Methods for the streamline calculation and for the estimation of transport resistance in fractures

Vesa Tukiainen

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### METHODS FOR THE STREAMLINE CALCULATION AND FOR THE ESTIMATION OF TRANSPORT RESISTANCE IN FRACTURES

**Vesa Tukiainen**

**Summary**

The flow of water is unevenly distributed in a single fracture and in a network of fractures. The most of the flow is often concentrated to few flow channels. The effect of matrix diffusion to the transport in fractures is related to the flow distribution in the fractures. In a single flow route, the integrated value of the flow rate per unit width along the route is a key parameter when assessing the effect of matrix diffusion. In TILA-99, for example, this parameter is called transport resistance. The flow distribution and the flow routes in the fractures can be identified with the help of the streamlines related to the flow field.

In this report different methods for the calculation of the streamlines in a single fracture or in a network of fractures are examined. The study was mainly done through a literature survey. Methods for the calculation of the transport resistance have also been examined. The aim of this study was to find a calculation method for the streamlines and for the approximation of the transport resistance that could be used in the current fracture network model at VTT Energy.

Direct solution of the stream function is possible only in a single two-dimensional fracture in the absence of sinks and sources. For the numerical solution Galerkin finite element method can be used. Stream function can not be defined for the three-dimensional fracture networks. Other examined methods that can be used in the fracture networks for the streamline calculation are based on the particle tracking in the approximated flow field. Different methods for the approximation of the flow field were examined. The method, which yields the most accurate streamlines and the easiest particle tracking scheme, is the mixed-hybrid finite element method.

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METHODS FOR THE STREAMLINE CALCULATION AND FOR THE
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ABSTRACT

The spent nuclear fuel will be placed to the repository situated at the depth of 500 m in the bedrock. If the canisters containing the fuel are somehow damaged, the radioactive nuclides are released to the surrounding bedrock. The main mechanisms in the transport of radionuclides are the advection along the water conducting fractures and diffusion and sorption to the rock matrix surrounding the fractures. The effect of these mechanisms to transport must be assessed by numerical modelling.

The flow of water is unevenly distributed in a single fracture and in a network of fractures. The most of the flow is often concentrated to few flow channels. The effect of matrix diffusion to the transport in fractures is related to the flow distribution in the fractures. In a single flow route, the integrated value of the flow rate per unit width along the route is a key parameter when assessing the effect of matrix diffusion. In TILA-99, for example, this parameter is called transport resistance. The flow distribution and the flow routes in the fractures can be identified with the help of the streamlines related to the flow field.

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Direct solution of the stream function is possible only in a single two-dimensional fracture in the absence of sinks and sources. For the numerical solution Galerkin finite element method can be used. Stream function can not be defined for the three-dimensional fracture networks. Other examined methods that can be used in the fracture networks for the streamline calculation are based on the particle tracking in the approximated flow field. Different methods for the approximation of the flow field were examined. The method, which yields the most accurate streamlines and the easiest particle tracking scheme, is the mixed-hybrid finite element method.

Key words: groundwater flow, advection, transport, transport resistance, streamline, stream function, matrix diffusion, sorption, numerical solution
VIRTAVIIVOJEN LASKENTAMENETELMÄT JA RAKOKULKEUTUMIS-VASTUKSEN ARVIOINTI

TIIVISTELMÄ

Käytetty ydinpoltoaine tullaan sijoittamaan loppusijoituskanistereissa kallioperään louhittavaan loppusijoitustilaan noin 500 m syvyyteen. Jos kanisterit vaurioituvat voivat radioaktiiviset aineet vapautua ympäröivään kallioperään. Radionuklidien pääasiallinen kulkeutumismekanisni rakolleessa kalliossa on advektio virtaavan veden mukana sekä diffuusio ja sorptio rakoja ymparoivan kallion huokoistilavuuteen. Nämä kulkeutumiseen vaikuttavien pidättymismekanismien vaikutus on arvioitava numeerisilla malleilla.


Tässä raportissa tutkitaan erilaisia menetelmiä virtaviivojen laskemiseksi yksittäisessä raossa ja rakoverkostossa. Tämä raportti perustuu pääasiassa kirjallisuuselle vikeyseen virtaviivojen laskentamenetelmistä, tämän lisäksi on kuitenkin myös tarkasteltu eri mahdollisuuksia kulkeutumisvastuksen määrättämiseksi. Tämän työn tarkoituksena on löytää virtaviivojen laskentamenetelmä, joka soveltuu käytettäväksi kulkeutumisvastuksen laskentaan rakoverkollilla rakataistussa virtauskentässä.


Avainsanat: pohjaveden virtaus, advektio, kulkeutuminen, kulkeutumisvastus, virtaviiva, virtafunktio, matriisidiffuusio, sorptio, numeerinen ratkaisu
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1 INTRODUCTION

The spent fuel of the Finnish nuclear power plants has to be placed in Finland. In the current disposal concept [Vieno & Nordman 1999] the spent fuel is encapsulated inside iron canisters that are covered by copper casing. These canisters are placed to the repository situated at the depth of 500 m in the bedrock. The space between the bedrock and the canisters is filled with the mixture of bentonite and crushed rock.

Assuming the canister is damaged by some way the radionuclides can migrate through the bentonite to the surrounding bedrock, which is the last natural barrier between the biosphere and the repository. The main mechanisms affecting in the radionuclide transport are the advection along the groundwater flowing in the fractures of the bedrock and a combination of diffusion and sorption in the rock matrix surrounding the fractures. When assessing the safety of the disposal the effect of these mechanisms must be somehow simulated.

The fractures are very heterogeneous and the hydraulic properties vary even in a single fracture. This means that the flow is unevenly distributed in a single fracture and in the network of many fractures. Most of the flow is concentrated to relatively small area of the total fracture area. This phenomenon is called flow channeling. The effect of matrix diffusion to the transport of radionuclides is related to the physical properties of the rock matrix and to the flow conditions in the fracture. When the flow rate per unit width in the fracture decreases, the effect of matrix diffusion to the transport increases. When we assess the effect of the matrix diffusion we need not only information about the properties of the rock matrix but also information about the flow distribution in a single fracture or in the fracture network. The flow distribution in the fractures can be examined with the help of the streamlines related to the flow field. When streamlines approach each other, the flow rate per unit width increases. When the streamlines draw away, the flow rate per unit width decreases. A single streamline defines also a path of a fluid particle. The calculation of the streamlines is therefore a natural way to define the flow distribution in the fracture. The effect of matrix diffusion in a single flow path is related to the integrated value of the flow rate per unit width along the flow path. This parameter is called the transport resistance of the flow path. The streamline approach enables the calculation of this parameter for different flow routes. In order to assess the effect of matrix diffusion to transport in a single fracture or in a network of fractures some numerical method for the determination of the streamlines and for the approximation of the transport resistance is needed.

In this study we examine different methods for the calculation of the streamlines in a single fracture or in a network of fractures. Especially we investigate the possibility to solve the stream function related to the flow field. The study is mainly done as a literature survey. We examine also methods to calculate the transport resistances of the calculated flow paths. VTT Energy currently uses numerical modeling package FRACMAN/MAFIC [Dershowitz, W. et. al. 1995, Miller, I. 1990] in the simulation of the flow in fracture networks. The applicability of the examined calculation methods to the fracture network modeling approach is also assessed.

In the next chapter we represent the traditional mathematical modeling concept for the fracture flow, The numerical solution method of the fracture flow case is also
introduced. The possibility to calculate directly the stream function is examined in
chapter three. A particle tracking method, which utilizes the FEM solution of the flow
field is introduced in chapter four. Some improved methods for the calculation of flow
field are examined in chapter five. In chapter six we introduce the transport resistance
and examine the calculation methods to approximate it from the numerical solution of
the flow field. The applicability of the different methods is assessed in chapter seven.
2 THE MODELLING OF GROUNDWATER FLOW

2.1 Mathematical model

The flow of water in bedrock is concentrated to the network of connected pores and fractures. In the mathematical description of groundwater flow the exact flow field in the pores is often ignored. Instead we examine the average flow on some macroscopic level. This approach is called continuum approach, where the bedrock is approximated as single continuum. Commonly used quantity in the description of the groundwater flow is hydraulic head. The hydraulic head $h$ for incompressible fluid is [Bear 1979, s. 62, Strack 1989]

$$ h(x, y, z) = z + \frac{p(x, y, z) - p_0}{\rho g}, \quad (1) $$

where

$h(x, y, z)$ is hydraulic head (m),

$p$ is pressure at point $(x, y, z)$ (Pa),

$p_0$ is some reference pressure (Pa),

$g$ is the acceleration of gravity (m/s$^2$),

$\rho$ is the density of water (kg/m$^3$),

$z$ is elevation over some reference level (m).

