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NAMMU (Release 6.4) Technical Overview

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1. INTRODUCTION

NAMMU is a software package for modelling groundwater flow and transport in porous media. It is powerful and flexible, with many options for customisation. The acronym NAMMU stands for ‘Numerical Assessment Method for Migration Underground’. NAMMU was also the name of the Sumerian goddess of the abyssal waters, whose name was expressed by the ideogram for ‘sea’ (Jacobson, 1949). This document provides a general overview of Release 6.4 of NAMMU, including a description of the equations solved and the numerical methods used. Additional more detailed information about the capabilities and potential applications of NAMMU is available from AEA Technology on request.

NAMMU has been developed by AEA Technology over a period of more than 15 years and has been verified extensively in international comparison exercises. It is developed under a rigorous quality system that conforms to the international standards ISO 9001 and TickIT (see also Section 6).

NAMMU can be used to model the following:

- groundwater flow in saturated and unsaturated conditions;
- saline groundwater flow with density dependent on concentration;
- coupled groundwater flow and heat transport with density dependent on temperature;
- saline groundwater flow and heat transport with density dependent on concentration and temperature;
- contaminant transport, including the effects of advection, dispersion and sorption;
- radioactive decay chains;
- 1D, 2D cross-sectional, 2D areal and 3D regions;
- steady-state and time-dependent behaviour;
- sensitivity to model parameters, using the adjoint sensitivity method.

NAMMU models have been used in the following applications:

- disposal of radioactive and toxic waste;
- regional groundwater flow;
- aquifer contamination;
- site investigation;
- pump test simulation;
- tracer tests;
- saline intrusion;
- risk assessment;
- design and evaluation of remediation strategies.

NAMMU is used in support of the radioactive waste disposal programmes of many countries throughout the world, by both the nuclear regulators and by national disposal organisations and consultants working for these organisations.

NAMMU has a wide range of facilities for specifying the model domain, the properties of the rocks, fluids and solutes within the domain, the equations to be solved and the output options required. The advanced 3D visualisation package, Avizier, is available for NAMMU. In addition to these standard facilities, many options are available that allow the user to customise the functionality of NAMMU for a particular project. For example, it is possible for the user to specify a site-specific relationship between fluid density, solute concentration, fluid temperature and pressure.

1.1 User Interface

Input to NAMMU is specified using a structured free-format input language, which has been designed to be readily comprehensible to the user. The input data specifies the finite-element grid (see subsection 4.1), the quantities of interest, (see subsections 2.1 and 4.2) the boundary conditions (see subsection 2.2), the processes that are to be modelled (see subsection 2.1) and the output required (see Section 5).

The input language allows the user to specify the execution of the program in a flexible manner. The individual components of a run (model generation, specification of processes to be modelled, output required etc) can be specified in any logical order and may appear more than once in any run. The results of a calculation may be saved for later post-processing or for use as an initial condition in a later calculation. An existing model may be modified and the results of a calculation may be interpolated from one finite-element grid to another.

The output from NAMMU currently takes three forms:

- text files containing information about the model, the performance of the solver and any output options requested;
- postscript graphics files;
- files for use with the Avizier visualisation package.

1.2 Availability

NAMMU is written in standard FORTRAN 77 and is therefore portable across a wide range of computers. NAMMU 6.4 is supported on a range of computer platforms, from desktop workstations to supercomputers.

Optional modules are available for some of the earlier releases of NAMMU.

- MATDIF: In fractured rocks, flow and hence advective transport of solutes is often confined to fractures, but the solutes may also access the immobile water in the rock matrix between the fractures by diffusion. MATDIF enables this process to be modelled.
- GEONAM enables flow and transport to be modelled in heterogeneous media, using a geostatistical Monte-Carlo approach.

NAMMU also forms part of the CONNECTFLOW package (Morris and Hartley, 1997), developed by AEA Technology, for modelling groundwater flow and transport in porous and fractured media.

Comprehensive technical support is available to users of NAMMU through a User Group (see subsection 1.3), organised by AEA Technology.

