundwater code.

The laboratory model of Äspö HRL, see Section 1, will be used for the simulations as we going to illustrate features that are believed to be important in real world applications.

7.2 Spatial and temporal discretisation errors

In this section results that show the magnitude of the discretisation errors, that can be expected in a real world application, will be presented. As we are interested in general trends and results, the estimated magnitudes will be based on the average of ten realisations of the background fracture network. This will also give a perspective on the discretisation error, as it can be compared to the variations due to different realisations.

It was stated in Section 3, that the smallest generated fracture size should be of the same size as the grid cells, i.e. $l_{\min} \approx \Delta$. In a grid independence study, it is however preferable to keep all parameters the same, except for the studied parameter Δ . For this reason l_{\min} is equal to 3 metres when flow rates are studied and 10 metres in the transport simulations.

Flow and Pressure

As a background to the grid independence study some general characteristics of the fracture network will be discussed. It was stated in Section 3, that an underlying assumption of the present method to represent a fracture network is that “large fractures are more important for the flow rate than small ones”. In Table 7-1 some calculations of the mean block, or domain, conductivity in the West to East direction are shown. As can be seen the block conductivity does not change a lot if l_{\min} is 5, 10 or 15 metres. In the following l_{\min} will be put to 3 metres, which ought to ensure that all fractures important for the flow simulation are included. Table 7-1 also shows that the block conductivity changes more when Δ is changed; this aspect will be analysed in detail below. Table 7-2 shows the block conductivity in different realisations for three of the values shown in Table 7-1. Different realisation can clearly result in rather different block conductivities. Block conductivities with only the major deterministic fracture zones present are shown in Table 7-3. There is no stochastic element in these simulations and there is hence no need for several realisations. Some grid dependence

is found for the South to North direction, while the two other directions show very little sensitivity to variations in Δ . We may also note that, for the West to East direction, the block conductivity is 30-50 % of the block conductivity shown in Table 7-1. The major fracture zones and the background fracture network thus have about the same significance for the flow rate.

The block conductivities in the West to East direction, as a function of Δ , are shown in Figure 7-1. Ten realisations of the background fracture network were generated to get the average values shown in the figures; l_{\min} was equal to 3 metres in all calculations. In the figure two graphs are shown. In the top one block conductivity is shown as a function of N_i , the number of cells in the coordinate direction studied.

This curve shows that the block conductivity approaches a certain value in an asymptotic manner; this is the normal behaviour in grid refinement studies. The lower figure shows the same data, but expressed as a function of Δ . The advantage of this representation is that it is possible to extrapolate the curve to $\Delta = 0.0$, and hence get an estimate of the discretisation error. At this stage we will only note that the error is around 10% (from extrapolation) for the solutions with $\Delta = 3$ metres.

Some illustrations of what happens when Δ is varied are given in Figures 7-2, and 7-3. In the first figure, the flow and pressure distributions for a mean pressure gradient from West to East are shown. The general impression from these figures is that a Δ equal to 3 metres resolves the major fracture zones (deterministic and stochastic) with high accuracy. For $\Delta = 10$ metres some of the details in the flow distribution are lost. One may also note that the pressure distributions are rather similar for $\Delta = 3$ and 10 metres. Figure 7-3 shows the conductivity fields for $\Delta = 3$ and 10 metres. The smaller Δ gives a fairly detailed picture of the fracture network.

Table 7-1. Block conductivity for a pressure gradient in the West to East direction, for various l_{\min} and Δ .

l_{\min}	Conductivity $\times 10^{-7}$ (m/s) for various Δ (m).			
	5	10	15	20
5	0.66	0.84	1.00	1.17
10	0.66	0.81	0.97	1.14
15	0.66	0.81	0.97	1.13
20	0.61	0.76	0.93	1.07

Table 7-2. Block conductivity for a pressure gradient in the West to East direction. Ten realisations based on $l_{\min} = 5$ metres and various Δ .

Realisation	Conductivity $\times 10^{-7}$ (m/s) for various Δ (m).		
	5	10	20
1	0.76	0.94	1.20
2	0.66	0.83	1.06
3	0.63	0.79	1.04
4	0.57	0.74	1.01
5	0.65	0.78	1.03
6	0.59	0.83	1.18
7	0.56	0.75	1.02
8	0.59	1.06	1.08
9	0.87	0.92	1.36
10	0.71	0.77	1.21

Table 7-3. Block conductivity in the three coordinate directions with only major deterministic fracture zones present, for various Δ .

Direction	Conductivity $\times 10^{-7}$ (m/s) for various Δ (m).				
	3	5	10	15	20
West-East	0.30	0.31	0.31	0.32	0.33
South-North	0.80	0.85	0.98	1.10	1.22
Low-High	4.26	4.22	4.23	4.22	4.26

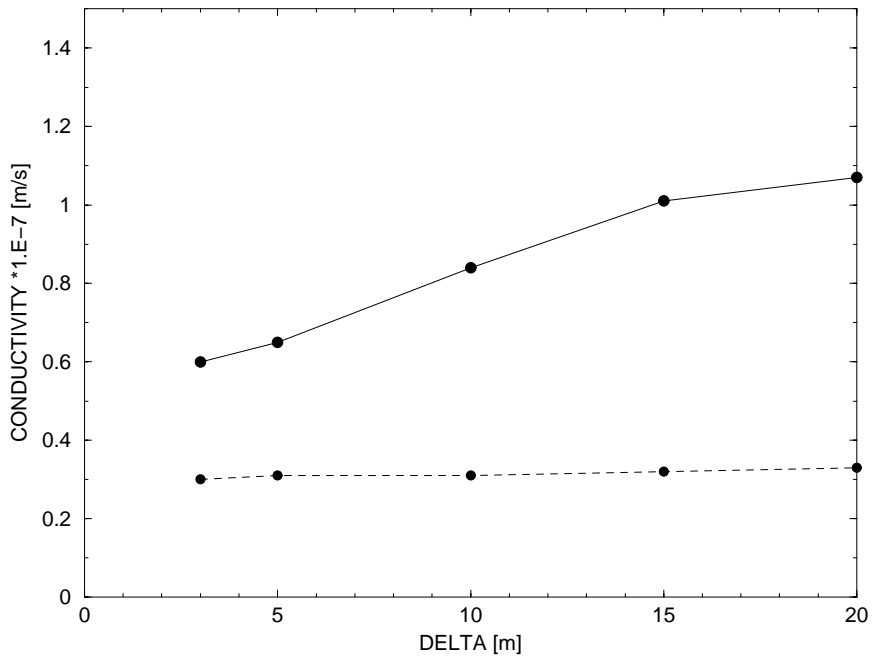
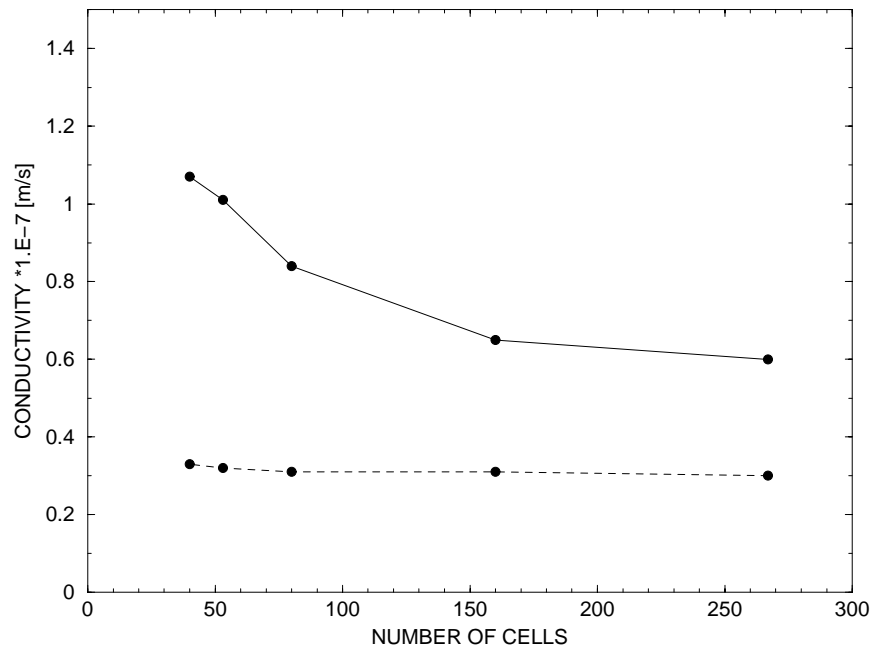
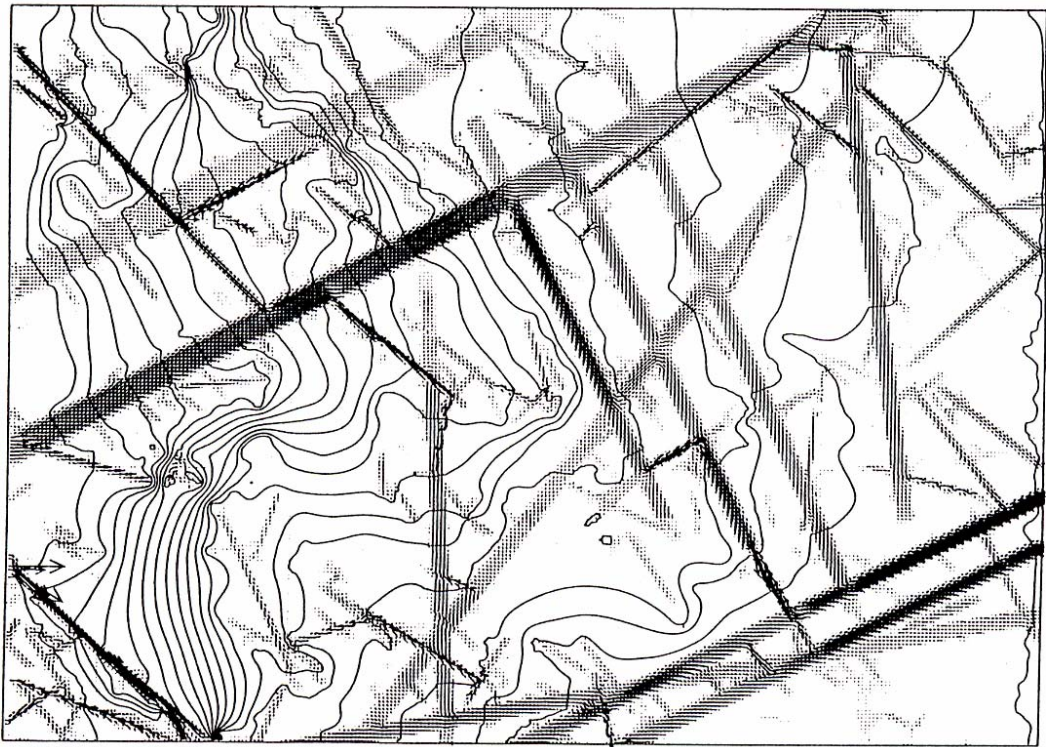


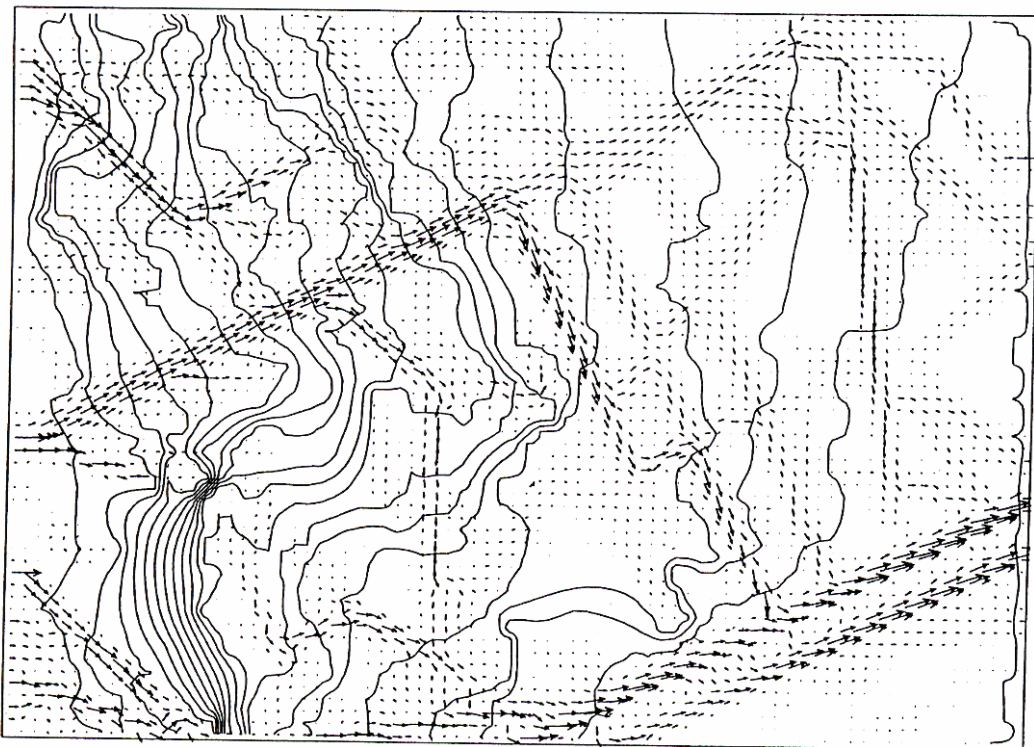
Figure 7-1. Block conductivity in the West to East direction as a function of the number of cells in the coordinate direction (top) and as a function of Δ .

(——) All fractures included.

(-----) Only major fracture zones.

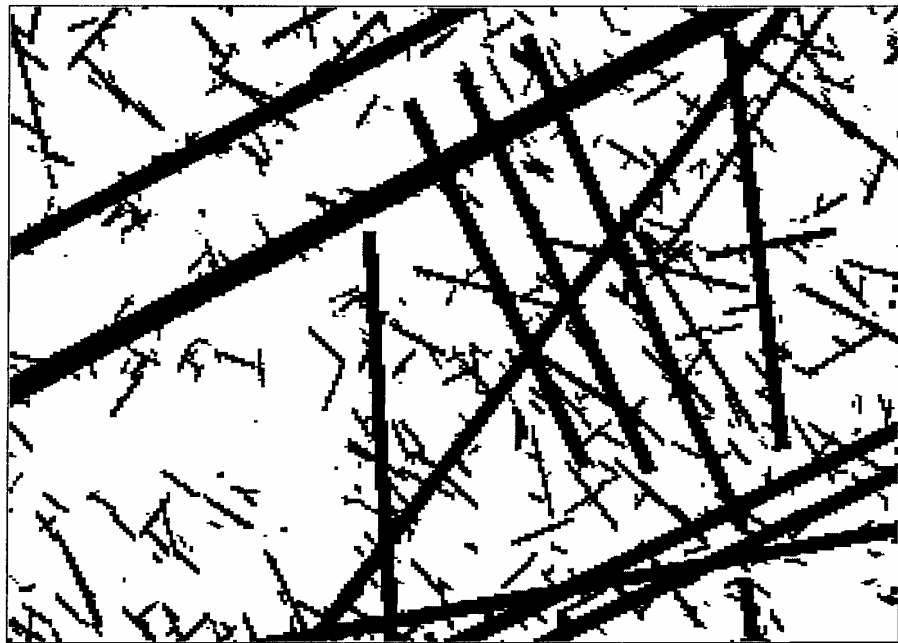


Scale: |-----| 100 m



Scale: |-----| 100 m

Figure 7-2. Flow and pressure distribution for a mean pressure gradient from West to East. Pressure distribution shown with 20 isolines. $\Delta = 3$ metres (top) and 10 metres.



Scale |-----| 100 m



Scale |-----| 100 m

Figure 7-3. Conductivity fields for $\Delta = 3$ metres (top) and 10 metres. All conductivities larger than 10^{-8} m/s shown.

Transport and Dispersion

Estimating the discretisation errors when simulating a tracer pulse that moves through the domain is more difficult, as we then have to consider the errors both in space and time. In order to simplify the analysis only flow in the West to East direction will be considered. As the flow simulations further indicate that $\Delta > 10$ metres produce quite “smeared” solutions, only $\Delta = 3, 5$ and 10 metres will be discussed.

The following situation is studied. In a steady flow field a tracer marks the water at the inlet (Western) boundary during a period of one year. After about fifteen years the pulse leaves through the Eastern boundary.

A typical breakthrough curve is shown in Figure 7-4. It is the concentration at the outlet, in fracture zone NE1, that is shown in the figure. The tracer will leave the domain through several fractures but the maximum flux is expected through NE1. Regarding l_{\min} it was argued in Section 3 that a good choice is to put it equal to Δ . However in a grid refinement study it is preferable to keep the geometry fixed and only vary Δ . For this reason l_{\min} will be put to the largest Δ , i.e. 10 metres, in the following calculations.

In the grid refinement study, we will use the maximum concentration at the outlet as a simple description of the breakthrough curve. The main result of the exercise is given in Figure 7-5. The smallest time step use, 0.25 months, is seen to be close to the time step independent solution (from an extrapolation). It is also interesting to note that $\Delta = 3$ and 5 metres give very similar results. Hence, with $\Delta = 3$ metres and $\Delta t = 0.25$ months, we are probably close to a grid independent (in space and time) solution. The $\Delta t : s$ discussed are of course related to the mean transport time, and hence to the prescribed mean head gradient.

In Figure 7-6 the tracer distribution after ten years is shown for two Δ . As can be seen, the main characteristics of the plume are quite well described in both grids. The breakthrough curves for the smallest time steps used are given in Figure 7-7. Also this figure indicates that $\Delta = 3$ metres resolves the transport problem with acceptable accuracy. The main difference between the three curves is the arrival time for the peak concentration. This difference is due to the increase in flow rate with Δ , as discussed above.

A concluding comment on the discretisation errors in the transport simulations shown may be in place. The breakthrough curves in Figure 7-7 mainly differs in the arrival times, which can be explained by the increase in flow rate with Δ (as discussed above). The peak value and the shape of the breakthrough curves are however very similar. This is a strong indication that the grid representation of the flow and porosity fields is based on sound principles. The flow field looks quite different for $\Delta = 3$ and 10 metres (see Figure 7-2) and the grid representation of the porosity fields is smeared in a similar way as the conductivity field (see Figure 7-3). Still the transport problem is solved in a similar way in both grids.

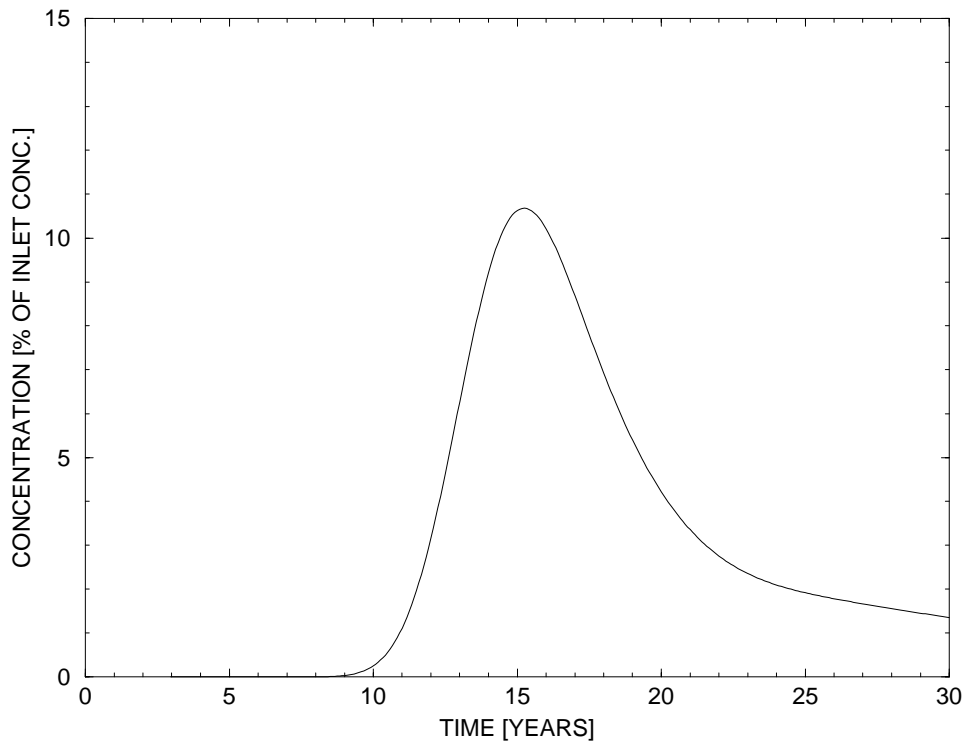


Figure 7-4. Breakthrough pulse through NE1 at the outlet boundary.
 $\Delta = 5$ metres, $\Delta t = 1$ month

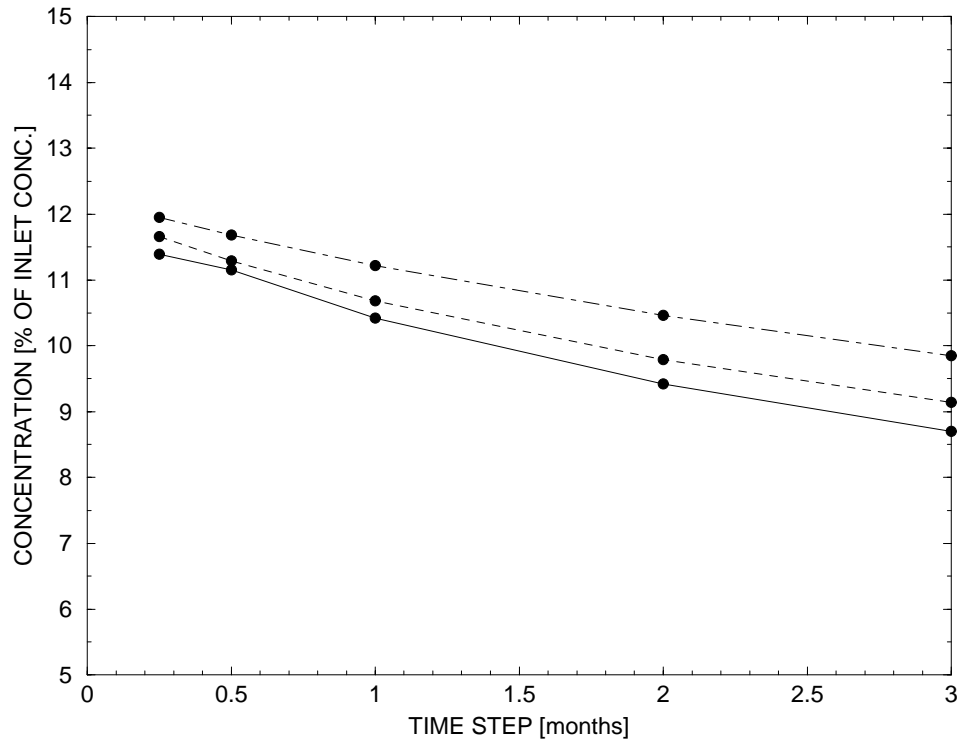


Figure 7-5. Maximum concentration in fracture zone NE1 at the outlet plane, as resolved by different Δ and Δt .

- (——) $\Delta = 3$ metres
- (- - - - -) $\Delta = 5$ metres
- (- · - · - ·) $\Delta = 10$ metres

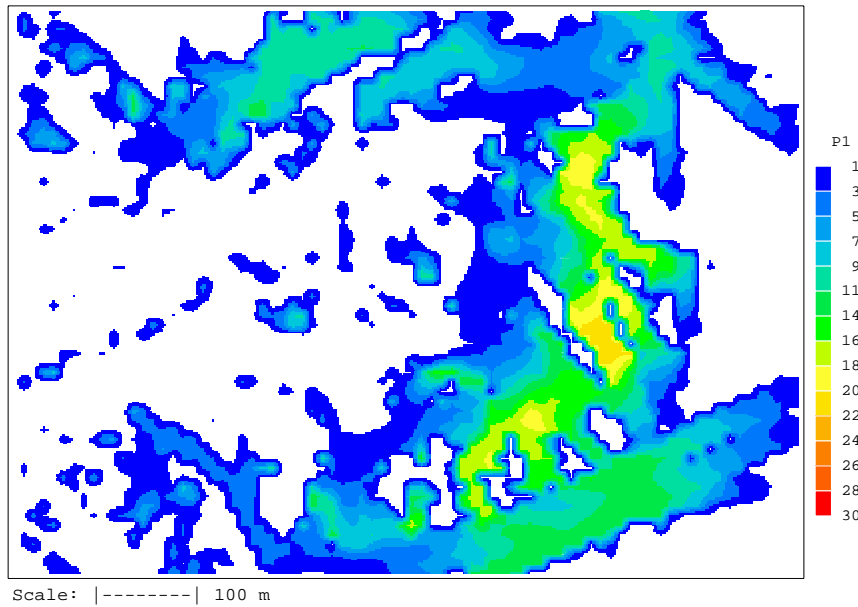
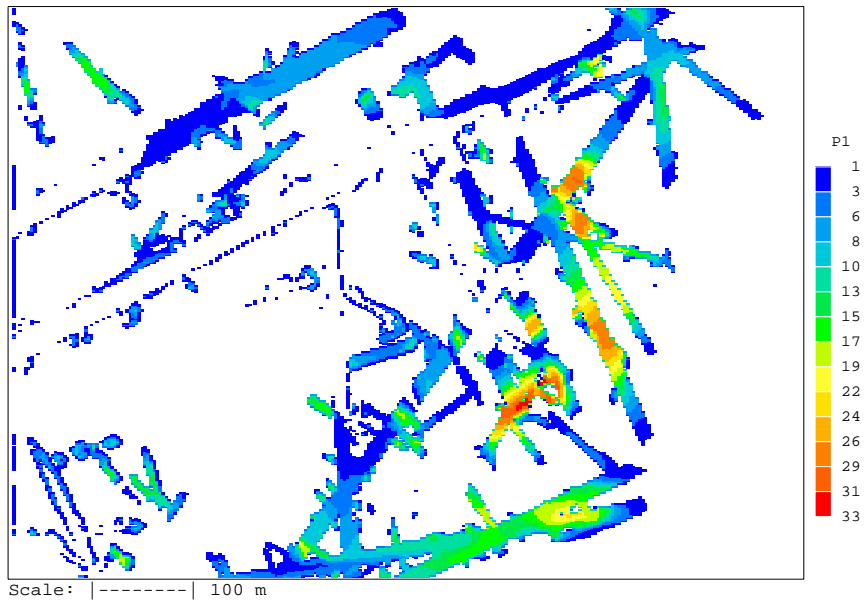


Figure 7-6. Tracer distribution after ten years.
 $\Delta = 3$ metres (top) and $\Delta = 10$ metres

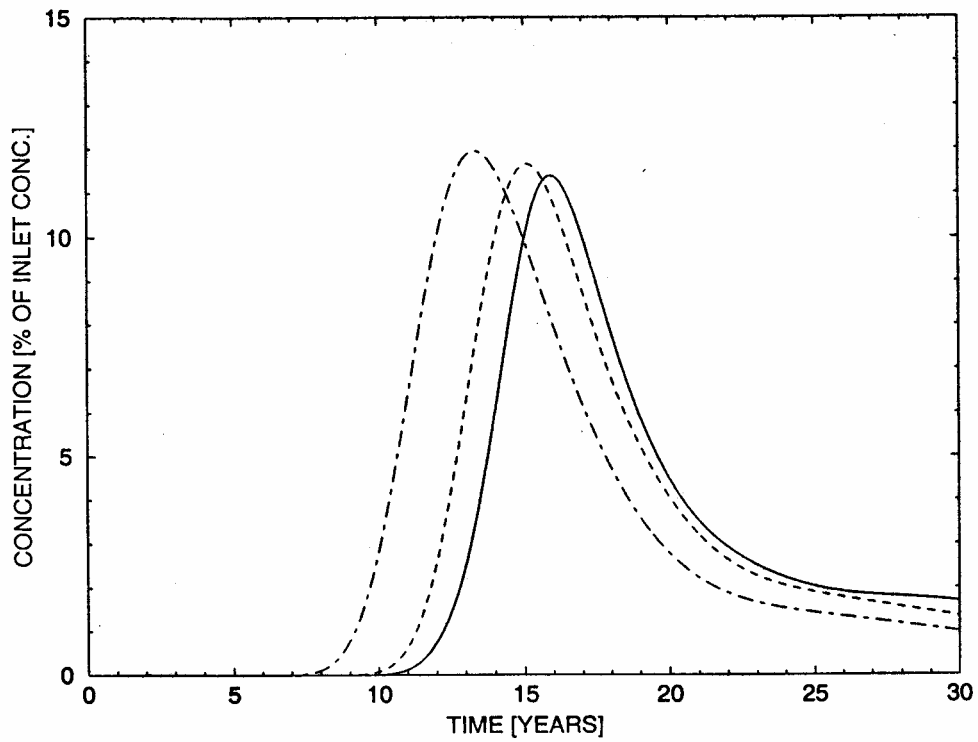


Figure 7-7. Breakthrough curves for $\Delta = 3$ metres (—), 5 metres (- - - -) and 10 metres (- · - · -). $\Delta t = 0.25$ months.

Conclusions

The objective of the work presented has been to estimate the discretisation error, in space and time, in simulations of flow and transport in a realistic fracture network. This has been done for a test case with a prescribed mean pressure gradient in a coordinate direction. The block conductivity and transport characteristics for such situations have been studied for a range of grid cell sizes, Δ , and time steps, Δt .

From the study the following main conclusions can be formulated:

- The space resolution, Δ , should be of the order of 1%, or smaller, of the domain size. For the test case studied the error, i.e. the difference between the actual and the estimated grid independent solution, in the block conductivity may then be around 10%.
- The estimated magnitude of the discretisation errors is regarded to be small in comparison to the uncertainty in input data (for example transmissivities and porosities).
- The minimum fracture size in the background fracture network should be comparable to the grid size. This ensures that all important flow channels are resolved and provides a natural link to a subgrid model (the subgrid model considers the dispersion effect due to all fractures smaller than the grid size).

7.3 Porosity and connectivity

In this section we will apply the porosity concepts to the laboratory model of the Äspö HRL.

In Section 3.6, some domain related porosity concepts were defined (θ_a , θ_c and θ_f). θ_f is the porosity based on "all volumes with a significant flow", i.e. stagnant parts have been removed from θ_c . As outlined in Section 3.8, some calculations are required to identify the stagnant volumes.

A typical sequence of calculations is shown in Table 7-4. For a head gradient of 10^{-3} , it is found that disregarding all cells with a maximum absolute cell wall flux of 3×10^{-11} m/s will result in a decrease of the average flux through the domain that is smaller than 1%. Note that the number of stagnant cells is not related to the flux value 3×10^{-11} m/s, as a different head gradient would result in another flux value; the 1% reduction limit will however still be valid.

Table 7-4. Determination of stagnant parts of the kinematic porosity field. The ratio Q/Q_m , where Q is the actual flow rate and Q_m the flow rate for θ_c , is determined for various limits on the absolute maximum flow rate through a cell wall, $|V_{\text{limit}}|$.

$ V_{\text{limit}} $ [m/s]	Q/Q_m [%]		
	East-West	North-South	High-Low
10^{-10}	93.7	96.9	99.0
5×10^{-11}	97.3	98.8	99.5
3×10^{-11}	99.0	99.5	99.7

Table 7-5. Kinematic porosity values based on total volume of domain and on volume of active cells.

Case	Porosity based on total volume	Number of active cells (%)	Porosity based on volume of active cells
All fractures included	1.19×10^{-4}	70	1.7×10^{-4}
Isolated fractures or clusters removed	1.13×10^{-4}	45	2.5×10^{-4}
Stagnant volumes and isolated fractures removed	1.09×10^{-4}	35	3.1×10^{-4}

In Figure 7-8 three porosity fields are shown; in the top one all generated fractures contribute to the porosity field, in the middle one all isolated volumes are disregarded and in the lower one also the stagnant volumes have been removed. It is clear that most of the flow is due to a limited number of fractures. Table 7-5 gives some further details. It is interesting to note that the porosity based on the total volume varies little between the cases listed. The explanation is that the isolated and stagnant parts of the porosity field are due to small fractures with low transmissivity and hence also low porosity. Figure 7-9 provides support for this explanation. When isolated and stagnant parts are removed 66% of all cells have a porosity of 10^{-8} , which is the prescribed lower limit.

A visualisation of the kinematic porosity (θ_c) and flow field is shown in Figure 7-10. The porosity is illustrated with an isosurface for a value of 3×10^{-5} , while the isosurface for the magnitude of the Darcy flux has a value of 3×10^{-11} m/s (this was the value that identified stagnant volumes). The flow direction is from west to east.

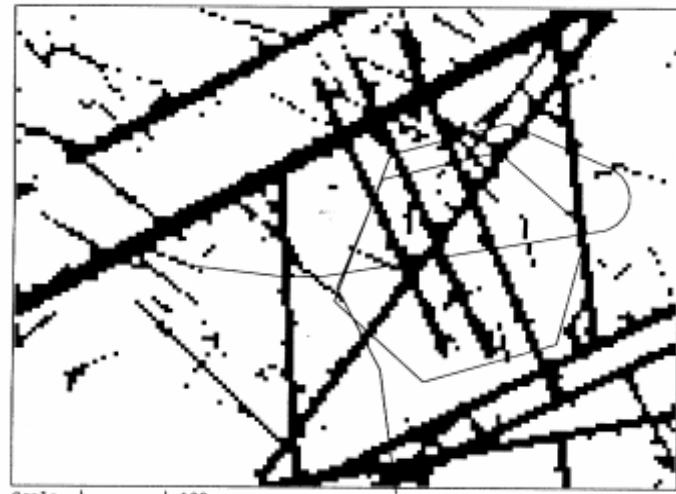
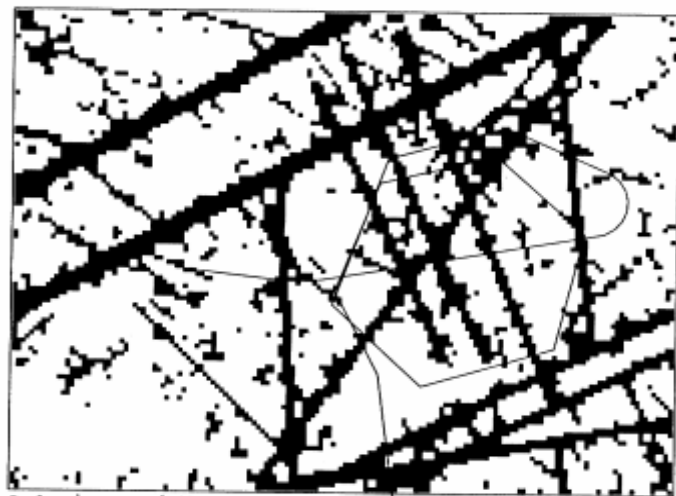


Figure 7-8. Kinematic porosity fields at a depth of 450 metres, based on all generated fractures (top), all connected fractures (middle) and all connected fractures disregarding stagnant volumes.