The analysis of the groundwater flow is based on Darcy's law

$$ \mathbf{q} = -K \nabla h, \quad (2) $$

where $K$ (m/s) is the hydraulic conductivity tensor of the porous medium and $\mathbf{q}$ is the specific discharge vector (m/s). $\mathbf{q}$ represents the volume of water flowing through unit area in unit time.

We assume that the water is incompressible and the flow is time independent. The continuity equation for incompressible flow at steady state is

$$ \nabla \cdot \mathbf{q} = Q_v, \quad (3) $$

where $Q_v$ is volumetric flow per unit volume coming from sources to the system (1/s). Inserting Darcy's law (2) to the continuity equation (3) we get the equation of the groundwater flow for incompressible fluid at steady state:

$$ \nabla \cdot (K \nabla h) = -Q_v. \quad (4) $$

Figure 1 describes a flow area, which is confined between two horizontal impermeable layers. If the horizontal dimensions are much larger than the vertical dimension, the flow is essentially two-dimensional. The hydraulic head is now the mean value taken in the vertical direction [Bear 1979, s. 71]:

...
Figure 1. Horizontal flow region between impermeable layers.

Darcy’s law for two-dimensional horizontal area is

\[ Q_w = -T \nabla h, \]

where \( Q_w \) is a vector representing the flow rate per unit width \((m^2/s)\). \( T = 2bK \) is the transmissivity tensor \((m^2/s)\). The equation of the groundwater flow is now

\[ \nabla \cdot (T \nabla h) = -Q_a, \]

where \( Q_a \) is volumetric flow per unit horizontal area coming from sources to the system \((m/s)\).

As the groundwater in fractured bedrock flows mainly through largest fractures, the modeling of the flow in the fractures is often needed. We first examine flow in a single fracture. Fracture aperture is much smaller than the other dimensions and fractures often have planar geometry. Therefore flow in the fracture is often essentially two-dimensional. As a first approximation the fracture can be conceptualized as void space between two smooth, parallel impermeable plates. Flow is assumed to be incompressible and at steady state. Flow is described by Navier-Stokes equation for viscous incompressible flow. The resulting velocity field is parabolic in the direction of the fracture aperture. Discharge per unit width in the direction of flow is then [Tukiainen 2000]

\[ Q_w = -\frac{(2b)^3 dp}{12\eta \ dx} = \frac{(2b)^3 \rho g \ dh}{12\eta \ dx}, \]

where \( 2b \) is the fracture aperture \((m)\) and \( \eta \) is dynamic viscosity of water \((kg/ms)\). As the magnitude of flow is proportional to the cube of the aperture, equation (8) is often
called cubic law in the literature. Comparing Darcy's law (6) and equation (8) it can be seen, that the transmissivity of constant aperture fracture is:

$$T = \frac{(2h)^3 \rho g}{12\eta}.$$  \hspace{1cm} (9)

In reality the fracture aperture is highly variable. If the cubic law holds also locally in the variable aperture fracture, equation (9) defines two-dimensional transmissivity field according to aperture variations. This transmissivity can then be used in equations (6) and (7). If we assume that there are no sources in the fracture then the equation (7) can be written in the form

$$\nabla \cdot (b^3(x, y) \nabla h) = 0.$$  \hspace{1cm} (10)

This equation is named as Reynolds equation in the literature. Majority of theoretical and simulation studies have postulated that local flow magnitudes are well described by the Reynolds equation [Assaf & Berkowitz 1998]. Therefore it can be assumed that equations (9), (7) and (6) can be used to describe the flow in the fracture.

Equation (7) needs some boundary conditions defined in the modeled domain boundary. Two types of boundary conditions can be defined:

$$h = \tilde{h}(\Gamma) \text{ on boundary } \Gamma_1,$$  \hspace{1cm} (11)

$$\mathbf{T} \cdot \nabla h \cdot \mathbf{n} = \tilde{Q}_w \text{ on boundary } \Gamma_2,$$  \hspace{1cm} (12)

where $$\Gamma_1$$ and $$\Gamma_2$$ are parts of the domain boundary $$\Gamma$$. Condition (11) represents the known hydraulic head at the boundary. In condition (12) $$\mathbf{n}$$ is unit normal vector of the boundary (direction outward) and $$\tilde{Q}_w$$ is discharge through the boundary to the modeled domain per unit width of the boundary ($$\text{m}^2/\text{s}$$).

The flow in the fracture network can basically be modeled with three-dimensional continuum approach, where areas of fractures have high hydraulic conductivity and rock matrix between fractures have vanishing hydraulic conductivity. Another alternative is discrete fracture network models [Dverstorp 1991, Nordqvist et al. 1992, Poteri & Laitinen 1996, Poteri & Laitinen 1999]. In these models the fractures are usually defined as a network of connected two-dimensional plates (Figure 2), which forms a route for the flow of groundwater. The properties and orientations of fractures can be deterministic or they can be constructed using stochastic methods. As the modeled fractures are essentially two-dimensional, equations (9), (7) and (6) can be used to describe the flow in the fractures.
2.2 Numerical solution with Galerkin finite element method

As fractures are heterogeneous and the geometry of the flow problem especially in the fracture network model is complicated, the equation of flow in the fracture or in the fracture network must be solved numerically. The most widely used numerical method for solving groundwater flow problems is the Galerkin finite element approach [Bear 1979, p. 146, Huyakorn 1983, p. 41]. Here we will give a brief review of the method and its application to the steady state flow equation (7) in two-dimensional fractures. In the finite element method the modeled domain is discretized to elements and nodes. In the Galerkin approach the hydraulic head is approximated by trial solution

$$\hat{h} = \sum_{j=1}^{N} h_j w_j(x_1, x_2),$$  \hspace{1cm} (13)

where $h_j$ are the unknown nodal values of hydraulic head and $w_j$ is the basis function associated with node $j$. The basis functions are defined such that $w_j$ is unity at node $j$ and zero at other nodes. The most common scheme is to use triangular elements and piecewise linear basis functions. Such basis function is shown in Figure 3.
The flow equation (7) can be written using operator $L$:

$$L(h) = \nabla \cdot T \nabla h + Q_a = 0.$$  \hspace{1cm} (14)

A solution of equation (7) is found by setting the residual resulting from the approximation (13) orthogonal to all $N$ basis functions:

$$\int_{\Omega} L(h) w_i d\Omega = 0 \quad i = 1, \ldots, N,$$  \hspace{1cm} (15)

where $\Omega$ is the modeled domain. Application of Green's theorem [Bear 1979, p. 149] to second derivative terms in (15) yields

$$\int_{\Omega} \sum_{n=1}^{2} \frac{\partial w_i}{\partial x_n} \sum_{m=1}^{2} T_{nm} \frac{\partial h}{\partial x_m} d\Omega - \int_{\Gamma} w_i \left( T \cdot \nabla h \right) \cdot n d\Gamma - \int_{\Omega} w_i Q_a d\Omega = 0 \quad i = 1, \ldots, N.$$  \hspace{1cm} (16)

If the flux boundary condition is defined for some boundary segment $\Gamma_3$, the boundary integral for that segment can be written in the form

$$\int_{\Gamma_3} w_i \left( T \cdot \nabla h \right) \cdot n d\Gamma_3 = \int_{\Gamma_3} \bar{Q}_a d\Gamma_3.$$  \hspace{1cm} (17)

If any boundary condition has not been defined over a boundary segment, it is assumed to be impermeable. We then substitute the trial solution (13) in (15) and calculate the integrals by summing the element contributions. The resulting equation can be written in matrix form

$$Ah = Q + \bar{Q},$$  \hspace{1cm} (18)
where vector $h$ contains the nodal values of the hydraulic head and the elements of matrix $A$ and vectors $Q$ and $\tilde{Q}$ are

$$A_{ij} = \sum_{e} \sum_{n,m=1}^{2} \frac{\partial w_j}{\partial x_n} \sum_{m=1}^{2} T_{nm} \frac{\partial w_i}{\partial x_m} d\Omega_e,$$

$$Q_i = \sum_{e} \int_{\Omega_e} w_i Q_a d\Omega_e,$$

$$\tilde{Q}_i = \sum_{e} \int_{\Gamma_2} w_i \tilde{Q}_w d\Gamma_2,$$

where subscript $e$ refers to different elements. In the boundary integral the summation is done over the elements that join at node $i$. The integrals are usually calculated assuming constant values of transmissivity tensor $T_{nm}$ and discharge $Q_a$ at elements and flux $\tilde{Q}_w$ at element edges. The last equation can be integrated over the boundary sections of the elements adjacent to the node $i$. Using linear basis functions we get

$$\tilde{Q}_i = \frac{1}{2} \tilde{Q}_w^1 l_i^1 + \frac{1}{2} \tilde{Q}_w^2 l_i^2,$$

where $\tilde{Q}_w^e$ is the specific discharge $(m^2/s)$ through the boundary of element $e$ adjacent to node $i$ and $l_e^i$ is the length of the boundary section of element $e$. The flux boundary condition (12) is therefore in practice given as nodal values $\tilde{Q}_i$. The prescribed head boundary condition (11) is given also as nodal values. It is implemented to the numerical scheme by manipulating the matrix $A$ and the right hand side of the equation (18). The head condition at a node is implemented by eliminating the corresponding matrix row and in the matrix $A$ and transferring the terms containing the fixed head values to the right hand side vector [Huyakorn 1983, p. 30].