1.3 The NAMMU User Group

Gaining full benefit from a powerful program such as NAMMU is a task that requires a high level of technical expertise. AEA Technology recognises this fact and, accordingly, runs training courses to help new users become familiar with the program and its use. In addition, AEA Technology has set up the NAMMU User Group in order to provide comprehensive technical support to NAMMU users. The support provided consists of updates of software and documentation, installation support by Internet, and consultancy by e-mail, telephone and fax. The User Group is an active community which provides users with a newsletter and occasional User Group meetings which act as a forum for users to discuss applications of the software, to provide feedback for future software developments and to hear about new developments.

NAMMU has been used by a significant number of organisations throughout the world, including the following:

- Department of the Environment, UK.
- United Kingdom Nirex Limited, UK.
- RM Consultants, UK.
- British Nuclear Fuels Limited (BNFL), UK.
- Golder Associates, UK.
- Entec, UK.
- British Geological Survey (BGS) Keyworth, UK.
- University of Bath, UK.
- University of Birmingham, UK.
- University of Edinburgh, UK.
- Gesellschaft fur Reaktorsicherheit (GRS), Germany.
- Federal Office for Radiation Protection (BfS), Germany.
- Federal Institute of Geosciences, Germany.
- Swedish Nuclear Fuel and Waste Management Company (SKB), Sweden.
- Swedish Nuclear Power Inspectorate (SKI), Sweden.
- Kemakta Consultants, Sweden.
- Conterra AB, Sweden.
- National Co-operative for the Disposal of Radioactive Waste (NAGRA), Switzerland.
- Colenco Power Consulting Ltd, Switzerland.
- Swiss Federal Institute of Technology, Switzerland.
- Diamo, Czech Republic.
- Korea Atomic Energy Research Institute (KAERI), South Korea.
- Korea Electric Power Corporation (KEPCO), South Korea.
- Hyundai Engineering and Construction Company, South Korea.
- Georgia Institute of Technology, USA.

1.4 Documentation

A comprehensive set of documentation has been produced for NAMMU. The following manuals are available for Release 6.4:

NAMMU Technical Overview (this document) This document provides a general technical overview of the software, including a description of the equations solved and the numerical methods used.

NAMMU User Guide This document describes how to prepare data for a NAMMU model, and how to interpret the output from a NAMMU calculation. This is demonstrated through a number of realistic examples.

NAMMU Installation and Running Guide This document describes how to install and run NAMMU on the various computer platforms supported.

NAMMU Reference Manual This document describes in detail the commands and keywords available in the NAMMU input language used to specify the model, the finite-element equations to be solved, and the post-processing required. This document is available in an electronic on-line form, which has the advantage of cross-referencing using hypertext links.

A bibliography is provided at the end of this report. It lists both material referenced in this report and some of the studies that have made use of NAMMU.

2. MATHEMATICAL MODELS

NAMMU can be used to model a wide range of groundwater flow and transport processes including:

- groundwater flow in saturated or unsaturated conditions;
- saline groundwater flow with groundwater density dependent on concentration;
- coupled groundwater flow and heat transport with groundwater density dependent on temperature;
- saline groundwater flow and heat transport with density dependent on concentration and temperature;
- contaminant transport, including the effects of advection, dispersion and sorption, and radioactive decay (for a single radionuclide or a chain);
- 1D, 2D cross-sectional, 2D areal and 3D regions;
- steady-state and time-dependent behaviour.

The mathematical models used to represent these processes are outlined below. The symbols used in the equations are defined in the Nomenclature and Units Section. Many of the parameters used in the equations are discussed in subsection 4.2.

