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FEFLOW: a finite element code for simulating groundwater flow, heat transfer and solute transport

L. Koskinen, M. Laitinen, J. Löfman, K. Meling, F. Mészáros
Technical Research Center of Finland, VTT Energy, P.O.Box 1604, 02044 VTT, Finland

Abstract

The FEFLOW code is a finite element program package developed at VTT Energy to model flow, solute transport and heat transfer in coupled and non-coupled, steady-state and transient situations, as well as in deterministic and stochastic modes.

The code offers a novel finite element technique to model groundwater phenomena in fractured crystalline rock. Linear and bi-quadratic one-, two- and three-dimensional finite elements can be used for describing engineered and natural bedrock structures. One of the solute transport models implemented in the package is capable of taking into account matrix diffusion as well. Highly convective cases are handled with different kinds of upwind schemes. The system of linear algebraic equations emerging from the standard Galerkin approximation can be solved with a direct frontal solver, as well as with an array of iterative solvers partly from the NSPCG package. The nonlinear algebraic equations resulting from coupled cases are solved with the Picard iterative approach with options for relaxation. The discretization of time is based on a simple finite difference scheme. For each result quantity to be determined, the code offers a wide selection of nodal boundary conditions including prescribed values, sources, sinks and/or fluxes. These may be constant or a function of time. Hydraulic properties of the bedrock features may also be constant or vary with depth. Besides the finite element analysis code the FEFLOW package comprises several programs to compute derived quantities (like flow paths and flow rates) and to facilitate generic modelling tasks.

The code has been tested in a series of test cases, and verified in the international HYDROCOIN project. Main application areas of the FEFLOW package have been site investigations and safety analyses undertaken by the Finnish power company Teollisuuden Voima/Posiva Oy operating two nuclear power plants. It has also been employed to simulate various hydraulic disturbances and solute transport phenomena in the Äspö Hard Rock Laboratory, Sweden.

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1 Introduction

Teollisuuden Voima/Posiva Oy carries out investigations and safety analyses concerning the fractured, crystalline bedrock for selected sites in Finland for the final disposal of spent nuclear fuel. Modelling the subsurface flow and other groundwater-related phenomena is a part of these investigations. In response to the specific needs of the modelling studies, the FEFLOW package was developed at VTT Energy.

Traditional approaches for describing the fractured rock media are commonly based on fracture network models or discretization of the domain for finite difference or finite element analyses. In the latter the large, deterministic fracture zones are usually implemented by introducing anisotropy for the cells/elements coinciding with the surface of the fracture zones.

Along with the common functionalities of a standard finite element analysis package, FEFLOW offers a novel approach in modelling the fractured rock media. In the finite element meshes various types of elements are used intermixed. Three-dimensional (3D) elements describe the rock blocks. Embedded in the 3D elements and defined by a subset of their nodes, 2D elements along the surfaces of identified fracture zones describe bedrock structures of primarily 2D nature. A set of advanced routines have been developed to facilitate the required element mesh creation process and consequently the addition or removal of embedded two-dimensional meshes can be performed flexibly. One-dimensional elements are used for modelling engineered structures like shafts, tunnels or repositories. Thus the geometry of the fracture zones, often decisive for the local groundwater regime, can be modelled with reasonable accuracy (Figure 1).

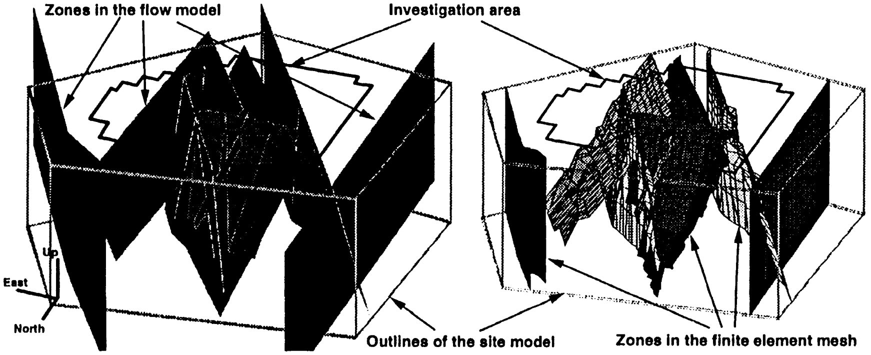

Figure 1. Modelling fracture zones with two-dimensional finite elements at the Kivetty site, Finland. Only a subset of all identified fracture zones is displayed.