The hydraulic head values at nodes are obtained by solving equation (18) by using some numerical solution method of the linear algebraic equations. The approximation of the specific discharge $Q_w$ can be calculated according to Darcy’s law (6). Insertion of (13) into the Darcy’s law yields

$$\tilde{Q}_w = -\sum_{j=1}^{N} h_j T \cdot \nabla w_j .$$

If the basis functions $w_j$ are piecewise linear, the approximation yields specific discharge, which is constant over the element. Additionally, the normal component of the specific discharge over the element edge is discontinuous between adjacent elements [Durlofsky 1994].

The previous definition of the Galerkin finite element method was defined for two-dimensional flow domain. The fracture network model is three-dimensional, although the discrete fractures are two-dimensional. The two-dimensional fractures can be
constructed from two-dimensional elements. As the integrals in equation (19) are calculated element by element, the Galerkin finite element method in two dimensions can be applied also to the fracture network model. The fracture network modeling package FRACMAN/MAFIC currently in use at VTT Energy uses also the Galerkin finite element method in the solving of the flow equation [Dershowitz, W. et. al. 1995, Miller, I. 1990].
3 STREAM FUNCTION FOR FRACTURE FLOW

Streamline is defined as a curve that is everywhere tangent to the fluid velocity field. In the case of the flow in two-dimensional fracture, it is therefore tangent to the specific discharge vector $Q_w$. The equation of streamline is [Bear 1979, p. 165]

$$Q_w \times ds = 0,$$

(22)

where $ds$ is an infinitesimal length along the streamline. In two dimensions the equation can be written in the form

$$(Q_w)_x \, dy - (Q_w)_y \, dx = 0,$$

(23)

where $x$ and $y$ are cartesian coordinates. We define a function $\psi = \psi(x, y)$, that is constant along streamline. Hence, along streamline

$$d\psi = \frac{\partial \psi}{\partial x} \, dx + \frac{\partial \psi}{\partial y} \, dy = 0.$$

(24)

Comparison of (23) and (24) leads to

$$\left[ \begin{array}{c} (Q_w)_x \\ (Q_w)_y \end{array} \right] = \pm \left[ \begin{array}{c} \frac{\partial \psi}{\partial y} \\ -\frac{\partial \psi}{\partial x} \end{array} \right].$$

(25)

The choice of the sign in the right hand side of equation (25) is arbitrary. Frind & Matanga [1985] have chosen the positive sign. The function $\psi$ is called stream function.

Stream tube is defined by the two bounding streamlines, where the stream function has constant values $\psi_e$ and $\psi_i = \psi_e + \Delta \psi$. It can be shown [Bear 1979, Frind & Matanga 1985] that the total discharge $\Delta Q$ (m$^3$/s) passing through the stream tube is $\Delta Q = \psi_e - \psi_i$. We can also write [Frind & Matanga 1985]

$$\psi(p) = \psi_e + \int_{p_0}^{p} \mathbf{Q}_w \cdot \mathbf{p} \, dp,$$

(26)

where integration is made along arbitrary path, $\mathbf{p}$ is unit normal vector of the path and $\psi_e$ is the value of the reference stream function at point $p_0$. Frind & Matanga [1985] have derived a differential equation for the stream function in two-dimensional domain. The equation has been derived assuming that there are neither sources nor sinks in the flow domain, the fluid is incompressible and the flow is at steady state. The discharge vector therefore fulfills the continuity equation.
Another assumption is that the driving force field $\nabla h$ is conservative and therefore satisfies
\[ \nabla \times \nabla h = 0. \] (28)
The derived equation for the stream function in the two-dimensional flow field is
\[ \nabla \cdot \left( \frac{T}{\det T} \nabla \psi \right) = 0. \] (29)
Bear [1979, p. 167] have also derived an analogous equation. It can be seen that equation (29) is formally same as equation (7) in the absence of sources. Boundary conditions are, however, defined differently. Dirichlet-type boundary condition can be defined according to equation (26) if the specific discharge is known at boundary:
\[ \psi(\Gamma) = \psi_0(\Gamma_0) + \int_{\Gamma_0} \mathbf{Q}_w \cdot \mathbf{n} d\Gamma \text{ on boundary } \Gamma, \] (30)
The reference level and position at the boundary can be chosen freely. Along impermeable boundary the stream function is constant. The normal vector $\mathbf{n}$ of the boundary depends on the integration path and direction. If $\mathbf{r}$ is the unit tangent vector of the boundary in the direction of integration, the components of $\mathbf{n}$ are $n_x = r_x$ and $n_y = -r_y$. Neumann-type boundary condition can be written in terms of the tangential component of the hydraulic gradient at the boundary:
\[ \left( \frac{T}{\det T} \nabla \psi \right) \cdot \mathbf{n} = \nabla h \cdot \mathbf{r} \text{ on boundary } \Gamma, \] (31)
where $\mathbf{r}$ is unit tangent vector of the boundary. $\mathbf{n}$ and $\mathbf{r}$ are related by $n_x = r_x$ and $n_y = -r_y$.
As equation (29) for the stream function is formally same as equation (7) for the hydraulic head, we can use the Galerkin finite element method to solve the stream function numerically. Application of the Galerkin method to (29) is done analogous to the case where the hydraulic head was solved. The resulting matrix equation is
\[ \mathbf{R} \Psi = \mathbf{f}, \] (32)
where the vector $\Psi$ contains the value of the stream function at the nodes, and the components of the matrix $\mathbf{R}$ and vector $\mathbf{f}$ are
\[ R_{ij} = \sum_c \int_{\Omega_c} \sum_{n,m=1}^{2} \frac{T_{mn}}{\det T} \frac{\partial \psi_i}{\partial x_n} \frac{\partial \psi_j}{\partial x_m} d\Omega_c, \]
\[ f_i = \sum_c \int_{\Gamma_c} (\nabla h \cdot \mathbf{r}) \psi_i d\Gamma. \] (33)
The specified specific discharges at the boundary are changed to nodal values of the stream function according to equation (30). The nodal values are implemented to the numerical scheme similarly as in the case where the hydraulic head was solved. Contours of equal stream function values coincide with the streamlines. After the values of the stream function at nodes have been obtained by solving the system (32), constant contours of stream function can be calculated. As the stream function in the case of the triangular elements is interpolated linearly between the nodes, the streamlines are straight lines over the elements. The usage of stream functions for obtaining streamlines is restricted to the simulation of flow in a single fracture in the absence of sources or sinks. Although the finite element solution for fracture networks uses two-dimensional elements, the flow is actually three-dimensional. The fracture intersections also act as sources or sinks for the flow in single fracture. Therefore the formulation of the two-dimensional stream function can not be used to calculate streamlines in fracture networks.
PARTICLE TRACKING IN THE TRADITIONAL SPECIFIC DISCHARGE FIELD

Assuming that the flow field is known, the path of a fluid particle can be followed. The path is a representation of a single streamline. The movement of the fluid particle can be described by the equation

\[
\frac{dx}{dt} = v(x),
\]

where \( x \) is the location vector and \( v \) is the fluid velocity vector. If velocity field is known, equation (34) completely defines the movement of the particle from the given initial position. Starting at \( x_0 \) at time \( t_0 \), the particle location at time \( t \) is

\[
x(t) = x(0) + \int_{t_0}^{t} v(\tau)d\tau,
\]

where \( v(\tau) \) is the particle velocity at time \( \tau \) as the particle moves along its trajectory. Usually there does not exist an analytical solution of the flow field, and integral must be evaluated numerically. The time integral is discretized to sufficiently small steps. Different numerical integration methods [Burden & Faires 1993] can be used. By using the simplest Euler integration method with constant time step we obtain

\[
x(t + \Delta t) = x(t) + v(t)\Delta t,
\]

where \( \Delta t \) is the constant time step. If the flow magnitudes are highly variable, it is necessary to adjust the time step according to local velocity [Wen & Gómez-Hernandez 1996]:

\[
\Delta t = \frac{\Delta s}{|v(t_1)|},
\]

where \( \Delta s \) is predefined constant displacement and \( v(t_1) \) is the local velocity at the start of the time step.