2.1 Equations

Underlying all of the models for groundwater flow is Darcy's law for flow in a porous medium,

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu} \cdot (\nabla P^R - (\rho_l - \rho_0)\mathbf{g}) , \tag{1}$$

and its extension to unsaturated flow,

$$\mathbf{q} = -\frac{k_r \mathbf{k}}{\mu} \cdot (\nabla P^R - (\rho_l - \rho_0)\mathbf{g}) . \tag{2}$$

These are combined with the appropriate equations for mass conservation,

$$\frac{\partial}{\partial t}(\phi \rho_l) + \nabla \cdot (\rho_l \mathbf{q}) = 0 , \tag{3}$$

or, for unsaturated flow,

$$\frac{\partial}{\partial t}(\phi S \rho_l) + \nabla \cdot (\rho_l \mathbf{q}) = 0 . \tag{4}$$

Alternatively, equation (3) can be written in terms of specific storage, *s*, in the form,

$$\frac{s}{g}\frac{\partial P^R}{\partial t} + \nabla \cdot (\rho_l \mathbf{q}) = 0 . \tag{5}$$

The flow equations given above are written in terms of the residual pressure, P^R. The residual pressure is related to the total pressure, P^T, by

$$P^R = P^T + \rho_0 g(z - z_0). \tag{6}$$

For some combinations of equation and numerical formulation (see also subsection 3.1), it is possible to input parameters such as boundary conditions to NAMMU in terms of P^T or, for constant density flow, in terms of the hydraulic head, h, which is defined by

$$h = \frac{P^R}{\rho_0 g}. \tag{7}$$

In all cases, it is possible to plot the results of the calculation in terms of P^R, P^T or h.

For calculations of the transport of a dense solute, heat or a passive solute, the groundwater flow equations (equations (1-5)) are combined with a transport equation. The resulting sets of equations are often non-linear.

In the case of groundwater flow coupled to the transport of a dense solute (by default, salt), the groundwater density is a function of the salinity. Transport of a dense solute is modelled using the equation

$$\frac{\partial}{\partial t}(\phi \rho_l C) + \nabla \cdot (\rho_l \mathbf{v} C) - \nabla \cdot (\phi \rho_l \mathbf{D} \cdot \nabla C) = 0. \tag{8}$$

This is basically a representation of conservation of the mass of solute.

In this case, equation (3) can be written in terms of specific storage, s, in the form,

$$\frac{s}{g}\frac{\partial P^R}{\partial t} + \phi \frac{\partial \rho_l}{\partial C}\frac{\partial C}{\partial t} + \nabla \cdot (\rho_l \mathbf{q}) = 0. \tag{9}$$

In the case of groundwater flow coupled to the transport of heat, the groundwater density is taken to be a function of the temperature. Transport of heat is modelled using the equations

$$(\rho c)_a \frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q} \cdot \nabla T - \Gamma_a \nabla^2 T = H, \tag{10}$$

for coupled groundwater flow and heat transport and

$$(\rho c)_a \frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q} \cdot \nabla T - \nabla \cdot (\mathbf{D}' \cdot \nabla T) = H, \tag{11}$$

for coupled groundwater flow, solute transport and heat transport. These equations basically represent conservation of energy.

Transport of a passive solute or contaminant, that is a solute that does not affect the groundwater density and viscosity and hence the flow, can also be modelled. Up to six solutes representing a radioactive decay chain can be handled. Transport of one of the solutes in such a decay chain is represented by the equations

$$\begin{aligned}\frac{\partial}{\partial t}(\phi R_\alpha N_\alpha) + \mathbf{q}\cdot\nabla N_\alpha - \nabla\cdot(\phi\mathbf{D}_\alpha \cdot\nabla N_\alpha) \\ = -\lambda_\alpha \phi R_\alpha N_\alpha + \lambda_{\alpha-1}\phi R_{\alpha-1}N_{\alpha-1} + \phi f_\alpha\end{aligned} \tag{12}$$

and,

$$\begin{aligned}\frac{\partial}{\partial t}(\phi S R_\alpha N_\alpha) + \mathbf{q}\cdot\nabla N_\alpha - \nabla\cdot(\phi S\mathbf{D}_\alpha \cdot\nabla N_\alpha) \\ = -\lambda_\alpha \phi S R_\alpha N_\alpha + \lambda_{\alpha-1}\phi S R_{\alpha-1}N_{\alpha-1} + \phi S f_\alpha\end{aligned} \tag{13}$$

for groundwater flow and unsaturated groundwater flow respectively. These equations, which correspond to conservation of mass for the solute, represent the processes of advection (transport with the flow), hydrodynamic dispersion (spreading about the flow) molecular diffusion, linear equilibrium sorption and radioactive decay and ingrowth.