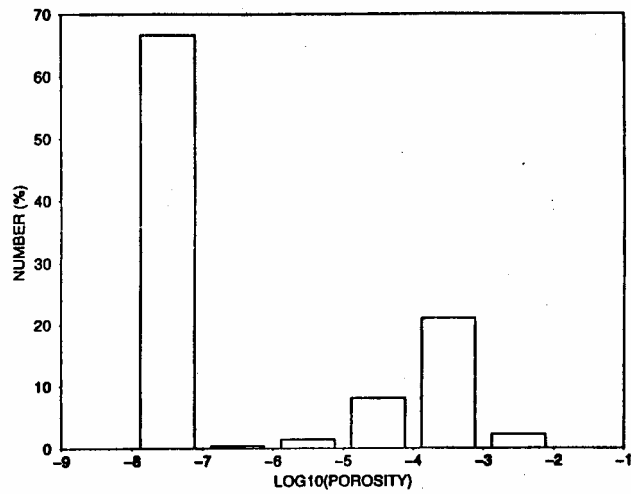
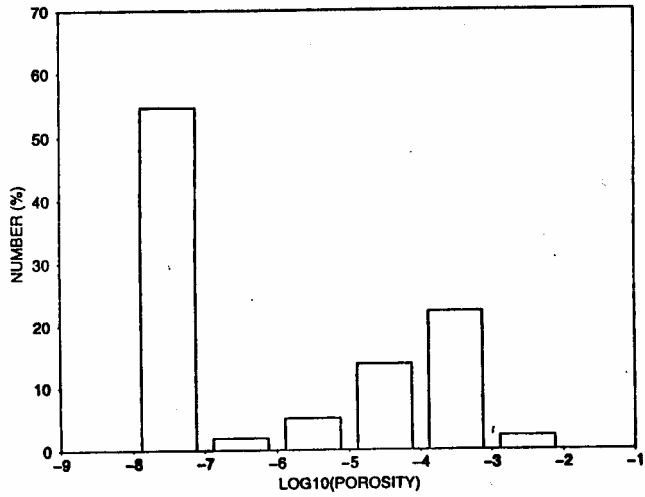
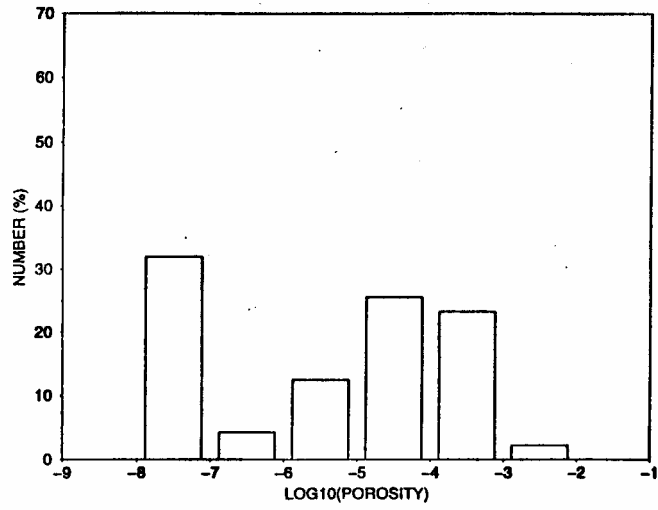


Figure 7-9. Porosity distribution in the computational grid. Number of cells with different kinematic porosity shown for the case where all generated fractures are kept (top), isolated fractures removed (middle) and isolated fractures and stagnant volumes removed.

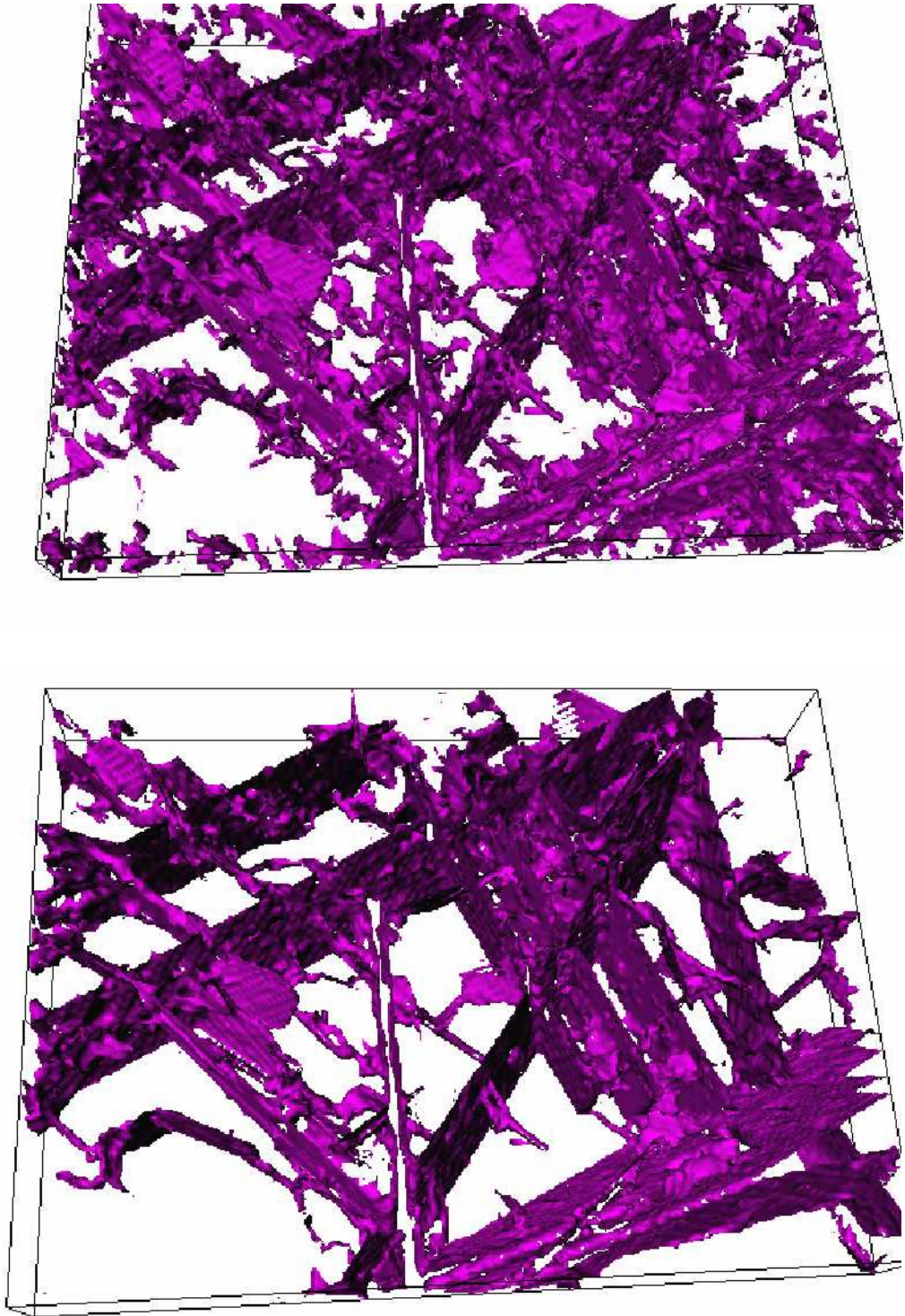


Figure 7-10. Illustration of porosity (top) and flow fields. Depth interval shown is 400 to 500 metres below ground level. The flow is from west to east. View from south.

Gravitational effects

At the Äspö HRL old water types (like Glacial water) have been found already at a depth of a few hundred metres. As discussed earlier, it is possible to explain the storage of water by a slow exchange with the storage volumes. Gravitational effects may however also contribute to the isolation of a water volume; salt water in the bottom of a fracture is not easily replaced by fresh water.

A qualitative study of the gravitational effects will be carried out. As in the previous case we specify a pressure gradient in the west to east direction. The inflow and outflow sections are however now limited to a 10 metres high horizontal band at a depth of 380 metres. The initial salinity in the domain is zero, while the inflowing water has a salinity that varies in time, according to Figure 7-11. The total integration time is 10 000 years. What one can expect is that the salt water will replace the water in the lower half of the domain, while some water with zero salinity may remain (note that the inflowing water always has a salinity $> 0\%$) in the upper half of the domain.

The result after 10 000 years of integration can be studied in Figure 7-11. The two vertical sections show the result with (top) and without gravity activated. Obviously gravity is a very important factor when storage of old water types is to be analysed.

A comment may be needed on the "horizontal band of 10 metres" giving the inflow and outflow boundaries. The salinity of the inflowing water is intended to illustrate different stages, with different salinities, of the Baltic Sea. In the present model set-up we do not simulate the contact with the Baltic Sea, as the top of the model domain is at a depth of 200 metres, and we are thus forced to specify "unrealistic" boundary conditions. It should however be noted that the purpose of the simulation is to illustrate the effect of density variations, in a qualitative way.

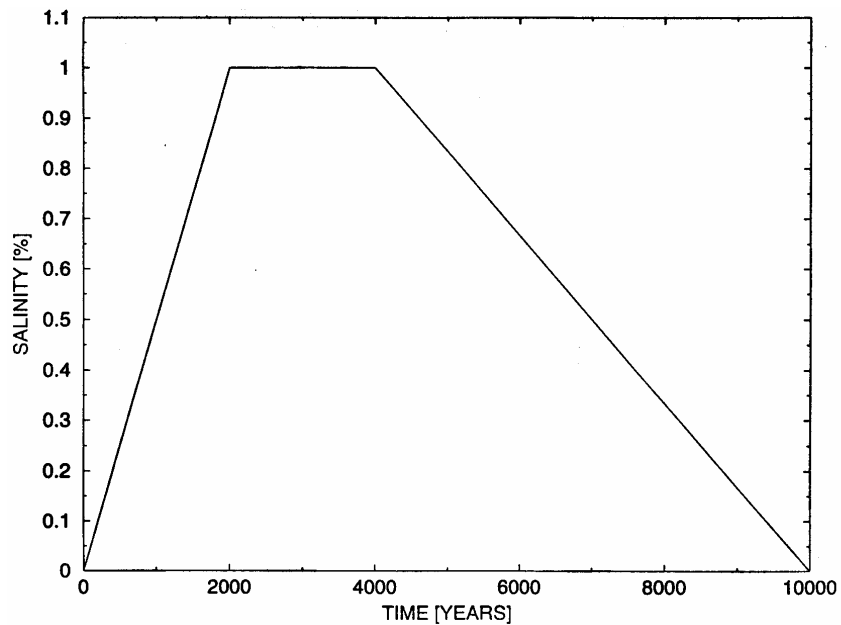
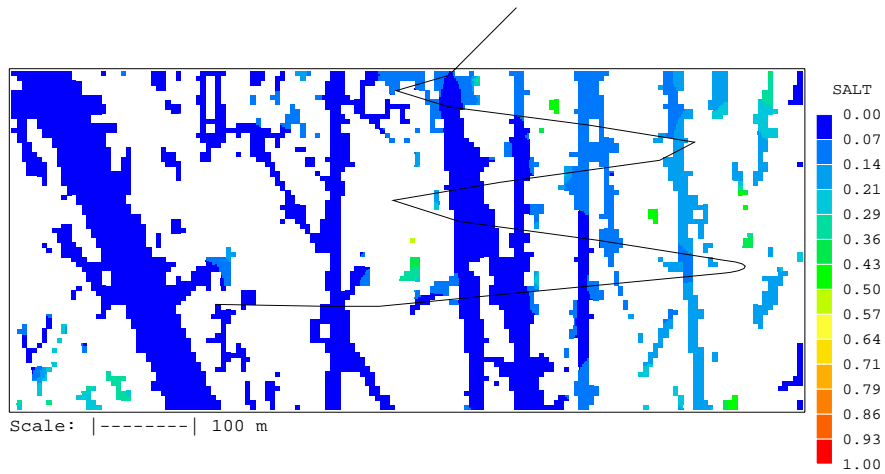
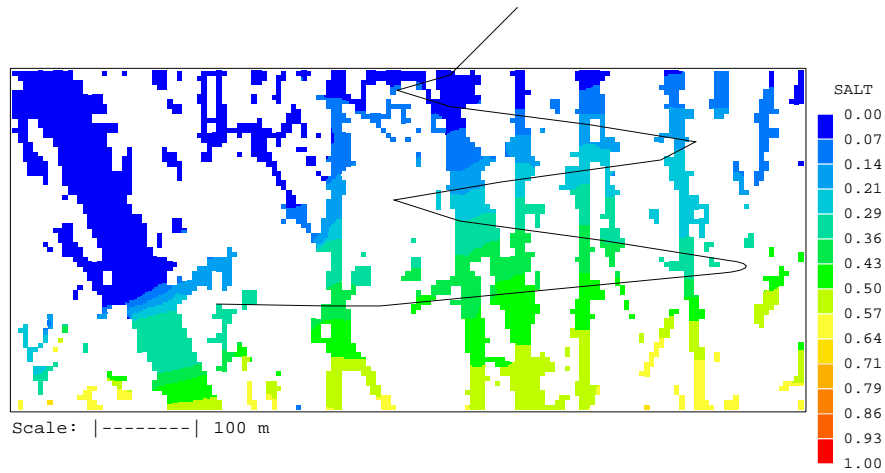


Figure 7-11. Effect of gravity. Vertical sections of salinity field after 10 000 years of integration with (top) and without gravity activated (middle). Salinity of inflowing water as a function of time (bottom).

Conclusions

The key feature of the GEHYCO method is that properties (conductivity, flow wetted surface and kinematic porosity) are defined for conductive elements that form a fracture network. The specific results from the present study can be summarised as follows:

- The fracture network generates a connected system of pore-space that we define as the kinematic porosity. Part of this porosity is defined as stagnant volumes, based on a flow criterion.
- Storage volumes are representing fractures smaller than the minimum fracture size in the network and all other volumes that exchange matter with the kinematic volumes by molecular diffusion only. Computationally storage volumes are simulated by the model FRAME.
- Simple test cases, generic studies and applications to the Äspö HRL demonstrate that the concepts are useful and easily employed in numerical models of the continuum type.

7.4 PARTRACK

Transport simulations can be based on two principally different methods, solving an advection/diffusion equation for the solute or tracking particles. In DarcyTools both methods are used. It is of course of value to base both methods on the same concepts and assumptions concerning the subgrid processes.

The particle tracking routine PARTRACK is described and tested in Svensson (2001a). That version was however based on a lognormal distribution of rate coefficients. FRAME, as described in this report, is based on power-law distributions, which are preferred as the general fracture network is based on such distributions.

As part of the general development of FRAME, a power-law distribution has also been introduced in PARTRACK. The objective of this section is to show some sample results that demonstrate that this has been achieved.

As PARTRACK is now based on FRAME, it will also use the same input parameters. For the results to be presented the following was specified: $\beta_t = 10$, $k = 1.8$ and $D_e = 10^{-10}$ m²/s (constant for the applications presented).

A one-dimensional channel with a steady state flow, with uniform velocity, is used. The length of the channel is 10 metres and the transport velocity 10^{-4} m/s. This gives an advective transport time of 10^5 s (≈ 28 hours). The concentration at the outlet as a function of time, i.e. the breakthrough curve (BTC), is used to illustrate the results.

In Figure 7-12, three BTC:s are shown. If no dispersion effects are active, all particles will arrive after about 27 hours. If Taylor dispersion is added an insignificant dispersion will result for $D_m = 10^{-10}$ m²/s. Decreasing D_m to 10^{-12} m²/s gives some dispersion as can be seen in Figure 7-12. If FRAME is added, the BTC will be significantly modified as can be expected.

Next we use the laboratory model in order to show a real world application. In the west to east flow considered, particles are released in fracture zone EW1, see Figure 1-1, and then tracked through the domain till they reach the eastern boundary. Figure 7-13 shows the flow paths generated by 100 particles. The main flow path is through EW1, changing to the NNW structures and leaving through NE1. Note that in this view from above, NE1 gives a wider impression, as this zone is not vertical. It is also worth noting that rather few flow channels are active in the transport.

The only objective of these simulations is to demonstrate that PARTRACK is now based on the subgrid model FRAME. More sensitivity studies and applications of this new version of PARTRACK will be presented elsewhere (for example in Task #6, initiated by the Äspö Task Force on modelling of groundwater flow and transport of solutes). Verification and Validation studies are also found in Report 2.

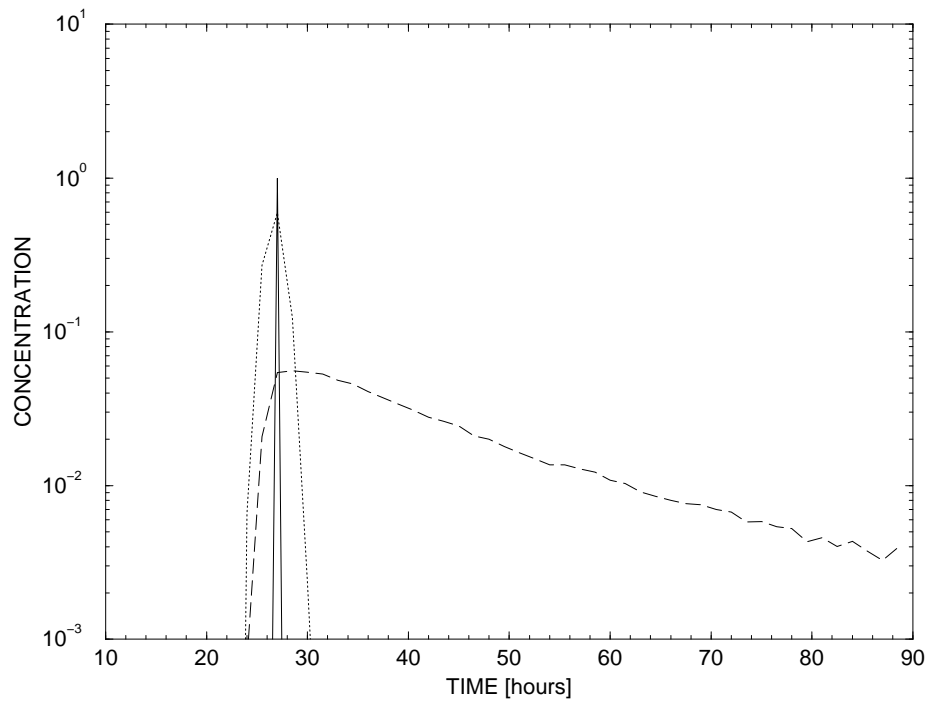


Figure 7-12. BTC:s in a one-dimensional channel.
 — No dispersion.
 Taylor dispersion added ($D_m = 10^{-12} \text{ m}^2/\text{s}$)
 - - - - - FRAME and Taylor dispersion added.

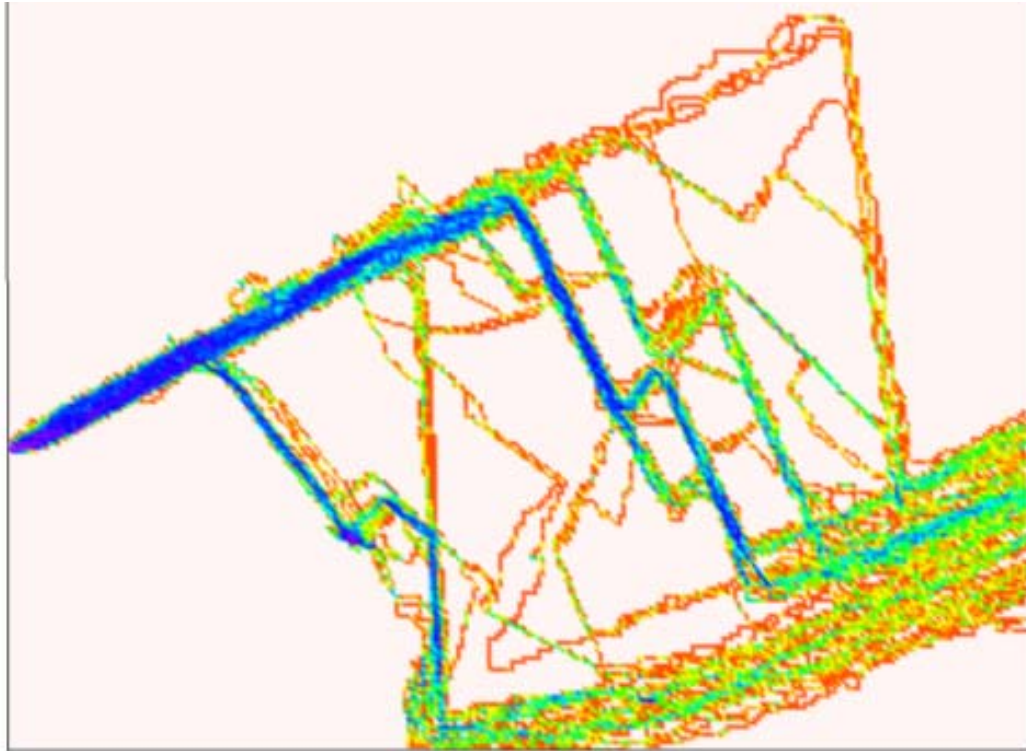


Figure 7-13. Flow channels formed by 100 particle tracks in a flow from west to east. Blue indicates high intensity of tracks, red low.

8 Discussion

Even if the main part of this report is, intentionally, short it may be difficult to “put the pieces together” and get a good grasp of DarcyTools. We will therefore use the discussion section to summarise the key features of DarcyTools and also to give a hint about possible future developments.

Key features

- **Mathematical model.** DarcyTools is based on conservation laws (mass, heat, momentum and massfractions) and state laws (density, porosity). The subgrid model utilise the multi-rate diffusion concept and the fracture network (resolved and subgrid) is based on fractal scaling laws.
- **Continuum model.** Even if a fracture network forms the basis of the approach, DarcyTools should be classified as a continuum porous-medium (CPM) model.
- **Fractures and fracture network.** Fractures and fracture zones are idealised as conductive elements, to which properties (conductivity, porosity and flow wetted surface) are ascribed. Empirical laws are used for the determination of these properties. The fracture network is based on fractal scaling laws and statistical distributions (random in space, Fisher distribution for orientation, etc).
- **GEHYCO.** This is the algorithm, based on the intersecting volume concept, that transforms the fracture network (with properties of conductive elements) to grid cell properties.
- **FRAME.** Subgrid processes are parameterised as “diffusive exchange with immobile zones”. FRAME uses the multi-rate diffusion model and fractal scaling laws, to formulate a simple and effective subgrid model.
- **SOLVE.** When the continuum model is generated, effective CFD-methods are used to solve the resulting finite-volume equations. DarcyTools uses the MIGAL-solver, which is a multigrid solver with the capability to solve coupled problems (like pressure and salinity) in a fully coupled way.
- **PARTRACK.** This particle tracking algorithm is fully integrated with DarcyTools and uses the same basic concepts as FRAME. PARTRACK can handle Taylor dispersion, sorption and matrix diffusion simultaneously in large 3D grids ($> 10^6$ cells).
- **Verification and Validation.** A large number and wide range of verification and validation studies have been carried out, see Report 2.

Version 3.0

The work leading to DarcyTools, Version 2.1 has been focused on the needs and requirements from the SKB Site Investigations. It is believed that V2.1 fulfils these requirements.

The development of V2.1 was not carefully planned and structured, simply because time did not allow it. Version 3.0 is intended to last longer (perhaps 3-5 years) and should hence be preceded by a more thorough investigation of expected future tasks.

A tentative suggestion, or guess, is that the following key words can describe the directions for work leading to Version 3.0:

- Repository stages. All stages in the construction and building (including the present Site Investigations) of the repository should be considered, as well as the long term behaviour after closure.
- Research tool. Hopefully DarcyTools will be useful for the research carried out at Äspö HRL and in the simulation projects defined by the Äspö Task Force on groundwater flow and transport of solutes.
- Technically it is expected that DarcyTools V3.0 will include an unstructured grid option and the capability to make use of multi-processor computers.

9 Conclusion

The main objective of this report is to provide the theoretical basis of DarcyTools. The main part of the report is written in a descriptive style, with the intention that also non-specialists in groundwater modelling may find it accessible. More detailed accounts of various topics are provided in appendices. Hopefully, the report still fulfills the objective stated.

It is the ambition to establish DarcyTools as a state of the art computer code for simulation of flow and transport in fractured and/or porous media. Many novel and powerful features have been introduced, but more work is needed before this ambition has been achieved.

10 References

AIAA Journal. 1998. Special issue, Vol. 36, No. 5, May 1998.

Andersson J., Hermansson J., Elert M., Gylling B., Moreno L., Selroos J-O. 1998. Derivation and treatment of the flow wetted surface and other geosphere parameters in the transport models FARF31 and COMP23 for use in safety assessment. SKB Report R-98-60.

Casey M., Wintergerste T. 2000. Best practice guidelines. ERCOFTAC Special Interest Group on "Quality and Trust in Industrial CFD".

Doe T., 1993. As referenced in Dershowitz et al. (1999)

Ferry M., 2002. MIGAL. See www.mfrdc.com

Fisher N. I., Lewis T., Embleton B. J. J., 1987. Statistical analysis of spherical data. Cambridge University Press.

Follin S. and Svensson U., 2002. The Laxemar project. SKB work in progress.

Forsmark T and Rhén I., 1999. Prototype Repository. Hydrogeology interference test campaign 1 after drill campaign 3. SKB International Progress Report IPR-00-07.

Forsmark T., Rhén I., Andersson C., 2001. Prototype Repository. Hydrology-deposition-and lead-through boreholes: Inflow measurements, hydraulic responses and hydraulic tests. SKB IPR-00-33.

Gómez-Hernández J.J., Hendricks Franssen H. J. W. M., Sahuquillo A. and Capilla J.E., 1999. Calibration of 3D transient groundwater flow models for fractured rock. Proceedings "Model CARE 99". International Conference on Calibration and reliability in groundwater modelling. Zürich, Switzerland, 20-23 September 1999.

Haggerty R. and Gorelick S.M., 1995. Multiple-rate mass transfer for modelling diffusion and surface reactions in media with pore-scale heterogeneity. *Water Resour. Res.*, 31 (10), pp 2383-2400.

Haggerty R., McKenna S. A. and Meigs C., 2000. On the late-time behavior of tracer breakthrough curves. *Water Resour. Res.*, Vol. 36, No.12, pp 3467-3479.

Harlow F. H. and Welch J.E., 1965. Numerical Calculation of Time-Dependent Viscous Incompressible Flow of Fluid with Free Surface. *Phys. Fluids*, vol. 8, p. 2182.

Jackson C. P., Andrew R. H. and Todman S., 2000. Self-consistency of heterogeneous continuum porous medium representation of a fractured medium. *Water Resources Res.*, 36(1), 189-202.

La Pointe P. R., Wallman P., Follin S., 1995. Estimation of effective block conductivities based on discrete network analyses using data from the Äspö site. SKB Technical Report TR-95-15.

- La Pointe P. R., Cladouhos T., Follin S., 1999.** Calculation of displacements on fractures intersecting canisters by earthquakes: Aberg, Beberg and Cberg examples. SKB Technical Report TR-99-03.
- Neretnieks I., 1993.** Solute transport in fractured rock -applications to radionuclide waste repositories. In "Flow and Contaminant Transport in Fractured Rock", 39-127. Academic Press, Inc.
- Niemi A., Kontio K., Kuusela-Lahtinen A., Vaittinen T., 1999.** Estimation of block conductivities from hydrologically calibrated fracture networks - description of methodology and application to Romuvaara investigation area. Posiva report 99-19.
- Outters N. and Shuttle D., 2000.** Sensitivity analysis of a discrete fracture network model for performance assessment of Aberg. SKB Report R-00-48.
- Patankar S.V., 1980.** Numerical heat transfer and fluid flow. Hemisphere Publishing Corporation, McGraw-Hill Book Company.
- Pozdniakov S.P., Tsang C.-F., 1999.** A semianalytical approach to spatial averaging of hydraulic conductivity in heterogeneous aquifers. J. Hydrol. 216, 78-98. R-99-03.
- Renard Ph. and de Marsily G., 1997.** Calculating equivalent permeability: a review. Advances in Water Res., 20 (5-6), 253-278.
- Rhén I. (ed), Gustafson G., Stanfors R., Wikberg P., 1997.** Äspö HRL - Geoscientific evaluation 1997/5. Models based on site characterization 1986-1995. SKB Technical Report TR-97-06.
- Sahimi M., 1995.** Flow and transport in porous media and fractured rock. VCH Verlagsgesellschaft mbH, Weinheim.
- Spalding D.B., 1981.** "A general purpose computer program for multi-dimensional one- and two-phase flow". Math. Comp. Sim., 8, 267-276. See also: <http://www.cham.co.uk>.
- Stanfors R., Rhén I., Tullborg E.-L., Wikberg P., 1999.** Overview of geological and hydrogeological conditions of the Äspö hard rock laboratory site. Appl. Geochem., 14, 819-834.
- Svensson U., 1991.** Groundwater flow at Äspö and changes due to the excavation of the laboratory. SKB PR 25-91-03.
- Svensson U., 1997a.** A regional analysis of groundwater flow and salinity distribution in the Äspö area. SKB Technical Report TR-97-09.
- Svensson U., 1997b.** A site scale analysis of groundwater flow and salinity distribution in the Äspö area. SKB Technical Report TR-97-17.
- Svensson U., 1999a.** Representation of fracture networks as gridcell conductivities. SKB Technical Report TR-99-25.
- Svensson U., 1999b.** A laboratory scale analysis of groundwater flow and salinity distribution in the Äspö area. SKB Technical Report TR-99-24.
- Svensson U., 2001.** PARTRACK. -A particle tracking algorithm for transport and dispersion of solutes in a sparsely fractured rock. SKB Report, R-01-16.

Svensson U., 2001. A continuum representation of fracture networks. Part I: Method and basic test cases. *Journal of Hydrology*, 250, pp 170-186.

Svensson U., 2001. A continuum representation of fracture networks. Part II: Application to the Äspö Hard Rock Laboratory. *Journal of Hydrology*, 250, pp 187-205.

Svensson U., Laaksoharju M. and Gurban Ioana., 2002. Impact of the tunnel construction on the groundwater system at Äspö. Task 5, Äspö Task Force on groundwater flow and transport of solutes. SKB International Progress Report IPR-02-25.

Svensson U. 2004. DarcyTools, Version 2.1 Verification and Validation, SKB report in progress.

Svensson U. and Ferry M. 2004. DarcyTools, Version 2.1 – User’s Guide. SKB report in progress.

Wen X.H., Gómez-Hernández J., 1996. Upscaling hydraulic conductivities in heterogeneous media: An overview. *J. Hydrol.* 183, ix-xxxii.

Winberg A., 1998. Äspö Hard Rock Laboratory. TRUE Block Scale Project. Scientific and technical status. Position report prepared for the 2nd TRUE Block Scale review meeting. SKB International Progress Report IPR-99-07.

Winberg A., 2000. TRUE Block Scale Project. Final report of the detailed characterisation stage. SKB International Cooperation Report ICR-00-02.

Winberg A., Andersson P., Hermansson J., Byegård J., Cvetkovic V., Birgersson L., 2000. Äspö Hard Rock Laboratory. Final report of the first stage of the tracer retention understanding experiments. SKB Technical Report TR-00-07.

APPENDIX A Numerical methods

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Numerical Methods

Introduction

DarcyTools computes fracture network flows using a continuum model in which the mass conservation equation (1) is associated to several mass fraction transport equations (2) for the salinity and/or particle mass concentrations, and to a heat transport equation (3). In relations (1), (2) and (3) r , u , v , w , T and C represent respectively the fluid density, the velocity components, the temperature and the mass fraction of the transported quantity. Q , Q_c and Q_T are source terms per unit volume of fluid mass (i.e. injection-withdrawal), of mass of transported quantity (e.g. local exchanges with the rock) and of heat (i.e. enthalpy).

$$\frac{\partial r \mathbf{q}}{\partial t} + \frac{\partial}{\partial x}(r u) + \frac{\partial}{\partial y}(r v) + \frac{\partial}{\partial z}(r w) = Q \quad (1)$$

$$\begin{aligned} \frac{\partial r \mathbf{q} C}{\partial t} + \frac{\partial}{\partial x} \left(r u C - r \mathbf{g} D_x \frac{\partial C}{\partial x} \right) \\ + \frac{\partial}{\partial y} \left(r v C - r \mathbf{g} D_y \frac{\partial C}{\partial y} \right) \\ + \frac{\partial}{\partial z} \left(r w C - r \mathbf{g} D_z \frac{\partial C}{\partial z} \right) = Q C + Q_c \end{aligned} \quad (2)$$

$$\begin{aligned}
& \frac{\partial (\mathbf{r}q c_p + (1 - \mathbf{q})c)T}{\partial t} + \frac{\partial}{\partial x} \left(\mathbf{r}u c_p T - \mathbf{I}_x \frac{\partial T}{\partial x} \right) \\
& + \frac{\partial}{\partial y} \left(\mathbf{r}v c_p T - \mathbf{I}_y \frac{\partial T}{\partial y} \right) \\
& + \frac{\partial}{\partial z} \left(\mathbf{r}w c_p T - \mathbf{I}_z \frac{\partial T}{\partial z} \right) = Q c_p T + Q_T
\end{aligned} \tag{3}$$

D_x , D_y and D_z are the normal terms of the diffusion-dispersion tensor. \mathbf{I}_x , \mathbf{I}_y and \mathbf{I}_z are the normal terms of the equivalent (i.e. rock with fluid) thermal conductivity tensor, c is the rock thermal capacity and c_p the specific heat of the fluid.

The mass conservation equation is turned into a pressure equation under the well known Darcy's assumption (4).

$$\begin{aligned}
\mathbf{r}u &= -\frac{K_x}{g} \frac{\partial P}{\partial x} \\
\mathbf{r}v &= -\frac{K_y}{g} \frac{\partial P}{\partial y} \\
\mathbf{r}w &= -\frac{K_z}{g} \frac{\partial P}{\partial z} - K_z (\mathbf{r} - \mathbf{r}_0)
\end{aligned} \tag{4}$$

where K_x , K_y and K_z are the local hydraulic conductivities in x, y and z direction, g the gravity acceleration, \mathbf{r}_0 a reference fluid density (8) and P the dynamic fluid pressure relative to the reference hydrostatic pressure.

$$P = p + \mathbf{r}_0 g z \tag{5}$$

The hydraulic conductivities K are related to the permeability k field through relation (6):

$$K = \frac{\mathbf{r}gk}{\mathbf{m}} \tag{6}$$

The fluid property like the dynamic viscosity \mathbf{m} , the density \mathbf{r} and the specific heat c_p are given by state laws:

$$\mathbf{m} = \mathbf{m}_0 \left[1 + a_1 (T - T_m) + a_2 (T - T_m)^2 \right]^{n_m} \quad (7)$$

$$\mathbf{r} = \mathbf{r}_0 \left[1 + \mathbf{a}_1 S + \mathbf{a}_2 S^2 - \mathbf{b}_1 (T - T_r) - \mathbf{b}_2 (T - T_r)^2 \right] \quad (8)$$

$$c_p = c_{p0} \left(1 + b_1 S + b_2 S^2 \right) \quad (9)$$

while the porosity \mathbf{q} and the compaction \mathbf{g} of the matrix are provided with the following dependencies:

$$\mathbf{q} = \mathbf{q}_0 \mathbf{g} \quad (10)$$

$$\mathbf{g} = 1 + (\mathbf{s}/\mathbf{q}_0) (P - P_0) / \mathbf{r} \mathbf{g} \quad (11)$$

In the above formulas S represents the salinity (salt mass fraction), \mathbf{q}_0 a reference porosity field given for a reference pressure field P_0 , \mathbf{s} the specific storativity field. n_m , a_i , b_i , \mathbf{a}_i , \mathbf{b}_i , \mathbf{m}_0 , \mathbf{r}_0 , c_{p0} , T_m and T_r are constants.

Finite Volume Integration

The finite volume method integrates equations (1), (2) and (3) over the six faces of a finite number of control volumes by converting volume integrals into surface integrals using Ostrogradsky's theorem:

$$\begin{aligned} \int_V \operatorname{div}(\vec{F}) dV &= \int_{A_e} \vec{F} \cdot \vec{n}_e dA + \int_{A_w} \vec{F} \cdot \vec{n}_w dA + \int_{A_n} \vec{F} \cdot \vec{n}_n dA + \\ &\int_{A_s} \vec{F} \cdot \vec{n}_s dA + \int_{A_t} \vec{F} \cdot \vec{n}_t dA + \int_{A_b} \vec{F} \cdot \vec{n}_b dA \end{aligned} \quad (12)$$

So that, according to the Mean Value Theorem:

$$\begin{aligned} \int_V \operatorname{div}(\vec{F}) dV &= A_e \vec{F}_e \cdot \vec{n}_e + A_w \vec{F}_w \cdot \vec{n}_w + A_n \vec{F}_n \cdot \vec{n}_n + \\ &A_s \vec{F}_s \cdot \vec{n}_s + A_t \vec{F}_t \cdot \vec{n}_t + A_b \vec{F}_b \cdot \vec{n}_b \end{aligned} \quad (13)$$

where, for example, A_e and n_e are respectively the area and the outside-normal of the “east” cell-face and where F_e is evaluated at east face center.