The current fracture network model in use in VTT Energy calculates the hydraulic head field using the previously introduced Galerkin finite element method. The model uses two-dimensional elements. The flow field is then calculated using the nodal values of the hydraulic head (equation (21)). The specific discharge and therefore the velocity is constant over the element. Path lines of fluid particles in this kind of flow field are straight lines over elements. The numerical integration is not needed, because when we know the starting point of a particle in an element, the exit point of the particle is completely defined. We simply draw a line parallel to the specific discharge vector and see, where the line crosses the edge of the element. This is the starting point of the fluid particle at the next element. In this way path lines can be tracked in a single fracture until the path crosses some fracture intersection. The properties of the approximated
specific discharge field might, however, lead to some problems during the path line construction. These problems must be handled by some heuristic methods. We next examine the problems and some methods to avoid them.

The approximated specific discharge field is discontinuous at element edges. In particular, the normal component of the specific discharge is discontinuous over the element edge. In some cases the normal components at adjacent elements can have opposite directions. This can happen in the vicinity of a sink [Herbert 1990], or at boundaries of elements having different hydraulic conductivities (transmissivities) [Cordes & Kinzelbach 1992]. As the fracture intersections act as line sinks, we can expect similar behavior also near the fracture intersections. The specific discharge vector can therefore be directed to the element edge, where the particle is coming to the element. If we use the previously introduced path line construction method, the particle is stuck to the element edge. These kind of artificial sinks can be avoided by extending the path line always over the element edge by a small amount [Herbert 1990]. Figure 4a shows an example of path line constructed by this method. The extension of the path line is exaggerated in the picture. Another alternative is shown in Figure 4b. When the particle encounters an element where the normal component of the specific discharge is outward directed, it is reflected back by a small amount and it is assigned a specific discharge parallel to the edge. The specific discharge vector can be for example the component of the original specific discharge parallel to the edge.

Problems can arise also at the fracture boundaries, which are impermeable. Due the approximations in the construction of the specific discharge field, the specific discharge vector is not necessary parallel to the impermeable boundary at the elements adjacent to the boundary. The tracked particles may therefore cross the impermeable boundaries and be lost. Herbert [1990] suggests a solution, where the particles are artificially displaced towards the fracture interior every time they cross the impermeable edge. The method is represented in Figure 5a. This method can lead to various artificial reflections in single element, if the element at the boundary has strong outward directed flow. The method can be slightly modified. The modification is shown in Figure 5b. The particle is similarly reflected back, but it is assigned a specific discharge vector parallel to the boundary. Therefore the method leads at most one reflection per element at the boundary. In both methods we must somehow be able to identify all the impermeable edges in the fracture network model from those that have real outflowing conditions.
The hydraulic head at the end point of a fracture intersection will often be lower than at all the surrounding nodes in the vicinity [Herbert 1990]. This might cause problems to tracked paths coming near to this artificial point sink. The tracked path might step back
and forth around the point sink and never reach the intersection. To prevent the loss of particles around these end nodes of intersections one can define a target area over the end point. If the particle crosses this target area, it is assumed to have reached the end of intersection. This kind of target area should be defined also for the real point sinks.

In the fracture intersections the flow path of a fluid particle is not uniquely defined if the flow out of the intersection is divided to many fractures. In the intersections some stochastic rule must therefore be used in determining which route the particle will follow. The particle tracking algorithm must be able to identify the element edges, which are fracture intersections. When the particle crosses the element edge, which is intersection, the tracking algorithm uses some stochastic method in determining to which element the particle continues. The method assigns transfer probabilities to the possible outlet elements. The simplest way is to define the transfer probabilities, which are proportional to the flow rates of the outlet elements. If the particle tracking is used in solute transport calculations, this kind of definition of transfer probabilities through fracture junctions is called complete-mixing theory [Park & Lee 1999]. As the elements at the intersection share a common edge, we can use the normal components of the elementwise specific discharges in the determination of the transfer probabilities. We first exclude the elements, from which the flow is coming to the intersection. For these elements

\[ Q'_w = Q'_w \cdot \mathbf{n}' > 0, \]

where \( Q'_w \) is the specific discharge vector of an element \((m^2/s)\) and \( \mathbf{n}' \) is the outward directed normal vector of the intersection edge. The transfer probabilities of the remaining outlet elements are calculated according to

\[ P(e) = \frac{Q'_w}{\sum_{j=1}^{m} Q'_w}, \]

where \( P(e) \) is the transfer probability to element \( e \) and \( m \) is the number of the possible outlet elements. When the particle tracking is used in the solute transport calculations, the complete mixing theory is valid for flows of very low Peclet number. For flows of very high Peclet number Park & Lee [1999] introduce streamline-routing theory, where the transfer probabilities are determined from the discharge conditions in the inlet branches as well as in the outlet branches.

By combining the basic particle tracking method and the heuristic rules the path of the particle can be tracked from some point of the inflow boundary until it reaches a fracture edge that belongs to the outflow boundary of the modeled domain.

We have seen that the traditional Galerkin approximation of the flow equation leads to discontinuous specific discharge field in the fractures or in the fracture network. The calculation of the streamlines using this field and particle tracking is possible. Various heuristic rules must, however, be used. The resulting path lines are therefore expected to be inaccurate. Because of the heuristic rules, the implementation of the particle tracking algorithm is also more difficult. In the next section we examine some methods, which
enable more accurate calculation of the specific discharge field than the traditional Galerkin method. The more accurate specific discharge field should lead to easier particle tracking scheme.
5 IMPROVED METHODS FOR THE APPROXIMATION OF THE SPECIFIC DISCHARGE FIELD

5.1 Application of Galerkin finite element method to Darcy’s law

Gour-Tsyh Yeh [1981] have proposed, that Galerkin finite element method could be applied to the Darcy’s law (6) after it has first been applied to the flow equation (7). This yields a specific discharge vector field, which is continuous at element edges. The approach of Yeh is presented here for flow in two-dimensional fracture. The nodal values of hydraulic head are first solved conventionally with Galerkin method. The trial solution for the components of the specific discharge vector is written in familiar form

\[
\hat{q}_n = \sum_{j=1}^{N} q_{nj} w_j (x_1, x_2) \quad n = 1,2, \quad (40)
\]

where \( n \) refers to the components of specific discharge vector \( q \). Here we use symbol \( q \) instead of \( Q_w \) to simplify the notation. Darcy’s law for the components of specific discharge vector is written using operator \( L \):

\[
L(q_n, h) = q_n + \sum_{m=1}^{2} T_{nm} \frac{\partial h}{\partial x_m} = 0 \quad (41)
\]

The solution of equation (41) is found by setting the residual resulting from the approximations (13) and (40) orthogonal to all \( N \) basis functions:

\[
\int_{\Omega} L(\hat{q}_n, \hat{h}) w_i d\Omega = 0 \quad i = 1, \ldots, N; \ n = 1,2. \quad (42)
\]

As a result we have matrix equation

\[
C q_n = u_n, \quad (43)
\]

where the vectors \( q_n (n=1,2) \) contain the nodal values of the components of the specific discharge \( q \). The components of matrix \( C \) and vector \( u_n \) are

\[
C_{ij} = \sum_{e} \int_{\Omega_e} w_i w_j d\Omega_e, \quad \tag{44}
\]

\[
u_{mi} = \sum_{e} \int_{\Omega_e} w_i \left[ \sum_{m=1}^{2} T_{nm} \frac{\partial}{\partial x_m} \left( \sum_{j=1}^{N} h_j w_j \right) \right] d\Omega_e. \quad (44)
\]
In the definition of $u_{ni}$, the expression inside the outer brackets can be identified as the component of the traditionally evaluated specific discharge at element $e$. Therefore we can write

$$u_{ni} = \sum_e w_i q_n^e d\Omega_e,$$  \hspace{1cm} \text{(45)}

where $q_n^e$ is the component of the specific discharge vector at element $e$ according to equation (21). Therefore the approach of Yeh actually transforms the traditional constant specific discharges at the elements $q_n^e$ to specific discharges at nodes $q_{nr}^e$. Additionally the components of specific discharge are linearly interpolated between nodes (for triangular elements). When we solve the equation (43) the nodal value $q_{nr}^e$ is actually the weighted average of the components $q_n^e$ at the elements surrounding the node.