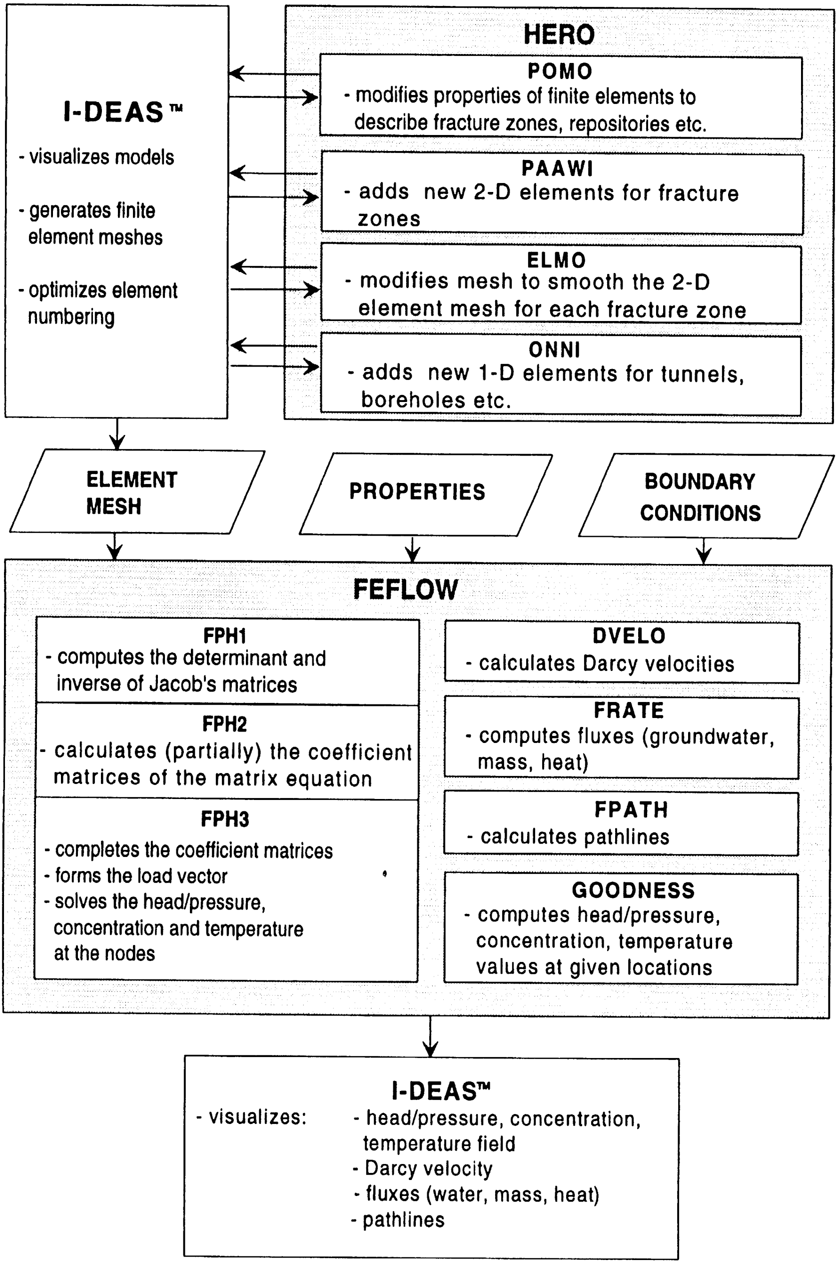

Figure 2. Components and data flow in the FEFLOW package.

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The most important inputs to the code are the geometry and the hydraulic properties of the bedrock structures, which are obtained from geological investigations, and the initial as well as the boundary conditions describing the prevailing hydraulic and other conditions affecting flow, transport and heat transfer.

Primary result quantities that are computed with the code are the hydraulic head/pressure, concentration and temperature fields, whilst derived result quantities are Darcy velocity, flow rates through specified surfaces and flow paths. The I-DEAS commercial finite element pre- and postprocessor and an array of in-house developed modelling tools facilitate the analysis of results (Figure 2).

The above three result quantities can also be coupled in any combination. Thus eg density-affected flow can be studied, when the density of the groundwater is assumed to vary according to the concentration of some dissolved matter in it, or due to a non-ignorable heat source. In the case of coupled problems nonlinearity of the algebraic equations is handled with the Picard iterative method with options for underrelaxation.

More information on the FEFLOW package and its applications are available at links on the WWW home page of VTT Energy:

http://www.vtt.fi/ene/enehome.htm

2 Model equations

The mathematical models of the phenomena taking place in subsurface flow that are implemented in the FEFLOW package take the form of partial differential equations. These are solved numerically with conventional Galerkin approximation, standard upwind method, streamline upwind Petrov-Galerkin (SUPG) method, or discontinuity capturing SUPG (Brooks & Hughes, 1992). The system of algebraic equations emerging from the above techniques are solved by a direct frontal method, or with an iterative solver (conjugate gradient method for the symmetric and a Lánczos method for non-symmetric problems from the NSPCG package (Oppe et al., 1988)). All problems are typically solved with the equivalent continuum (EC) approach, but for certain transport problems the dual-porosity (DP) concept has also been implemented.