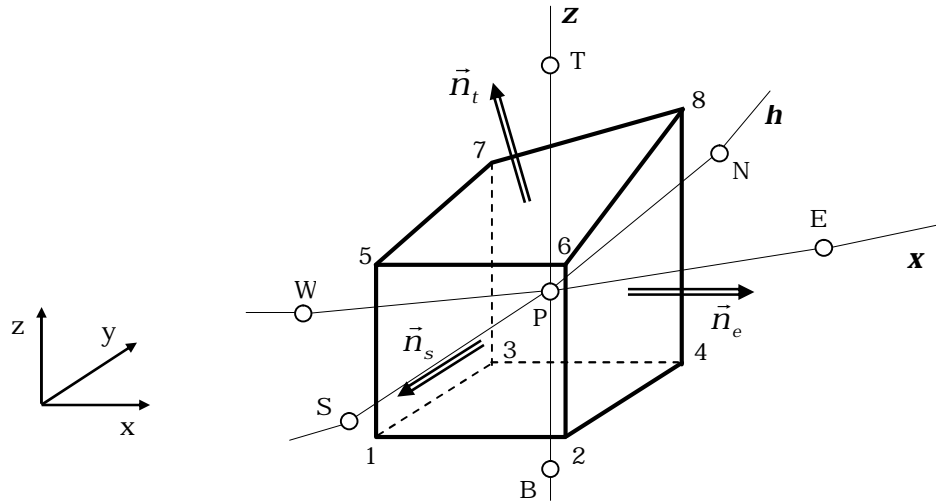


Figure 1 : Control volumes, normals and vertex labeling

Grid arrangement

Among the common grid arrangements, DarcyTools uses the “node-centered” arrangement in which the pressure and the scalar variables (mass fractions) are located at center of grid cells. The main advantage of this formulation is that the control volumes coincide with the grid cells and that the cell vertices are directly defined by grid nodes.

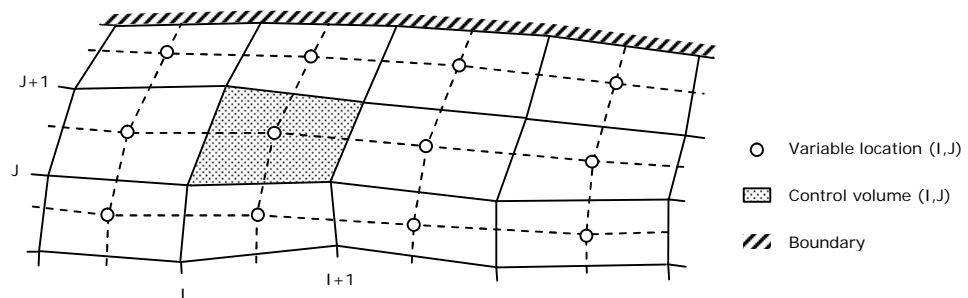


Figure 2 : Node-centered arrangement labeling

The main drawback is that, for stretched meshes, the faces of control volumes are not located mid-way between variable locations (see Figure 3) and require

more sophisticated interpolations for second order accurate discretisation of convective fluxes. A second drawback is that the algorithm or the grid definition for embedded grids interpolations is more complicated than for the “cell-centered” arrangement.

Stability

The strength of the finite volume integration is its conservative formulation for which any flux getting out from a control volume is automatically entering the neighboring volume. Nevertheless this strength may be a drawback when considering the convergence process. Given a bounded conservative scheme, the convective term interpolation at east cell face can be written:

$$\vec{F} \cdot \vec{n} \Big|_e = \mathbf{f}_e \mathbf{r} \vec{u} \cdot \vec{n} \Big|_e = (\mathbf{a}_e \mathbf{f}_E + (1 - \mathbf{a}_e) \mathbf{f}_P) \mathbf{r} \vec{u} \cdot \vec{n} \Big|_e \tag{14}$$

where the value of \mathbf{a}_e depends on u to ensure the monotony and remains in the interval $[0,1]$ to ensure the boundness of the scheme. The subscripts e , E , and P indicate respectively the east face value, the east variable and the center variable.

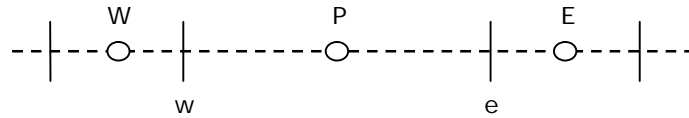


Figure 3 : East-West stencil labeling

Therefore, for the convective term of the transport equation (2), applying relation (14) to approximate the integrals of relation (12) leads to the following algebraic relation:

$$\int_V \text{div}(\mathbf{r} \vec{u} \mathbf{f}) dV = \left(\int_V \text{div}(\mathbf{r} \vec{u}) dV - \sum_{nb} a_{nb} \right) \mathbf{f}_P + \sum_{nb} a_{nb} \mathbf{f}_{nb} \tag{15}$$

Because of (1) and for stationary problem with no internal mass source term, relation (15) apparently leads to a central coefficient (applied to \mathbf{f}_P) equal to the opposite sum of neighboring coefficients. This property, even if not necessary, is highly desirable for stability. Unfortunately, during the convergence process, relation (1) may be temporarily highly unsatisfied. Hence, in spite of the

bounded form (14) the discretisation of the transport equation from (2) may become unstable. For this reason, DarcyTools substitutes the source term CQ of equation (2) by its evaluation from relation (1) and finally solves equations (16) and (17) instead of (2) and (3).

$$\begin{aligned}
\mathbf{r}q \frac{\partial C}{\partial t} + \frac{\partial}{\partial x} \left(\mathbf{r}uC - \mathbf{r}gD_x \frac{\partial C}{\partial x} \right) \\
+ \frac{\partial}{\partial y} \left(\mathbf{r}vC - \mathbf{r}gD_y \frac{\partial C}{\partial y} \right) \\
+ \frac{\partial}{\partial z} \left(\mathbf{r}wC - \mathbf{r}gD_z \frac{\partial C}{\partial z} \right) = \left(\frac{\partial \mathbf{r}u}{\partial x} + \frac{\partial \mathbf{r}v}{\partial y} + \frac{\partial \mathbf{r}w}{\partial z} \right) C + Q_c
\end{aligned} \tag{16}$$

$$\begin{aligned}
\mathbf{r}q \frac{\partial c_p T}{\partial t} + \frac{\partial (1-\mathbf{q})cT}{\partial t} \\
+ \frac{\partial}{\partial x} \left(\mathbf{r}uc_p T - I_x \frac{\partial T}{\partial x} \right) \\
+ \frac{\partial}{\partial y} \left(\mathbf{r}vc_p T - I_y \frac{\partial T}{\partial y} \right) \\
+ \frac{\partial}{\partial z} \left(\mathbf{r}wc_p T - I_z \frac{\partial T}{\partial z} \right) = \left(\frac{\partial \mathbf{r}u}{\partial x} + \frac{\partial \mathbf{r}v}{\partial y} + \frac{\partial \mathbf{r}w}{\partial z} \right) c_p T + Q_T
\end{aligned} \tag{17}$$

The main advantage of this technique is to ensure a central coefficient always equal to the opposite sum of neighboring coefficients. A second advantage is that the source terms (CQ and $c_p QT$) due to fluid mass source disappears from relation (16) and (17). This simplifies the implementation of boundary conditions since the internal mass source terms have to be specified only once: for the mass conservation equation (1). In return, the mass fractions C must be specified where the fluid mass source Q is positive (no necessary condition when $Q < 0$). It should also be noted that, for time varying density or porosity, the time derivative term lost its conservative form.

Spatial scheme

Also for stability reason, the fluxes discretisation in space must involved both convective and diffusive terms in order to produce positive coefficients. Then, considering the face f separating two control volumes,

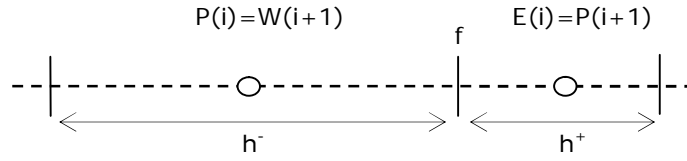


Figure 4 : East-West face flux labeling

DarcyTools uses the hybrid scheme to express the fluxes as:

$$F_f = c\mathbf{f}_f - d\mathbf{f}_{,xf} = -a^+ \mathbf{f}_{E(i)} + a^- \mathbf{f}_{P(i)} = -a^+ \mathbf{f}_{P(i+1)} + a^- \mathbf{f}_{W(i-1)} \quad (18)$$

$$\begin{cases} a^+ = a^- - c \\ a^- = \max\left(0, c, \frac{h^+c + 2d}{h^+ + h^-}\right) \end{cases} \quad (19)$$

with the faces values linearly interpolated as:

$$\mathbf{f}_f = \frac{h^- \mathbf{f}_{E(i)} + h^+ \mathbf{f}_{P(i)}}{h^+ + h^-} = \frac{h^- \mathbf{f}_{P(i+1)} + h^+ \mathbf{f}_{W(i-1)}}{h^+ + h^-} \quad (20)$$

Time derivative

To ensure the precision of time dependent simulations, DarcyTools implements two different implicit time schemes. The default one is the Euler first order implicit scheme given by:

$$\left. \frac{\partial \mathbf{f}}{\partial t} \right|_n = \frac{\mathbf{f}_n - \mathbf{f}_{n-1}}{t_n - t_{n-1}} \quad (21)$$

The alternative is a second order implicit scheme that differentiates a parabola forced through solutions at three non-equally spaced time levels:

$$\left. \frac{\partial \mathbf{f}}{\partial t} \right|_n = \frac{2\Delta t_1 + \Delta t_2}{\Delta t_1(\Delta t_1 + \Delta t_2)} \mathbf{f}_n - \frac{\Delta t_1 + \Delta t_2}{\Delta t_1 \Delta t_2} \mathbf{f}_{n-1} + \frac{\Delta t_1}{\Delta t_1(\Delta t_1 + \Delta t_2)} \mathbf{f}_{n-2} \quad (22)$$

where Δt_1 and Δt_2 represent respectively the time steps $t_n - t_{n-1}$ and $t_{n-1} - t_{n-2}$.

Algebraic Set of Equations

After the discretisation step, equation (1) as well as all the equations (16) can be written with the general algebraic form:

$$a_p \mathbf{f}_p = \sum_{nb} a_{nb} \mathbf{f}_{nb} + S_f \quad (23)$$

where a_p and a_{nb} are positive coefficients and where a_p , because of the transient term, is greater than the sum of the neighboring coefficients a_{nb} . Whenever it is possible, if the source term operator S_f depends on the solution field \mathbf{f} DarcyTools increases the diagonal dominance of the operator by rewriting it as follows:

$$S_f = Q_{src} - Q_{phi} \mathbf{f}_p \quad \text{with} \quad Q_{phi} > 0 \quad (24)$$

and by including Q_{phi} into the central coefficient.

$$(a_p + Q_{phi}) \mathbf{f}_p = \sum_{nb} a_{nb} \mathbf{f}_{nb} + Q_{src} \quad (25)$$

This linearization of the operator source term is also a practical way for users to fix different kind of boundary conditions. For example, setting a *BIG* value in Q_{phi} and a *BIGxVAL* value in Q_{src} becomes equivalent to the Dirichlet boundary condition: $\mathbf{f} = VAL$. Setting Q_{src} to VQ and Q_{phi} to zero is also the easiest way to specify an inlet fluid mass flux in the pressure equation (1) When an inlet fluid mass is set ($Q > 0$) it can also be of interest to specify only the inlet salinity instead of fixing the mean cell value by a Dirichlet condition. In that case the implicit input must be removed by setting Q_{phi} to VQ and the effective input forced by setting Q_{src} to VQS_{in} .

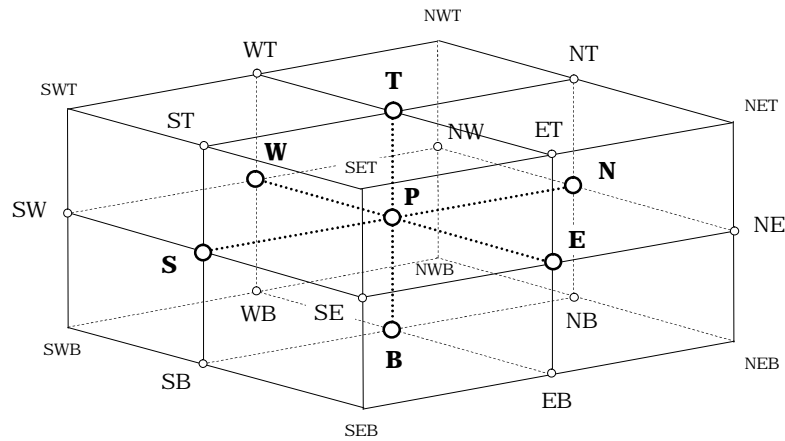


Figure 5 : 3-D discretisation stencil labeling

BFC Discretisation

When the computational domain is meshed by a Boundary Fitted Coordinate (BFC) grid, a generalized coordinate space (x, h, z) is introduced to link the (I, J, K) location indexes to the spatial domain (x, y, z) .

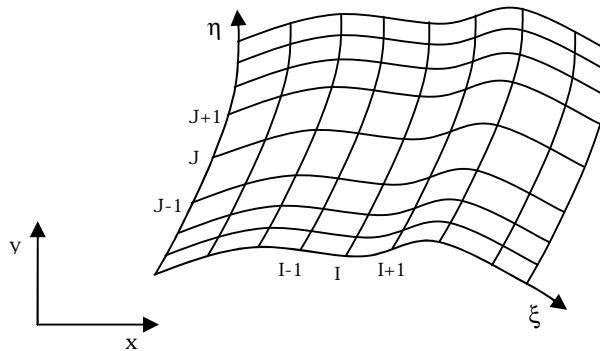


Figure 6 : Curvilinear BFC grid transformation

A continuum metric transformation can be introduced between the generalized coordinate space (x, h, z) and the physical space (x, y, z) as follows:

$$\begin{bmatrix} b_1^1 & b_1^2 & b_1^3 \\ b_2^1 & b_2^2 & b_2^3 \\ b_3^1 & b_3^2 & b_3^3 \end{bmatrix} = \begin{bmatrix} \frac{\partial y}{\partial \mathbf{h}} \frac{\partial z}{\partial \mathbf{z}} - \frac{\partial z}{\partial \mathbf{h}} \frac{\partial y}{\partial \mathbf{z}} & \frac{\partial z}{\partial \mathbf{x}} \frac{\partial y}{\partial \mathbf{z}} - \frac{\partial y}{\partial \mathbf{x}} \frac{\partial z}{\partial \mathbf{z}} & \frac{\partial y}{\partial \mathbf{x}} \frac{\partial z}{\partial \mathbf{h}} - \frac{\partial z}{\partial \mathbf{x}} \frac{\partial y}{\partial \mathbf{h}} \\ \frac{\partial x}{\partial \mathbf{z}} \frac{\partial z}{\partial \mathbf{h}} - \frac{\partial x}{\partial \mathbf{h}} \frac{\partial z}{\partial \mathbf{z}} & \frac{\partial x}{\partial \mathbf{x}} \frac{\partial z}{\partial \mathbf{z}} - \frac{\partial z}{\partial \mathbf{x}} \frac{\partial x}{\partial \mathbf{z}} & \frac{\partial z}{\partial \mathbf{x}} \frac{\partial x}{\partial \mathbf{h}} - \frac{\partial x}{\partial \mathbf{x}} \frac{\partial z}{\partial \mathbf{h}} \\ \frac{\partial x}{\partial \mathbf{h}} \frac{\partial y}{\partial \mathbf{z}} - \frac{\partial y}{\partial \mathbf{h}} \frac{\partial x}{\partial \mathbf{z}} & \frac{\partial y}{\partial \mathbf{x}} \frac{\partial x}{\partial \mathbf{z}} - \frac{\partial x}{\partial \mathbf{x}} \frac{\partial y}{\partial \mathbf{z}} & \frac{\partial x}{\partial \mathbf{x}} \frac{\partial y}{\partial \mathbf{h}} - \frac{\partial y}{\partial \mathbf{x}} \frac{\partial x}{\partial \mathbf{h}} \end{bmatrix} \quad (26)$$

$$J = \frac{\partial x}{\partial \mathbf{x}} \left(\frac{\partial y}{\partial \mathbf{h}} \frac{\partial z}{\partial \mathbf{z}} - \frac{\partial z}{\partial \mathbf{h}} \frac{\partial y}{\partial \mathbf{z}} \right) + \frac{\partial x}{\partial \mathbf{h}} \left(\frac{\partial z}{\partial \mathbf{x}} \frac{\partial y}{\partial \mathbf{z}} - \frac{\partial y}{\partial \mathbf{x}} \frac{\partial z}{\partial \mathbf{z}} \right) + \frac{\partial x}{\partial \mathbf{z}} \left(\frac{\partial y}{\partial \mathbf{x}} \frac{\partial z}{\partial \mathbf{h}} - \frac{\partial z}{\partial \mathbf{x}} \frac{\partial y}{\partial \mathbf{h}} \right) \quad (27)$$

With the above notations (26) and (27), the areas and normals appearing in relation (12) are given by:

$$\begin{aligned} A_e \bar{\mathbf{n}}_e &= b_{1e}^1 \bar{x} + b_{1e}^2 \bar{y} + b_{1e}^3 \bar{z} & A_w \bar{\mathbf{n}}_w &= b_{1w}^1 \bar{x} + b_{1w}^2 \bar{y} + b_{1w}^3 \bar{z} \\ A_n \bar{\mathbf{n}}_n &= b_{2n}^1 \bar{x} + b_{2n}^2 \bar{y} + b_{2n}^3 \bar{z} & A_s \bar{\mathbf{n}}_s &= b_{2s}^1 \bar{x} + b_{2s}^2 \bar{y} + b_{2s}^3 \bar{z} \\ A_t \bar{\mathbf{n}}_t &= b_{3t}^1 \bar{x} + b_{3t}^2 \bar{y} + b_{3t}^3 \bar{z} & A_b \bar{\mathbf{n}}_b &= b_{3b}^1 \bar{x} + b_{3b}^2 \bar{y} + b_{3b}^3 \bar{z} \end{aligned} \quad (28)$$

With curvilinear coordinates the evaluation partial derivatives of governing equations in X , Y and Z direction is not straightforward because variables are not distributed along X , Y or Z coordinate-lines but along the \mathbf{x} , \mathbf{h} and \mathbf{z} lines of the transformed space. Nevertheless, with the continuum metric transformation, they are given by:

$$\begin{bmatrix} \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \\ \frac{\partial \mathbf{f}}{\partial \mathbf{y}} \\ \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \end{bmatrix} = \frac{1}{J} \begin{bmatrix} b_1^1 & b_1^2 & b_1^3 \\ b_2^1 & b_2^2 & b_2^3 \\ b_3^1 & b_3^2 & b_3^3 \end{bmatrix} \begin{bmatrix} \frac{\partial \mathbf{f}}{\partial \mathbf{h}} \\ \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \\ \frac{\partial \mathbf{f}}{\partial \mathbf{z}} \end{bmatrix} \quad (29)$$

Finally the governing equations are written as follows:

$$\begin{aligned}
& J \frac{\partial \mathbf{r}q}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \left(-\frac{K_{11}}{g} \frac{\partial P}{\partial \mathbf{x}} \right) + \\
& \frac{\partial}{\partial \mathbf{h}} \left(-\frac{K_{22}}{g} \frac{\partial P}{\partial \mathbf{h}} \right) + \\
& \frac{\partial}{\partial \mathbf{z}} \left(-\frac{K_{33}}{g} \frac{\partial P}{\partial \mathbf{z}} \right) = JQ + S_{DM}
\end{aligned} \tag{30}$$

$$\begin{aligned}
& J\mathbf{r}q \frac{\partial C}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \left(\mathbf{r}UAC - \mathbf{r}gD_{11} \frac{\partial C}{\partial \mathbf{x}} \right) + \\
& \frac{\partial}{\partial \mathbf{h}} \left(\mathbf{r}VAC - \mathbf{r}gD_{22} \frac{\partial C}{\partial \mathbf{h}} \right) + \\
& \frac{\partial}{\partial \mathbf{z}} \left(\mathbf{r}WAC - \mathbf{r}gD_{33} \frac{\partial C}{\partial \mathbf{z}} \right) = \left(\frac{\partial \mathbf{r}U}{\partial \mathbf{x}} + \frac{\partial \mathbf{r}V}{\partial \mathbf{h}} + \frac{\partial \mathbf{r}W}{\partial \mathbf{z}} \right) C + JQ_C + S_{DC}
\end{aligned} \tag{31}$$

$$\begin{aligned}
& J\mathbf{r}q \frac{\partial c_p T}{\partial t} + J \frac{\partial (1-q)cT}{\partial t} \\
& + \frac{\partial}{\partial \mathbf{x}} \left(\mathbf{r}UAc_p T - \mathbf{I}_{11} \frac{\partial T}{\partial \mathbf{x}} \right) \\
& + \frac{\partial}{\partial \mathbf{h}} \left(\mathbf{r}VAc_p T - \mathbf{I}_{22} \frac{\partial T}{\partial \mathbf{h}} \right) \\
& + \frac{\partial}{\partial \mathbf{z}} \left(\mathbf{r}WAc_p T - \mathbf{I}_{33} \frac{\partial T}{\partial \mathbf{z}} \right) = \left(\frac{\partial \mathbf{r}U}{\partial \mathbf{x}} + \frac{\partial \mathbf{r}V}{\partial \mathbf{h}} + \frac{\partial \mathbf{r}W}{\partial \mathbf{z}} \right) c_p T + JQ_T + S_{DT}
\end{aligned} \tag{32}$$

Those equations keep their primary form but differ from (1), (16) and (17) in that the diffusion coefficients K , D and I change for:

$$\begin{aligned}
D_{11} &= \frac{1}{J} (b_1^1 b_1^1 D_x + b_2^1 b_2^1 D_y + b_3^1 b_3^1 D_z) \\
D_{22} &= \frac{1}{J} (b_1^2 b_1^2 D_x + b_2^2 b_2^2 D_y + b_3^2 b_3^2 D_z) \\
D_{33} &= \frac{1}{J} (b_1^3 b_1^3 D_x + b_2^3 b_2^3 D_y + b_3^3 b_3^3 D_z)
\end{aligned} \tag{33}$$

$$\begin{aligned}
K_{11} &= \frac{1}{J} (b_1^1 b_1^1 K_x + b_2^1 b_2^1 K_y + b_3^1 b_3^1 K_z) \\
K_{22} &= \frac{1}{J} (b_1^2 b_1^2 K_x + b_2^2 b_2^2 K_y + b_3^2 b_3^2 K_z) \\
K_{33} &= \frac{1}{J} (b_1^3 b_1^3 K_x + b_2^3 b_2^3 K_y + b_3^3 b_3^3 K_z)
\end{aligned} \tag{34}$$

$$\begin{aligned}
I_{11} &= \frac{1}{J} (b_1^1 b_1^1 I_x + b_2^1 b_2^1 I_y + b_3^1 b_3^1 I_z) \\
I_{22} &= \frac{1}{J} (b_1^2 b_1^2 I_x + b_2^2 b_2^2 I_y + b_3^2 b_3^2 I_z) \\
I_{33} &= \frac{1}{J} (b_1^3 b_1^3 I_x + b_2^3 b_2^3 I_y + b_3^3 b_3^3 I_z)
\end{aligned} \tag{35}$$

in that buoyancy terms appear (see S_{DM}) in each direction with:

$$\begin{aligned}
K_1 &= b_3^1 K_z \\
K_2 &= b_3^2 K_z \\
K_3 &= b_3^3 K_z
\end{aligned} \tag{36}$$

in that mass fluxes are given by:

$$\begin{aligned}
\mathbf{r}UA &= -K_1(\mathbf{r} - \mathbf{r}_0) - \frac{K_{11}}{g} \frac{\partial P}{\partial \mathbf{x}} - \frac{K_{12}}{g} \frac{\partial P}{\partial \mathbf{h}} - \frac{K_{13}}{g} \frac{\partial P}{\partial \mathbf{z}} \\
\mathbf{r}VA &= -K_2(\mathbf{r} - \mathbf{r}_0) - \frac{K_{21}}{g} \frac{\partial P}{\partial \mathbf{x}} - \frac{K_{22}}{g} \frac{\partial P}{\partial \mathbf{h}} - \frac{K_{23}}{g} \frac{\partial P}{\partial \mathbf{z}} \\
\mathbf{r}WA &= -K_3(\mathbf{r} - \mathbf{r}_0) - \frac{K_{31}}{g} \frac{\partial P}{\partial \mathbf{x}} - \frac{K_{32}}{g} \frac{\partial P}{\partial \mathbf{h}} - \frac{K_{33}}{g} \frac{\partial P}{\partial \mathbf{z}}
\end{aligned} \tag{37}$$

and in that cross derivatives now appear. In spite of the indirect coupling they introduce between (30) and (31) these new derivatives are explicitly treated in separated sources terms S_{DM} and S_{DC} in order not to enlarge the algebraic stencil. Their magnitude reduces to zero when the curvilinear coordinate lines are orthogonal and the diffusion is isotropic.

$$\begin{aligned}
S_{DM} = & \frac{\partial}{\partial \mathbf{x}} \left(\frac{K_{12}}{g} \frac{\partial P}{\partial \mathbf{h}} + \frac{K_{13}}{g} \frac{\partial P}{\partial \mathbf{z}} + K_1 (\mathbf{r} - \mathbf{r}_0) \right) + \\
& \frac{\partial}{\partial \mathbf{h}} \left(\frac{K_{21}}{g} \frac{\partial P}{\partial \mathbf{x}} + \frac{K_{23}}{g} \frac{\partial P}{\partial \mathbf{z}} + K_2 (\mathbf{r} - \mathbf{r}_0) \right) + \\
& \frac{\partial}{\partial \mathbf{z}} \left(\frac{K_{31}}{g} \frac{\partial P}{\partial \mathbf{x}} + \frac{K_{32}}{g} \frac{\partial P}{\partial \mathbf{h}} + K_3 (\mathbf{r} - \mathbf{r}_0) \right) +
\end{aligned} \tag{38}$$

$$\begin{aligned}
S_{DC} = & \frac{\partial}{\partial \mathbf{x}} \left(\mathbf{r}gD_{12} \frac{\partial C}{\partial \mathbf{h}} + \mathbf{r}gD_{13} \frac{\partial C}{\partial \mathbf{z}} \right) + \\
& \frac{\partial}{\partial \mathbf{h}} \left(\mathbf{r}gD_{21} \frac{\partial C}{\partial \mathbf{x}} + \mathbf{r}gD_{23} \frac{\partial C}{\partial \mathbf{z}} \right) + \\
& \frac{\partial}{\partial \mathbf{z}} \left(\mathbf{r}gD_{32} \frac{\partial C}{\partial \mathbf{h}} + \mathbf{r}gD_{31} \frac{\partial C}{\partial \mathbf{x}} \right)
\end{aligned} \tag{39}$$

$$\begin{aligned}
S_{DT} = & \frac{\partial}{\partial \mathbf{x}} \left(\mathbf{l}_{12} \frac{\partial T}{\partial \mathbf{h}} + \mathbf{l}_{13} \frac{\partial T}{\partial \mathbf{z}} \right) + \\
& \frac{\partial}{\partial \mathbf{h}} \left(\mathbf{l}_{21} \frac{\partial T}{\partial \mathbf{x}} + \mathbf{l}_{23} \frac{\partial T}{\partial \mathbf{z}} \right) + \\
& \frac{\partial}{\partial \mathbf{z}} \left(\mathbf{l}_{32} \frac{\partial T}{\partial \mathbf{h}} + \mathbf{l}_{31} \frac{\partial T}{\partial \mathbf{x}} \right)
\end{aligned} \tag{40}$$

The cross derivative diffusion coefficients are given by:

$$\begin{aligned}
K_{12} = K_{21} &= \frac{1}{J} (b_1^1 b_1^2 K_x + b_2^1 b_2^2 K_y + b_3^1 b_3^2 K_z) \\
K_{23} = K_{32} &= \frac{1}{J} (b_1^2 b_1^3 K_x + b_2^2 b_2^3 K_y + b_3^2 b_3^3 K_z) \\
K_{13} = K_{31} &= \frac{1}{J} (b_1^1 b_1^3 K_x + b_2^1 b_2^3 K_y + b_3^1 b_3^3 K_z)
\end{aligned} \tag{41}$$

$$\begin{aligned}
D_{12} = D_{21} &= \frac{1}{J} (b_1^1 b_1^2 D_x + b_2^1 b_2^2 D_y + b_3^1 b_3^2 D_z) \\
D_{23} = D_{32} &= \frac{1}{J} (b_1^2 b_1^3 D_x + b_2^2 b_2^3 D_y + b_3^2 b_3^3 D_z) \\
D_{13} = D_{31} &= \frac{1}{J} (b_1^1 b_1^3 D_x + b_2^1 b_2^3 D_y + b_3^1 b_3^3 D_z)
\end{aligned} \tag{42}$$

$$\begin{aligned}
I_{12} = I_{21} &= \frac{1}{J} (b_1^1 b_1^2 I_x + b_2^1 b_2^2 I_y + b_3^1 b_3^2 I_z) \\
I_{23} = I_{32} &= \frac{1}{J} (b_1^2 b_1^3 I_x + b_2^2 b_2^3 I_y + b_3^2 b_3^3 I_z) \\
I_{13} = I_{31} &= \frac{1}{J} (b_1^1 b_1^3 I_x + b_2^1 b_2^3 I_y + b_3^1 b_3^3 I_z)
\end{aligned} \tag{43}$$

BFC:s Discretisation

The use of Boundary Fitted Coordinate (BFC) grids requires a lot of memory to store the 31 arrays of the metric and the 9 property arrays per control volume. Moreover, the computation of the multiple cross derivatives is an expensive task that should be avoided when unnecessary. For this reasons, DarcyTools also uses a Simplified BFC formulation (BFC:s) in which X and Y are Cartesian coordinates depending only on I and J indexes respectively and Z is a floating coordinate. A first simplification concerns the areas and normals involved in relation (12):

$$\begin{aligned}
A_e \bar{n}_e &= h_y f_{3e} \bar{x} & A_w \bar{n}_w &= -h_y f_{3w} \bar{x} \\
A_n \bar{n}_n &= h_x f_{3n} \bar{y} & A_s \bar{n}_s &= -h_x f_{3s} \bar{y} \\
A_t \bar{n}_t &= -h_y f_{1t} \bar{x} - h_x f_{2t} \bar{y} + h_x h_y \bar{z} & A_b \bar{n}_b &= h_y f_{1b} \bar{x} + h_x f_{2b} \bar{y} - h_x h_y \bar{z}
\end{aligned} \tag{44}$$

where h_x and h_y are the spatial steps in X and Y directions and where functions f_1 , f_2 and f_3 are the discrete expressions of the Z coordinate transformed derivatives (see Figure 1 for notation):

$$\begin{aligned}
f_{1t} &= \frac{1}{2} (z_6 + z_8 - z_5 - z_7) & f_{1b} &= \frac{1}{2} (z_2 + z_4 - z_1 - z_3) \\
f_{2t} &= \frac{1}{2} (z_7 + z_8 - z_5 - z_6) & f_{2b} &= \frac{1}{2} (z_3 + z_4 - z_1 - z_2) \\
f_{3e} &= \frac{1}{2} (z_6 + z_8 - z_2 - z_4) & f_{3w} &= \frac{1}{2} (z_5 + z_7 - z_1 - z_3) \\
f_{3n} &= \frac{1}{2} (z_7 + z_8 - z_3 - z_4) & f_{3s} &= \frac{1}{2} (z_5 + z_6 - z_1 - z_2)
\end{aligned} \tag{45}$$

The volume of control volume is given by:

$$V = \frac{h_x h_y}{4} (z_5 + z_6 + z_7 + z_8 - z_1 - z_2 - z_3 - z_4) \tag{46}$$

The finite volume integrated governing equations become:

$$\begin{aligned}
V \frac{\partial \mathbf{r}q}{\partial t} & - h_y f_{3e} \frac{K_{xe}}{g} \frac{\partial P}{\partial x} \Big|_e + h_y f_{3w} \frac{K_{xw}}{g} \frac{\partial P}{\partial x} \Big|_w \\
& - h_x f_{3n} \frac{K_{yn}}{g} \frac{\partial P}{\partial y} \Big|_n + h_x f_{3s} \frac{K_{ys}}{g} \frac{\partial P}{\partial y} \Big|_s \\
& - h_x h_y \frac{K_{zt}}{g} \frac{\partial P}{\partial z} \Big|_t + h_x h_y \frac{K_{zb}}{g} \frac{\partial P}{\partial z} \Big|_b = VQ + S_{DM}
\end{aligned} \tag{47}$$

$$\begin{aligned}
V \mathbf{r}q \frac{\partial C}{\partial t} & - h_y f_{3e} \mathbf{r}_e \mathbf{g}_e D_{xe} \frac{\partial C}{\partial x} \Big|_e + h_y f_{3w} \mathbf{r}_w \mathbf{g}_w D_{xw} \frac{\partial C}{\partial x} \Big|_w \\
& - h_x f_{3n} \mathbf{r}_n \mathbf{g}_n D_{yn} \frac{\partial C}{\partial y} \Big|_n + h_x f_{3s} \mathbf{r}_s \mathbf{g}_s D_{ys} \frac{\partial C}{\partial y} \Big|_s \\
& - h_x h_y \mathbf{r}_t \mathbf{g}_t D_{zt} \frac{\partial C}{\partial z} \Big|_t + h_x h_y \mathbf{r}_b \mathbf{g}_b D_{zb} \frac{\partial C}{\partial z} \Big|_b \\
& + \mathbf{r}UA_e (C_e - C_p) - \mathbf{r}UA_w (C_w - C_p) \\
& + \mathbf{r}VA_n (C_n - C_p) - \mathbf{r}VA_s (C_s - C_p) \\
& + \mathbf{r}WA_t (C_t - C_p) - \mathbf{r}UA_b (C_b - C_p) = VQ_C + S_{DC}
\end{aligned} \tag{48}$$

$$\begin{aligned}
V \mathbf{r}q \frac{\partial c_p T}{\partial t} & + V \frac{\partial (1-q)cT}{\partial t} \\
& - h_y f_{3e} \mathbf{l}_{xe} \frac{\partial T}{\partial x} \Big|_e + h_y f_{3w} \mathbf{l}_{xw} \frac{\partial T}{\partial x} \Big|_w \\
& - h_x f_{3n} \mathbf{l}_{yn} \frac{\partial T}{\partial y} \Big|_n + h_x f_{3s} \mathbf{l}_{ys} \frac{\partial T}{\partial y} \Big|_s \\
& - h_x h_y \mathbf{l}_{zt} \frac{\partial T}{\partial z} \Big|_t + h_x h_y \mathbf{l}_{zb} \frac{\partial T}{\partial z} \Big|_b \\
& + \mathbf{r}UA_e (c_{pe} T_e - c_p T_p) - \mathbf{r}UA_w (c_{pw} T_w - c_p T_p) \\
& + \mathbf{r}VA_n (c_{pn} T_n - c_p T_p) - \mathbf{r}VA_s (c_{ps} T_s - c_p T_p) \\
& + \mathbf{r}WA_t (c_{pt} T_t - c_p T_p) - \mathbf{r}UA_b (c_{pb} T_b - c_p T_p) = VQ_T + S_{DT}
\end{aligned} \tag{49}$$

with explicit sources terms:

$$\begin{aligned}
 S_{DM} = & -h_y f_{1t} \frac{K_{xt}}{g} \frac{\partial P}{\partial x} \Big|_t - h_x f_{2t} \frac{K_{yt}}{g} \frac{\partial P}{\partial y} \Big|_t + h_x h_y K_{zt} (\mathbf{r}_t - \mathbf{r}_0) \\
 & + h_y f_{1b} \frac{K_{xb}}{g} \frac{\partial P}{\partial x} \Big|_b + h_x f_{2b} \frac{K_{yb}}{g} \frac{\partial P}{\partial y} \Big|_b - h_x h_y K_{zb} (\mathbf{r}_b - \mathbf{r}_0)
 \end{aligned} \tag{50}$$

$$\begin{aligned}
 S_{DC} = & -h_y f_{1t} \mathbf{r}_t \mathbf{g}_t D_{xt} \frac{\partial C}{\partial x} \Big|_t - h_x f_{2t} \mathbf{r}_t \mathbf{g}_t D_{yt} \frac{\partial C}{\partial y} \Big|_t \\
 & + h_y f_{1b} \mathbf{r}_b \mathbf{g}_b D_{xb} \frac{\partial C}{\partial x} \Big|_b + h_x f_{2b} \mathbf{r}_b \mathbf{g}_b D_{yb} \frac{\partial C}{\partial y} \Big|_b
 \end{aligned} \tag{51}$$

$$\begin{aligned}
 S_{DT} = & -h_y f_{1t} \mathbf{I}_{xt} \frac{\partial T}{\partial x} \Big|_t - h_x f_{2t} \mathbf{I}_{yt} \frac{\partial T}{\partial y} \Big|_t \\
 & + h_y f_{1b} \mathbf{I}_{xb} \frac{\partial T}{\partial x} \Big|_b + h_x f_{2b} \mathbf{I}_{yb} \frac{\partial T}{\partial y} \Big|_b
 \end{aligned} \tag{52}$$

and mass fluxes given by:

$$\begin{aligned}
 \mathbf{r}UA &= -h_y f_3 \frac{K_x}{g} \frac{\partial P}{\partial x} \\
 \mathbf{r}VA &= -h_x f_3 \frac{K_y}{g} \frac{\partial P}{\partial y} \\
 \mathbf{r}WA &= -h_x h_y \frac{K_z}{g} \frac{\partial P}{\partial z} - h_x h_y K_z (\mathbf{r} - \mathbf{r}_0) + h_y f_1 \frac{K_x}{g} \frac{\partial P}{\partial x} + h_x f_2 \frac{K_y}{g} \frac{\partial P}{\partial y}
 \end{aligned} \tag{53}$$

The second simplification of the BFC:s formulation concerns the normal derivative along Z direction. Due to the vertical east-west and north-south faces this derivative reduces to:

$$\frac{\partial \mathbf{f}}{\partial z} \Big|_t = \frac{\mathbf{f}_T - \mathbf{f}_P}{z_{CT} - z_{CP}} \tag{54}$$

where z_c represents the Z coordinate of variable locations, i.e. of the centers of control volumes:

$$z_c = \frac{1}{8}(z_1 + z_2 + z_3 + z_4 + z_5 + z_6 + z_7 + z_8) \quad (55)$$

Like with BFC formulation X and Y derivatives suffer of non-alignment with the \mathbf{x} and \mathbf{h} lines connecting variable locations. For example, the X derivative at center of east face is:

$$\left. \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right|_e = \frac{(\mathbf{f}_{E^*} - \mathbf{f}_{P^*})}{\mathbf{x}_E - \mathbf{x}_P} \quad (56)$$

Where the points E^* and P^* are the projections of the points E and P on X direction at the altitude z_f of the face center.