The specific discharge and therefore the fluid velocity are a linear function of the coordinates. We can write the components of the velocity inside the 2-dimensional triangular element in the form

$$v_x (x,y) = a_x + b_x x + c_x y,$$

$$v_y (x,y) = a_y + b_y x + c_y y,$$  \hspace{1cm} \text{(46)}

where $x$ and $y$ are the local cartesian coordinates of the element and the constant coefficients $a_x, b_x, c_x, a_y, b_y$, and $c_y$ depend on the nodal values of the velocity components and on the geometry of the element.

The equation of motion for the fluid particle inside an element can be written in the form

$$\begin{bmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{bmatrix} = \begin{bmatrix} b_x & c_x \\ b_y & c_y \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} a_x \\ a_y \end{bmatrix}$$  \hspace{1cm} \text{(47)}

Equation (47) is a nonhomogeneous linear system of first order differential equations with constant coefficients. Different analytical solutions for the system can be found depending on the values of the constant coefficients [Kreyszig 1993, s. 186]. With this analytical solution the path of the particle inside the element can be accurately tracked. Of course the path of the particle can be defined also by integrating equation (47) numerically.

In the fracture network model the nodes, which belong to the fracture intersections have adjacent elements from different fractures. The traditionally calculated specific discharge vectors of these elements lie always on the plane of the element. The weighted average of these vectors generally is not parallel to any of the fracture planes. Therefore the calculated velocities at the nodes in the fracture intersections point to the
space between the fractures. As specific discharges are interpolated linearly between the
nodes, also the specific discharges in the elements adjacent to the intersections are not
parallel to the fracture plane. This leads to a clearly unphysical flow field at the
elements adjacent to fracture intersections. When these specific discharges are used in
the particle tracking the particles move to the undefined area between the fracture
planes. The particle tracking must be handled therefore separately in these elements. We
can for example use the traditional constant elementwise specific discharges at the
elements adjacent to the intersections. This might still lead problems in the particle
tracking, as was introduced in the previous chapter.

5.2 Postprocessing of the elementwise specific discharge field

Cordes and Kinzelbach [1992] have introduced a method, which uses the traditional
constant specific discharges at elements in the construction of a new, more accurate
specific discharge field. Here the method is introduced for two-dimensional triangular
elements. Each triangular element is divided to four subelements by drawing straight
lines between the centers of the adjacent element edges (Figure 6). The values of the
original elementwise discharge vectors are assigned to the center subelements of each
element. The aim is then to find the specific discharges of other subelements.

\[ \sum_{i=1}^{M} Q^i = R , \]
where $R$ is source discharge (m³/s) at the node and $Q'$ is the discharge (m³/s) through patch boundary section of subelement $s$. $M$ is the number of subelements in the patch. Positive discharge means flux directed outward from the node. The discharges through the patch boundaries can be calculated according to the known specific discharge vectors at center subelements:

$$Q' = q_e \cdot n^{s1} \cdot l^{s1},$$  \hspace{1cm} (49)

where

$n^{s1}$ is the outward directed unit normal vector of the patch boundary section of subelement $s$,

$q_e$ is the discharge vector in the adjacent center subelement,

$l^{s1}$ is the length of the patch boundary section.

Patches are used in the calculation of the specific discharges of subelements around the interior nodes of the finite element domain. In the calculation it is assumed, that the nodes contain no sources ($R_\pi = 0$). The aim is to find the specific discharges in the subelements, so that the normal components are continuous at the subelement edges. This continuity is possible, if there is no source at the node related to the patch. The continuity relations for the patch boundary sections are

$$q_s n^{s1} + q_s n^{s1} = \frac{Q'}{l^{s1}} \quad s = 1, ..., M.$$  \hspace{1cm} (50)

The continuity relations between the subelement edges inside the patch are

$$q_s n^{s2} + q_s n^{s2} + q_s n^{s3} + q_s n^{s3} = 0 \quad s = 1, ..., M - 1,$$

$$q_s n^{s2} + q_s n^{s2} + q_s n^{s3} + q_s n^{s3} = 0.$$  \hspace{1cm} (51)

In these relations $q_s$, $q_s$ are the components of the specific discharge vector in a subelement, $n_{\pi}^{s_i}$, $n_{\pi}^{s_i}$ are the components of the outward directed unit normal vector of subelement edge $i$ and $l_i$ is the length of subelement edge $i$. Index $s$ refers to the subelements. The edges of the subelement are numbered by clockwise rotation starting from the patch boundary section (Figure 6). The numbering of the subelements is done also clockwise. Continuity relations (50) and (51) form a system of $2M$ equations, of which $2M - 1$ are independent. Therefore one more equation is needed for obtaining unique vectors $Q$. This equation is obtained from the validity of equation (28) in a weak sense over the patch:

$$\oint_T T^{-1} q \cdot dX = 0,$$  \hspace{1cm} (52)

where $X$ is a closed path around a node. The parts of the closed path in subelements are chosen parallel to the patch boundary sections as shown in Figure 7. This gives the last equation
The specific discharges at the subelements can now be obtained by solving equations (50), (51) and (53), which form a system of 2M+1 linear equations.

The system of equations is not needed for the nodes at the finite element domain boundaries, where the normal component of specific discharge has been used as a boundary condition. (At impermeable boundaries this component is zero). The flux boundary condition in finite element scheme is usually given as nodal values $Q_i$ of discharge (m$^3$/s). According to equation (19) this nodal value can be interpreted as an integral of constant fluxes through the boundary sections of adjacent elements. The relation between the nodal value of discharge and the fluxes through boundary sections of adjacent elements is given by equation (20). This equation can be used in calculating the fluxes $\tilde{Q}_{\alpha \beta}$ through element edges at the boundary.

The specific discharge $q_i^s$ of the subelement can be uniquely defined, if we know the normal components of the specific discharge on two edges. For those subelements, which have one common edge with the boundary, the specific discharge can be uniquely defined from the two known flux values at two edges. An example of a patch at boundary is shown in Figure 8. The discharge vector $q_i^s$ of the subelement 1 can be calculated using the known discharge $\tilde{Q}^1_i$ to the adjacent center subelement and boundary flux $\tilde{Q}_{\alpha 1}^i$. The specific discharge of subelement 2 can be obtained using the calculated $q_1^s$ and known discharge $\tilde{Q}^2_i$ and so on.
Cordes and Kinzelbach defined the usage of the patches in two-dimensional domain. In the fracture network model this definition is applicable for the nodes that do not lie at fracture intersections. The nodes at intersections have common elements from different fracture planes. An example of the intersection of two fractures is shown in Figure 9. The elements from the fracture planes that are connected to the same single node have been drawn. Analogous to the previous two-dimensional analysis the patch around the node at an intersection is formed of all subelements in contact with the node. The patch around the node in Figure 9 is shown in Figure 10. The equations for the definition of the specific discharges at the subelements are somewhat modified. The continuity relations for the patch boundary sections remain unchanged (equation (50)). The continuity relations for the subelement edges inside the patch remain unchanged for the element edges, that are not fracture intersection lines:

\[
q_x^s n_x^s + q_y^s n_y^s + q_x^{s+1} n_x^{(s+1)} + q_y^{s+1} n_y^{(s+1)} = 0, \tag{54}
\]

where subelements \( s \) and \( s+1 \) are at the same fracture plane and the edge between the subelements is not an intersection. The equations for the edges that lie on the intersection are obtained assuming mass conservation at the intersection. In Figure 10 four subelements share an edge, that is an intersection. The discharges and therefore the normal components of the specific discharges through the subelement edge must sum to zero, if mass is conserved:

\[
\sum_{s=1}^{4} q^s \cdot n^s = 0, \tag{55}
\]

where \( n^s \) is the outward directed unit normal vector of subelement \( s \). This equation is formed for every subelement edge that is a fracture intersection (for two edges in the case of Figure 10). In general, the summation is made over all subelements, which have common edge at intersection.