With regard to the global system matrix associated to the model, large symmetric problems (flow modelling) as well as strongly non-symmetric cases (material transport in the presence of hydraulic disturbances causing convection) can be handled with FEFLOW efficiently. The package has been streamlined and made available on various computer hardware architectures to process a large number of cases for sensitivity analyses, model calibrations and transient analyses.

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2.1 Flow equations

In case the density of the groundwater is constant, the flow equation is solved for the hydraulic head h [m] (Bear, 1979):

$$\nabla(\boldsymbol{K}\nabla h) - Q = S_s \frac{\partial h}{\partial t} \tag{1}$$

where: $\boldsymbol{K}$ is the hydraulic conductivity tensor [m/s],
Q is the flow rate per unit volume as sources and sinks [1/s],
S_s is the specific storage [1/m] and
t is time [s].

Simulations taking into account the varying density of water are based on the flow equation describing the pressure p [Pa]:

$$\nabla\left(\frac{\rho \boldsymbol{k}}{\mu}\nabla(p + \rho g z)\right) - \rho Q = \phi \frac{\partial \rho}{\partial t} \tag{2}$$

where: ρ is the density of water [kg/m^3],
$\boldsymbol{k}$ is the permeability tensor [m^2],
μ is the viscosity of the water [kg/m/s],
g is the gravitational acceleration (9.81 m/s^2),
z is the elevation relative to the reference plane [m] and
ϕ is the total porosity [-].

2.2 Transport equations

Two distinctly different concepts have so far been implemented in the FEFLOW package for solute transport. The EC model (Huyakorn & Pinder, 1983) describes the concentration c [kg/m^3] as:

$$\nabla(\boldsymbol{D}\nabla c) - \nabla(\boldsymbol{q}c) + Q_{in}c_{in} - Q_{out}c = \phi_f \frac{\partial c}{\partial t} \tag{3}$$

where: c is the concentration [kg/m^3],
$\boldsymbol{D}$ is the dispersion tensor (incl. convection and diffusion [m^2/s],

$\boldsymbol{q}$ is the Darcy velocity [m/s],
Q_{in} is the the term for sources [1/s],
c_{in} is the concentration in the inflowing water [kg/m^3],
Q_{out} is the term for sinks [1/s] and
ϕ_f is the flow porosity [–].

In DP model (Huyakorn et al. 1983) the computational domain is decomposed into fractures with flowing water (Equation 4) and matrix blocks with stagnant water (Equation 5), in which the concentration c is described as:

$$\nabla(\boldsymbol{D}\nabla c) - \nabla(\boldsymbol{q}c) + Q_{in}c_{in} - Q_{out}c - (1-\phi_f)\Gamma = \phi_f \frac{\partial c}{\partial t} \qquad (4)$$

and

$$\frac{\partial}{\partial z'}(D'_e \frac{\partial c'}{\partial z'}) = \phi' \frac{\partial c'}{\partial t} \qquad (5)$$

where: Γ is mass transfer term

$$\Gamma = -\frac{1}{a}(D'_e \frac{\partial c'}{\partial z'} \mid_{z=0}) \qquad (6)$$

a is the half thickness of the matrix block [m],
c' is the concentration in the matrix blocks [m^3/s],
D'_e is the effective diffusion coefficient [m^2/s] and
ϕ' is the the porosity in the matrix blocks [–].

2.3 Heat transfer

FEFLOW offers the concept suggested by Huyakorn & Pinder (1983) for modelling the distribution of temperature T [K]:

$$\nabla(\lambda\nabla T) - \nabla(\rho_w c_w \boldsymbol{q} T) + \rho_{in} Q_{in} c_{w,in} T_{in} - \rho_w Q_{out} c_w T - H = \\ = \frac{\partial}{\partial t}((\rho c)_{rw} T) \qquad (7)$$

in which

$$(\rho c)_{rw} = (1-\phi)\rho_r c_r + \phi\rho_w c_w \tag{8}$$

where: $\boldsymbol{\lambda}$ is the heat conductivity tensor [W/m/K],
ρ_w is the density of water [kg/m^3],
ρ_r is the density of rock [kg/m^3],
ρ_{in} is the density of the inflowing water [kg/m^3],
c_w is the specific heat of the water [J/kg/K],
c_r is the specific heat of the rock [J/kg/K],
T_{in} is the temperature of the inflowing water [K] and
H is the heat source [W/m^3].