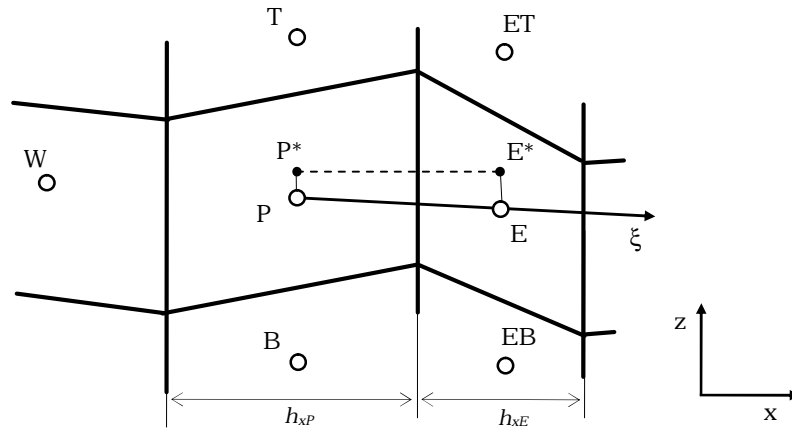


Figure 7 : East face partial X derivative labeling

Because the E^* and P^* values are not directly known, DarcyTools approximates them by:

$$\mathbf{f}_{E^*} = \mathbf{f}_E + (z_f - z_E) \left. \frac{\partial \mathbf{f}}{\partial z} \right|_E \quad \mathbf{f}_{P^*} = \mathbf{f}_P + (z_f - z_P) \left. \frac{\partial \mathbf{f}}{\partial z} \right|_P \quad (57)$$

Therefore, since Z derivatives are straightforward, partial X derivative at east face becomes:

$$\left. \frac{\partial \mathbf{f}}{\partial x} \right|_e = \frac{\mathbf{f}_E - \mathbf{f}_P}{x_E - x_P} + \frac{z_f - z_E}{x_E - x_P} \left(\frac{\mathbf{f}_{ET} - \mathbf{f}_{EB}}{z_{ET} - z_{EB}} \right) + \frac{z_P - z_f}{x_E - x_P} \left(\frac{\mathbf{f}_T - \mathbf{f}_B}{z_T - z_B} \right) \quad (58)$$

Again, like with BFC formulation, the top and bottom diffusive fluxes involve cross derivatives since face normals are not vertical.

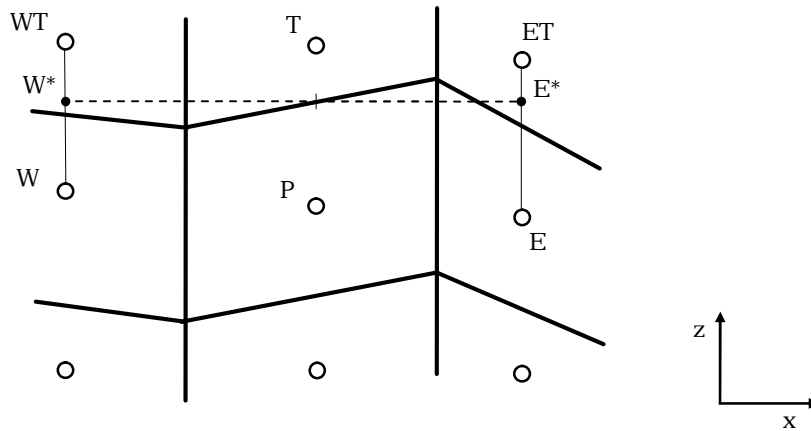


Figure 8 : Top face partial X derivative labeling

DarcyTools approximates these cross derivatives as follows:

$$\left. \frac{\partial \mathbf{f}}{\partial x} \right|_t = \frac{(\mathbf{f}_{E^*} - \mathbf{f}_{W^*})}{x_E - x_W} \quad (59)$$

where the E^* and W^* values are linearly interpolated as before:

$$\mathbf{f}_{E^*} = \mathbf{f}_E + (z_f - z_E) \left. \frac{\partial \mathbf{f}}{\partial z} \right|_E \quad \mathbf{f}_{W^*} = \mathbf{f}_W + (z_f - z_P) \left. \frac{\partial \mathbf{f}}{\partial z} \right|_W \quad (60)$$

z_f is now the top face center's altitude. The partial X derivative at top face finally becomes:

$$\left. \frac{\partial \mathbf{f}}{\partial x} \right|_t = \frac{z_f - z_E}{x_E - x_W} \left(\frac{\mathbf{f}_{ET} - \mathbf{f}_E}{z_{ET} - z_E} \right) - \frac{z_f - z_W}{x_E - x_W} \left(\frac{\mathbf{f}_{WT} - \mathbf{f}_W}{z_{WT} - z_T} \right) \quad (61)$$

At boundaries, extreme points in relation (61) are replaced by central points. For example for $l=1$, W and WT are respectively replaced by P and T . For two dimensional (Y - Z) and (X - Z) problems partial X and Y derivatives at top and bottom faces are respectively ignored.

Cartesian Discretisation

The fastest and the less memory consuming formulation in DarcyTools is the Cartesian grid formulation for which the X , Y and Z coordinates of grid nodes depend only on I , J and K indexes respectively. Many simplifications are therefore possible and, in particular, areas and normals of relation (12) become:

$$\begin{aligned} A_e \vec{n}_e &= h_y h_z \vec{x} & A_w \vec{n}_w &= -h_y h_z \vec{x} \\ A_n \vec{n}_n &= h_x h_z \vec{y} & A_s \vec{n}_s &= -h_x h_z \vec{y} \\ A_t \vec{n}_t &= h_x h_y \vec{z} & A_b \vec{n}_b &= -h_x h_y \vec{z} \end{aligned} \quad (62)$$

so that the governing equations do not contain any cross derivatives in additional explicit sources terms and simplify to:

$$\begin{aligned} h_x h_y h_z \frac{\partial \mathbf{r} \mathbf{q}}{\partial t} &- h_y h_z \frac{K_{xe}}{g} \frac{\partial P}{\partial x} \Big|_e + h_y h_z \frac{K_{xw}}{g} \frac{\partial P}{\partial x} \Big|_w \\ &- h_x h_z \frac{K_{yn}}{g} \frac{\partial P}{\partial y} \Big|_n + h_x h_z \frac{K_{ys}}{g} \frac{\partial P}{\partial y} \Big|_s \\ &- h_x h_y \frac{K_{zt}}{g} \frac{\partial P}{\partial z} \Big|_t + h_x h_y \frac{K_{zb}}{g} \frac{\partial P}{\partial z} \Big|_b = h_x h_y h_z Q + S_{DM} \end{aligned} \quad (63)$$

$$\begin{aligned}
& h_x h_y h_z \mathbf{r} \mathbf{q} \frac{\partial C}{\partial t} - h_y h_z \mathbf{r}_e \mathbf{g}_e D_{xe} \frac{\partial C}{\partial x} \Big|_e + h_y h_z \mathbf{r}_w \mathbf{g}_w D_{xw} \frac{\partial C}{\partial x} \Big|_w \\
& - h_x h_z \mathbf{r}_n \mathbf{g}_n D_{yn} \frac{\partial C}{\partial y} \Big|_n + h_x h_z \mathbf{r}_s \mathbf{g}_s D_{ys} \frac{\partial C}{\partial y} \Big|_s \\
& - h_x h_y \mathbf{r}_t \mathbf{g}_t D_{zt} \frac{\partial C}{\partial z} \Big|_t + h_x h_y \mathbf{r}_b \mathbf{g}_b D_{zb} \frac{\partial C}{\partial z} \Big|_b \\
& + \mathbf{r} U A_e (C_e - C_p) - \mathbf{r} U A_w (C_w - C_p) \\
& + \mathbf{r} V A_n (C_n - C_p) - \mathbf{r} V A_s (C_s - C_p) \\
& + \mathbf{r} W A_t (C_t - C_p) - \mathbf{r} U A_b (C_b - C_p) = h_x h_y h_z Q_C
\end{aligned} \tag{64}$$

$$\begin{aligned}
& h_x h_y h_z \mathbf{r} \mathbf{q} \frac{\partial c_p T}{\partial t} + h_x h_y h_z \frac{\partial (1 - \mathbf{q}) c T}{\partial t} \\
& - h_y h_z \mathbf{I}_{xe} \frac{\partial T}{\partial x} \Big|_e + h_y h_z \mathbf{I}_{xw} \frac{\partial T}{\partial x} \Big|_w \\
& - h_x h_z \mathbf{I}_{yn} \frac{\partial T}{\partial y} \Big|_n + h_x h_z \mathbf{I}_{ys} \frac{\partial T}{\partial y} \Big|_s \\
& - h_x h_y \mathbf{I}_{zt} \frac{\partial T}{\partial z} \Big|_t + h_x h_y \mathbf{I}_{zb} \frac{\partial T}{\partial z} \Big|_b \\
& + \mathbf{r} U A_e (c_{pe} T_e - c_p T_p) - \mathbf{r} U A_w (c_{pw} T_w - c_p T_p) \\
& + \mathbf{r} V A_n (c_{pn} T_n - c_p T_p) - \mathbf{r} V A_s (c_{ps} T_s - c_p T_p) \\
& + \mathbf{r} W A_t (c_{pt} T_t - c_p T_p) - \mathbf{r} U A_b (c_{pb} T_b - c_p T_p) = h_x h_y h_z Q_T
\end{aligned} \tag{65}$$

where the only additional source term is given by:

$$S_{DM} = h_x h_y K_{zt} (\mathbf{r}_t - \mathbf{r}_0) - h_x h_y K_{zb} (\mathbf{r}_b - \mathbf{r}_0) \tag{66}$$

the mass fluxes by:

$$\begin{aligned}
rUA &= -h_y h_z \frac{K_x}{g} \frac{\partial P}{\partial x} \\
rVA &= -h_x h_z \frac{K_y}{g} \frac{\partial P}{\partial y} \\
rWA &= -h_x h_y \frac{K_z}{g} \frac{\partial P}{\partial z} - h_x h_y K_z (\mathbf{r} - \mathbf{r}_0)
\end{aligned} \tag{67}$$

and the normal partial derivatives by:

$$\begin{aligned}
\left. \frac{\partial f}{\partial x} \right|_e &= \frac{f_E - f_P}{x_E - x_P} & \left. \frac{\partial f}{\partial x} \right|_w &= \frac{f_W - f_P}{x_W - x_P} \\
\left. \frac{\partial f}{\partial y} \right|_n &= \frac{f_N - f_P}{y_N - y_P} & \left. \frac{\partial f}{\partial y} \right|_s &= \frac{f_S - f_P}{y_S - y_P} \\
\left. \frac{\partial f}{\partial z} \right|_t &= \frac{f_T - f_P}{z_T - z_P} & \left. \frac{\partial f}{\partial z} \right|_b &= \frac{f_B - f_P}{z_B - z_P}
\end{aligned} \tag{68}$$

Embedded Grids Strategy

To reduce the amount of computational work when high resolution of the fractured network is needed, DarcyTools applies an embedded grids strategy. Starting from a large domain, local block refinements are embedded in one or several parent grid footprints.

Child (embedded) grids are defined by three refining factors so that every parent cell of the footprint is subdivided into f_I , f_J and f_K child cells in the I , J and K direction respectively (f_I , f_J and f_K being integer values). An additional plane of cells is also used where boundaries of the footprint do not coincide with the parent grid boundaries (Figure 9). DarcyTools uses these cells to specify Dirichlet boundary conditions to the embedded grid problem from the parent grid solution.

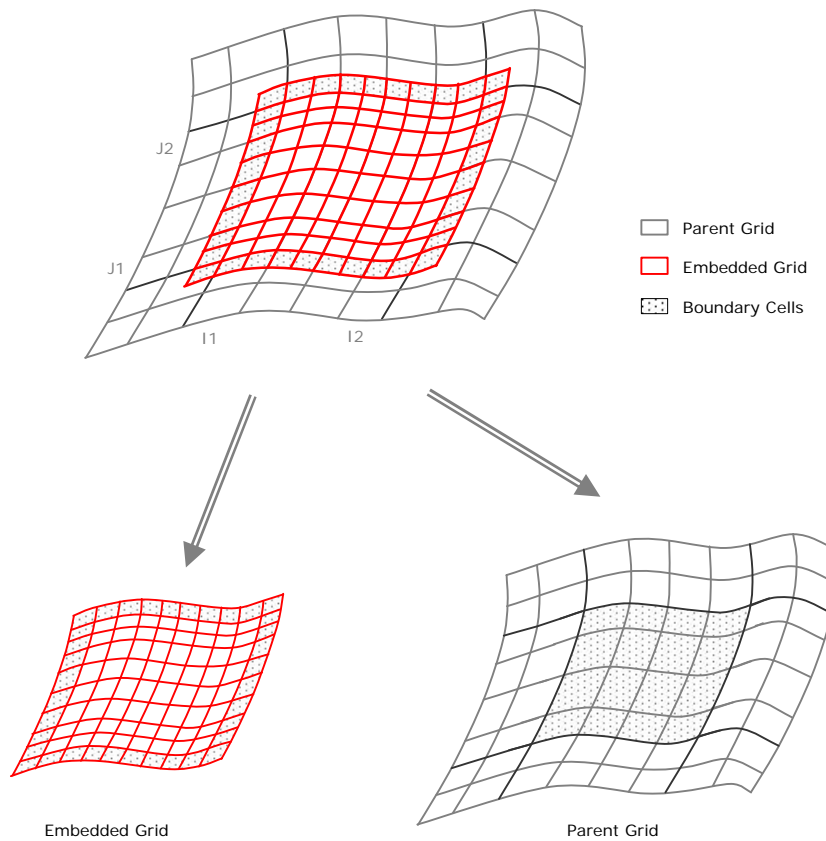


Figure 9 : Footprint and embedded grid arrangement

To solve the interdependence of grid solutions, DarcyTools starts by solving the most embedded grid solution with Dirichlet boundary conditions on the additional cell planes. The fixed values are obtained from a tri-linear interpolation of the parent grid node values. Actually, DarcyTools uses the parent grid node values because the location of child cell grid centers is linearly defined from the parent grid nodes and not from the parent grid cell centers. The advantage of this procedure is that it is faster compare to a fully non linear interpolation procedure but the drawback is that the parent grid node values themselves have to be interpolated from the parent solution. For this DarcyTools implements an inverse volume weighting such as:

$$f_v = \left(\sum \frac{1}{Vol_i} f_i \right) / \left(\sum \frac{1}{Vol_i} \right) \tag{69}$$

Then, given the child solutions, the parent grid solution is computed outside the footprints with fixed fluxes boundary conditions on cells at footprints' borders (e.g. $I=I1-1$ or $I=I2+1$). The fixed fluxes are obtained by summation of the

child grids fluxes entering the additional cells in order not to lose the conservative property of the finite volume procedure.

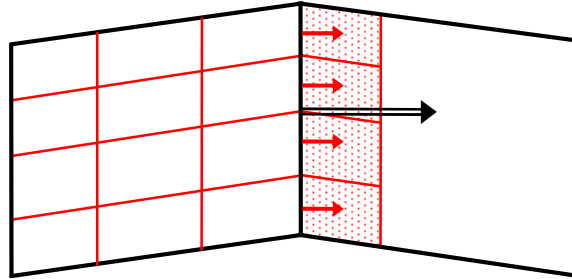


Figure 10 : Fluxes transfer from child to parent grids

For interpolation purpose, the footprints values of the parent grid are also fixed at mean values of the child grids solutions. Mean values are obtained by a volume weighting of the $f_i \times f_j \times f_k$ child grid cells embedded in each parent cell.

$$\mathbf{f}_v = \left(\sum Vol_i \mathbf{f}_i \right) / \left(\sum Vol_i \right) \quad (70)$$

Finally, the interdependence of grid solutions is solved by completing iterations until the boundary conditions and the residuals converged on each grid.

Users will note that DarcyTools also implements an alternative for parent grid boundary conditions in which the footprint fluxes are not fixed but only the footprint values, and that, because of boundary conditions on the parent footprints, the mass sources terms must be specified on the most embedded grids only when occurring on a footprint and on the parent grid otherwise (additional boundary cells of the embedded grids must be considered as laying outside the footprints).

Coupled Procedure

Density driven flows are problems in which the governing partial differential equations may be strongly coupled with instabilities arising from nonlinearities. To reliably and efficiently solve this kind of challenging flows DarcyTools uses the MIGAL solver capabilities and allows for example a fully coupled solution of the pressure-salinity coupling. For this purpose, the buoyancy terms appearing in the fluid mass conservation equation is implicitly treated instead of being

included into the additional source term S_{DM} (38), (50) and (66) using the density state law:

$$\mathbf{r} - \mathbf{r}_0 = \mathbf{r}_0 \mathbf{a} S \quad (71)$$

For stability reason, the face salinity involved in this transformation is approximated by its upwind the value (e.g. S_t is substituted by S_p). The algebraic set of equations resulting from the coupled system follows the same form than the single variable generic equation (23) but coefficients are now 2x2 matrixes:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}_p \begin{bmatrix} P \\ C \end{bmatrix}_p = \sum_{nb} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}_{nb} \begin{bmatrix} P \\ C \end{bmatrix}_{nb} + \begin{bmatrix} S_p \\ S_c \end{bmatrix} \quad (72)$$

The practice of coupled solutions between pressure and salinity showed that low diffusivity field requires special treatment for convergence. For this purpose, instead of solving the linearized operator resulting from the discrete form of the governing equations, DarcyTools solves iteratively an approximated defect correction operator:

$$A^* \mathbf{df} = S - A\mathbf{f} \quad (73)$$

where A represents the original operator, \mathbf{f} a solution guess $(P,C)^T$ and \mathbf{df} the correction such as:

$$\mathbf{f}^{new} = \mathbf{f} + \mathbf{df} \quad (74)$$

The operator A^* is initially set to the original operator A but can be modified to stabilize the global convergence.

MIGAL solver

DarcyTools uses the MIGAL algebraic multi-grid solver to solve the successive algebraic sets of equations resulting from discretisation. This use sums up in a single call to the routine MIGAL and in the possibility of programming several routines for efficiency control: NLINS, SETRELAX or SETDOMI.

The basics

The set of linear equations (23) or (72) resulting of the discretisation of the continuity and the transport equations can be expressed as:

$$A x = S \tag{75}$$

where A represents the matrix of coefficients, x the variables array and S the right hand side vector of source terms.

There are several well-established iterative schemes to solve this set of linear equations. These include Jacobi, Gauss-Seidel, incomplete LU factorization, etc. But, each of them has a rate of convergence depending on the condition number of the matrix A . Hence, as the number of cells will increase, and because of the elliptic nature of the diffusion operator contained in the equation, the condition number of the matrix will increase and the rate of convergence will deteriorate. Further, a characteristic of all these iterative schemes is that the initial rate of convergence is rapid for the first iterations, and deteriorates as the iterations progress. It can be shown that the cause of this slow convergence is primarily the sluggish rate of convergence of the low frequency errors that are present in the solution. As the grid refined, these low frequency errors dominate the overall rate of convergence.

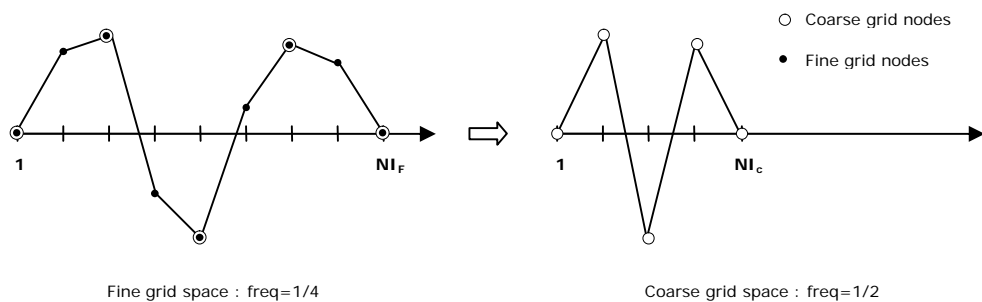


Figure 11: Fine to coarse grid error frequency mutation.

Hence, the concept of the multi-grid technique as implemented by MIGAL is as follows. Given the fact that the low frequencies converge slowly, it is possible to accelerate their rate of convergence by making them behave as high frequencies on coarser grids. For this, the basic principle consists in working on a subset of the fine grid points (e.g. keeping only odd or even nodes) to reduce the number of points and automatically raise the error signal frequency in the transformed grid space (see Figure 11).

MIGAL proceeds as follows. Consider that we initiate a solution on a given fine grid. A few iterations are then performed on this fine grid to obtain an estimation x_F . For these iterations, the convergence is usually fast.

$$x_F = \tilde{A}^{-1}S \tag{76}$$

The notation (\sim) means \tilde{A}^{-1} is not the inverse of matrix A but only an approximate (e.g. few relaxations of an iterative solver). Subsequently, the convergence begins to worsen so that the calculations are switches to a coarser grid with the aim of improving the fine grid estimation x_F at lower cost. For that, the residuals and the corresponding defect correction operator are formed on the fine grid and interpolated ("restricted") to the next coarse grid by:

$$R A dx_F = R (S - Ax_F) \tag{77}$$

where the restriction operator R (e.g. pure injection) is a $(NI_c \times NI_F)$ matrix that shorten the dimension of the right hand side from NI_F to NI_c .

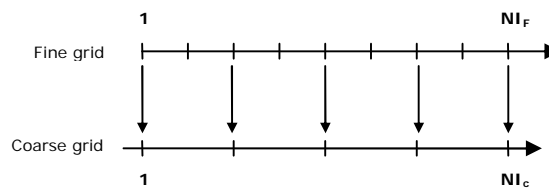


Figure 12 : Pure injection restriction.

At this point a second operator is introduced to shorten the left hand side of the operator. It is done by changing the fine grid correction variable dx_F for a coarse grid variable named dx_c so that the former can be interpolated ("prolongated") from the latter by:

$$dx_F = P dx_c \tag{78}$$

where the prolongation operator P (e.g. linear interpolation) is a $(NI_F \times NI_C)$ matrix that reduces the coarse grid operator size to $(NI_C \times NI_C)$

$$(R \ A \ P) \mathbf{dx}_c = R (S - Ax_F) \tag{79}$$

Once the coarse grid operator (RAP) is formed, a few iterations are performed to obtain \mathbf{dx}_c to the required accuracy and the fine grid correction is retrieved using (78).

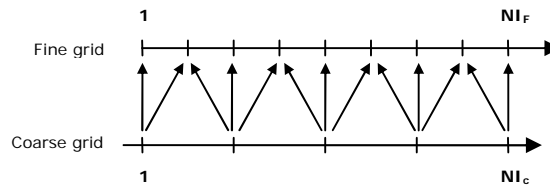


Figure 13: Linear prolongation.

Of course, since the error spectrum contains a wide range of frequencies, it is necessary to consider a number of coarse grids and to successively build the coarse operator of the coarse operators. On the coarsest grid, which must be a small grid, a direct solver can be used or, like with MIGAL, the necessary number of iterations can be performed. Finally the manner in which the grids are visited can vary.

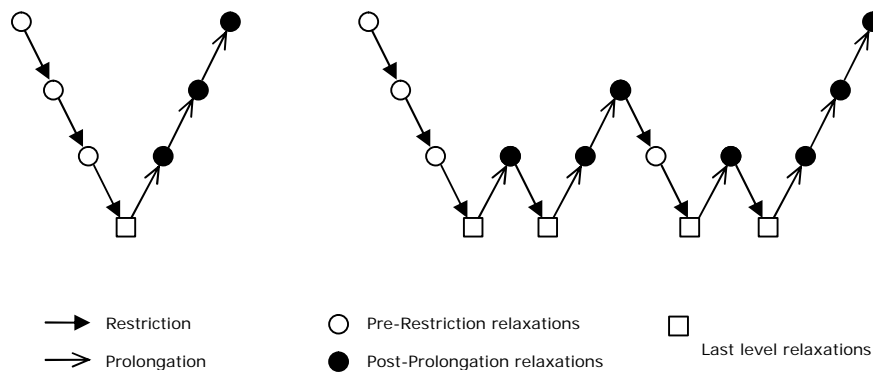


Figure 14 : V and W multi-grid cycles

In the simplest case, called V-cycle, each grid is visited in turn on the downward and upward legs of a V-cycle. On each grid a number of iterations are performed and the next grid is visited. With the W-cycle, each grid is visited in turn on the downward leg of the a W-cycle, then after that the correction is prolonged by one level, the error is again restricted to the lower level and the correction prolonged up to the next upper level (see Figure 14). The iterations can be done during both the restriction part of the cycle (downward limb) and during the prolongation part (upward limb).

GMRES acceleration

The emphasis of basic multi-grid procedures is to improve the performance of the classical iterative solver (smoother) by adapting the operator to their intrinsic capabilities. This technique encounters some limits when the coefficients are highly anisotropic and when the mesh aspect ratios are quite large but the ILUO smoother of MIGAL has demonstrated to be robust enough in many 3D applications. The main difficulty of the flows processed by DarcyTools comes from the sharp spatial variations of the coefficients that couple the high and low frequencies error components during the restriction/prolongation procedure and finally deteriorate the overall performance. To fight this wavelength coupling problem DarcyTools may use MIGAL as a GMRES preconditioner.

The GMRES method is a projection method based that consists in finding the optimal solution of the system (75) that belongs to the m -th Krylov subspace K_m .

$$K_m = \text{span} \left\{ r_0, AM^{-1}r_0, [AM^{-1}]^2 r_0, \dots, [AM^{-1}]^{m-1} r_0 \right\} \quad (80)$$

where r_0 is the initial residual of (75) and where M^{-1} is a right preconditioning matrix whose function is to lower the condition number of the algebraic set of equations.

$$AM^{-1}u = S, \quad u = Mx \quad (81)$$

For a given dimension m , the MIGAL-GMRES algorithm involves an Arnoldi loop that constructs an orthogonal basis of the right-preconditioned Krylov subspace by a modified Gram-Schmidt process, in which the new vector to be orthogonalized is obtained from the previous vector of the process.

1. **Start:** Choose x_0 and a dimension m of the Krylov subspaces and initialize a $(m+1) \times m$ matrix H to zero
2. **Arnoldi process:**
 - Compute $r_0 = S - Ax_0$, $b = \|r_0\|$ and $v_1 = r_0/b$
 - For $j=1, \dots, m$
 - Compute $z_j = M^{-1} v_j$
 - Compute $w = A z_j$
 - For $i=1, \dots, j$

$$H_{i,j} = (w, v_i)$$

$$w = w - H_{i,j} v_i$$
 - Compute $h_{j+1,j} = \|w\|$ and $v_{j+1} = w/h_{j+1,j}$
 - Define $Z_m = [z_1, \dots, z_m]$
3. **From the approximate solution:** Compute $x_m = x_0 + Z_m y_m$ where $y_m = \operatorname{argmin}_y \|be_1 - Hy\|$ and $e_1 = [1, 0, \dots, 0]^T$
4. **Restart:** if satisfied stop, else set $x_0 = x_m$ and goto 2.

Figure 15 : MIGAL-GMRES algorithm

The preconditioning matrix is only involved in the $z = M^{-1}v$ products and does not need to be explicitly formulated. Instead, since relation (81) shows that $M=A$ is the best preconditioning choice, some multi-grid cycles of MIGAL are advantageously used to compute an approximated value of z as being the solution of $Az=v$.

The drawback is that, since M now changes for each vector z depending on the convergence of MIGAL, it is necessary to store the orthogonal basis Z_m to retrieve the solution x_m . Therefore, since reaching an expected level of accuracy usually involves large sub-spaces, the method may become impractical because of large memory and computational requirements. For this reason MIGAL use a restarted GMRES procedure (step 4. Figure 1) which limits the Krylov-subspace basis to a given size and iterates the initial estimation x_0 .

MIGAL preconditions the Krylov subspace by one multi-grid cycle. To increase this number of preconditioning cycles users may specify the parameter IPRECO in the MIGAL parameters list. For particularly difficult problems it is possible, on coarse grid levels, to replace the ILU(0) smoother by a GMRES ILU(0) preconditioned smoother. For this users have to stipulate the size of the desired Krylov subspace by setting the parameter IGMS to any non-zero value. The coarse grid smoother then becomes a GMRES solver right-preconditioned by NBPRER or NBRELAX ILU(0) relaxations depending of the limb of the multi-grid cycle actually performed. For flexibility, the IGMS parameter may be set independently of IGMRES, i.e. that MIGAL can implement different combinations of the multi-grid and GMRES algorithms.

SOLVER	NBGRID	IGMRES	IPRECO	IGMS
ILU(0)	1	0	-	0
GMRES not-preconditioned	1	n	0	0
GMRES ILU(0) preconditioned	1	n	n	0
Multi-grid[ILU(0)]*	n	0	-	0
GMRES multi-grid[ILU(0)] preconditioned	n	n	n	0
Multi-grid[GMRES-ILU(0) preconditioned]	n	0	-	n
GMRES multi-grid[GMRES-ILU(0) preconditioned] preconditioned	n	n	n	n

Figure 16 : Multi-grid/GMRES possible combinations. (*)=default

APPENDIX B Some aspects of using the multirate model with a power law distribution of rates

Some aspects of using the multirate model with a power law distribution of rates

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1 Introduction

This paper deals with some aspects of using the multirate model of the immobile zone with a power law distribution of first-order rates. For an introduction to the subject, see Refs. 1 and 2. Sections 2, 3, 4 and 5 have a mathematical character and mainly discuss the relation between power law distributions for diffusion rates and first-order rates. The main conclusion is that the two power law distributions will have the same exponent if some conditions are fulfilled, a fact which was briefly mentioned in Ref. 2. Section 6 describes how the power law distribution for diffusion rate can be obtained starting from a power law distribution for fracture size and many other assumptions. Finally, Section 7 suggests how the theory presented in the earlier sections can be applied to computer simulations of tracer motion in fractured rock.

Many of the ideas in the paper originate from Refs. 1 and 2. Urban Svensson has contributed with basic ideas for Sections 6 and 7, while I have concentrated on mathematical issues.

2 The base of the model for the immobile zone

Consider a region of fractured rock. The fractures are filled with water (apart from possible solid material). A tracer is dissolved in the water at varying concentration. Water and tracer particles are subject to diffusion in the entire water-filled volume. Let the mobile zone be the part of the water-filled volume where also advection can occur. The mobile zone is assumed to be connected. (This means that a water or tracer particle anywhere in the zone can travel through the zone by means of advection or diffusion to any other location in the zone.) Let the immobile zone be the parts of the water-filled volume which do not belong to the mobile zone but which are accessible to particles in the mobile zone by means of diffusion. (There can also be parts of the water-filled volume which are inaccessible to water and

tracer in the mobile zone, and which we shall not consider further.) The solid material surrounding both the mobile and immobile zones can adsorb tracer particles. Adsorbed particles are still regarded as being located in the respective zones.

Consider a volume of water belonging to the mobile or immobile zone. Assume that the concentration of tracer in the water is uniform in the volume and that the dissolved and adsorbed tracer are in equilibrium. Let us form the ratio of the amount of tracer, dissolved and adsorbed, to the concentration of tracer in the water. (If there is no adsorption, the ratio is equal to the volume of the water.) With the capacity of the volume I mean this ratio. (I hope I use the term correctly.)

The total capacity ratio β_{tot} is the ratio of the capacity of the immobile zone to the capacity of the mobile zone. When the mobile and immobile zones are in equilibrium, the ratio of the amount of tracer in the immobile zone to that in the mobile zone is equal to β_{tot} .

According to the multirate model described in Ref. 1, the immobile zone can be modelled as a continuous spectrum of first-order boxes. Each box is characterized by a first-order rate $\alpha > 0$, and the probability that a tracer particle in the box will leave the box and enter the mobile zone during a time interval dt is αdt , regardless of the particle's history. The capacity ratio density function $b(\alpha) \geq 0$ specifies how the total capacity ratio β_{tot} is distributed over the spectrum of boxes. The capacity ratio for the boxes with rates in the interval $(\alpha, \alpha + d\alpha)$ is $b(\alpha) d\alpha$, and

$$\int_0^{\infty} b(\alpha) d\alpha = \beta_{\text{tot}}. \quad (1)$$

This means that when the mobile zone and all the first-order boxes are in equilibrium, the ratio of the amount of tracer in the boxes with rates in the interval $(\alpha, \alpha + d\alpha)$ to the amount of tracer in the mobile zone is $b(\alpha) d\alpha$. It is possible to conclude from this that if the tracer particles have an equilibrium distribution within the mobile zone, the probability that a randomly chosen particle in the mobile zone will enter any of the boxes with rates in the interval $(\alpha, \alpha + d\alpha)$ during a time interval dt is $b(\alpha) d\alpha \alpha dt$, regardless of whether the mobile zone is in equilibrium with the first-order boxes.