In the case of the patch in Figure 10 we have eight equations according to continuity relations (50) of all eight patch boundary sections. The subelement edges inside the patch that belong to a single fracture plane give 4 more equations (equation (54)). Using (55) for the edges at fracture intersections gives two equations. As we have \( 2 \times 8 = 16 \)
unknown components of specific discharge, two more equations are needed. If we assume the validity of equation (52) separately on each fracture plane, we get two last equations needed. The integration paths through the subelements in the same fracture plane are defined as in Figure 7, parallel to the patch boundaries.

Figure 9. The elements at the intersection of horizontal and vertical fracture around single node.

Figure 10. A patch formed of subelements from two fracture planes.

The method of Cordes and Kinzelbach produces a specific discharge field that is constant at the subelements. The path lines are straight lines through the subelements and we can use similar particle tracking scheme than in the traditional Galerkin finite element method. As the normal component of the specific discharge is continuous at element edges we avoid the artificial sinks at element edges and the problems at impermeable boundaries.
The equations for the patches at fracture intersections were examined only for an intersection of two fractures. The geometry was also simple. If several fractures cross at the intersection it is possible that the equations for the specific discharges at subelements can not be defined. The effect of multiple fractures and complex geometries can be investigated in the future if needed. One way to avoid difficulties at intersections is to define specific discharges at subelements connected to intersections equal to original constant specific discharge defined over whole element.

5.3 Mixed finite element method

In the mixed finite element method [Chavent & Roberts 1991, Mosé et al. 1994, Durlofsky 1994, Kaasschieter 1995, Cirpka et al. 1999] the hydraulic head and the specific discharge are approximated simultaneously. The mathematical principles of the method are generally in the examined literature introduced for a two-dimensional flow system. The method is in this study first applied to the two-dimensional flow in a single fracture. The modelled domain is divided to triangular elements. On each element \( E \) \( h \) and \( Q_w \) are approximated by

1. \( h_E' \) an approximation of mean \( h \) on \( E \)
2. \( Th_E \) an approximation of the mean \( h \) on each edge \( \Gamma_i \) of \( E \), \( i=1,\ldots,3 \)
3. \( q_E \) an approximation of \( Q_w \) that belongs to the Raviart-Thomas space of lower order.

On \( E \) the \( q_E \) has the following properties:

1. \( \nabla \cdot q_E \) is constant over \( E \)
2. \( q_E \cdot n_{\Gamma_i} \) is constant over the element edge \( \Gamma_i \), \( n_{\Gamma_i} \) being the unit exterior normal vector of the edge \( \Gamma_i \)
3. Any vector field \( q_E \) is perfectly determined by the knowledge of its flux (discharge) \( Q_{E_i} \) (m\(^3\)/s) through the element edges \( \Gamma_i \), \( i=1,\ldots,3 \).

We define vectorial basis functions \( w_i \) by

\[
\int_{\Gamma_i} w_i \cdot n_{E_j} d\Gamma = \delta_{ij},
\]

(56)

where \( \delta_{ij} \) is the Kronecker delta. The vector function \( w_i \) has unit flux through the edge \( \Gamma_i \) and zero flux through the others. The vector components are therefore presented in [1/m]. It has also property

\[
\int_E \nabla \cdot w_i dA = \sum_{j=1}^{3} \int_{\Gamma_j} w_i \cdot n_{E_j} = 1.
\]

(57)
Any triangle can be mapped to the reference triangle shown in Figure 11a using the affine transformation [Chavent & Roberts 1991]. The vectorial basis functions \( w_i \) for the reference element are visualized in Figure 11b.

**Figure 11.** Reference triangle and the visualization of the basis functions \( w_i \) in the element [Chavent & Roberts 1991]

With these basis functions and fluxes \( Q_E \) we can write the approximation \( q_E \):

\[
q_E = \sum_{j=1}^{3} Q_E w_j .
\]

For the numerical solution, the Darcy's law is written in the form

\[
L(Q_n, h) = T^{-1} \cdot Q_n + \nabla h = 0 .
\]

A solution of equation (59) is found by setting the residual resulting from the approximations \( q_E, Th_E \) and \( h_E \) orthogonal to all basis functions \( w_i \) in element:

\[
\int_{E} L(q_E, h_E, Th_E, i) \cdot w_i dA = 0 \quad i = 1, \ldots, 3 .
\]

With the help of Green's theorem [Bear 1979, p. 149] equation (60) can be written in the form

\[
\int_{E} (T^{-1} \cdot q_E) \cdot w_i dA = h_E \int_{E} \nabla \cdot w_i dA - \sum_{j=1}^{3} Th_E \int_{r_j} w_i \cdot n_E d\Gamma \quad i = 1, \ldots, 3 .
\]

Using the properties of \( w_i \) and inserting the approximation (58) in (61) yields
\[
\sum_{j=1}^{3} Q_{Ej} \int_{E} \left( T^{-1} \cdot w_j \right) \cdot w_i dA = h_{Ei} - T h_{Ei} \quad i = 1, \ldots, 3.
\]  
(62)

The approximated continuity equation is simply integrated over the element:

\[
\int_{E} \nabla \cdot q_{E} dA = \int_{E} Q_{a} dA.
\]  
(63)

Using the definition (58) for \(q_{E}\) yields

\[
\sum_{i=1}^{3} Q_{Ei} = Q_{E},
\]  
(64)

where \(Q_{E}\) is the total discharge (\(m^3/s\)) coming from the sources to the element area.

The continuity of the hydraulic head is required at element edges:

\[
T h_{Ei} = T h_{E' i},
\]  
(65)

for every edge \(i\) (in global numbering of the edges), \(E\) and \(E'\) being adjacent elements. The continuity of fluxes requires

\[
Q_{Ei} + Q_{E'i} = 0.
\]  
(66)

Equations (62), (64), (65) and (66) are the basic equations for the unknowns \(h_{E}, T h_{E}\) and \(Q_{E}\) at element level. These equations are used to form the linear system of equations at global level. The calculations are fully presented by Chavent and Roberts [1991]. Two distinct formulations can be separated.

In the mixed formulation the hydraulic head at elements \(h_{E}\) and the fluxes over element edges \(Q_{E}\) are forced to be the main unknowns to be solved. The number of unknowns is \(N+M\), where \(N\) is the total number of element edges and \(M\) is the number of elements. The coefficient matrix of the system of equations is symmetric but not positive definite and therefore the system cannot be solved numerically by standard linear algebra algorithms [Chavent & Roberts 1991].

In the mixed-hybrid formulation the values of the hydraulic head at element edges \(T h_{E}\) are forced to be the main unknowns. There are \(N\) unknowns in the global matrix equation. The coefficient matrix of the system is symmetric and positive definite and the system can be solved by standard methods. Fluxes \(Q_{E}\) can then be calculated through postprocessing at element level. The specific discharge field can be easily calculated using equation (58) after the fluxes \(Q_{E}\) are known.

When we apply the mixed element method to the fracture network model equations (62), (64), (65) and (66) are valid at the elements and element edges in the middle of fracture planes. At the fracture intersections, equations (65) and (66) must be modified.
to take into account all elements connected to intersection line. At intersections equation (65) is written in the form

\[ Th_{\infty} = Th_{E_i} \quad E = 2, m, \]  

(67)

where \( m \) is the number of the elements sharing a common edge, \( i \) refers to the global edge number and \( E \) to elements adjacent to the edge. In (67) the elements related to edge \( i \) are numbered from 1 to \( m \). Assuming conservation of mass at the intersection equation (66) is written in the form

\[ \sum_{E=1}^{m} Q_{E_i} = 0. \]  

(68)

In (68) the elements related to edge \( i \) are numbered from 1 to \( m \).

As the global system of equations is easier to solve in the mixed-hybrid formulation than in the mixed formulation, the mixed-hybrid formulation should be preferred. The derivation of the global equations is also different for the fracture networks than for the strictly two-dimensional case because we must use equations (67) and (68) instead of (65) and (66). Following the procedure of Chavent and Roberts [1991] it was found that the global equations for the fracture network can be derived much easier in the mixed-hybrid than in the mixed formulation. In fact, the global matrices can be calculated element by element similarly for the fracture network and for the single two-dimensional fracture. The boundary conditions of prescribed head or flux can be given naturally at the element edges at boundaries. Therefore the mixed-hybrid formulation can be easily used in the fracture network model.