It is also possible to model flow in a 2D areal model of an aquifer overlain by a confining layer using a vertically integrated form of equation (3). The resulting equation is

$$\nabla\cdot(b\rho_l\mathbf{q}) = Q \tag{14}$$

where b is the effective thickness of the aquifer and is given by

$$b = z_t - z_b,\ \text{if } \frac{P^R}{\rho_l g} \geq z_t \quad \text{(confined aquifer)} \tag{15}$$

$$b = \frac{P^R}{\rho_l g} - z_b,\ \text{if } \frac{P^R}{\rho_l g} < z_t \quad \text{(unconfined aquifer),} \tag{16}$$

where z_t and z_b are the elevations of the top and bottom of the aquifer, respectively.

The source term, Q, accounts for infiltration, I, when modelling an unconfined aquifer. When modelling a confined aquifer, Q, accounts for leakage and is given by,

$$Q = \frac{\rho_l k_v}{\mu}\left(\frac{\rho_l g z_s - P^R}{z_s - z_t}\right). \tag{17}$$

NAMMU also includes an option to specify the flow and transport equations being solved. This is done through FORTRAN subroutines that define the equations. It is a very powerful facility for the advanced user.

2.2 Boundary Conditions

The equations presented above represent the flow and transport processes within the modelled domain. Appropriate boundary conditions have also to be specified before a calculation can be carried out. NAMMU supports a wide range of types of boundary condition, which may be constant or may vary in space and/or time. The most commonly used are Dirichlet (or specified value), Neuman (or specified flux) and zero dispersive flux. If the user does not specify boundary conditions on part of the boundary then suitable default boundary conditions are imposed. With the exception of the mixed-element formulation for groundwater flow (see subsection 3.1), the default boundary condition is that the flux of groundwater, salinity, heat or solute is zero.

3. NUMERICAL METHODS

3.1 Spatial Discretisation

NAMMU uses the finite-element approach for spatial discretisation. This is a powerful approach that is particularly suited to numerical modelling in domains that are complicated geometrically, such as the domains that represent geological structures with many faults. The basic idea of the approach is that the domain is represented as the combination of ‘finite elements’ that have a simple geometric shape (such as triangles or quadrilaterals in 2D and tetrahedra, triangular prisms or cuboids in 3D). These elements may also be distorted by simple mappings. The possibility of using triangular and tetrahedral elements in particular, provides much more flexibility in accurately representing the domain than is possible using the cuboid blocks of a simple finite-difference method.

On each finite element, the quantities of interest, such as the residual pressure, are represented by simple polynomial functions that interpolate between the values at certain special points called nodes. The possibility of using polynomials of higher order than linear enables numerical schemes that have a high order of accuracy to be easily developed.

NAMMU has a library of many different finite elements, including linear and quadratic triangles and bi-linear and bi-quadratic quadrilaterals in 2D and linear and quadratic tetrahedra and tri-linear and tri-quadratic prisms and cuboids in 3D. The library also includes variants of the so-called ‘mixed elements’ (see below). This provides considerable flexibility in representing the domain.

There are several approaches to the finite-element method, which all lead to similar equations. In NAMMU, the Galerkin finite-element method (Ciarlet 1978, Mitchell and Wait 1977, Zienkeiwicz 1977) is used to carry out the spatial discretisation of the equations (see Winters and Jackson, 1984, for a brief NAMMU-specific discussion). The finite-element method starts from an integral form of the equations.