It may seem natural to divide the immobile zone into a spectrum of parts characterized by their sizes. (This could be done if we modelled the immobile zone as a collection of square fractures extending perpendicularly from the mobile zone, for example.) We shall however use a characteristic diffusion rate $\alpha_d > 0$ instead of the size as the characterizing variable in the spectrum. (It is usual to assume that there is a simple relationship between size and diffusion rate, as we will do in Section 6 using Formula 37.) Let us introduce the capacity ratio density function $b_d(\alpha_d) \geq 0$ to specify the distribution of the total capacity ratio β_{tot} over the new spectrum. I.e.,

the capacity ratio for the parts of the immobile zone whose diffusion rates belong to the interval $(\alpha_d, \alpha_d + d\alpha_d)$ is $b_d(\alpha_d) d\alpha_d$, and

$$\int_0^\infty b_d(\alpha_d) d\alpha_d = \beta_{\text{tot}}. \quad (2)$$

For fixed diffusion rate α_d , let us model the corresponding part of the immobile zone with a multirate model specified by $b_{\text{fo}|d}(\alpha | \alpha_d) \geq 0$ (“fo” for “first order”), where

$$\int_0^\infty b_{\text{fo}|d}(\alpha | \alpha_d) d\alpha = 1. \quad (3)$$

The multirate model for the entire immobile zone (all α_d) will then be specified by

$$b(\alpha) = \int_0^\infty b_{\text{fo}|d}(\alpha | \alpha_d) b_d(\alpha_d) d\alpha_d. \quad (4)$$

(Some of the terminology and notation in this section is inspired by probability theory.)

3 A power law distribution for the diffusion rate

In Ref. 2 a power law distribution for the diffusion rate α_d is suggested (among a few other distributions). Power law distributions occur in connection with fractals and are therefore theoretically attractive. The distribution is given by the formula

$$b_d(\alpha_d) = \begin{cases} \frac{\beta_{\text{tot}}}{I(\alpha_{d,\text{min}}, \alpha_{d,\text{max}}, k-2)} \alpha_d^{k-3}, & \alpha_{d,\text{min}} < \alpha_d < \alpha_{d,\text{max}}, \\ 0 & \text{otherwise,} \end{cases} \quad (5)$$

where

$$I(x_{\text{min}}, x_{\text{max}}, p) = \int_{x_{\text{min}}}^{x_{\text{max}}} x^{p-1} dx = \begin{cases} \ln \frac{x_{\text{max}}}{x_{\text{min}}}, & p = 0, \\ \frac{x_{\text{max}}^p - x_{\text{min}}^p}{p}, & p \neq 0. \end{cases} \quad (6)$$

The exponent $k-3$ has been chosen in conformance with Formula (27a) in Ref. 2.

4 Multirate models for fixed diffusion rate

In this section we shall study multirate models for the part of the immobile zone corresponding to a fixed diffusion rate α_d . In other words, we shall study $b_{\text{fo|d}}(\alpha | \alpha_d)$.

$b_{\text{fo|d}}(\alpha | \alpha_d)$ may or may not have properties P_1 and $P_2(k)$, which are defined as follows. k is a given real number.

P_1 : There exists a function $f(\xi)$ such that

$$b_{\text{fo|d}}(\alpha | \alpha_d) = \frac{f(\alpha/\alpha_d)}{\alpha_d} \quad (7)$$

for all α_d and α .

$P_2(k)$: The integral

$$\int_0^\infty f(\xi)\xi^{2-k} d\xi, \quad k \neq 2, \quad (8)$$

or the integral

$$\int_0^\infty f(\xi) \ln \xi d\xi, \quad k = 2, \quad (9)$$

converges at both 0 and ∞ . (There is thus a different variant of this condition for each of the cases $k \neq 2$ and $k = 2$.)

If $b_{\text{fo|d}}(\alpha | \alpha_d)$ has property P_1 , the function $f(\xi)$ is uniquely determined. It is defined for all $\xi > 0$, $f(\xi) \geq 0$ for all $\xi > 0$, and

$$\int_0^\infty f(\xi) d\xi = 1. \quad (10)$$

Therefore, if $k = 2$, the integral in Formula 8 will converge. If $b_{\text{fo|d}}(\alpha | \alpha_d)$ has properties P_1 and $P_2(k)$, let us define

$$\xi_{\text{mean}}(k) = \begin{cases} \left(\int_0^\infty f(\xi)\xi^{2-k} d\xi \right)^{1/(2-k)}, & k \neq 2, \\ \exp \int_0^\infty f(\xi) \ln \xi d\xi, & k = 2. \end{cases} \quad (11)$$

The definitions etc. in this paragraph will be used in Section 5.

We shall now study three kinds of immobile zones, in order to get examples of what $b_{\text{fo|d}}(\alpha | \alpha_d)$ can look like.

Consider a narrow and thin fracture which extends straightly a distance a from the mobile zone into the surrounding material. Let us assume that the fracture has constant cross-section area along its entire length. If there

is any solid material in the fracture, it is assumed to be homogeneously distributed. Let D_a be the apparent diffusivity for tracer particles in the fracture. Let us choose the ratio D_a/a^2 as the characteristic diffusion rate α_d of the fracture. Let us assume that the immobile zone consists entirely of such fractures. The fractures may have different a and D_a values and therefore different α_d values. The part of the immobile zone consisting of fractures with a given α_d value then has the multirate model specified by

$$b_{\text{fo|d}}(\alpha | \alpha_d) = \sum_{j=1}^{\infty} \frac{8}{(2j-1)^2\pi^2} \delta\left(\alpha - \frac{(2j-1)^2\pi^2}{4}\alpha_d\right), \quad (12)$$

where δ is the Dirac delta function. Immobile zone diffusion to which this formula applies is called layered diffusion (in finite layers).

If the cross-section area of a fracture is not constant along the fracture's length but proportional to the distance to the dead end of the fracture (i.e., the end which is not in contact with the mobile zone), then the term cylindrical diffusion is used, and the multirate model is specified by

$$b_{\text{fo|d}}(\alpha | \alpha_d) = \sum_{j=1}^{\infty} \frac{4}{u_j^2} \delta(\alpha - u_j^2\alpha_d). \quad (13)$$

u_j here denotes the j th solution of $J_0(u_j) = 0$, where J_0 is a Bessel function of the first kind. It should be noted that $u_{j+1} - u_j \approx \pi$ for large j .

If the cross-section area is proportional to the square of the distance to the dead end, the term spherical diffusion is used, and the formula is

$$b_{\text{fo|d}}(\alpha | \alpha_d) = \sum_{j=1}^{\infty} \frac{6}{j^2\pi^2} \delta(\alpha - j^2\pi^2\alpha_d). \quad (14)$$

Formulas 12, 13 and 14 have been taken from Table 1 in Ref. 2, although the notation has been changed somewhat.

We shall now investigate how the formulas for layered, cylindrical and spherical diffusion are related to properties P_1 and $P_2(k)$.

It is rather easy to show that the three formulas all have property P_1 . Therefore to each formula there is a corresponding function $f(\xi)$. For each formula, $f(\xi) = 0$ for small ξ , and therefore the integrals in Formulas 8 and 9 converge at 0 for all k . Moreover, $f(\xi) = O(\xi^{-3/2})$ on average (loosely speaking) for large ξ , and therefore the two integrals converge at ∞ for all $k > 3/2$. Thus, the three formulas all have property $P_2(k)$ for all $k > 3/2$.

Property P_1 means that $b_{\text{fo|d}}(\alpha | \alpha_d)$, when viewed as a function of α , is equal for all α_d except for stretching and contraction. P_1 therefore indicates some kind of scale-invariance with respect to α_d . Small ξ correspond to low first-order rates α and therefore to slow first-order boxes, i.e. boxes where particles stay for a long time on average once they have entered. For fixed α_d

the immobile zone fractures in the three diffusion models have finite length, or more precisely, they have a fixed D_a/a^2 ratio, and therefore it is natural that there is a limit to how slow first-order boxes there are, or equivalently, that $f(\xi) = 0$ for small ξ . Large ξ , on the other hand, correspond to high rates α and fast first-order boxes. $f(\xi)$'s $O(\xi^{-3/2})$ behaviour for large ξ is common to the three diffusion models, although the shapes of the fractures vary between the models. Fast boxes in the multirate model mostly have to do with particles that leave the immobile zone fractures soon after they have entered them, probably not diffusing far into the fractures. The fractures do not vary much in cross-section area in the parts nearest to the mobile zone, and therefore it is perhaps natural that all three diffusion models exhibit the same $O(\xi^{-3/2})$ behaviour for large ξ .

From the discussion in the previous two paragraphs we can draw the following conclusions. Consider the class of diffusion models where $b_{\text{fo|d}}(\alpha | \alpha_d)$ has properties P_1 and $P_2(k)$ for $k > 3/2$. The models for layered, cylindrical and spherical diffusion belong to this class. The three models are probably members of a rather large group of diffusion models which seem to be realistic from a mathematical point of view and which belong to the class.

5 The multirate model for the entire immobile zone

There are two ways to obtain $b(\alpha)$, which specifies the multirate model for the entire immobile zone. The first way is to choose some suitable $b(\alpha)$ without consideration of $b_d(\alpha_d)$ and $b_{\text{fo|d}}(\alpha | \alpha_d)$. The second way is to choose $b_d(\alpha_d)$ and $b_{\text{fo|d}}(\alpha | \alpha_d)$ first and then use Formula 4 to calculate $b(\alpha)$.

When $b(\alpha)$ is obtained the first way, a power law distribution is a possible choice, as suggested in Ref. 2. $b(\alpha)$ will then be given by the formula

$$b(\alpha) = \begin{cases} \frac{\beta_{\text{tot}}}{I(\alpha_{\min}, \alpha_{\max}, k-2)} \alpha^{k-3}, & \alpha_{\min} < \alpha < \alpha_{\max}, \\ 0 & \text{otherwise.} \end{cases} \quad (15)$$

Note the similarity to Formula 5.

We shall now see what $b(\alpha)$ will look like when it is obtained the second way, provided that certain conditions are fulfilled.

We shall assume that $b_d(\alpha_d)$ is given by Formula 5 and that $b_{\text{fo|d}}(\alpha | \alpha_d)$ has properties P_1 and $P_2(k)$ as defined in Section 4. The k in $P_2(k)$ shall be

the same as in Formula 5. Using Formulas 4 and 5 and property P_1 we get

$$\begin{aligned}
b(\alpha) &= \int_0^\infty b_{\text{fo|d}}(\alpha | \alpha_d) b_d(\alpha_d) d\alpha_d \\
&= \int_{\alpha_d, \min}^{\alpha_d, \max} \frac{f(\alpha/\alpha_d)}{\alpha_d} \frac{\beta_{\text{tot}}}{I(\alpha_d, \min, \alpha_d, \max, k-2)} \alpha_d^{k-3} d\alpha_d \\
&= \left[\xi = \frac{\alpha}{\alpha_d}, \quad \alpha_d = \frac{\alpha}{\xi}, \quad d\alpha_d = -\frac{\alpha d\xi}{\xi^2} \right] \\
&= \int_{\alpha/\alpha_d, \min}^{\alpha/\alpha_d, \max} \frac{f(\xi)}{\alpha/\xi} \frac{\beta_{\text{tot}}}{I(\alpha_d, \min, \alpha_d, \max, k-2)} \left(\frac{\alpha}{\xi}\right)^{k-3} \left(-\frac{\alpha d\xi}{\xi^2}\right) \\
&= \frac{\beta_{\text{tot}}}{I(\alpha_d, \min, \alpha_d, \max, k-2)} \alpha^{k-3} \int_{\alpha/\alpha_d, \max}^{\alpha/\alpha_d, \min} f(\xi) \xi^{2-k} d\xi. \quad (16)
\end{aligned}$$

Had the integral in the last term not been dependent on α , $b(\alpha)$ would have been proportional to α^{k-3} . Let us therefore study the integral more closely.

Let $\epsilon > 0$ be some small number. Property $P_2(k)$ implies that there are numbers ξ_{\min} and ξ_{\max} with $0 < \xi_{\min} \leq \xi_{\max}$ such that

$$\int_0^{\xi'} f(\xi) \xi^{2-k} d\xi < \epsilon \int_0^\infty f(\xi) \xi^{2-k} d\xi \quad (17)$$

for all ξ' with $0 < \xi' < \xi_{\min}$ and

$$\int_{\xi'}^\infty f(\xi) \xi^{2-k} d\xi < \epsilon \int_0^\infty f(\xi) \xi^{2-k} d\xi \quad (18)$$

for all $\xi' > \xi_{\max}$. If also $\xi_{\max} \alpha_{d, \min} < \xi_{\min} \alpha_{d, \max}$, then

$$\frac{\int_{\alpha/\alpha_d, \max}^{\alpha/\alpha_d, \min} f(\xi) \xi^{2-k} d\xi}{\int_0^\infty f(\xi) \xi^{2-k} d\xi} \in \begin{cases} [0, \epsilon), & 0 < \alpha < \xi_{\min} \alpha_{d, \min}, \\ [0, 1], & \xi_{\min} \alpha_{d, \min} \leq \alpha \leq \xi_{\max} \alpha_{d, \min}, \\ (1 - 2\epsilon, 1], & \xi_{\max} \alpha_{d, \min} < \alpha < \xi_{\min} \alpha_{d, \max}, \\ [0, 1], & \xi_{\min} \alpha_{d, \max} \leq \alpha \leq \xi_{\max} \alpha_{d, \max}, \\ [0, \epsilon), & \xi_{\max} \alpha_{d, \max} < \alpha. \end{cases} \quad (19)$$

This formula suggests that the numerator integral could be approximated by a function which is equal to the denominator integral when α belongs to some interval and equal to 0 outside the interval.

Let us assume that ξ_{\min} and ξ_{\max} can be chosen so that they satisfy the following two conditions in addition to those already given. ξ_{\min} and ξ_{\max} shall not be too far apart, in order that the intervals $\xi_{\min} \alpha_{d, \min} \leq \alpha \leq$

$\xi_{\max}\alpha_{d,\min}$ and $\xi_{\min}\alpha_{d,\max} \leq \alpha \leq \xi_{\max}\alpha_{d,\max}$ in Formula 19 shall not be too wide. The relation $\xi_{\min} \leq \xi_{\text{mean}}(k) \leq \xi_{\max}$ shall hold, where $\xi_{\text{mean}}(k)$ was defined by Formula 11. If such ξ_{\min} and ξ_{\max} can be found, then the numerator integral can be approximated as described with the interval being $\xi_{\text{mean}}(k)\alpha_{d,\min} < \alpha < \xi_{\text{mean}}(k)\alpha_{d,\max}$. $b(\alpha)$ can consequently be approximated by the function

$$b_{\text{appr}}(\alpha) = \begin{cases} \frac{\beta_{\text{tot}}}{I(\alpha_{d,\min}, \alpha_{d,\max}, k-2)} \alpha^{k-3} \int_0^\infty f(\xi) \xi^{2-k} d\xi, & \xi_{\text{mean}}(k)\alpha_{d,\min} < \alpha < \xi_{\text{mean}}(k)\alpha_{d,\max}, \\ 0 & \text{otherwise,} \end{cases} \quad (20)$$

which thanks to the definition of $\xi_{\text{mean}}(k)$ can also be written

$$b_{\text{appr}}(\alpha) = \begin{cases} \frac{\beta_{\text{tot}}}{I(\xi_{\text{mean}}(k)\alpha_{d,\min}, \xi_{\text{mean}}(k)\alpha_{d,\max}, k-2)} \alpha^{k-3}, & \xi_{\text{mean}}(k)\alpha_{d,\min} < \alpha < \xi_{\text{mean}}(k)\alpha_{d,\max}, \\ 0 & \text{otherwise.} \end{cases} \quad (21)$$

This choice of $b_{\text{appr}}(\alpha)$ has the advantages that the intervals in Formulas 5 and 21 are equally wide in a logarithmic sense and that

$$\int_0^\infty b_{\text{appr}}(\alpha) d\alpha = \int_0^\infty b(\alpha) d\alpha = \beta_{\text{tot}}. \quad (22)$$

Note the similarity between Formulas 5, 15 and 21.

The definition of $\xi_{\text{mean}}(k)$ in Formula 11, case $k \neq 2$, was chosen in order that Formula 22 should hold. When $k = 2$, Formula 22 would hold regardless of the value of $\xi_{\text{mean}}(k)$. The definition of $\xi_{\text{mean}}(k)$ in Formula 11, case $k = 2$, was chosen because

$$\lim_{k \rightarrow 2} \left(\int_0^\infty f(\xi) \xi^{2-k} d\xi \right)^{1/(2-k)} = \exp \int_0^\infty f(\xi) \ln \xi d\xi. \quad (23)$$

Let us summarize our results about the second way of obtaining $b(\alpha)$ as follows. Assume that $b(\alpha)$ is calculated from $b_d(\alpha_d)$ and $b_{\text{fo|d}}(\alpha | \alpha_d)$ using Formula 4. Assume that $b_d(\alpha_d)$ is given by Formula 5 and that $b_{\text{fo|d}}(\alpha | \alpha_d)$ has properties P_1 and $P_2(k)$, where k is the same as in Formula 5. Let $\xi_{\text{mean}}(k)$ be defined by Formula 11. Let $\epsilon > 0$ be some suitably small number. Assume that ξ_{\min} and ξ_{\max} can be chosen so that they are not too far apart and satisfy the conditions $0 < \xi_{\min} \leq \xi_{\text{mean}}(k) \leq \xi_{\max}$ and $\xi_{\max}\alpha_{d,\min} < \xi_{\min}\alpha_{d,\max}$ as well as the condition stated using Formulas 17 and 18. Then

$$b(\alpha) = \frac{\beta_{\text{tot}}}{I(\alpha_{d,\min}, \alpha_{d,\max}, k-2)} \alpha^{k-3} \int_{\alpha/\alpha_{d,\max}}^{\alpha/\alpha_{d,\min}} f(\xi) \xi^{2-k} d\xi, \quad (24)$$

where the integral satisfies Formula 19. Moreover, $b(\alpha)$ can be approximated by the function

$$b_{\text{appr}}(\alpha) = \begin{cases} \frac{\beta_{\text{tot}}}{I(\xi_{\text{mean}}(k)\alpha_{\text{d,min}}, \xi_{\text{mean}}(k)\alpha_{\text{d,max}}, k-2)} \alpha^{k-3}, & \xi_{\text{mean}}(k)\alpha_{\text{d,min}} < \alpha < \xi_{\text{mean}}(k)\alpha_{\text{d,max}}, \\ 0 & \text{otherwise,} \end{cases} \quad (25)$$

where $b_{\text{appr}}(\alpha)$ satisfies Formula 22.

6 A derivation of the power law distribution for diffusion rate from fracture properties

In this section we shall see how the power law distribution for diffusion rate, as given by Formula 5, can be obtained starting from a power law distribution for fracture size and other assumptions. There are many assumptions made in this section, and some of them are perhaps not realistic.

We assume that fractures are randomly and homogeneously distributed in the solid material surrounding the mobile zone. We assume that a length scale a can in some manner be associated with each fracture. The number $d^2 N$ of fractures with centres within a volume dV of surrounding material and with length scales in the interval $(a, a + da)$ is assumed to satisfy the power law formula

$$d^2 N \begin{cases} \propto a^{-D_f-1} da dV, & a_{\text{min}} < a < a_{\text{max}}, \\ = 0 & \text{otherwise,} \end{cases} \quad (26)$$

where “ \propto ” denotes proportionality. (Regarding the designation D_f see the end of this section.)

It is reasonable to assume that a fracture intersects the mobile zone if the distance from the centre of the fracture to the mobile zone is in the order of a or less. The number $d^2 N_{\text{im}}$ of fractures intersecting an area dA_m of the mobile zone and with length scales in the interval $(a, a + da)$ is therefore assumed to satisfy

$$d^2 N_{\text{im}} \propto a^{-D_f-1} da a dA_m = a^{-D_f} da dA_m. \quad (27)$$

(From now on, we do not mention the condition $a_{\text{min}} < a < a_{\text{max}}$ explicitly.)

To simplify the discussion we shall assume that the fractures in the material surrounding the mobile zone are not in direct contact with each other. (However, those of the fractures which intersect the mobile zone are in indirect contact with each other via the zone.) We shall also assume that fractures which intersect the mobile zone and which have the same length scale a have equal properties in other respects too.

In a fracture intersecting the mobile zone, let the immobile zone volume denote the volume of water in the fracture which is accessible to water and tracer in the mobile zone. The immobile zone is formed by the immobile zone volumes of all the fractures intersecting the mobile zone.

Consider the assumption that the volume of a fracture intersecting the mobile zone is proportional to $a^{\gamma+2}$. This should be the case if the length, width and thickness of the fracture were proportional to a , a and a^γ , respectively. We shall however instead assume that the capacity of the immobile zone volume of the fracture is proportional to $a^{\gamma+2}$. This assumption is perhaps less realistic, but it is necessary if we want to arrive at a power law distribution for the diffusion rate. Consider again the fractures intersecting the area dA_m of the mobile zone and with length scales in the interval $(a, a + da)$. It follows from our assumption (and from Formula 27) that the capacity $R_{im} d^2V_{im}$ of the immobile zone volume of these fractures satisfies

$$R_{im} d^2V_{im} \propto a^{\gamma+2} a^{-D_f} da dA_m = a^{\gamma-D_f+2} da dA_m. \quad (28)$$

(R_{im} and d^2V_{im} are explained in the following paragraph.)

Let R_m and $R_{im,tot}$ be the retardation factors for the mobile and immobile zones, respectively. The retardation factor for a zone specifies the ratio of the total amount of tracer (both dissolved and adsorbed) to the amount of dissolved tracer in the zone at equilibrium. Let dV_m be the volume of the mobile zone corresponding to the area dA_m . dA_m/dV_m is thus the area-to-volume ratio of the mobile zone. Let dV_{im} be the volume of the immobile zone in contact with the area dA_m of the mobile zone. The capacities of the two volumes can be expressed as $R_m dV_m$ and $R_{im,tot} dV_{im}$, which leads to the formula

$$\beta_{tot} = \frac{R_{im,tot} dV_{im}}{R_m dV_m}. \quad (29)$$

The analogous formula for the part of the immobile zone with length scales in the interval $(a, a + da)$ is

$$b_a(a) da = \frac{R_{im} d^2V_{im}}{R_m dV_m}, \quad (30)$$

where R_{im} may depend on a . We have here introduced the capacity ratio density function $b_a(a)$, which specifies how the total capacity ratio β_{tot} is distributed over the spectrum of length scales a . As usual,

$$\int_0^\infty b_a(a) da = \beta_{tot}. \quad (31)$$

Multiplication of Formulas 28 and 30 yields

$$b_a(a) \propto \frac{dA_m}{R_m dV_m} a^{\gamma-D_f+2}. \quad (32)$$

From Formulas 31 and 32 we get

$$\beta_{\text{tot}} \propto \frac{dA_m}{R_m dV_m} \quad (33)$$

and

$$b_a(a) = \begin{cases} \frac{\beta_{\text{tot}}}{I(a_{\min}, a_{\max}, \gamma - D_f + 3)} a^{\gamma - D_f + 2}, & a_{\min} < a < a_{\max}, \\ 0 & \text{otherwise,} \end{cases} \quad (34)$$

where we have taken the condition $a_{\min} < a < a_{\max}$ in Formula 26 into account.

We shall now set up a relation between a and the diffusion rate α_d (Formula 37), and using this relation we shall transform Formula 34 into the sought formula for the diffusion rate distribution $b_d(\alpha_d)$ (Formula 39).

As in Section 4 and in Ref. 2 we shall use the relation

$$\alpha_d \propto \frac{D_a}{a^2}, \quad (35)$$

where D_a is the apparent diffusivity in a fracture of the immobile zone. We shall also assume that

$$D_a \propto a^\Psi. \quad (36)$$

Combining these two formulas yields

$$\alpha_d \propto a^{\Psi-2}. \quad (37)$$

We also have the relation

$$b_d(\alpha_d)|d\alpha_d| = b_a(a)|da|, \quad (38)$$

as both sides express the same capacity ratio in different ways. (Absolute values have been taken since $d\alpha_d$ and da may have equal or opposite signs depending on Ψ .) With routine calculations, where Formulas 37 and 38 are used, we can transform Formula 34 into

$$b_d(\alpha_d) = \begin{cases} \frac{\beta_{\text{tot}}}{I(\alpha_{d,\min}, \alpha_{d,\max}, k - 2)} \alpha_d^{k-3}, & \alpha_{d,\min} < \alpha_d < \alpha_{d,\max}, \\ 0 & \text{otherwise,} \end{cases} \quad (39)$$

where

$$\frac{\alpha_{d,\max}}{\alpha_{d,\min}} = \left(\frac{a_{\max}}{a_{\min}} \right)^{|2-\Psi|} \quad (40)$$

(the exact values of $\alpha_{d,\min}$ and $\alpha_{d,\max}$ depend on the implicit proportionality constant in Formula 37),

$$k = \frac{D_f - \gamma - 2\Psi + 1}{2 - \Psi}, \quad (41)$$

and (from Formula 33)

$$\beta_{\text{tot}} \propto \frac{dA_m}{R_m dV_m}. \quad (42)$$

As Formula 39 is the same as Formula 5, we have now reached our goal to derive Formula 5 from our assumptions. Formulas 40, 41 and 42 can be used to calculate the parameters in Formula 5.

(In Ref. 3, Sections 3.1 and 5.7.2, and Ref. 4, Section 2.2.1, the designations D_f and D are used, respectively, and they are said to denote fractal dimension. Let us neglect fracture thickness in the present section's model of the fractures in the material surrounding the mobile zone, so that the fractures are regarded as surfaces with area proportional to a^2 . I believe that the use of D_f in this model is then similar to the use of D_f and D in Refs. 3 and 4. Probably there exist one or more exact definitions of the concept fractal dimension in the mathematical literature. I am not sure whether the use of D_f and D in the present section and Refs. 3 and 4 is in accord with those definitions.)

7 Practical use of the multirate model in computer simulations of tracer motion

In this section it will be discussed how the multirate model with a power law distribution can be included in computer simulations of tracer motion in fractured rock.

We assume that the domain of rock where tracer motion is to be simulated is divided into cells by a computational grid, as is usual in numerical calculations. We further assume that the domain can be divided into a number of subdomains, each consisting of a group of cells. The properties of the immobile zone are assumed to be similar in cells which belong to the same subdomain. What is meant by this similarity will be specified further on.

Section 2 starts, "consider a region of fractured rock". This region is the setting for all of Sections 2, 3, 4 and 5. In connection with the concepts introduced in the previous paragraph, it is suitable to assume that the region refers to any one of the cells. If we look at Section 2, β_{tot} , $b(\alpha)$, $b_d(\alpha_d)$ and $b_{\text{fo|d}}(\alpha | \alpha_d)$ then all refer to this cell. If we consider the entire domain, there is one β_{tot} , one $b(\alpha)$, one $b_d(\alpha_d)$ and one $b_{\text{fo|d}}(\alpha | \alpha_d)$ for each cell. However, as we have assumed that the cells of a subdomain have similar immobile zone properties, we shall assume that $b_{\text{fo|d}}(\alpha | \alpha_d)$ is equal in

all cells of the subdomain, while $b(\alpha)$ and $b_d(\alpha_d)$ are proportional to β_{tot} within the subdomain. In other words, each of the three functions $b(\alpha)/\beta_{\text{tot}}$, $b_d(\alpha_d)/\beta_{\text{tot}}$ and $b_{\text{fo|d}}(\alpha | \alpha_d)$ is equal for all cells in a subdomain but may vary between subdomains. In Section 3, $\alpha_{\text{d,min}}$, $\alpha_{\text{d,max}}$ and k are assumed to be constant within a subdomain, while β_{tot} and $b_d(\alpha_d)$ may vary between cells. It follows from Formula 5 that $b_d(\alpha_d)$ is proportional to β_{tot} within the subdomain. Regarding Section 4 it is sufficient to say that $b_{\text{fo|d}}(\alpha | \alpha_d)$ is assumed not to vary between the cells of a subdomain. In Section 5 two ways to obtain $b(\alpha)$ are discussed. In the paragraph about the first way, α_{min} , α_{max} and k are assumed to be constant and $b(\alpha)$ proportional to β_{tot} within a subdomain. What has been said above about Sections 3 and 4 is true also for the part of Section 5 discussing the second way.

Section 6 can also be read with the domain, subdomains and cells in mind. a_{min} , a_{max} , $\alpha_{\text{d,min}}$, $\alpha_{\text{d,max}}$, D_f , γ , Ψ , k and $R_{\text{im,tot}}$ should then be assumed to be constant within each subdomain. R_{im} and D_a may vary with a , but for fixed a they should be constant within a subdomain. The implicit proportionality constants in all the proportionality relations (i.e., formulas including “ \propto ”) in the section are also assumed to be constant within each subdomain. The number of fractures $d^2 N_{\text{im}}$, the area dA_m and the volumes dV_m , dV_{im} and $d^2 V_{\text{im}}$ are assumed to refer to any one cell and may vary between cells. dA_m is the area of the part of the mobile zone which belongs to the cell, for example. (However, it is better to assume that dV and $d^2 N$ in Formula 26 refer to an arbitrary volume within a subdomain.) R_m , β_{tot} , $b_a(a)$ and $b_d(\alpha_d)$ are also assumed to refer to a cell and may vary between cells. Formulas 34 and 39 show that $b_a(a)$ and $b_d(\alpha_d)$ are proportional to β_{tot} within a subdomain.

We shall now discuss possible ways to choose a multirate model for inclusion in computer simulations of tracer motion.

The task amounts to choosing a function $b(\alpha)$ for each cell. We shall treat each subdomain separately, so let us focus on one subdomain. Let us decide that each $b(\alpha)$ shall be of the form given in Formula 15. As has already been said, α_{min} , α_{max} and k are assumed to be constant within the subdomain while β_{tot} may vary from cell to cell. The remaining problem is to choose these parameters. When doing this it is possible to use more or less of the theory presented in this paper. If as much as possible of the theory is to be used, we can proceed as follows.

Following Section 6, we assume that dA_m , dV_m and R_m are somehow known for each cell in the subdomain. β_{tot} can then be calculated for each cell using Formula 42, provided that we can somehow choose the implicit proportionality constant. (If dA_m and dV_m are known for each cell, a possible way to calculate R_m is to use the relation $(R_m - 1) dV_m \propto dA_m$.) Let us also assume that the constants a_{min} , a_{max} , D_f , γ and Ψ are known, as well as the implicit proportionality constant in Formula 37. $\alpha_{\text{d,min}}$ and $\alpha_{\text{d,max}}$ can then be calculated using Formula 37, and k using Formula 41. $b_d(\alpha_d)$

for each cell will then be given by Formula 39 or Formula 5.

Following Section 4, we must choose $b_{\text{fo|d}}(\alpha | \alpha_d)$, which should be the same for all cells in the subdomain. $b_{\text{fo|d}}(\alpha | \alpha_d)$ should have properties P_1 and $P_2(k)$. Formulas 12, 13 and 14 are possible choices, provided that $k > 3/2$. (The choice of $b_{\text{fo|d}}(\alpha | \alpha_d)$ may influence the already mentioned choice of the implicit proportionality constant in Formula 37.) $\xi_{\text{mean}}(k)$ should also be calculated using Formula 11. I believe that this calculation may have to be done numerically.

Now we have both $b_d(\alpha_d)$ and $b_{\text{fo|d}}(\alpha | \alpha_d)$, and $b(\alpha)$ could then be calculated using Formula 4. But then $b(\alpha)$ would not generally have the form given in Formula 15. However, if the conditions stated in Section 5 are fulfilled, we can use $b_{\text{appr}}(\alpha)$ given by Formula 21 instead of the $b(\alpha)$ of Formula 4. The sought α_{min} and α_{max} will then be given by $\alpha_{\text{min}} = \xi_{\text{mean}}(k)\alpha_{d,\text{min}}$ and $\alpha_{\text{max}} = \xi_{\text{mean}}(k)\alpha_{d,\text{max}}$. We have already obtained k and β_{tot} , and therefore we now know all parameters for the multirate model for the subdomain.

References

1. R. Haggerty and S. M. Gorelick. Multiple-rate mass transfer for modeling diffusion and surface reactions in media with pore-scale heterogeneity. *Water Resources Research*, 31(10):2383–2400, 1995.
2. R. Haggerty, S. A. McKenna and L. C. Meigs. On the late-time behavior of tracer test breakthrough curves. *Water Resources Research*, 36(12):3467–3479, 2000.
3. M. Sahimi. *Flow and Transport in Porous Media and Fractured Rock. From Classical Methods to Modern Approaches*. VCH Verlagsgesellschaft mbH, Weinheim, 1995.
4. P. R. LaPointe, T. Cladouhos and S. Follin. *Calculation of displacements on fractures intersecting canisters induced by earthquakes: Aberg, Beberg and Ceberg examples*. Technical Report TR-99-03. Svensk Kärnbränslehantering AB, Stockholm, January 1999.

APPENDIX C A numerical method for generating a two-dimensional set of random numbers with a certain multivariate normal distribution

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This report describes a numerical method for generating a two-dimensional set of random numbers with a multivariate normal distribution characterized by a certain covariance structure.

A reader who only wants to learn the numerical method and the character of the random numbers that can be calculated using it can read Chapters 1–8 straight through and skip the appendices. A reader who is also interested in derivations should read the entire report, in which case the following order is recommended: Chapters 1–3, Appendix A, Chapters 4–7, Appendix B, Chapter 8, Appendix C.

In this chapter we shall introduce the concept of multivariate normal distribution.

Let n and m be non-negative integers, and let a_{ij} , $1 \leq i \leq n$, $1 \leq j \leq m$, and b_i , $1 \leq i \leq n$, be real numbers. Consider the joint probability distribution of the n stochastic variables $Y_i = \sum_{j=1}^m a_{ij} X_j + b_i$, $1 \leq i \leq n$, where X_j , $1 \leq j \leq m$, are independent stochastic variables with a standard normal distribution, i.e. a normal distribution with expected value 0 and standard deviation 1. This joint probability distribution will depend on the choice of n , m , a_{ij} , $1 \leq i \leq n$, $1 \leq j \leq m$, and b_i , $1 \leq i \leq n$.

Now consider the totality of joint probability distributions obtained from all possible choices of n , m , a_{ij} , $1 \leq i \leq n$, $1 \leq j \leq m$, and b_i , $1 \leq i \leq n$, as described in the previous paragraph. These distributions are called “multivariate normal distributions”.

The following theorem is an elementary result about multivariate normal distributions: Let n be a non-negative integer, let X_i , $1 \leq i \leq n$, be stochastic variables with a multivariate normal distribution, and let also Y_i , $1 \leq i \leq n$, be stochastic variables with a multivariate normal distribution. If $E[X_i] = E[Y_i]$, $1 \leq i \leq n$, and $\text{Cov}(X_{i_1}, X_{i_2}) = \text{Cov}(Y_{i_1}, Y_{i_2})$, $1 \leq i_1, i_2 \leq n$, then the two multivariate normal distributions are the same. In other words, a multivariate normal distribution is completely characterized by its expected values and covariances.

Multivariate normal distributions are discussed in Ross (1985), p. 65–68.

DEFINITION SET 1

The definitions in this chapter shall be valid in some parts of the report. In those parts, it will be explicitly stated that the definitions in this chapter shall be valid.

Let x_0, y_0, a and b be real numbers which satisfy $a, b > 0$ and $x_0^2 + y_0^2 = a^2 - b^2$.

Define the quadratic form Q by letting

$$Q(x, y) = \frac{(b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2}{a^2b^2}$$

for all real numbers x and y .