In the absence of sources the specific discharge \( q_e \) is constant at the element, and path lines are parallel straight lines through the elements. If there are sources, the path lines are not necessarily parallel, but a single path line is still a straight line over element [Kaasschieter 1995]. Similar particle tracking scheme can therefore be used than in the Galerkin finite element method. As the normal component of the specific discharge is continuous at element edges we avoid the artificial sinks at element edges and the problems at impermeable boundaries.
6 THE APPROXIMATION OF TRANSPORT RESISTANCE

6.1 Conceptual model for the transport of radionuclides and the meaning of transport resistance

The connected fractures at the bedrock are the main routes of the transport of radionuclides from the repository to the biosphere. The most significant processes in the transport are the advection of groundwater in the fractures and the interaction of radionuclides and the surrounding rock. The radionuclides are retarded by the diffusion into the rock and by the sorption on the surfaces of the fractures.

The conceptual transport model used in the safety assessment (e.g. TILA-99 (Vieno & Nordman 1999)) is based on the transport of radionuclides through a network of fractures [Poteri & Laitinen 1999]. The flow paths through the fracture network are one-dimensional and properties of the surrounding rock are assumed homogeneous. The radionuclides are retarded to the fracture surfaces and diffused to the rock matrix. The transport of a stable radionuclide species is described by the equations

\[
R_u \frac{\partial C(x,z,t)}{\partial t} = -\nu \frac{\partial C(x,z,t)}{\partial x} + D_e \frac{2}{2b} \frac{\partial C(x,z,t)}{\partial z} \bigg|_{z=0},
\]

\[
R_p \frac{\partial C(x,z,t)}{\partial t} = D_e \frac{\partial^2 C(x,z,t)}{\partial z^2},
\]

where
- \( C(x,z,t) \) is the concentration in the water (mol/m³),
- \( \nu \) is the velocity of groundwater in the fracture (m/s),
- \( 2b \) is the aperture of the fracture (m),
- \( R_u \) is the retardation coefficient of the fracture surface,
- \( R_p \) is the retardation coefficient in the rock matrix,
- \( D_e \) is the effective diffusion coefficient of the rock matrix (m²/s),
- \( \epsilon_p \) is the porosity of the rock matrix,
- \( x \) is the distance along the fracture (m),
- \( z \) is the distance into the rock matrix from the surface of the fracture (m),
- \( t \) is the time (s).

The matrix is assumed to be infinite. Assuming an initial condition of a delta-function at the inlet equations (69) have an analytical solution at the fracture:

\[
\frac{\dot{m}(x,0,t)}{m_0} = u \frac{u^2}{\sqrt{\pi} (t - R_u t_w)^2},
\]

where \( \dot{m}(x,0,t) \) is the flux of radionuclides (mol/s), \( m_0 \) is the initial inventory in the delta pulse (mol), \( t_w = x/\nu \) is the groundwater transit time (s) and the parameter \( u \) is
where \( W \) is the width of the flow channel (m) and \( Q \) is the flow rate (m\(^3\)/s). The term \( R_{f_c} \) only shifts the output pulse to later time and in the safety assessment this effect is not taken into account. The flux of nuclides at the fracture therefore depends only on the parameter \( u \). The last part \( Wx/Q \) depends on the flow geometry and the flow rate. Replacing \( x \) with the length \( L \) of the fracture we get the transport resistance of the fracture \( WL/Q \).

### 6.2 The transport resistance of a flow path

We first consider transport through two sequential fractures, which have different \( u \)-parameters \( u_1 \) and \( u_r \). We assume initial condition of a delta function at the inlet of the first fracture. The output flux at the outlet of the second fracture can be calculated by taking the output flux of the first fracture as input to the second fracture. The output flux of the second fracture can be calculated by convoluting the response function of the second fracture (equation (70) with parameter \( u_r \)) and the response function of the first fracture (equation (70) with parameter \( u_1 \)) [Poteri & Laitinen 1999].

In the calculation of the convolution, the transit times \( t_w \) are excluded. The Convolution integral is calculated using Laplace transform. The Laplace transform of the convolution integral is the product of the Laplace transforms of the individual functions in the integrand [Kreyszig 1995, s. 294]:

\[
&L \left\{ \frac{-u_1^2}{\sqrt{\pi t^2}} \right\} L \left\{ \frac{-u_r^2}{\sqrt{\pi t^2}} \right\} = e^{-2u_1\sqrt{w}} e^{-2u_r\sqrt{w}} = e^{-2(u_1+u_r)\sqrt{w}},
\]

where \( L \) is the Laplace operator and \( w \) is the Laplace transform variable. From (72) it can be seen, that the output flux from the second fracture can be calculated using equation (70), where the effective \( u \)-parameter is the sum of the parameters of the individual fractures. Therefore the \( u \)-parameters of sequential routes can be added to give the effective \( u \)-parameter of the whole route.

The fractures in the bedrock are, however, very heterogeneous. The local transmissivities in fracture can differ by orders of magnitude. This means that the flow is channeled in single fracture and in the whole fracture network. Only few channels might govern the total flux. The determination of the effective \( u \)-parameter of the main flow routes is therefore important in the safety assessment. We further assume that the rock matrix is homogeneous along the flow route. Then only the effective value of the \( WL/Q \) along the flow route must be determined. In this study we examine the calculation of the effective \( WL/Q \)-value of some flow path in general. Assuming that the
flow path consists of infinitely many small flow tubes we can calculate the effective transport resistance according to

\[
\left( \frac{WL}{Q} \right)_{\text{eff}} = \lim_{n \to \infty} \sum_{i=1}^{n} \frac{W_i L_i}{Q_i} = \frac{W}{Q} \int_{Q} dl = \int_{Q_w} \frac{dl}{Q}. 
\]  

(73)

The effective transport resistance of a flow path is the integrated value of \( W/Q \) along the path \( l \). The calculation of this integral depends on the method with which the path lines are constructed.

### 6.3 Calculation of the transport resistance using the stream function

If the flow is examined in a single fracture in the absence of sources or sinks, the stream function can be calculated with Galerkin finite element method. As a result we have the stream function, which is piecewise linear over the triangular elements. The contours of equal stream function levels, which are the streamlines of the flow, can be constructed using some contouring algorithm. We assume that we can construct the contours of the stream function, which differ from each other by the constant value \( \Delta \psi \) (Figure 12). The area confined by adjacent streamlines is interpreted as a stream tube. According to the theory of the stream function the flow rate in the stream tube is \( \Delta Q = \Delta \psi \). We define also the centerline of a stream tube. The centerline is a streamline where the stream function differs by absolute value of \( \Delta \psi/2 \) from the value of the stream function in the confining streamlines. We also define the width of the stream tube to be perpendicular to the centerline. This width varies along the stream tube in general. As the flow rate is constant through the stream tube, we can calculate the effective values of the \( W/Q \) for the stream tube by integrating the width of the stream tube along the center line \( l \):

\[
\left( \frac{WL}{Q} \right)_{\text{eff}} = \frac{1}{\Delta Q} \int W dl. 
\]  

(74)

The exact numerical methods for the streamline construction, centerline construction and the calculation of the integral (74) can be investigated in the future.
6.4 Calculation of the transport resistance using constant elementwise specific discharges

We assume that some flow path has been successfully constructed using constant elementwise specific discharges. These specific discharges can be obtained from the conventional Galerkin finite element approximation or from the previously introduced postprocessing method of Gordes & Kinzelbach [1992]. In the mixed element method the specific discharges are also constant at the elements in the absence of sinks or sources. According to equation (73) the effective $WL/Q$-value can be calculated as an integral along the flow path. Because the path line is a straight line over the element and the specific discharge is constant at the elements (see Figure 13), the effective $WL/Q$-value of the path line can be approximated with

$$
\left(\frac{WL}{Q}\right)_{\text{eff}} = \sum \frac{\Delta l^e}{Q^e},
$$

(75)

where $\Delta l^e$ is the length of the straight flow path through the element and the summation is made along the path line.
Figure 13. A Piece of a flow path through piecewise constant specific discharge field.