The region to be modelled is divided up into elements, which have a simple geometric shape. NAMMU uses triangles and quadrilaterals in two dimensions and tetrahedra, triangular prisms and hexahedra in three dimensions (see above). The dependent variables in the problem are then approximated by functions, which have a simple polynomial behaviour on each of the elements. The discretised equations are a discrete form of the integral equations. The final result is a set of coupled, possibly non-linear, algebraic equations for a steady-state problem, and a set of coupled, possibly non-linear, ordinary differential equations in time for a transient problem (see, for example, Mitchell and Wait, 1977). Temporal discretisation of the equations in NAMMU is described in subsection 3.2. The equations are solved using the methods described in subsection 3.3.

Two formulations of the various groundwater flow equations have been implemented in NAMMU. In the so-called standard formulation, the basic quantity that is represented using finite elements is the residual pressure. This formulation is used with the standard elements (linear and quadratic triangles and bi-linear and bi-quadratic quadrilaterals in 2D and linear and linear and quadratic tetrahedra and tri-linear and tri-quadratic prisms and cuboids in 3D). It is a widely used approach.

In the so-called mixed-element formulation, both the residual pressure and the mass flux are represented using finite elements. This approach is less widely used than the standard formulation. It has a lower order of accuracy than the standard formulation using bi- or tri-quadratic elements. However, it has one particular advantage. It ensures that the normal component of the mass-flux vector is continuous across any interface within the modelling region, as is the case for the underlying equations, whereas the standard formulation does not preserve this property. This feature of the mixed-element formulation is particularly beneficial when the quantity of primary interest is the velocity field, for example when calculating pathlines, or performing transport calculations. In particular, it is often the case that numerically calculated pathlines can become stuck in the flow field obtained using the standard formulation on relatively coarse grids.

A remark must be made about the treatment of advection in NAMMU. Many authors recommend the use of upstream weighting, the finite-element equivalent of upwind differencing which is often used for finite-difference discretisations of advection-diffusion equations. Upwinding often removes the numerical instabilities associated with a straightforward application of the Galerkin method to the advective terms. However, there is a price to be paid - upwinding introduces a numerical dispersion effect which amounts to dispersion with a dispersion length closely related to the mesh spacing. This leads to the total amount of dispersion in the model being a function of the refinement, which may be undesirable. Therefore, in NAMMU the amount of dispersion in the calculation is made explicit by using a consistent Galerkin approach for the advective terms (Gresho and Lee, 1981). If numerical instabilities appear, the user has two alternatives: either refine the mesh in the regions of high gradients so that the instabilities disappear or are reduced to an acceptable level, or increase the physical dispersion lengths to stabilise the calculation.

3.2 Temporal Discretisation

In NAMMU, the spatial discretisation is carried out using the Galerkin finite-element method (see subsection 3.1). For time-dependent problems, the application of this method leads to a set of coupled, possibly non-linear, ordinary differential equations. There are two basic methods available in NAMMU for integrating these ordinary differential equations:

- the Crank-Nicholson method;
- Gear’s method (see, for example, Byrne and Hindmarsh, 1975).

The Crank-Nicholson method contains a parameter, q, that controls the degree of implicitness of the method. The scheme is implicit for all values of q except 0 (for which it is equivalent to the explicit forward Euler scheme), and first-order accurate for all values except 0.5 for which it is second order accurate. For $q = 1$ (fully implicit), the method is a backward-difference scheme (backward Euler). Although this scheme is only first-order accurate, it has the merit of being very stable, and is recommended for use in many cases. Indeed, it often may be unconditionally stable, allowing, in principle, the use of very large timesteps, although this may not give a very accurate description of the time evolution of the system. It may be appropriate for problems with a single time scale such as radionuclide transport in advection dominated flows. The explicit forward Euler scheme ($q = 0$) and the second-order accurate scheme ($q = 0.5$) are only conditionally stable; that is there are constraints on the size of the timesteps, which depend on the size of the finite elements. If these constraints are exceeded, the numerical solution will diverge.