Definition set 1 shall be valid in this chapter.

In this chapter we shall become a little familiar with the quadratic form Q .

With regard to the result of Section A.2, it is clear that $Q(x, y) \geq 0$ for all x and y , equality holding precisely when $x, y = 0$.

In Section A.4 it is shown that the equation $Q(x, y) = 1$ describes an ellipse with foci $(-x_0, -y_0)$ and (x_0, y_0) and half axis lengths a and b .

More generally, in Section A.5 it is shown that for every real number $d > 0$ the equation $Q(x, y) = d^2$ describes an ellipse which has the same centre, orientation and shape but which is d times as large as the one described by $Q(x, y) = 1$.

Definition set 1 shall be valid in this chapter.

Consider the following problem: Let n_r and n_k be non-negative integers.

Construct a numerical method for generating random numbers

H_{rk} , $1 \leq r \leq n_r$, $1 \leq k \leq n_k$, (H_{rk} are treated formally as stochastic variables here)

which have a multivariate normal distribution characterized by

$$E[H_{rk}] = 0, \quad 1 \leq r \leq n_r, \quad 1 \leq k \leq n_k,$$

$$\text{Cov}(H_{r_1 k_1}, H_{r_2 k_2}) = \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right), \quad 1 \leq r_1, r_2 \leq n_r, \quad 1 \leq k_1, k_2 \leq n_k.$$

We shall not give an exact solution to this problem in the report. However, in Chapter 6 a variant of this problem where the covariances are only specified approximately will be given, and in Chapter 8 a solution to this approximate problem will be given.

Definition set 1 shall be valid in this chapter.

The approximate version of the numerical problem is the following: Let n_r and n_k be non-negative integers, and let \mathbf{e} be a positive real number. Construct a numerical method for generating random numbers H_{rk} , $1 \leq r \leq n_r$, $1 \leq k \leq n_k$, which have a multivariate normal distribution which satisfies

$$E[H_{rk}] = 0, \quad 1 \leq r \leq n_r, \quad 1 \leq k \leq n_k,$$

$$\text{Var}(H_{rk}) = 1, \quad 1 \leq r \leq n_r, \quad 1 \leq k \leq n_k,$$

$$\left| \text{Cov}(H_{r_1 k_1}, H_{r_2 k_2}) - \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \right| \leq \mathbf{e}, \quad 1 \leq r_1, r_2 \leq n_r, \quad 1 \leq k_1, k_2 \leq n_k.$$

DEFINITION SET 2

The definitions in this chapter shall be valid in some parts of the report. In those parts, it will be explicitly stated that the definitions in this chapter shall be valid.

The definitions in this chapter are given under the assumption that definition set 1 is valid, as the entities introduced there are referred to here. In those parts of the report where definition set 2 will be valid, definition set 1 will also be valid.

Numbers which can be written as integers divided by 2 we shall call “half-integers”. (If this is a standard term I do not know.) As Z normally denotes the set of integers, let $Z_{1/2}$ denote the set of half-integers. If e.g. r_0 is a half-integer variable and r_{0l} and r_{0h} are half-integers, the expression $r_{0l} \leq r_0 \leq r_{0h} (1/2)$ shall mean that r_0 shall assume all half-integer values from r_{0l} to r_{0h} .

Let x_h and y_h be non-negative half-integers.

Let

$$M_n = \left\{ (x, y) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}} \mid |x| \leq x_h \wedge |y| \leq y_h \right\},$$

$$M_f = \left\{ (x, y) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}} \mid |x| > x_h \vee |y| > y_h \right\},$$

i.e. M_n is the set of those half-integer pairs in which the absolute value of the first half-integer is less than or equal to x_h and the absolute value of the second half-integer is less than or equal to y_h , and M_f is the set of those half-integer pairs that do not belong to M_n . “n” and “f” stand for “near” and “far”, respectively.

In the report expressions like $(r, k) - M_n$, where r and k are integers, will occur. $(r, k) - M_n$ means the set of half-integer pairs which can be written as differences between (r, k) and elements in M_n .

Let

$$s_n = \sqrt{\sum_{(x,y) \in M_n} \exp(-2Q(x, y))},$$

$$s_f = \sqrt{\sum_{(x,y) \in M_f} \exp(-2Q(x, y))}.$$

In the sum in the definition of \mathbf{s}_n , the term $\exp(-2Q(0, 0)) = \exp(-2 \times 0) = 1$ is always present, and all terms are positive, so $\mathbf{s}_n \geq 1$. The definition of \mathbf{s}_f is correct because the infinite series converges, which is shown in Section B.4.

Definition sets 1 and 2 shall be valid in this chapter. We also keep the definitions from Chapter 6.

The following is a solution to the approximate numerical problem:

Let

$$d = \max \left(\frac{1}{\sqrt{2} \times b}, \frac{1}{2\sqrt{2} \times b} + \sqrt{\max \left(0, \ln \frac{2\sqrt{pab}}{\min \left(\frac{e}{3}, \frac{1}{2} \right)} \right)} \right),$$

and let x_h and y_h be the smallest half-integers that still satisfy

$$x_h \geq d\sqrt{b^2 + x_0^2} - \frac{1}{4}, \quad y_h \geq d\sqrt{b^2 + y_0^2} - \frac{1}{4}.$$

Let $F_{r_0 k_0}$, $1 - x_h \leq r_0 \leq n_r + x_h(1/2)$, $1 - y_h \leq k_0 \leq n_k + y_h(1/2)$, be independent random numbers with a standard normal distribution — these can be easily generated on a computer. Let

$$H_{rk} = \frac{\sum_{(r_0, k_0) \in (r, k) - M_n} (\exp(-Q(r - r_0, k - k_0)) \times F_{r_0 k_0})}{S_n}, \quad 1 \leq r \leq n_r, 1 \leq k \leq n_k.$$

The joint probability distribution of the H_{rk} will then meet the specifications given in Chapter 6.

A derivation of this solution is given in Appendix C.

APPENDIX A: PROPERTIES OF THE QUADRATIC FORM Q

A.1 Introduction

Throughout this appendix, definition set 1 shall be valid.

In this appendix, various properties of the quadratic form Q will be deduced. The results of the appendix are used in different parts of the report.

A.2

$$(x^2 + y^2)/a^2 \leq Q(x, y) \leq (x^2 + y^2)/b^2$$

In this section we shall show that

$$\frac{x^2 + y^2}{a^2} \leq Q(x, y) \leq \frac{x^2 + y^2}{b^2}$$

for all real numbers x and y .

Indeed, we have

$$-(y_0x - x_0y)^2 \leq 0 \leq (x_0x + y_0y)^2$$

$$-y_0^2x^2 + 2x_0y_0xy - x_0^2y^2 \leq 0 \leq x_0^2x^2 + 2x_0y_0xy + y_0^2y^2$$

$$b^2(x^2 + y^2) \leq (b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2 \leq (b^2 + x_0^2 + y_0^2)(x^2 + y^2)$$

$$b^2(x^2 + y^2) \leq (b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2 \leq a^2(x^2 + y^2)$$

$$\frac{x^2 + y^2}{a^2} \leq Q(x, y) \leq \frac{x^2 + y^2}{b^2}.$$

A.3

$$x^2 \leq (b^2 + x_0^2)Q(x, y) \text{ and } y^2 \leq (b^2 + y_0^2)Q(x, y)$$

In this section we shall show that

$$x^2 \leq (b^2 + x_0^2)Q(x, y), \quad y^2 \leq (b^2 + y_0^2)Q(x, y)$$

for all real numbers x and y .

To show the first inequality, we have

$$\frac{(b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2}{a^2b^2} = Q(x, y)$$

$$\frac{(b^2 + x_0^2)((b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2)}{a^2b^2} = (b^2 + x_0^2)Q(x, y)$$

$$\frac{(b^2 + x_0^2 + y_0^2)b^2x^2 + x_0^2y_0^2x^2 - 2(b^2 + x_0^2)x_0y_0xy + (b^2 + x_0^2)^2y^2}{a^2b^2} = (b^2 + x_0^2)Q(x, y)$$

$$\frac{a^2b^2x^2 + (x_0y_0x - (b^2 + x_0^2)y)^2}{a^2b^2} = (b^2 + x_0^2)Q(x, y)$$

$$x^2 \leq (b^2 + x_0^2)Q(x, y).$$

The second inequality can be shown analogously.

A.4 $Q(x, y) = 1$ describes an ellipse

In this section we shall show that the equation $Q(x, y) = 1$ describes an ellipse with foci $(-x_0, -y_0)$ and (x_0, y_0) and half-axis lengths a and b .

Consider the following sequence of equations:

$$Q(x, y) = 1$$

$$\Downarrow$$

$$(b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2 = a^2b^2$$

$$\Downarrow$$

$$(a^2 - x_0^2)x^2 - 2x_0y_0xy + (a^2 - y_0^2)y^2 = a^2(a^2 - x_0^2 - y_0^2)$$

$$\Downarrow$$

$$a^2(x^2 \pm 2x_0x + x_0^2 + y^2 \pm 2y_0y + y_0^2) = a^4 \pm 2a^2(x_0x + y_0y) + x_0^2x^2 + 2x_0y_0xy + y_0^2y^2$$

$$\Downarrow$$

$$a^2((x \pm x_0)^2 + (y \pm y_0)^2) = (a^2 \pm (x_0x + y_0y))^2$$

$$\Uparrow$$

$$a\sqrt{(x \pm x_0)^2 + (y \pm y_0)^2} = a^2 \pm (x_0x + y_0y)$$

$$\Downarrow$$

$$4a\sqrt{(x \pm x_0)^2 + (y \pm y_0)^2} = 4a^2 + (x \pm x_0)^2 + (y \pm y_0)^2 - (x \mp x_0)^2 - (y \mp y_0)^2$$

$$\Downarrow$$

$$\begin{aligned}
& 2a\left(\sqrt{(x+x_0)^2+(y+y_0)^2}+\sqrt{(x-x_0)^2+(y-y_0)^2}+\right. \\
& \left.+\sqrt{(x\pm x_0)^2+(y\pm y_0)^2}-\sqrt{(x\mp x_0)^2+(y\mp y_0)^2}\right)= \\
& =4a^2+\left(\sqrt{(x\pm x_0)^2+(y\pm y_0)^2}-\sqrt{(x\mp x_0)^2+(y\mp y_0)^2}\right)\times \\
& \times\left(\sqrt{(x+x_0)^2+(y+y_0)^2}+\sqrt{(x-x_0)^2+(y-y_0)^2}\right) \\
& \quad \Downarrow \\
& 0=\left(2a-\sqrt{(x\pm x_0)^2+(y\pm y_0)^2}+\sqrt{(x\mp x_0)^2+(y\mp y_0)^2}\right)\times \\
& \times\left(2a-\sqrt{(x+x_0)^2+(y+y_0)^2}-\sqrt{(x-x_0)^2+(y-y_0)^2}\right) \\
& \quad \Uparrow \\
& 0=2a-\sqrt{(x+x_0)^2+(y+y_0)^2}-\sqrt{(x-x_0)^2+(y-y_0)^2} \\
& \quad \Downarrow \\
& \sqrt{(x+x_0)^2+(y+y_0)^2}+\sqrt{(x-x_0)^2+(y-y_0)^2}=2a
\end{aligned}$$

Obvious equivalences and implications have been indicated with arrows. Each equation containing “ \pm ” or “ \mp ” signs is to be regarded as the statement that both versions of the equation hold. Because of the direction of the two implication arrows, it is clear that the last equation in the sequence implies the first one. However, the first one also implies the last one, which we shall show here. Start by assuming that the first equation holds. Then the fifth equation must also hold. Moreover, in Section A.2 it is shown that $(x^2+y^2)/a^2 \leq Q(x,y)$. As $Q(x,y)=1$, we have $\sqrt{x^2+y^2} \leq a$. As $x_0^2+y_0^2=a^2-b^2$, we also have $\sqrt{x_0^2+y_0^2} \leq a$. Now the Schwarz inequality gives us $|x_0x+y_0y| \leq \sqrt{x_0^2+y_0^2} \times \sqrt{x^2+y^2} \leq a \times a = a^2$, which in turn yields $0 \leq a^2 \pm (x_0x+y_0y)$. Together with this fact, the fifth equation gives us the sixth one. Adding together the two versions of this equation and dividing the sum equation by a directly gives us the last equation.

As the first and the last equation in the sequence are thus equivalent, it only remains to show that the last equation describes the specified ellipse.

An ellipse can be defined as the set of those points whose distances to two given points, the foci of the ellipse, have a constant given sum. This is indeed expressed by the last equation of the sequence, if $(-x_0,-y_0)$ and (x_0,y_0) are the foci and $2a$

is the total distance. Imagining an ellipse, one can see that the total distance is equal to the length of the long axis of the ellipse, and one can also see that half the interfocal distance, half the short axis and half the given total distance form a right triangle. The half long axis length must therefore be a , and the half short axis length must be $\sqrt{a^2 - \left(\sqrt{x_0^2 + y_0^2}\right)^2} = \sqrt{a^2 - x_0^2 - y_0^2} = b$.

A.5 $Q(x, y) = d^2$ also describes an ellipse

In this section we shall show that for every real number $d > 0$ the equation $Q(x, y) = d^2$ describes an ellipse which has the same centre $(x, y = 0)$, orientation and shape but which is d times as large as the one described by $Q(x, y) = 1$. (The ellipse $Q(x, y) = 1$ is discussed in the previous section.)

We can convince ourselves that the ellipse mentioned which is d times as large as the $Q(x, y) = 1$ one, must be described by the equation $Q(x/d, y/d) = 1$. However, this equation is equivalent to $Q(x, y) = d^2$, which is easily seen on inspection of the definition of Q .

A.6 Linear transformation between (x, y) and (ξ, η) coordinates

In this section we shall introduce a coordinate transformation and determine some of its properties.

Define

$$t_{x\xi} = \frac{b^2 + x_0^2 + ab}{a + b}, \quad t_{x\eta} = \frac{x_0 y_0}{a + b},$$

$$t_{y\xi} = \frac{x_0 y_0}{a + b}, \quad t_{y\eta} = \frac{b^2 + y_0^2 + ab}{a + b},$$

and introduce a linear transformation from new coordinates ξ and η to the old ones x and y by

$$x = t_{x\xi}\xi + t_{x\eta}\eta, \quad y = t_{y\xi}\xi + t_{y\eta}\eta.$$

The area scale of the transformation is

$$\begin{aligned} t_{x\xi}t_{y\eta} - t_{x\eta}t_{y\xi} &= \\ &= \frac{(b^2 + x_0^2 + ab)(b^2 + y_0^2 + ab) - x_0 y_0 x_0 y_0}{(a + b)^2} = \end{aligned}$$

$$\begin{aligned}
&= \frac{(b^2 + x_0^2 + y_0^2 + b^2 + ab)ab + (b^2 + x_0^2 + y_0^2)b^2}{(a+b)^2} = \\
&= \frac{(a^2 + b^2 + ab)ab + a^2b^2}{(a+b)^2} = \frac{(a^2 + 2ab + b^2)ab}{(a+b)^2} = ab.
\end{aligned}$$

I.e., if a variable substitution in a double integral is to be made, the formula

$$dx dy = ab d\mathbf{x}d\mathbf{h}$$

should be used.

We have

$$\begin{aligned}
t_{yh}x - t_{xh}y &= t_{yh}(t_{xx}\mathbf{x} + t_{xh}\mathbf{h}) - t_{xh}(t_{yx}\mathbf{x} + t_{yh}\mathbf{h}) = \\
&= (t_{xx}t_{yh} - t_{xh}t_{yx})\mathbf{x} = ab\mathbf{x}, \\
-t_{yx}x + t_{xx}y &= -t_{yx}(t_{xx}\mathbf{x} + t_{xh}\mathbf{h}) + t_{xx}(t_{yx}\mathbf{x} + t_{yh}\mathbf{h}) = \\
&= (t_{xx}t_{yh} - t_{xh}t_{yx})\mathbf{h} = ab\mathbf{h},
\end{aligned}$$

so the inverse transformation is given by

$$\mathbf{x} = \frac{t_{yh}x - t_{xh}y}{ab}, \quad \mathbf{h} = \frac{-t_{yx}x + t_{xx}y}{ab}.$$

We have

$$\begin{aligned}
t_{xx}^2 + t_{xh}^2 &= \frac{(b^2 + x_0^2 + ab)^2 + (x_0y_0)^2}{(a+b)^2} = \\
&= \frac{(b^2 + x_0^2)(b^2 + 2ab) + (b^2 + x_0^2)x_0^2 + a^2b^2 + x_0^2y_0^2}{(a+b)^2} = \\
&= \frac{(b^2 + x_0^2)(b^2 + 2ab) + (b^2 + x_0^2 + y_0^2)x_0^2 + a^2b^2}{(a+b)^2} = \\
&= \frac{(b^2 + x_0^2)(b^2 + 2ab) + a^2x_0^2 + a^2b^2}{(a+b)^2} =
\end{aligned}$$

$$\begin{aligned}
&= \frac{(b^2 + x_0^2)(a^2 + 2ab + b^2)}{(a+b)^2} = b^2 + x_0^2, \\
t_{xx}t_{yx} + t_{xh}t_{yh} &= \frac{(b^2 + x_0^2 + ab)x_0y_0 + x_0y_0(b^2 + y_0^2 + ab)}{(a+b)^2} = \\
&= \frac{(b^2 + x_0^2 + y_0^2 + 2ab + b^2)x_0y_0}{(a+b)^2} = \frac{(a^2 + 2ab + b^2)x_0y_0}{(a+b)^2} = x_0y_0, \\
t_{yx}^2 + t_{yh}^2 &= \frac{(x_0y_0)^2 + (b^2 + y_0^2 + ab)^2}{(a+b)^2} = \\
&= \frac{x_0^2y_0^2 + (b^2 + y_0^2)(b^2 + 2ab) + (b^2 + y_0^2)y_0^2 + a^2b^2}{(a+b)^2} = \\
&= \frac{(b^2 + y_0^2)(b^2 + 2ab) + (b^2 + x_0^2 + y_0^2)y_0^2 + a^2b^2}{(a+b)^2} = \\
&= \frac{(b^2 + y_0^2)(b^2 + 2ab) + a^2y_0^2 + a^2b^2}{(a+b)^2} = \\
&= \frac{(b^2 + y_0^2)(a^2 + 2ab + b^2)}{(a+b)^2} = b^2 + y_0^2,
\end{aligned}$$

and therefore

$$\begin{aligned}
\mathbf{x}^2 + \mathbf{h}^2 &= \left(\frac{t_{yh}x - t_{xh}y}{ab} \right)^2 + \left(\frac{-t_{yx}x + t_{xx}y}{ab} \right)^2 = \\
&= \frac{(t_{yx}^2 + t_{yh}^2)x^2 - 2(t_{xx}t_{yx} + t_{xh}t_{yh})xy + (t_{xx}^2 + t_{xh}^2)y^2}{a^2b^2} = \\
&= \frac{(b^2 + y_0^2)x^2 - 2x_0y_0xy + (b^2 + x_0^2)y^2}{a^2b^2} = Q(x, y).
\end{aligned}$$

A.7 Identity with four Q

In this section we shall show that

$$Q(x_1 + x_2, y_1 + y_2) + Q(x_2 - x_1, y_2 - y_1) = 2(Q(x_1, y_1) + Q(x_2, y_2))$$

for all real numbers x_1, y_1, x_2 and y_2 .

Using the coordinate transformation in Section A.6, we let (x_1, y_1) and (x_2, y_2) correspond to $(\mathbf{x}_1, \mathbf{h}_1)$ and $(\mathbf{x}_2, \mathbf{h}_2)$, respectively. As the transformation is linear, $(x_1 + x_2, y_1 + y_2)$ and $(x_2 - x_1, y_2 - y_1)$ will then correspond to $(\mathbf{x}_1 + \mathbf{x}_2, \mathbf{h}_1 + \mathbf{h}_2)$ and $(\mathbf{x}_2 - \mathbf{x}_1, \mathbf{h}_2 - \mathbf{h}_1)$, respectively. With the new coordinates the above equation can be written

$$(\mathbf{x}_1 + \mathbf{x}_2)^2 + (\mathbf{h}_1 + \mathbf{h}_2)^2 + (\mathbf{x}_2 - \mathbf{x}_1)^2 + (\mathbf{h}_2 - \mathbf{h}_1)^2 = 2(\mathbf{x}_1^2 + \mathbf{h}_1^2 + \mathbf{x}_2^2 + \mathbf{h}_2^2),$$

which is an obvious identity.

A.8 Triangle inequality with Q

In this section we shall show that

$$\left| \sqrt{Q(x_2, y_2)} - \sqrt{Q(x_1, y_1)} \right| \leq \sqrt{Q(x_2 - x_1, y_2 - y_1)},$$

$$\sqrt{Q(x_1 + x_2, y_1 + y_2)} \leq \sqrt{Q(x_1, y_1)} + \sqrt{Q(x_2, y_2)}$$

for all real numbers x_1, y_1, x_2 and y_2 .

Changing to new coordinates as in the previous section, the above inequalities can be written

$$\left| \sqrt{\mathbf{x}_2^2 + \mathbf{h}_2^2} - \sqrt{\mathbf{x}_1^2 + \mathbf{h}_1^2} \right| \leq \sqrt{(\mathbf{x}_2 - \mathbf{x}_1)^2 + (\mathbf{h}_2 - \mathbf{h}_1)^2},$$

$$\sqrt{(\mathbf{x}_1 + \mathbf{x}_2)^2 + (\mathbf{h}_1 + \mathbf{h}_2)^2} \leq \sqrt{\mathbf{x}_1^2 + \mathbf{h}_1^2} + \sqrt{\mathbf{x}_2^2 + \mathbf{h}_2^2}.$$

These inequalities are the well-known triangle inequality in two dimensions, which we do not prove here.

APPENDIX B: PROPERTIES OF S_f

B.1 Introduction

Throughout this appendix, definition sets 1 and 2 shall be valid.

In this appendix, a few properties of S_f will be deduced. The results of the appendix are used in Chapter 7 and Appendix C.

B.2 An upper estimation of an integral

In this section we shall show that if c and d are real numbers which satisfy $0 < c \leq d/2$, then

$$\begin{aligned} & \iint_{Q(x,y) \geq d^2} \exp\left(-2\left(\sqrt{Q(x,y)} - c\right)^2\right) \times dx dy \leq \\ & \leq pab \exp\left(-2(d-c)^2\right). \end{aligned}$$

Indeed, we have

$$\begin{aligned} & \iint_{Q(x,y) \geq d^2} \exp\left(-2\left(\sqrt{Q(x,y)} - c\right)^2\right) \times dx dy = \\ & = [\text{substitution from } x, y \text{ to } \mathbf{x}, \mathbf{h} \text{ as described in Section A.6}] = \\ & = \iint_{x^2+h^2 \geq d^2} \exp\left(-2\left(\sqrt{x^2+h^2} - c\right)^2\right) \times ab d\mathbf{x}d\mathbf{h} = \\ & = [\mathbf{x} = r \cos \mathbf{j}, \mathbf{h} = r \sin \mathbf{j}, d\mathbf{x}d\mathbf{h} = r d\mathbf{j} dr] = \\ & = ab \int_d^\infty \int_0^{2p} \exp\left(-2(r-c)^2\right) \times r d\mathbf{j} dr = \\ & = 2pab \int_d^\infty \frac{r}{r-c} (r-c) \exp\left(-2(r-c)^2\right) \times dr \leq \\ & \leq pab \int_d^\infty 4(r-c) \exp\left(-2(r-c)^2\right) \times dr = \end{aligned}$$

$$= \mathbf{pab} \left[- \exp(-2(\mathbf{r} - c)^2) \right]_d^\infty = \mathbf{pab} \exp(-2(d - c)^2),$$

because $\mathbf{r}/(\mathbf{r} - c) \leq 2$ when $\mathbf{r} \geq 2c$.

B.3 A sufficient condition that $\mathbf{s}_f \leq d$

In this section we shall show that for any given real number $\mathbf{d} > 0$, if we choose the real number d and the half-integers x_h and y_h so that they satisfy

$$d \geq \frac{1}{\sqrt{2} \times b}, \quad 4\mathbf{pab} \exp\left(-2\left(d - \frac{1}{2\sqrt{2} \times b}\right)^2\right) \leq \mathbf{d}^2,$$

$$x_h + \frac{1}{4} \geq d\sqrt{b^2 + x_0^2}, \quad y_h + \frac{1}{4} \geq d\sqrt{b^2 + y_0^2},$$

then $\mathbf{s}_f \leq \mathbf{d}$.

Indeed, we have

$$\begin{aligned} \mathbf{s}_f^2 &= \sum_{(x', y') \in M_f} \exp(-2Q(x', y')) = \\ &= \sum_{(x', y') \in M_f} 4 \int_{y' - \frac{1}{4}}^{y' + \frac{1}{4}} \int_{x' - \frac{1}{4}}^{x' + \frac{1}{4}} \exp(-2Q(x', y')) \times dx dy \leq \\ &\leq [\text{comment 1}] \leq \\ &\leq 4 \sum_{(x', y') \in M_f} \int_{y' - \frac{1}{4}}^{y' + \frac{1}{4}} \int_{x' - \frac{1}{4}}^{x' + \frac{1}{4}} \exp\left(-2\left(\sqrt{Q(x, y)} - \frac{1}{2\sqrt{2} \times b}\right)^2\right) \times dx dy = \\ &= 4 \iint_{|x| \geq x_h + \frac{1}{4} \vee |y| \geq y_h + \frac{1}{4}} \exp\left(-2\left(\sqrt{Q(x, y)} - \frac{1}{2\sqrt{2} \times b}\right)^2\right) \times dx dy \leq \\ &\leq [\text{comment 2}] \leq \\ &\leq 4 \iint_{Q(x, y) \geq d^2} \exp\left(-2\left(\sqrt{Q(x, y)} - \frac{1}{2\sqrt{2} \times b}\right)^2\right) \times dx dy \leq \end{aligned}$$

$$\leq [\text{comment 3}] \leq 4\mathbf{pab} \exp\left(-2\left(d - \frac{1}{2\sqrt{2}\times b}\right)^2\right) \leq \mathbf{d}^2,$$

i.e. $\mathbf{s}_f \leq \mathbf{d}$. However, some of the above steps need comments:

Comment 1. Because $|x - x'| \leq 1/4$ and $|y - y'| \leq 1/4$, $(x - x')^2 + (y - y')^2 \leq 1/8$. According to Section A.2, $Q(x - x', y - y') \leq ((x - x')^2 + (y - y')^2)/b^2$. According to Section A.8, $\sqrt{Q(x', y')} \geq |\sqrt{Q(x, y)} - \sqrt{Q(x - x', y - y')}|$. Using these facts, we have

$$\begin{aligned} \sqrt{Q(x', y')} &\geq |\sqrt{Q(x, y)} - \sqrt{Q(x - x', y - y')}| \geq \\ &\geq \sqrt{Q(x, y)} - \sqrt{Q(x - x', y - y')} \geq \sqrt{Q(x, y)} - \frac{\sqrt{(x - x')^2 + (y - y')^2}}{b} \geq \\ &\geq \sqrt{Q(x, y)} - \frac{1}{2\sqrt{2}\times b}. \end{aligned}$$

Because $(x', y') \in M_f$, $|x'| > x_h$ or $|y'| > y_h$. As x', x_h, y' and y_h are half-integers, $|x'| \geq x_h + 1/2$ or $|y'| \geq y_h + 1/2$ must hold. As $|x - x'| \leq 1/4$ and $|y - y'| \leq 1/4$, $|x| \geq x_h + 1/4$ or $|y| \geq y_h + 1/4$ must hold. According to comment 2, then $Q(x, y) \geq d^2$ must hold. As d satisfies $d \geq 1/(\sqrt{2}\times b)$, we have

$$\sqrt{Q(x, y)} \geq d \geq \frac{1}{\sqrt{2}\times b} > \frac{1}{2\sqrt{2}\times b}.$$

The above inequality $\sqrt{Q(x', y')} \geq \sqrt{Q(x, y)} - 1/(2\sqrt{2}\times b)$ can therefore be squared, and we obtain

$$Q(x', y') \geq \left(\sqrt{Q(x, y)} - \frac{1}{2\sqrt{2}\times b}\right)^2.$$

Comment 2. We shall show that if $|x| \geq x_h + 1/4$ or $|y| \geq y_h + 1/4$, then $Q(x, y) \geq d^2$. In fact, remembering that $x_h + 1/4 \geq d\sqrt{b^2 + x_0^2}$ and $y_h + 1/4 \geq d\sqrt{b^2 + y_0^2}$, we can conclude that $x^2/(b^2 + x_0^2) \geq d^2$ or $y^2/(b^2 + y_0^2) \geq d^2$. However, according to Section A.3 $Q(x, y)$ is greater than or equal to both $x^2/(b^2 + x_0^2)$ and $y^2/(b^2 + y_0^2)$. Therefore $Q(x, y) \geq d^2$ must hold in both cases.

Comment 3. The inequality follows directly from what is shown in Section B.2.

B.4 \mathbf{s}_f is finite for all x_h and y_h

Consider the definition of \mathbf{s}_f :

$$\mathbf{s}_f = \sqrt{\sum_{(x,y) \in M_f} \exp(-2Q(x,y))}.$$

In order that the definition shall be valid, it is necessary that the infinite series in the definition converges. This is indeed the case, as we shall show in this section.

For any choice of the non-negative half-integers x_h and y_h , M_f will contain all but a finite number of the elements of $Z_{1/2} \times Z_{1/2}$. Therefore, either the series will converge for all choices of x_h and y_h , or it will diverge for all choices. But in Section B.3 it was shown that if sufficiently large x_h and y_h values are chosen, the series will converge. Thus, the series will converge for all choices of x_h and y_h .

APPENDIX C: DERIVATION OF THE SOLUTION TO THE APPROXIMATE NUMERICAL PROBLEM

Definition sets 1 and 2 as well as the definitions made in Chapters 6 and 8 shall be valid in this appendix.

In this appendix we shall show that the numerical method described in Chapter 8 really is a solution to the approximate numerical problem stated in Chapter 6. The derivation will be given in four parts.

Part 1. We shall show that the H_{rk} have a multivariate normal distribution.

This is really the case, as the H_{rk} are linear combinations of a set of independent random numbers with a standard normal distribution.

Part 2. We shall show that $E[H_{rk}] = 0$, $1 \leq r \leq n_r$, $1 \leq k \leq n_k$.

This is the case because the H_{rk} are linear combinations of a set of random numbers with expected value 0.

Part 3. We shall show that $\text{Var}(H_{rk}) = 1$, $1 \leq r \leq n_r$, $1 \leq k \leq n_k$.

As the $F_{r_0k_0}$ are independent and have variance 1, we have

$$\begin{aligned} \text{Var}(H_{rk}) &= \text{Var} \left(\frac{\sum_{(r_0, k_0) \in (r, k) - M_n} (\exp(-Q(r - r_0, k - k_0)) \times F_{r_0k_0})}{\mathbf{s}_n} \right) = \\ &= \frac{\sum_{(r_0, k_0) \in (r, k) - M_n} (\exp(-Q(r - r_0, k - k_0)))^2 \text{Var}(F_{r_0k_0})}{\mathbf{s}_n^2} = \\ &= \frac{\sum_{(x, y) \in M_n} \exp(-2Q(x, y))}{\mathbf{s}_n^2} = 1. \end{aligned}$$

Part 4. We shall show that

$$\left| \text{Cov}(H_{r_1k_1}, H_{r_2k_2}) - \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \right| \leq \mathbf{e}, \quad 1 \leq r_1, r_2 \leq n_r, 1 \leq k_1, k_2 \leq n_k.$$

This part of the derivation of the numerical method is rather complicated. We shall derive the inequality in a single sequence of inequalities and equalities. After that, some of the steps in the sequence will be commented.

$$\begin{aligned}
& \left| \text{Cov}(H_{r_1 k_1}, H_{r_2 k_2}) - \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \right| = \\
& = \left| \text{Cov}(H_{r_1 k_1}, H_{r_2 k_2}) - \frac{\mathbf{s}_n^2 + \mathbf{s}_f^2}{\mathbf{s}_n^2} \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \right| + \\
& + \frac{\mathbf{s}_f^2}{\mathbf{s}_n^2} \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \Big| = \\
& = [\text{comments 1-2}] = \\
& = \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_n)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2} - \\
& - \frac{\sum_{(r_0, k_0) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}}} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2} + \\
& + \frac{\mathbf{s}_f^2}{\mathbf{s}_n^2} \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \Big| = \\
& = \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_f)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2} - \\
& - \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_f) \cap ((r_2, k_2) - M_n)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2} - \\
& - \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_f) \cap ((r_2, k_2) - M_f)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2} +
\end{aligned}$$

$$\begin{aligned}
& + \frac{\mathbf{s}_f^2}{\mathbf{s}_n^2} \exp \left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2} \right) \Big| \leq \\
& \leq [\text{triangle inequality + comments 3-4}] \leq \\
& \leq \frac{\mathbf{s}_n \mathbf{s}_f}{\mathbf{s}_n^2} + \frac{\mathbf{s}_f \mathbf{s}_n}{\mathbf{s}_n^2} + \frac{\mathbf{s}_f^2}{\mathbf{s}_n^2} + \frac{\mathbf{s}_f^2}{\mathbf{s}_n^2} = \frac{\mathbf{s}_f}{\mathbf{s}_n} \left(2 + 2 \frac{\mathbf{s}_f}{\mathbf{s}_n} \right) \leq [\text{comments 5-6}] \leq \\
& \leq \frac{\mathbf{e}}{1} \left(2 + 2 \times \frac{1}{2} \right) = \mathbf{e}
\end{aligned}$$

Comment 1. We shall show that

$$\begin{aligned}
& \text{Cov}(H_{r_1 k_1}, H_{r_2 k_2}) = \\
& = \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_n)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2}.
\end{aligned}$$

The $F_{r_0 k_0}$ are independent and have variance 1, so $\text{Cov}(F_{r_{01} k_{01}}, F_{r_{02} k_{02}})$ is equal to 1 when $(r_{01}, k_{01}) = (r_{02}, k_{02})$ and 0 otherwise. Therefore we have

$$\begin{aligned}
& \text{Cov}(H_{r_1 k_1}, H_{r_2 k_2}) = \\
& = \text{Cov} \left(\frac{\sum_{(r_0, k_0) \in (r_1, k_1) - M_n} (\exp(-Q(r_1 - r_0, k_1 - k_0)) \times F_{r_0 k_0})}{\mathbf{s}_n}, \right. \\
& \left. \frac{\sum_{(r_0, k_0) \in (r_2, k_2) - M_n} (\exp(-Q(r_2 - r_0, k_2 - k_0)) \times F_{r_0 k_0})}{\mathbf{s}_n} \right) = \\
& = \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_n)} (\exp(-Q(r_1 - r_0, k_1 - k_0)) \times \exp(-Q(r_2 - r_0, k_2 - k_0)))}{\mathbf{s}_n^2} =
\end{aligned}$$

$$= \frac{\sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_n)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0))}{\mathbf{s}_n^2}.$$

Comment 2. We shall show that

$$\begin{aligned} & \sum_{(r_0, k_0) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}}} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0)) = \\ & = (\mathbf{s}_n^2 + \mathbf{s}_f^2) \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right). \end{aligned}$$

From the definition of Q it is easy to see that $2Q((r_2 - r_1)/2, (k_2 - k_1)/2) = Q(r_2 - r_1, k_2 - k_1)/2$. This fact together with the result of Section A.7 gives us

$$\begin{aligned} & Q(r_1 - r_0, k_1 - k_0) + Q(r_2 - r_0, k_2 - k_0) = \\ & = 2\left(Q\left(\frac{r_2 - r_1}{2}, \frac{k_2 - k_1}{2}\right) + Q\left(\frac{r_1 + r_2}{2} - r_0, \frac{k_1 + k_2}{2} - k_0\right)\right) = \\ & = \frac{Q(r_2 - r_1, k_2 - k_1)}{2} + 2Q\left(\frac{r_1 + r_2}{2} - r_0, \frac{k_1 + k_2}{2} - k_0\right). \end{aligned}$$

This identity enables us to conclude that

$$\begin{aligned} & \sum_{(r_0, k_0) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}}} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0)) = \\ & = \sum_{(r_0, k_0) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}}} \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2} - 2Q\left(\frac{r_1 + r_2}{2} - r_0, \frac{k_1 + k_2}{2} - k_0\right)\right) = \\ & = \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \times \sum_{(x, y) \in Z_{\frac{1}{2}} \times Z_{\frac{1}{2}}} \exp(-2Q(x, y)) = \\ & = \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right) \times \left(\sum_{(x, y) \in M_n} \exp(-2Q(x, y)) + \sum_{(x, y) \in M_f} \exp(-2Q(x, y))\right) = \\ & = (\mathbf{s}_n^2 + \mathbf{s}_f^2) \exp\left(-\frac{Q(r_2 - r_1, k_2 - k_1)}{2}\right). \end{aligned}$$

Comment 3. We shall show that the three sums on the left side of the inequality sign are less than or equal to $\mathbf{s}_n \mathbf{s}_f$, $\mathbf{s}_f \mathbf{s}_n$ and \mathbf{s}_f^2 , respectively.