2.4 Coupling the flow, transport and heat transfer

In coupled analyses certain parameters of an equation depend on the result quantity of the other equation, and the outcome is obtained by iteration. These parameters are:

- the density:

$$\rho = \rho_0 + a_c c + a_T(T - T_0) \tag{9}$$

- the viscosity:

$$\mu = \mu(T) \tag{10}$$

- the Darcy velocity:

$$\boldsymbol{q} = -\frac{\boldsymbol{k}}{\mu}(p + \rho g z) \tag{11}$$

- the dispersion tensor:

$$\boldsymbol{D_{ij}} = \varepsilon_T|\boldsymbol{q}|\delta_{ij} + (\varepsilon_L - \varepsilon_T)\frac{q_i q_j}{|\boldsymbol{q}|} + D_e, \qquad i,j = 1,2,3 \tag{12}$$

- the heat conductivity tensor:

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}(\boldsymbol{q}) \tag{13}$$

where: ρ_0 is the density of the fresh water [kg/m^3],
a_c is the coefficient of density dependence of solute concentration [–],
a_T is the thermal expansion coefficient [kg/m^3/K],
ε_T is the transversal dispersion length [m],
ε_L is the longitudinal dispersion length [m],
δ_{ij} is the Kronecker delta function [–], and
D_e is the effective diffusion coefficient [m^2/s].

3 Applications

The FEFLOW package has been employed in numerous site characterization studies (eg Taivassalo & Mészáros, 1994), safety analyses (eg Vieno et al., 1992) and in various projects of the Äspö Hard Rock Laboratory in Sweden (eg Taivassalo et al., 1994, Löfman & Taivassalo 1995). These sites typically included 20-40 fracture zones with complex geometries and properties affecting flow and solute transport.

3.1 TVO/Posiva site investigations

In a former phase of site characterization works that was completed in 1992, three sites had to be selected from five (Kivetty, Olkiluoto, Romuvaara, Syyry and Veitsivaara) for further studies. Groundwater flow modelling was part of these investigations, and was expected to produce the following measures:

- hydraulic headfield over the investigation area,
- average groundwater flux (calculated at 100, 500 and 900 m),
- Darcy velocity and
- groundwater flow routes.

On the basis of geological investigations finite element models were built for all the sites on both regional and site scales. Field measurements of the hydraulic properties, as well as of the hydraulic responses to pumping tests facilitated the calibration of these models. Sensitivity analyses were used to establish the importance of uncertainties associated to the input data for the models. Finally, the uncertainties of the model output were discussed, also indicating a plausible range for the quantities of interest.

Kivetty, Olkiluoto and Romuvaara are the present candidate locations for a possible future spent fuel repository and more detailed site investigations have continued at these sites since 1993. The FEFLOW code has been further developed, and is currently employed in simulations addressing the saline subsurface waters at the Olkiluoto site.

3.2 Äspö HRL projects

The Äspö Hard Rock Laboratory was initiated by SKB (Sweden), and is now a joint international effort to study subsurface phenomena and deep rock behaviour.

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The FEFLOW package has so far been employed in the following modelling works:

- a six-borehole pumping test (the withdrawal holes were pumped consecutively)
- simulating the hydraulic impact of the excavation of the access tunnel and shafts to the underground laboratory
- simulating the development of the freshwater lens under the island of Äspö caused by the land uplift that Scandinavia currently experiences, and
- a multiple-hole tracer retention understanding experiment.

4 Concluding remarks

The idea of modelling large, deterministic fracture zones with sets of 2D elements proved successful in numerous analyses, and has become an established modelling technology at VTT Energy. Comparison with other approaches (Gustafson & Ström, 1995) shows that complex problems can be addressed with the FEFLOW package efficiently both in terms of the quality of results and the modelling effort required for them. As well as the basic concept of the package, the following four, more general issues of methodology are highlighted.

Frequent communication with field investigators who produce the data used as model input has always proved particularly fruitful in the conceptualization phase.

Quality assurance calls for computer-readable input data for building models of any complexity. Batch (ie non-interactive) processing of as many phases of the modelling work from model development through simulations to postprocessing as possible may also contribute to reliable and reproducible results.

Large, nonetheless numerically simpler problems, like modelling hydraulic disturbances of the groundwater regime especially of transient nature can be handled effectively with the iterative solvers developed for symmetric, sparse systems. However, modelling more complicated phenomena, like convection-dominated material transport, may require a direct solver to obtain reliable results.

In order to understand the model output, post-processing the results from several aspects with tools ranging from simple summary tables to sophisticated visualization software is indispensable.

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