If we use the specific discharges obtained from the Galerkin finite element solution in the particle tracking, we might encounter some problems that were discussed in Chapter four. Heuristic rules must be used at impermeable boundaries and at the element edges where the normal components of the specific discharges at adjacent elements have opposite directions. These rules must be taken into account when the approximation of the transport resistance along the simulated path line is calculated. We assume that we use the heuristic rules shown in Figures 4b and 5b. As a result the path line in an element consists of two straight parts shown in Figures 14a and 14b. The element contribution to the transport resistance can be calculated as a sum over the two separate parts of the path line:

\[
\left( \frac{WL}{Q} \right)_{\text{element}} = \frac{\Delta l'^{e}}{Q_w} + \frac{\Delta l'^{e}}{Q_{w,p}},
\]

(76)

where \(\Delta l'^{e}\) and \(\Delta l'^{e}\) are the lengths of the two straight parts of the flow path and \(Q_{w,p}\) is the magnitude of the component of the specific discharge along the reflecting element edge.
Figure 14. A Flow path through an element at element edge and at impermeable boundary when heuristic rules are used in path line calculation.
7 CONCLUSIONS

We have examined different methods for the calculation of the path lines in the two-dimensional fracture or in the three-dimensional fracture network. In this chapter we represent a summary of the methods and assess their applicability to path line construction and to the calculation of the effective $WL/Q$-values of the constructed flow paths.

The direct computation of the stream function is the most natural way to define the streamlines of the flow field. The method is applicable only to calculations in a single fracture in the absence of sinks and sources, and can not be used in three-dimensional fracture networks. The equation for the stream function is analogous to the flow equation for hydraulic head and can be solved similarly by Galerkin finite element method. The boundary conditions are defined slightly differently. Therefore the stream function calculation is easy to implement to the already existing fracture network code. The calculation of the $WL/Q$-values of the stream tubes confined by the adjacent streamlines has real physical meaning as the stream tubes can be interpreted as separate flow channels. If we need analyses of flow channeling and $WL/Q$-calculations in a single fracture, the stream function approach is the most natural choice. Presumably we more often need to examine flow and transport in the fracture networks and alternate methods must be used.

In all alternate methods the path line construction is based on particle tracking but the numerical approximation of the specific discharge field varies. The starting point is the current numerical fracture network model in VTT Energy. When comparing the methods we should inspect the following attributes:

- The need of heuristic rules in particle tracking
- The easiness to implement the method to the current fracture network code
- The applicability at the fracture intersections
- The numerical accuracy of the constructed path lines
- The computational effort needed
- The calculation of the $WL/Q$-values of the constructed path lines

The first alternative is to track particles in the specific discharge field based on the Galerkin finite element approximation of the hydraulic head field. As the specific discharges are constant over the elements the path lines of the tracked particles are straight lines through the elements. The basic particle tracking algorithm is therefore easy to implement. The discontinuity of the specific discharges at element edges causes, however, problems to the basic algorithm and some heuristic rules must be used to prevent the particles getting lost during the tracking. The problems and the heuristic rules were discussed in Chapter 4. The current fracture network code [Miller 1990] already includes the basic particle tracking algorithm, and the heuristic rule for the element edges inside the modeled domain (Figure 4b). Also the stochastic tracking at fracture intersections according to equation (39) is included in the code. The only change needed is therefore the implementation of the heuristic rule at the impermeable fracture boundaries (Figure 5b). The integration of the $WL/Q$-value along the piecewise straight flow path is straightforward and can be done during the particle tracking. As
part of the particle tracking algorithm is already implemented in the used code, it should be tested before trying other alternatives.

Yeh [1981] introduces a method, which yields a continuous specific discharge field to the whole modelled domain. In the method the hydraulic head field is first solved conventionally with the Galerkin finite element method. The approximated head is inserted then in the Darcy’s law for the components of the specific discharges and the approximation for the components is obtained again by the Galerkin method. The changes to the current code include the forming of the global matrix $C$ and vectors $u_0$. It is supposed that this can be done by modifying the already existing routines of the current code. The equations can be then solved by the current solver of the code. The particle tracking in the continuous specific discharge field can be done by some numerical integration technique, which must also be implemented. In the tracking no problems are encountered in the fracture planes, as the specific discharge field is continuous. The specific discharge field at the elements adjacent to fracture intersections is, however, unphysical, as the specific discharge generally is not parallel to fracture plane. Tracking algorithm must therefore use the traditional constant specific discharges at these elements. Therefore the identification of the elements adjacent to intersections must also be implemented to the code. The $WLQ$-values of the flow path can be presumably integrated easily during the tracking process. As the method has four times more unknowns as the current method for the calculation of head field the computational effort is also approximately four times larger. The accuracy of the path lines should be increased compared to the current method, as the flow field is continuous.

In the postprocessing method of Cordes and Kinzelbach [1992] the triangular elements are divided to four subelements. New, more accurate specific discharge field is then constructed to the subelements using the traditional constant elementwise specific discharges. The resulting specific discharges are constant over the subelements. The path lines are straight lines through the subelements and we can use similar particle tracking scheme than in the traditional Galerkin finite element method. As the normal component of the specific discharge is continuous at element edges we avoid the artificial sinks at element edges and the problems at impermeable boundaries. The method can be used also at the fracture intersections of two fractures. Its applicability in the intersections of more complex geometries is, however, not necessarily true. The integration of the $WLQ$-value along the piecewise straight flow path is straightforward and can be done during the particle tracking. The implementation of the method to the current code is not necessarily easy: We must define the subelement division, numbering of the subelements, numbering of the subelements edges and connections of the subelements. For every node we must form a patch and the system of equations for the unknown components of the specific discharge. If this system is formed for every node the computational effort is not negligible. According to Mose et al. [1994] the computational effort compared to the traditional Galerkin method in the 400x400 two-dimensional mesh is increased by over a factor of four.

In the mixed finite element method the Darcy’s law and the continuity equation are approximated simultaneously. At element level the used unknowns are the mean hydraulic head at the element, mean hydraulic heads at element edges and fluxes through the element edges. These fluxes and vectorial basis functions define a specific
discharge field that has continuous normal component over the element edges. The proper method for the forming of the global equations in the case of the fracture network is the mixed-hybrid formulation, where the hydraulic head values at element edges are forced to be the main unknowns. After the head values are solved, the fluxes through element edges can be defined through postprocessing at the element level. As a result we have a specific discharge field that can be used in the particle tracking everywhere in the fracture network, also at the elements adjacent to the fracture intersections. Path lines are straight lines through the elements and the basic particle tracking scheme can be used. However, the stochastic rule at the intersections must still be used. The calculation of the $WL/Q$-values of the flow paths is also similar than in the traditionally obtained specific discharge field. The implementation of the mixed-hybrid finite element method to the current code is relatively straightforward. As it is still an element method, the mesh generation and element property definitions are done mainly as before. The only real change is that the hydraulic heads are defined at element edges, and therefore we must define the edge numbering and element edge connections. The forming of the global equations must also be implemented. The equations can be solved by the current solver of the code. The calculations of the specific discharges at element level must also be implemented. Most of the work probably consists of the formulation of the routines, which calculate the global equations. Mosé et al. [1994] have compared the postprocessing method of Cordes and Kinzelbach [1992] and the mixed hybrid method in terms of both accuracy and computational effort by calculating various two-dimensional test cases without sinks or sources. They compare the streamlines obtained by the two methods to the Galerkin finite element approximation of the stream function. Their conclusion is that the mixed-hybrid method is superior to the postprocessing method in terms of both accuracy and computational effort. This means that the mixed method yields more accurate results with the same or smaller computational effort than the postprocessing method. The superiority increases when the heterogeneity of the flow system increases. The numerical simulations also show that the mixed hybrid method gives identical results to the stream function solution in the same computational mesh. This is not a coincidence since Kaasschieter [1995] states that also theoretically the mixed method is equivalent to the stream function solution by the Galerkin finite element method. Therefore the mixed element method can be considered as a generalization of the stream function approach for problems with sinks or sources and for three-dimensional problems. As such the mixed element method is also clearly superior to the method of Yeh.

We can now draw conclusions about the applicability of the different methods. The optimal choice depends on the amount of work we can put on the development of the current fracture network code. The amount of work is directly related to the importance of the path line construction and the estimation of the transport resistance in the safety assessment of the spent nuclear fuel disposal. If the calculations are often needed the implementation work is not an important factor and we should choose the best alternative in terms of accuracy and computational effort. If the calculations are seldom needed we should choose the alternative that needs least implementation work. Therefore the mixed method is clearly the best choice if the calculation of the path lines and the transport resistance is of great importance in the future. Otherwise the traditional particle tracking with heuristic rules should be used. In any case the already existing particle tracking algorithm in the current fracture network model should be tested.
REFERENCES