We shall only derive the first of these three inequalities here, as the other two can be derived analogously.

$$\begin{aligned}
& \sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_f)} \exp(-Q(r_1 - r_0, k_1 - k_0) - Q(r_2 - r_0, k_2 - k_0)) = \\
& = \sum_{(r_0, k_0) \in ((r_1, k_1) - M_n) \cap ((r_2, k_2) - M_f)} (\exp(-Q(r_1 - r_0, k_1 - k_0)) \times \exp(-Q(r_2 - r_0, k_2 - k_0))) \leq \\
& \leq [\text{Schwarz inequality}] \leq \\
& \leq \sqrt{\sum_{(r_0, k_0) \in (r_1, k_1) - M_n} (\exp(-Q(r_1 - r_0, k_1 - k_0)))^2} \times \\
& \times \sqrt{\sum_{(r_0, k_0) \in (r_2, k_2) - M_f} (\exp(-Q(r_2 - r_0, k_2 - k_0)))^2} = \\
& = \sqrt{\sum_{(x, y) \in M_n} \exp(-2Q(x, y))} \times \sqrt{\sum_{(x, y) \in M_f} \exp(-2Q(x, y))} = \\
& = \mathbf{s}_n \mathbf{s}_f
\end{aligned}$$

Comment 4. We shall show that $\exp(-Q(r_2 - r_1, k_2 - k_1)/2) \leq 1$.

It is sufficient to note that $Q(r_2 - r_1, k_2 - k_1) \geq 0$, which follows from the result of Section A.2.

Comment 5. $\mathbf{s}_n \geq 1$, as we noted in Chapter 7.

Comment 6. We shall convince ourselves that $\mathbf{s}_f \leq \mathbf{e}/3$ and $\mathbf{s}_f \leq 1/2$.

The conditions on d , x_h and y_h given in Chapter 8 imply that

$$d \geq \frac{1}{\sqrt{2} \times b}, \quad 4 \mathbf{p} a b \exp\left(-2\left(d - \frac{1}{2\sqrt{2} \times b}\right)^2\right) \leq \left(\min\left(\frac{\mathbf{e}}{3}, \frac{1}{2}\right)\right)^2,$$

$$x_h + \frac{1}{4} \geq d \sqrt{b^2 + x_0^2}, \quad y_h + \frac{1}{4} \geq d \sqrt{b^2 + y_0^2}.$$

According to Section B.3, then $\mathbf{s}_f \leq \min(\mathbf{e}/3, 1/2)$.

REFERENCE

Ross, Sheldon M.

(1985). Introduction to Probability Models, 3rd ed. Academic Press, Inc., Orlando, Florida.

APPENDIX D Generation of random points with a Fisher distribution

Generation of random points with a Fisher distribution

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13th March 2003

1 The Fisher distribution

The Fisher distribution is a probability distribution for the location of a point \mathbf{V} on a unit sphere. (We let points be represented by their position vectors from the centre of the sphere.) The distribution has two parameters, the location parameter $\boldsymbol{\lambda}$, which is a point on the sphere, and the concentration parameter κ , which is a real number. If dS is the area of an infinitesimally small portion of the sphere around a point \mathbf{v} on the sphere, the probability that \mathbf{V} will belong to this portion is

$$\frac{\kappa}{4\pi \sinh \kappa} e^{\kappa \boldsymbol{\lambda} \cdot \mathbf{v}} dS. \quad (1)$$

From now on we shall assume that $\boldsymbol{\lambda} = (0, 0, 1)$ for simplicity. The formula then takes the form

$$\frac{\kappa}{4\pi \sinh \kappa} e^{\kappa w} dS, \quad (2)$$

where $\mathbf{v} = (u, v, w)$.

The total probability is obtained by integrating Formula 2 around the unit sphere. Let us check that the total probability equals 1. Let $u = \sin \theta \cos \phi$, $v = \sin \theta \sin \phi$, $w = \cos \theta$. We get

$$\begin{aligned} \int_0^\pi \int_0^{2\pi} e^{\kappa \cos \theta} \sin \theta d\phi d\theta &= 2\pi \left[-\frac{1}{\kappa} e^{\kappa \cos \theta} \right]_0^\pi = -\frac{2\pi}{\kappa} (e^{\kappa \cos \pi} - e^{\kappa \cos 0}) \\ &= -\frac{2\pi}{\kappa} (e^{-\kappa} - e^\kappa) = \frac{4\pi \sinh \kappa}{\kappa}, \quad (3) \end{aligned}$$

which is correct.

The three above formulas, as well as other formulas in this paper, are not valid in the case $\kappa = 0$. E.g., 1 should be substituted for $(\sinh \kappa)/\kappa$ when $\kappa = 0$. In order not to distract the reader (or the author) from the main subject, the case $\kappa = 0$ will normally not be treated specially.

2 A generation method from the literature

The following straightforward method to generate random points with a Fisher distribution on a computer is described in essence on p. 59 in Ref. 1. Because \mathbf{V} 's spherical coordinates Θ and Φ are independent random variables, they can be generated independently. Θ and Φ are calculated using the formulas $\Theta = F_{\Theta}^{-1}(U_{\Theta})$ and $\Phi = F_{\Phi}^{-1}(U_{\Phi})$, where F_{Θ} and F_{Φ} are the cumulative distribution functions of Θ and Φ , and where U_{Θ} and U_{Φ} are independent random numbers uniformly distributed over the interval $(0, 1)$.

There is however a possible disadvantage with this method, as we shall see now.

For simplicity, let us study the case $\kappa = 0$, where the Fisher distribution is equal to a uniform distribution on the sphere. In this case $\Theta = F_{\Theta}^{-1}(U_{\Theta}) = \arccos(1 - 2U_{\Theta})$ and $\Phi = F_{\Phi}^{-1}(U_{\Phi}) = 2\pi U_{\Phi}$. On a computer U_{Θ} and U_{Φ} will be calculated by a random number generator. For numerical reasons U_{Θ} and U_{Φ} will have a discrete rather than a continuous distribution. It is realistic to assume that the possible U_{Θ} and U_{Φ} values will be closely and more or less evenly spaced numbers in the interval $(0, 1)$. (We shall not dwell on whether the endpoints 0 and 1 are possible values.) The distribution of generated points on the sphere will also be discrete. As the derivative of F_{Θ}^{-1} is very large near 0 and 1, the points will not be so closely spaced in the θ direction near the poles of the sphere. On the other hand, the points will be very closely spaced in the ϕ direction, as a small change in ϕ corresponds to a much smaller change in location near the poles.

Whether the not-so-close spacing of points in the θ direction near the poles is a disadvantage or not depends on the application in which the generated points are used.

A possible solution to the problem is to calculate U_{Θ} with a double precision random number generator, if one is available. (We assume then that single precision is used otherwise in the program.) U_{Θ} 's increased resolution will be enough to compensate for the large derivative of F_{Θ}^{-1} near 0 and 1. I have not tried this solution in a computer program.

3 A generation method developed by the author

In this section another method to generate random points with a Fisher distribution will be described. I developed the method in 1998–1999. I also wrote a subroutine to generate Fisher-distributed random points based on the method. The subroutine has been used at Computer-aided Fluid Engineering AB.

Let $\mathbf{r} = (x, y, z)$ denote an arbitrary point in space, and (unless $x = y = z = 0$) let $\mathbf{v} = (u, v, w)$ be its projection onto the unit sphere defined by $\mathbf{v} = \mathbf{r}/|\mathbf{r}|$. With spherical coordinates r, θ, ϕ we have $x = r \sin \theta \cos \phi$,

$y = r \sin \theta \sin \phi$, $z = r \cos \theta$, and $u = \sin \theta \cos \phi$, $v = \sin \theta \sin \phi$, $w = \cos \theta$.

Let D_1 be the three-dimensional domain consisting of all points \mathbf{r} which satisfy

$$0 < r \leq e^{(\kappa w - |\kappa|)/3}. \quad (4)$$

Consider a surface element dS around a point \mathbf{v} on the sphere. The volume of the part of D_1 projected onto dS is

$$\frac{e^{\kappa w - |\kappa|}}{3} dS. \quad (5)$$

Let \mathbf{R} be a random point uniformly distributed within D_1 , and let $\mathbf{V} = \mathbf{R}/|\mathbf{R}|$ be its projection onto the sphere. Because the volume given by Formula 5 is proportional to the probability given by Formula 2, \mathbf{V} will have a Fisher distribution.

We can generate \mathbf{R} uniformly distributed within D_1 by generating \mathbf{R} uniformly distributed within the larger domain D_2 defined by

$$|x|, |y| \leq \sqrt{\frac{2}{1 + \sqrt{1 + (2\kappa/3)^2}}}, \quad |z| \leq 1, \quad (6)$$

and keeping \mathbf{R} only if it is located within D_1 . It remains to show (1) that D_1 is a subset of D_2 , and (2) that the volume ratio of D_1 to D_2 is large enough that \mathbf{R} can be kept often enough.

As a preparation for showing (1), we shall first calculate $\sin \theta$ for that θ in the interval $0 \leq \theta \leq \pi$ which maximizes the expression

$$e^{(\kappa \cos \theta - |\kappa|)/3} \sin \theta. \quad (7)$$

As the expression is positive in the interior of the interval and 0 at the endpoints, the maximum must be attained when the derivative is 0.

$$\frac{d}{d\theta} (e^{(\kappa \cos \theta - |\kappa|)/3} \sin \theta) = 0 \quad (8)$$

$$e^{(\kappa \cos \theta - |\kappa|)/3} \left(\cos \theta - \frac{\kappa}{3} \sin^2 \theta \right) = 0 \quad (9)$$

$$\cos \theta = \frac{\kappa}{3} \sin^2 \theta \quad (10)$$

$$1 - \sin^2 \theta = \left(\frac{\kappa}{3} \right)^2 \sin^4 \theta \quad (11)$$

$$\sin^{-4} \theta - \sin^{-2} \theta - \left(\frac{\kappa}{3} \right)^2 = 0 \quad (12)$$

$$\sin^{-2} \theta = \frac{1}{2} (\pm) \sqrt{\frac{1}{4} + \left(\frac{\kappa}{3} \right)^2} \quad (13)$$

$$\sin \theta = \sqrt{\frac{2}{1 + \sqrt{1 + (2\kappa/3)^2}}} \quad (14)$$

Let θ_0 denote the θ which maximizes Formula 7.

To show (1), we shall show that any point \mathbf{r} belonging to D_1 also belongs to D_2 . In other words, we shall show that if \mathbf{r} satisfies Formula 4, then \mathbf{r} also satisfies Formula 6. And this is indeed the case, because if \mathbf{r} satisfies Formula 4, then

$$\begin{aligned} |x|, |y| &\leq r \sin \theta \leq e^{(\kappa w - |\kappa|)/3} \sin \theta = e^{(\kappa \cos \theta - |\kappa|)/3} \sin \theta \\ &\leq e^{(\kappa \cos \theta_0 - |\kappa|)/3} \sin \theta_0 \leq \sin \theta_0 = \sqrt{\frac{2}{1 + \sqrt{1 + (2\kappa/3)^2}}} \end{aligned} \quad (15)$$

and

$$|z| \leq r \leq e^{(\kappa w - |\kappa|)/3} \leq 1. \quad (16)$$

To show (2), let us first calculate the volumes of D_1 and D_2 . We obtain the volume of D_1 by integrating Formula 5 around the unit sphere and using Formula 3. The volume is

$$\begin{aligned} \int_0^\pi \int_0^{2\pi} \frac{e^{\kappa \cos \theta - |\kappa|}}{3} \sin \theta \, d\phi \, d\theta &= \frac{e^{-|\kappa|}}{3} \int_0^\pi \int_0^{2\pi} e^{\kappa \cos \theta} \sin \theta \, d\phi \, d\theta \\ &= \frac{e^{-|\kappa|}}{3} \cdot \frac{4\pi \sinh \kappa}{\kappa} = \frac{e^{-|\kappa|}}{3} \cdot \frac{4\pi \sinh |\kappa|}{|\kappa|} = \frac{2\pi(1 - e^{-2|\kappa|})}{3|\kappa|}. \end{aligned} \quad (17)$$

From Formula 6 the volume of D_2 is found to be

$$\frac{16}{1 + \sqrt{1 + (2\kappa/3)^2}}. \quad (18)$$

The following inequality shows that the volume ratio of D_1 to D_2 is greater than $\pi/36$ for all κ .

$$\begin{aligned} \frac{2\pi(1 - e^{-2|\kappa|})}{3|\kappa|} \bigg/ \frac{16}{1 + \sqrt{1 + (2\kappa/3)^2}} &= \frac{\pi(1 - e^{-2|\kappa|})(1 + \sqrt{1 + (2\kappa/3)^2})}{24|\kappa|} \\ &> \frac{\pi(1 - e^{-2|\kappa|})(1 + 2|\kappa|/3)}{24|\kappa|} = \frac{\pi[(1 + 2|\kappa|/3) - (1 + 2|\kappa|/3)e^{-2|\kappa|}]}{24|\kappa|} \\ &> \frac{\pi[(1 + 2|\kappa|/3) - 1]}{24|\kappa|} = \frac{\pi}{36} \end{aligned} \quad (19)$$

It is easy to show that the volume ratio equals $\pi/6$ when $\kappa = 0$, and that it approaches $\pi/36$ when $\kappa \rightarrow \pm\infty$. The volume ratio therefore varies with κ , but it is always greater than $\pi/36$. We have thus shown (2).

Let us summarize the method to generate Fisher-distributed random points described in this section. Generate three random numbers uniformly distributed e.g. over $(0, 1)$. Calculate from these numbers a random point \mathbf{R} uniformly distributed within D_2 , which is defined by Formula 6. If \mathbf{R} belongs to D_1 , defined by Formula 4, keep it, otherwise discard it and repeat the process until an \mathbf{R} belonging to D_1 has been found. Calculate $\mathbf{V} = \mathbf{R}/|\mathbf{R}|$. \mathbf{V} is then our random point with a Fisher distribution.

It is evident that the method described in this section does not have the possible disadvantage of the method in Section 2. As long as $|\kappa|$ is not large, the method should work well from all reasonable aspects (possibly except for speed). To be specific, I think that the method should work well at least for $|\kappa| < 20$ or so. (The choice of 20 as the limit will not be explained here.) I am not sure how well the method works numerically for larger $|\kappa|$.

Reference

1. N. I. Fisher, T. Lewis, B. J. J. Embleton. *Statistical analysis of spherical data*. First paperback edition. Cambridge university press, Cambridge, 1993.

Appendix E Deriving estimates of the flow wetted surface in DarcyTools

1 INTRODUCTION

A substance dissolved in water (hereafter called a tracer) can be transported through a rock volume, provided there is a system of connected fractures and a flow through these. The tracer may enter crossing fractures, with or without a flow, and may also diffuse into the rock matrix. The strength of the diffusive process is related to the flow rate and the flow wetted surface (to be defined below) as it is through this surface matrix diffusion and diffusion into smaller fractures take place.

An up to date review of how the flow wetted surface (FWS) can be derived or estimated is given by Andersson et al. (1998) and there is hence no need to give an extensive background here. An account of how the FWS is derived in Discrete Fracture Network (DFN) models is given by Outters and Shuttle (2000).

The present analysis will be concerned with how the FWS can be derived in the stochastic continuum model DarcyTools. In DarcyTools the rock volume is divided into a regular system of computational cells and the key question is hence how the FWS can be estimated for such a cell. In Figure E-1 the situation is illustrated, schematically. If, as an illustration, we assume that the cell has the dimensions $1 \times 1 \times 1 \text{ m}^3$, the channel shown may have a surface area of $1 \times 0.5 \text{ m}^2$. The FWS would then be 1 m^2 , as an exposed area is found on both sides of the channel. It is clear from this illustration that the FWS can not be much larger than $2 \text{ m}^2/\text{m}^3$, if the simple channel model with two bounding surfaces is accepted. However, the surface may be very irregular and may also comprise parallel channels and the upper limit of $2 \text{ m}^2/\text{m}^3$ is hence only a “rough guide”.

When a tracer travels through the channel illustrated in Figure E-1, it may exchange matter by diffusion with the rock volume exposed by the FWS. The significance of this exchange can be expected to be related to two parameters: the FWS per unit volume of water in the channel, a_w , and the residence time, t . The exchange will increase with both these parameters and a new variable the F -quotient (Andersson et al., 1998) has been introduced for this product:

$$F = a_w \times t \tag{E-1}$$

By simple algebra it is possible to write Equation E-1 as:

$$F = a_r L / q$$

where L is the cell dimension, a_r the FWS per unit rock volume and q the Darcy velocity. The present report will mainly be concerned with a_r and F , determined locally for a cell or integrated along a flow channel. The objective of this appendix is hence to demonstrate how the FWS and F -quotient can be determined in DarcyTools.

STORAGE VOLUMES

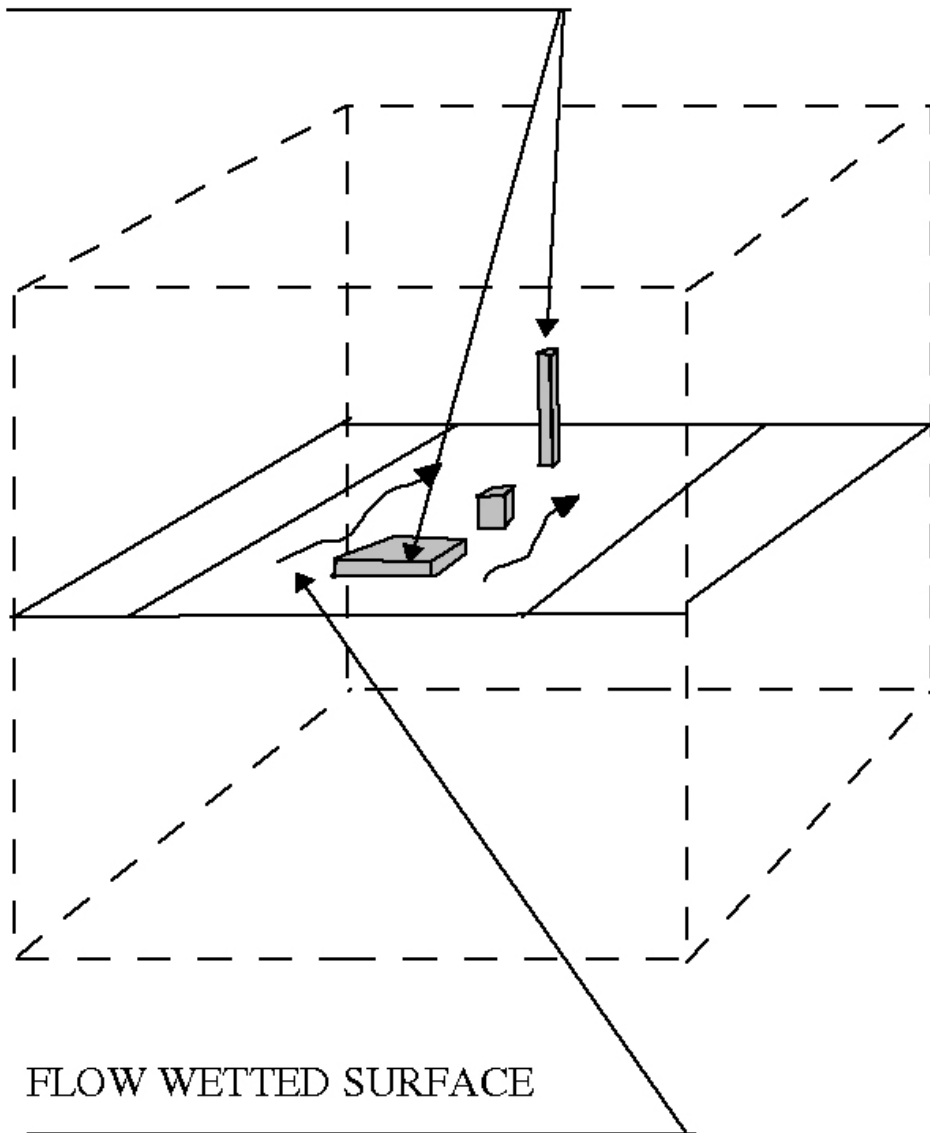


Figure E-1. Illustration of a computational cell with a channel with flow.

2 EVALUATED METHODS

Three different ways of calculating the FWS, for a computational cell, in DarcyTools will be investigated; these will now be described.

2.1 GEHYCO METHOD

The general method used in DarcyTools to derive hydraulic properties is called GEHYCO (GEneral HYdraulic COnditions). The central idea is to calculate “how much of a conductive element that intersects a computational cell and let that volume generate a contribution to the cell property in question”. A full account of this method can be found in Svensson (2001b).

It is also possible to determine how much of a fracture surface that intersects a cell and let this “intersecting surface” give a contribution to the FWS in the cell. This method is hence conceptually straight forward and does not involve any further assumptions than those involved in the specification and generation of the fracture network.

2.2 P_{32} METHOD

When the background fracture network is generated, a power law distribution is assumed for the intensity, i.e. number of fractures in a size interval per unit volume. It is straight forward to use this power law to calculate the expected number of fractures for a number of length intervals and hence obtain the total surface area per unit volume, P_{32} .

In Table E-1 the contributions from different size groups are given together with the total area P_{32} . As can be seen, fractures down to a length-scale of three metres are assumed to contribute to P_{32} . The reason for choosing three metres as the lower limit, is that the cell size in the model simulations to be presented is three metres; the assumption being that all flow channels are picked up by the fracture network and grid chosen.

When the global P_{32} has been determined, we need to distribute the surface to each cell. This is done with the kinematic porosity as a weighting factor, as cell porosity values are available from GEHYCO. Finally we note that the local a_r value is twice the local P_{32} value. An underlying assumption of this method is that the local a_r -value is directly proportional to the local kinematic porosity; this is no more than an assumption.

Table E-1. Estimate of global P_{32} value from a power law for fracture intensity. The Laboratory scale model (Svensson, 1999) is used for the estimates.

Fracture set	Length interval [m]	Number, excluding isolated fractures	P_{32}	ΣP_{32}
Determ zones			0.014	0.014
1	160-320	12	0.004	0.018
2	80-160	70	0.004	0.022
3	40-80	425	0.007	0.029
4	20-40	2050	0.008	0.037
5	10-20	9150	0.009	0.046
6	5-10	38800	0.008	0.054
7	3-5	95600	0.006	0.060
				0.06

2.3 APERTURE METHOD

The third method to be evaluated derives the FWS by the following steps:

- A conductivity is available at each of the six cell walls.
- A transmissivity can be obtained by multiplying with the cell dimension, Δ .
- Use the relation between transport aperture and transmissivity ($e_T = 2.0T^{0.6}$) presented in Appendix H to calculate e_T , based on six cell wall values.
- The free volume in the cell is given by $\theta_k \Delta^3$, where θ_k is the kinematic porosity, and the area can hence be calculated as:

$$a_r = 2.0 \frac{\theta_k \Delta^3}{e_T} \quad (\text{E-2})$$

The method apparently involves a number of assumptions that can not easily be evaluated.

3 RESULTS

In the evaluation of the methods a slightly modified version of the Laboratory scale model (Svensson, 1999) will be used. One modification is that the cell size is put to 3 metres (instead of 5 metres) and another that only a simple forcing (flow from west to east) will be used. The Äspö HRL is not included in the model and all flow channels will hence start at the western boundary and leave through the eastern one.

3.1 FWS VALUES IN CELLS

We start by discussing the global mean values of a_r , see Table E-2, and the corresponding histograms, see Figure E-2. Starting with the mean values, it is clear that all three estimates are in fair agreement and are also in agreement with the mean value of $0.1 \text{ m}^2/\text{m}^3$ suggested by Andersson et al. (1998). The distributions are however different, as can be seen in the histograms, see Figure E-2.

First it should be explained that the bar $0.5 - 1.0 \times 10^{-2}$ represents all cells with an a_r less than $10^{-2} \text{ m}^2/\text{m}^3$. Roughly two thirds of all cells have a very small a_r . This is due to the fact that the same fraction of cells is not intersected by any fracture and hence get zero porosity and zero a_r . From the histograms one may also note that all three methods generate most “active” a_r -values in the two intervals $0.1 \rightarrow 0.5$ and $0.5 \rightarrow 1.0$. It is also worth noting that method three (aperture based) generates very few cells with an a_r -value greater than 1.0.

3.2 FWS VALUES ALONG FLOW CHANNELS

The global a_r -values are not of much relevance, as it is the FWS along flow channels that will affect the exchange with the rock matrix. For this reason we will study the correlation between the cell Darcy velocity and cell a_r -value, for the simple flow situation described above, see Figure E-3. At a first glance the result may look rather similar for the three methods; a closer examination reveals however some interesting differences:

- Method three shows a weak correlation between the Darcy velocity, q , and a_r . If a_r does not increase with q this implies that e_T increases with q , as a larger q should be correlated with a larger “channel cross section area”.
- Method two shows a linear increase of a_r with q . The interpretation of this behaviour is that “a doubling of q doubles the width of the channel, with e_T kept constant”.

Table E-2. Global mean values of a_r for the three methods evaluated.

a_r (m^2/m^3)	Method		
	GEHYCO	P_{32}	Aperture
	0.12	0.13	0.18

- Method one can be viewed as being in between these two extremes and perhaps be interpreted as “increased q is correlated with an increase in both width and aperture of the channel”.

A tentative conclusion is that method one is the more realistic one, from this point of view.

Next we study the variation of a_r along a streamtube. This requires that flow paths are calculated. In DarcyTools this is carried out in the submodel PARTRACK (Svensson, 2001a). In the west to east flow considered, particles are released in fracture zone EW1, see Figure 1-2, and then tracked through the domain till they reach the eastern boundary. Figure E-4 shows the flow paths generated by 100 particles. The main flow path is through EW1, changing to the NNW structures and leaving through NE1. Note that in this view from above, NE1 gives a wider impression as this zone is not vertical. It is also worth noting that rather few flow channels are active in the transport.

Figure E-5 shows the variation of a_r for one flow path. The same trends as in Figure E-3 can be identified, i.e. method three generates a fairly constant a_r , method two shows the largest variations and method one is somewhere in between.

3.3 F-QUOTIENTS ALONG FLOW CHANNELS

Figure E-6 shows the variation of the cell F -quotients ($F_i = a_{r,i}\Delta/q_i$) along a flow path. The same differences between the methods as for a_r can be expected, but the implications for the F -quotients are a little bit different:

- In method three a_r is fairly constant and this is probably the reason for the rather small variation seen in this figure.
- Method two was found to give a correlation between a_r and q . It is hence not surprising that the F -quotient is fairly constant for long periods.
- Method one has a weaker correlation between a_r and q and hence shows a larger variability.

In Outters and Shuttle (2000) the integrated F -quotient along a flow path versus time was analysed. In that report also a curve was fitted to the results from the numerical model. Here, this curve will be used for comparisons with the three methods analysed in the present report. The F -quotient was hence summed up along a flow path; this was done for one hundred particles and the result can be studied in Figure E-7. The following should be noted:

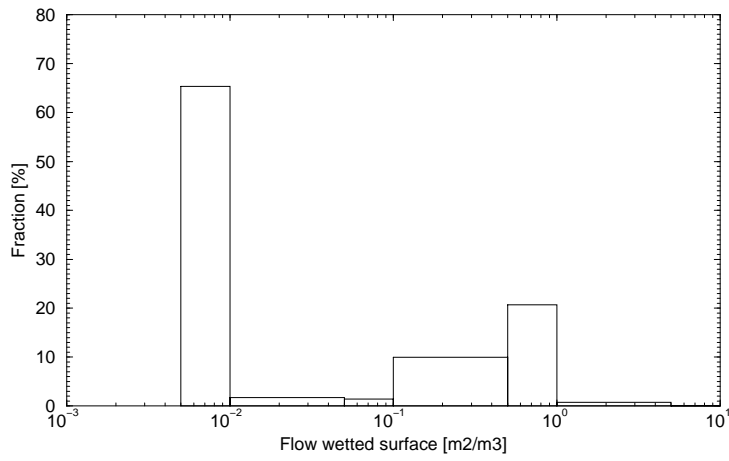
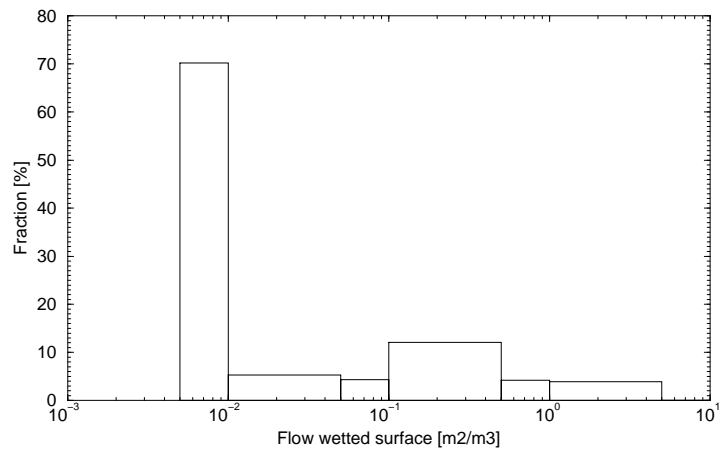
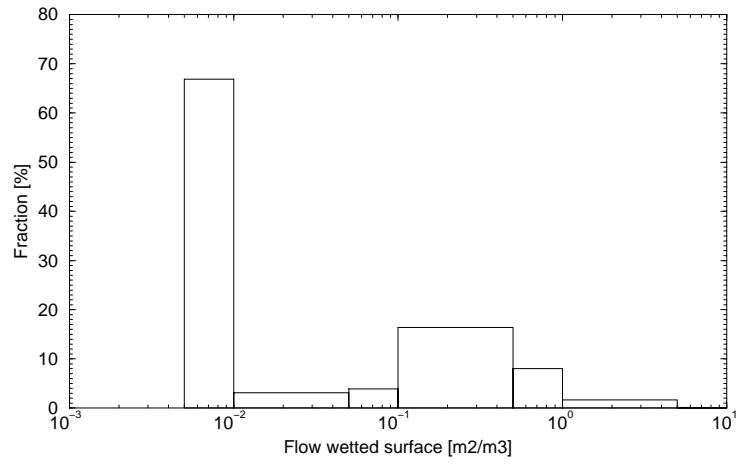


Figure E-2. Histograms of a_r [m^2/m^3]. Method one (top), two (middle) and three (bottom).

- All results are in fair agreement with Outters and Shuttle (2000) (straight line in the figures). The fact that the present results are generally below the straight line can be explained by a somewhat higher P_{32} -value used in the model by Outters and Shuttle. Method three, which has the highest average a_r , is closest to the straight line.
- Method two, which has a strong correlation between a_r and q , gives the smallest spread around the mean value.

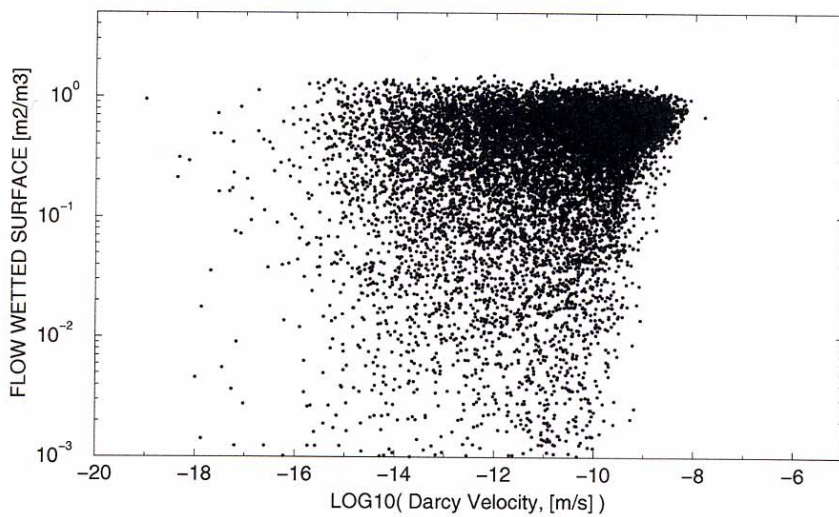
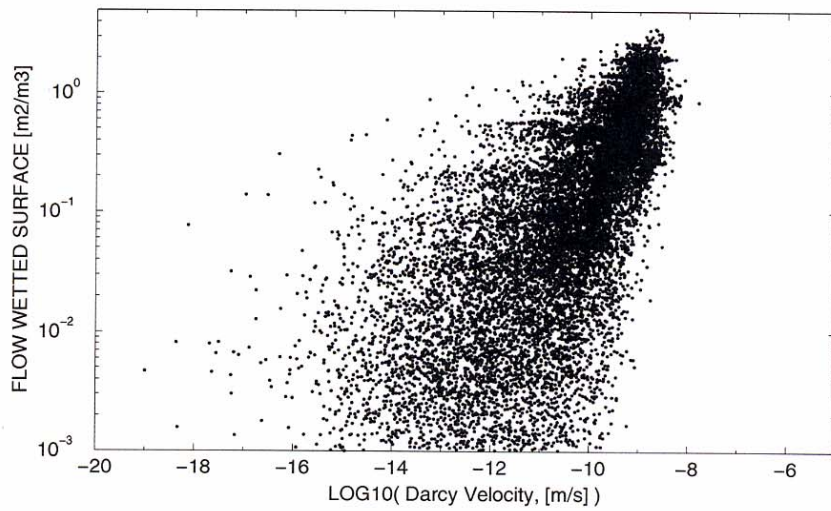
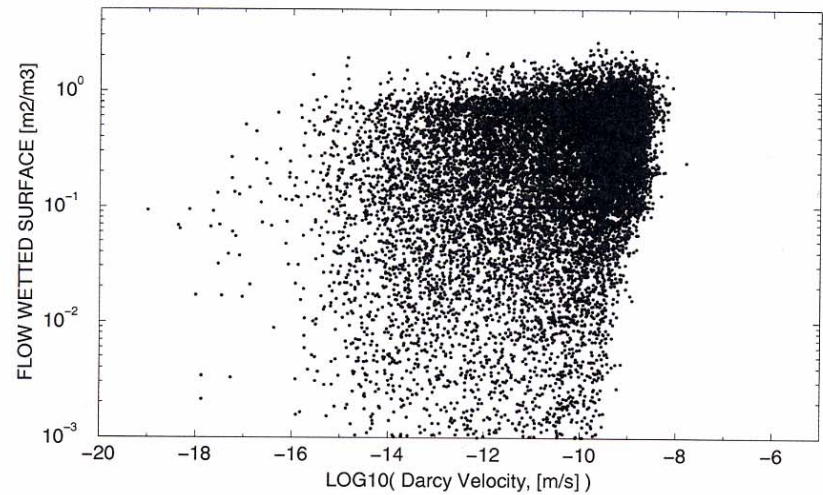


Figure E-3. Correlation between flow wetted surface a_r , and Darcy velocity, q . Method one (top), two (middle) and three (bottom).

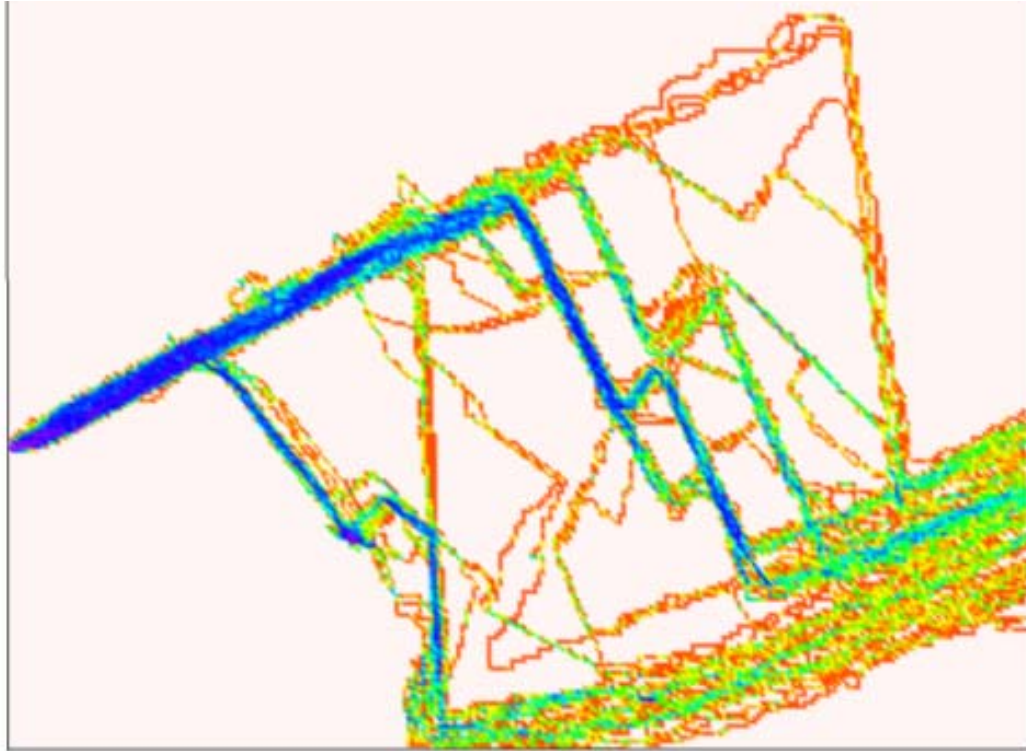


Figure E-4. Flow channels formed by 100 particle tracks in a flow from west to east. Blue indicates high intensity of tracks, red low.

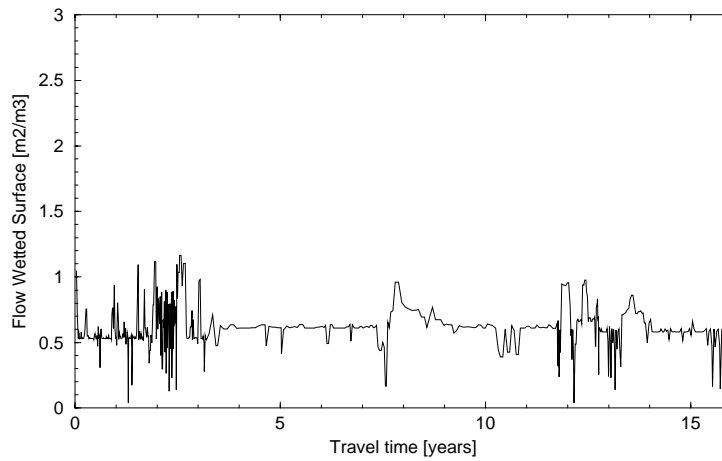
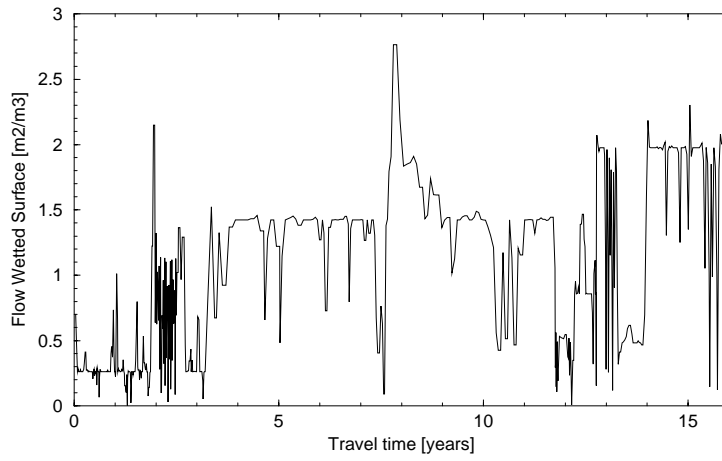
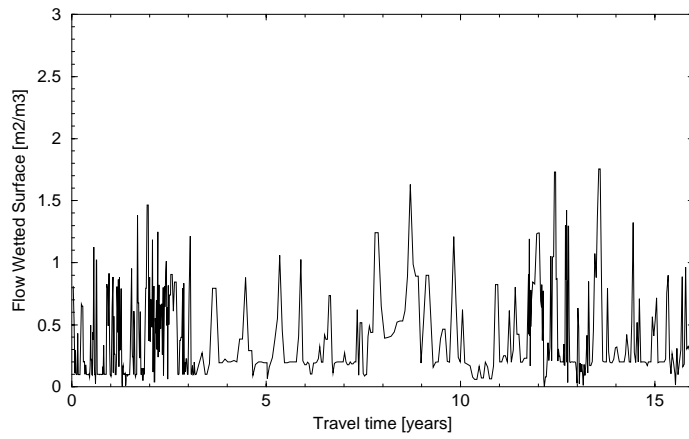


Figure E-5. Variation of a_r along a single flow path. Method one (top), two (middle) and three (bottom).

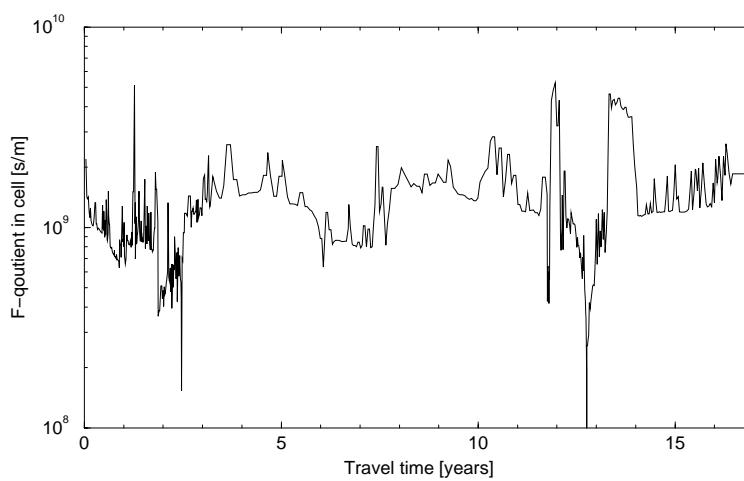
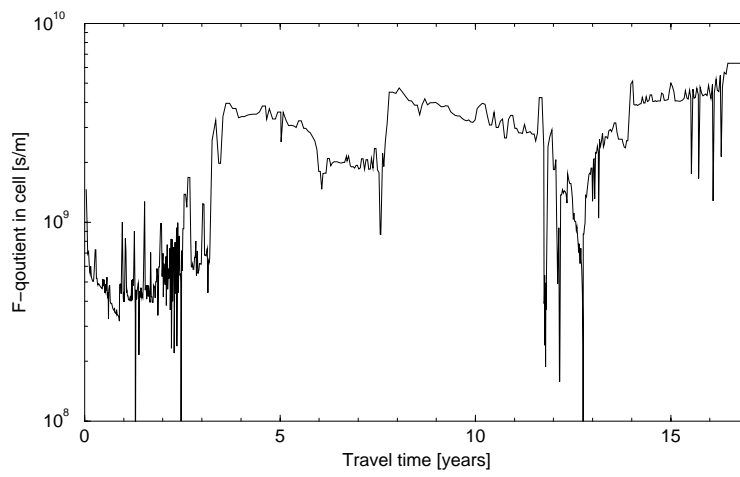
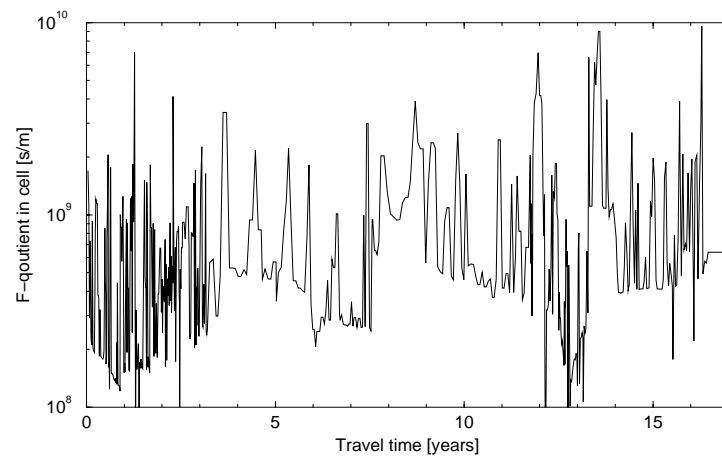


Figure E-6. *F-quotients along a flow path. Method one (top), two (middle) and three (bottom).*

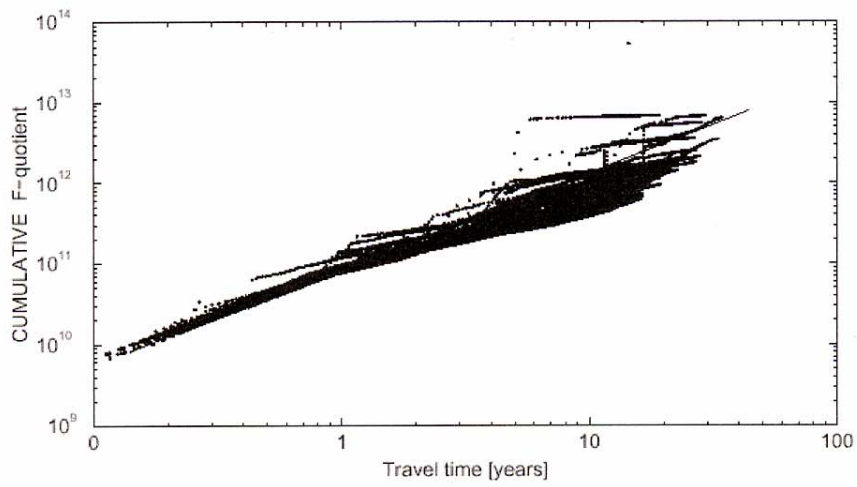
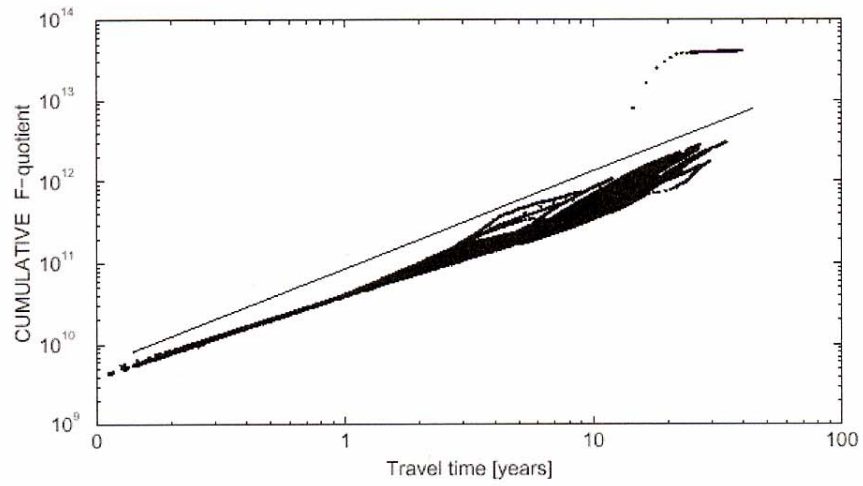
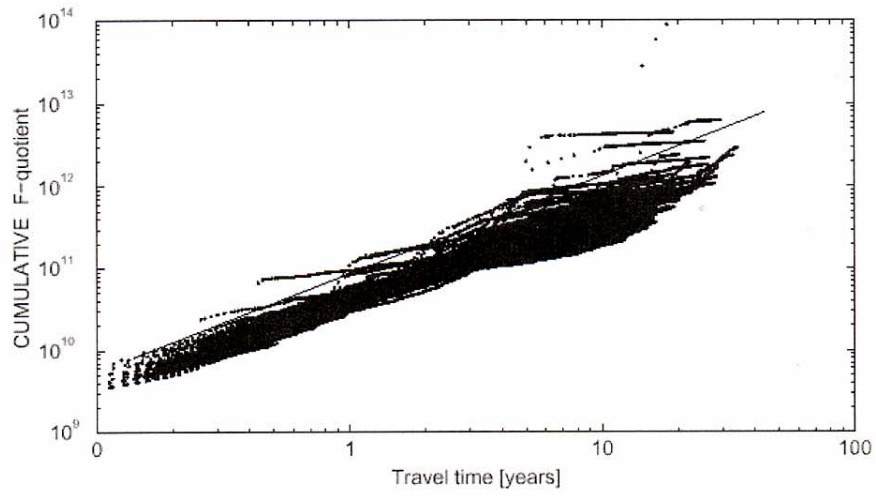


Figure E-7. Integrated F -quotients along flow paths. Straight line gives the result from Outters and Shuttle (2000). Method one (top), two (middle) and three (bottom).

4 DISCUSSION AND CONCLUSIONS

The present analysis assumes that all fractures and fracture zones have a simple geometric shape, i.e. the bounding surfaces are two parallel planes. This is of course a gross simplification that needs to be taken into account when the results are evaluated. The following points should also be considered:

- The a_r values determined give *all* the surface area in a cell. It may well be the case that only a fraction of this area is in direct contact with the flowing water.
- On the other hand, a real fracture is not made up of two parallel planes, but may be highly irregular, which increases the possibly active surface (as compared to the assumptions made in this report).
- A steady flow field was used in the present analysis. In reality one may expect transient “pulses” on a variety of times scales; from tidal effects, yearly groundwater level variations to periods with an inland ice on the very long time scale. These transients may disperse a tracer within a fracture plane and also activate fractures that otherwise could not be reached by the tracer. A larger flow wetted surface would hence be the result.

The a_r -values derived should hence more be considered as index of a flow wetted surface, rather than an absolute estimate of the magnitude.

In Andersson et al. (1998) four topics are suggested, as having the potential to improve our understanding of the flow related migration parameters:

- develop the theoretical understanding of migration and matrix diffusion,
- study the effect of diffusion into stagnant or low flow zones in a single fracture,
- migration modelling directly in the flow codes,
- exploring for further evidence of matrix diffusion from tracer tests, static diffusion tests, geology and geochemistry.

This project has not been focused on these suggestions, but it may be the case that DarcyTools, with the features introduced in this report (FRAME and FWS-derivations), goes some way towards these goals. Presently PA-studies use global estimates of FWS in estimates of the F-quotients. It is possible to get some perspective on these estimates from the present study. In Figure E-8, the integrated F-quotients for 100 particles using two methods are compared. In one of the methods we use the global estimate of a_r , while the other method use the local cell values. If the two methods were giving equal results, the points should fall on the straight line in Figure E-8. This is not the case, the method using local cell values gives a significantly larger variation of F-quotients.

With the precautions mentioned above in mind, the following conclusions from the study are formulated:

- Three partly independent methods to estimate the flow wetted surface from the groundwater code DarcyTools have been evaluated. All three methods

give global estimates of a_r that are in fair agreement and these are also in agreement with the expected value for the Äspö HRL (Andersson et al., 1998).

- Method one, which is based on the GEHYCO technique, is considered to be the best choice as it directly calculates a_r from the fracture network without any additional assumptions.

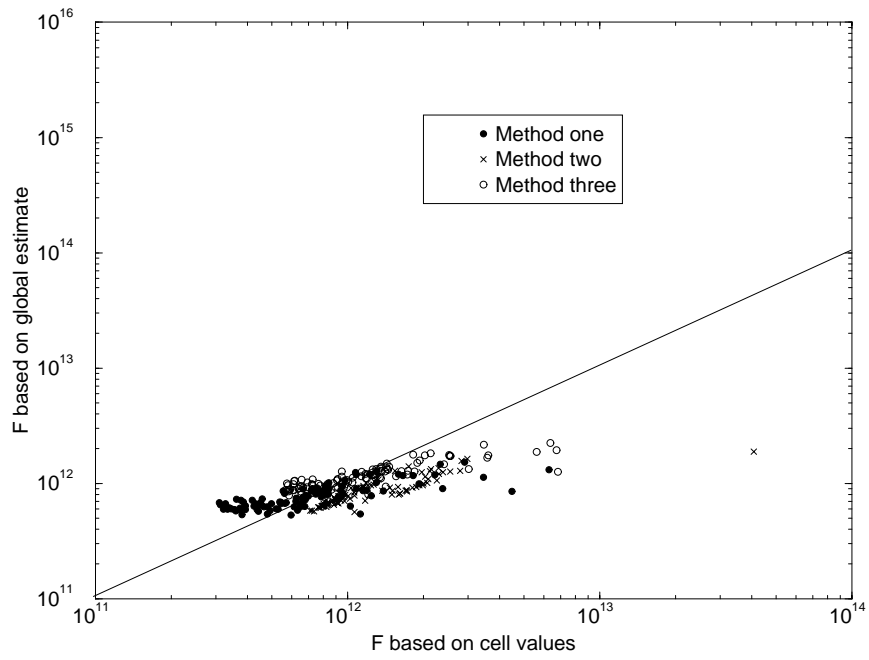


Figure E-8. *F-quotients determined with local and global FWS values.*

Appendix F Empirical relations for the determination of fracture properties

Introduction

It is necessary to specify the properties of the conductive elements, even if some of the required information is uncertain or unknown.

The relations to be presented are not claimed to be the “best possible input data”, but merely represent what is presently available (a more complete compilation is needed).

Transmissivity-fracture size

The following relation was found in a calibration study for the laboratory domain considered also in this report (see Report 2):

$$T = \begin{cases} 10^{-5} (l/100)^2 & [m^2 / s] \text{ for } l \leq 100 \text{ metres} \\ 10^{-5} & [m^2 / s] \text{ for } l > 100 \text{ metres} \end{cases} \quad (\text{F-1})$$

This relation is shown in Figure F-1 (labelled LABM (99)) together with data from field investigations (Åspö Major zones, Prototype Repository, TRUE Feature A, TRUE Block Scale) and some mean values from simulation models (DFN Aberg, DFN TRUE Block Scale). As already mentioned, the compilation is far from complete and we will restrain from any firm statements. However, relation (F-1) does not seem to contradict the information compiled.

Transmissivity-transport aperture

The transport aperture, e_T , will be used to calculate the kinematic porosity of a conductive element. In Figure F-2 one experimental curve (Rhén et al., 1997), one curve used in other models (Doe, 1993) and the relation resulting from the cubic law are shown. The solid line is given by:

$$e_T = 2.0T^{0.6} \quad (\text{F-2})$$

This relation is regarded as a good compromise, based on the following arguments:

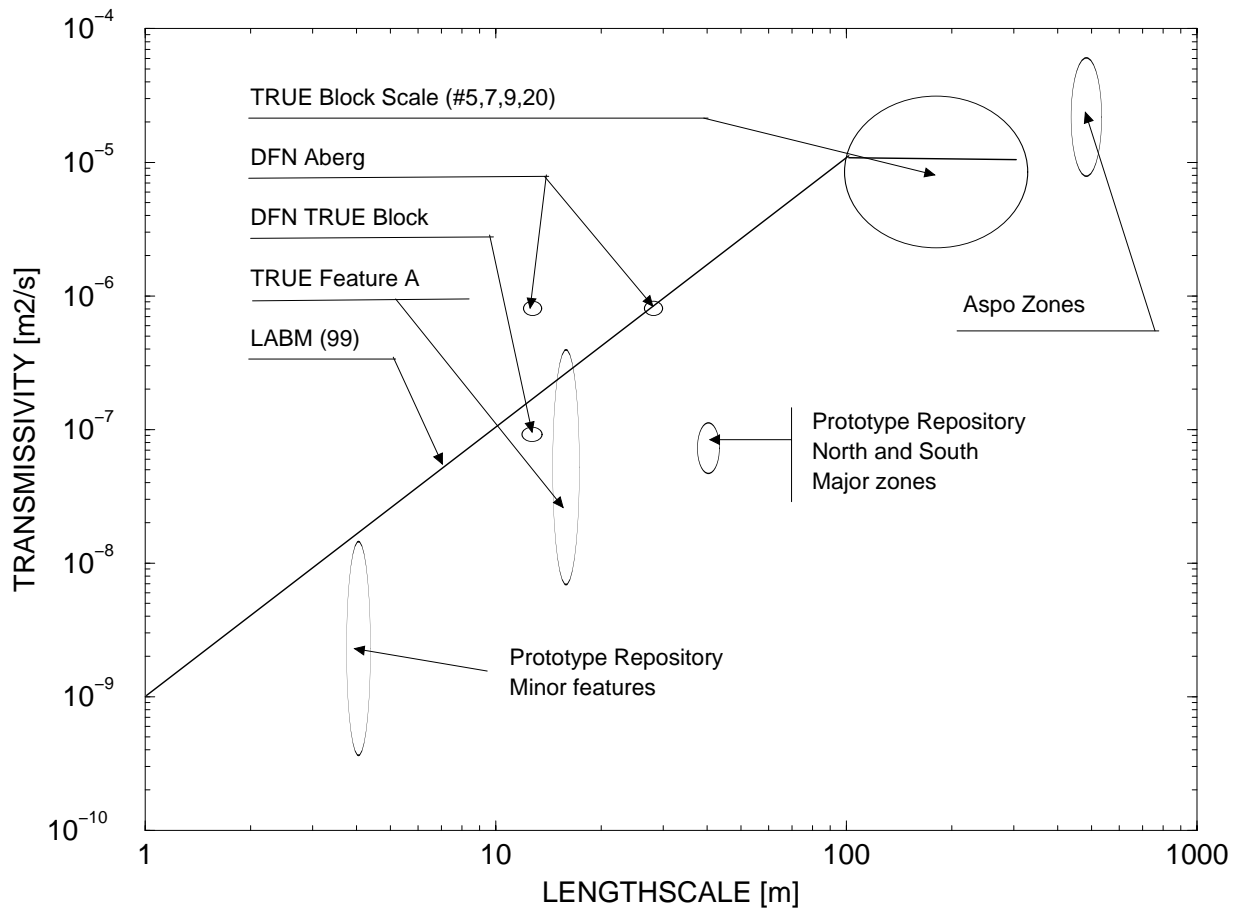


Figure F-1. Relation between fracture size and transmissivity.

Compiled data:

- TRUE BLOCK fractures (#5, 7, 9, 20) (Winberg, 1998)
- TRUE Feature A (Winberg et al., 2000)
- Äspö. Major fracture zones NNW* (Rhén et al., 1997)
- Prototype Repository. South and North major zones and minor zones (Forsmark and Rhén, 2000)
- DFN, Aberg (Dershowitz et al., 1999)
- DFN, TRUE Block Scale (Winberg, 2000)

- The curve by Rhén et al. (1997) is mainly based on fracture zones with relatively high transmissivity.
- The curve by Doe (1993) is mostly used for transmissivities in the range $10^{-7} \rightarrow 10^{-5} \text{ m}^2 / \text{s}$.
- The cubic law applies to “single opening fractures” and is hence best suited for small transmissivities.

It should once again be pointed out that the only purpose of this compilation is to show that the relation used, Equation (F-2), is in fair agreement with some easily compiled information.

Fracture size-thickness

It will be assumed that fractures are squares with dimension $L \times L \text{ m}^2$ and that the fracture thickness, b , is 1% of the fracture length scale, L . Field data from Äspö, (see Figure F-3), do not seem to contradict this relation. The definition of “fracture thickness” is given in Section 3.3.

Diffusion coefficients

Effective molecular diffusion in a conductive element should be proportional to the product of the kinematic porosity and the diffusivity value in the pore water (Neretnieks, 1993). The proportionality constant is related to the properties of the pore space (constrictivity and tortuosity).

In DarcyTools, we will simply assume that the diffusion coefficient for a conductive element is equal to the product of the kinematic porosity and the diffusion value in pure water.

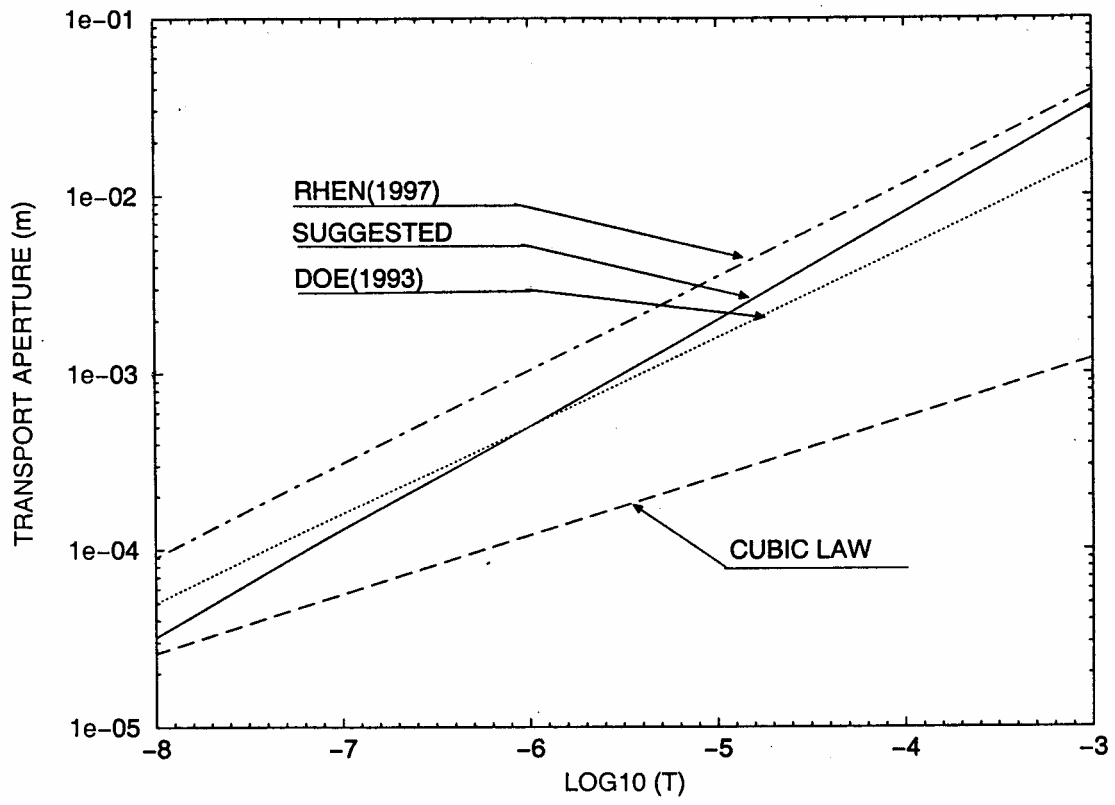


Figure F-2. Relation between fracture transmissivity and transport aperture.

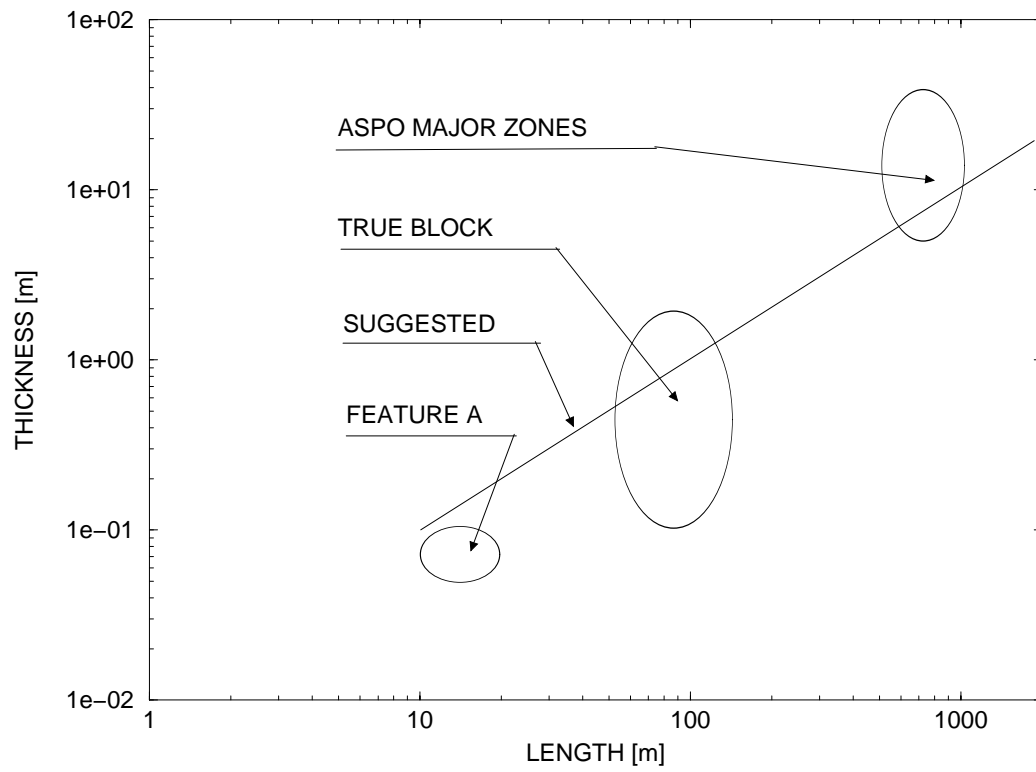


Figure F-3. Relation between fracture thickness and length.

Compiled data:

- Äspö (zones NNW*) (Rhén et al., 1997)
- TRUE BLOCK (Winberg, 1998)
- Feature A (Winberg et al., 2000)

**Appendix G. Some simple calculations
illustrating the GEHYCO method**

Some simple calculations illustrating the GEHYCO method

Calculations (which can be done without a computer) for a 2D case will be presented, with the objective to illustrate the basic idea of GEHYCO. The case to be discussed concerns a conductive element that runs at an angle of 45° to the coordinate directions and has a thickness, b_e , comparable to the grid size, Δ , see Figure G-1. The exact flux, Q_a , from cell centre (2, 2) to cell centre (3, 3) is given by:

$$Q_a = K_e b_e \frac{dh}{\sqrt{2}\Delta} \quad (\text{G-1})$$

where K_e is the element conductivity and dh the head difference. In the grid representation there will be two flow paths between the points in question. The velocity cell conductivity, K_c , is calculated as the "element conductivity times the intersecting volume divided by the cell volume" according to the basic principle of the method, thus:

$$K_c = K_e \frac{\sqrt{2}\Delta b_e}{2\Delta^2} = K_e \frac{b_e \sqrt{2}}{2\Delta} \quad (\text{G-2})$$

for both the velocity cell between (2, 2) and (3, 2) and the cell between (3, 2) and (3, 3). The head gradient from point (2, 2) to (3, 2) is thus $dh/2\Delta$. We can now formulate the flux, as represented in the grid, as:

$$Q_c = K_e \frac{b_e \sqrt{2}\Delta}{2\Delta} \frac{dh}{2\Delta} = \frac{K_e b_e}{2} \frac{dh}{\sqrt{2}\Delta} \quad (\text{G-3})$$

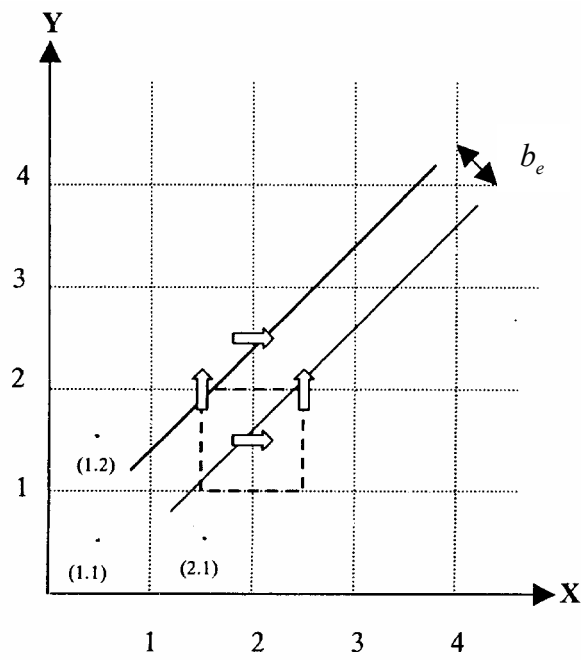


Figure G-1. Illustration of how flow and transport is simulated on the grid.

As we have two flow paths between the points, it is found that the grid representation gives the same flux as the exact solution.

Next we consider the transport time between the two points in question. Analytically it is easily calculated as the distance divided by the pore velocity:

$$t = \frac{\sqrt{2}\Delta}{U_D/n_e} = \frac{\theta_e\Delta\sqrt{2}}{K_e \frac{dh}{\sqrt{2}\Delta}} = \frac{2\theta_e\Delta^2}{K_e dh} \quad (\text{G-4})$$

where t is the transport time, U_D the Darcy velocity and θ_e the kinematic porosity. When estimating the transport time in the grid representation of the element, it is instructive to think of a particle that travels the distance. If we further accept that the residence time of the particle in a cell is equal to the free volume of the cell divided by the flow rate through the cell, the following calculations can be carried out. First one should note that the particle has to move through the grid in the "staggered arrangement", i.e. from (2,2) to (3,2), or (2,3), and then to (3,3). The two pathways have the same transport time and we only need to consider one of them. The two cells in question (2,2) and (3,2) have however different free volumes and through flows and we need to calculate the residence time for each and add the times.

$$\text{Cell (2,2): } t_{2,2} = \frac{\theta_e V_i}{Q} \quad (\text{G-5})$$

Where V_i is the intersecting volume and Q is the flow rate through cell (2.2). After some algebra it is found that:

$$t_{2,2} = \frac{\sqrt{2}}{2} \frac{\theta_e \Delta}{K_e dh} (2\sqrt{2}\Delta - b_e) \quad (\text{G-6})$$

Cell (3,2): By the same procedure it is found that:

$$t_{3,2} = \frac{\sqrt{2}}{2} \frac{\theta_e \Delta}{K_e dh} b_e \quad (\text{G-7})$$

By adding these two residence times, it is found that the transport time in the grid representation is equal to the analytical solution (Equation G-4).

Diffusive transport can be regarded as a combination of the two cases, flow and transport, discussed. First one should note that the diffusive flux is analogue to the Darcy flux, if the head gradient is replaced by the concentration gradient and the conductivity by the diffusion coefficient. It is clear that diffusion coefficients thus need to be evaluated at cell walls. If the diffusive term is part of an advection/diffusion equation for a scalar, we should evaluate the balance equation for a scalar control volume, see Figure 3-3. It is thus the free volume of the scalar cell, discussed already, that is affected by the fluxes at the cell walls. Hence, solving an advection/diffusion equation for a scalar quantity, does not require any new elements in the grid representation.

The calculations presented intend to illustrate how the properties of the conductive elements are represented in the grid. It is of course reassuring that the method gives correct result for the simple case studied, but it is not a proof that the method is exact. In fact, see Svensson (1999a) and Svensson (2001), it is well established that some fracture orientations, in relation to the grid, give an error in the simulated flow and transport times. This error has also been found to depend on the thickness of the element in relation to the grid size (b_e / Δ). Estimating this error is one of the main issues in the verification studies, see Report 2.