Three variants of the Crank-Nicholson scheme are included in NAMMU:

- a version with a fixed time step size;
- a very fast fully implicit version for linear problems. This is particularly suitable for contaminant transport calculations;
- a version in which the timestep size is chosen automatically at each time step to ensure convergence. This version is particularly recommended for calculations of coupled groundwater flow and transport of salinity (and possibly heat).

Gear’s method is a variable-timestep variable-order scheme, based on a predictor-corrector algorithm. At each time step, the size of the time step and the order of the difference scheme are selected to try to maximise the size of the time step subject to satisfying a specified accuracy criterion, the error in the step being estimated from the difference between the predictor and corrector. The corrector schemes used are the backward difference schemes of order one to five, which are generally very stable. The scheme is particularly appropriate for use on problems that are what is called ‘stiff’, that is in simple terms, the behaviour of the system involves components with a wide range of time scales. For example, Gear’s method may be a good scheme to use for modelling coupled groundwater flow and transport of heat from a radioactive waste repository, which constitutes a decaying heat source.

3.3 Solution Methods and Treatment of Non-linearities

In general, spatial and temporal discretisation of a problem gives rise to large, non-linear, coupled, algebraic systems of equations. In NAMMU, non-linearities are treated using the Newton-Raphson iterative method. This is a powerful technique for solving non-linear equations and converges very rapidly (quadratically) provided the initial guess is sufficiently close to the solution of the equations. Solution of a linear problem is equivalent to using the Newton-Raphson method with a single iteration.

For non-linear transient problems, the solution at the previous timestep is often a sufficiently good initial guess, since one does not want the solution to change too much over a single time step for reasons of accuracy.

For highly non-linear steady-state problems, it is not always easy to find a sufficiently good initial guess. In such cases, parameter-stepping may be effective. Parameter-stepping is a technique in which the solution of a hard non-linear problem is approached via a sequence of related problems, starting from a problem that is easy to solve. At each step the parameters of the system are changed slightly and the solution at the previous step is used as the initial guess for the Newton-Raphson iterations. Parameter-stepping is a very powerful technique.

The Newton-Raphson method requires a linear system of equations to be solved at each stage of the iterative procedure. These linear systems are large and sparse and have a structure that is determined by the underlying finite-element discretisation. In NAMMU, an efficient implementation of the Frontal Method (Duff and Scott 1993, Hood 1976, Irons 1975) is used to solve linear systems. The Frontal Method is a variant of Gaussian elimination that exploits the structure of the equations to solve the system using a relatively small amount of memory, without the need to assemble the full matrix for the system in memory. Gaussian elimination has the advantage of being a very robust method.

4. MODEL

4.1 The Finite-element Mesh

Various facilities have been implemented in NAMMU to try to make grid generation as simple as possible. The principal approach used in NAMMU for generating grids is based on the concept of ‘patches’, which are then subdivided into elements. A patch is a region of a simple shape bounded by straight lines, either a triangle or a quadrilateral in 2D and a (possibly distorted) triangular prism or a (possibly distorted) cuboid in 3D. It is specified by the positions of its corners, and is subdivided into a number of finite elements. In two dimensions, an extension of this approach, has been developed using the concept of ‘polygons’, which are regions with many sides. These are first subdivided into patches, which are then subdivided into elements.

The use of patches, and polygons in particular, enables grids to be generated with a minimum of input data. It also makes it very simple to change the refinement of a grid because the user does not have to calculate the locations of all of the individual elements. Figures 4.1 to 4.3 illustrate some of the types of grid that can be generated using the standard grid generation facilities available within NAMMU.

Options are available for representing faults and engineered features, such as boreholes, tunnels and drifts, in the grid.

In NAMMU, each element is assigned to a rock unit. This assignment associates certain physical properties, for example, the permeability, with the element. A rock unit is comprised of one or more finite elements. In NAMMU 6.4, a model may contain up to 500 different rock units.

NAMMU also includes an option for the user to specify the finite-element grid through a user-specified FORTRAN subroutine. This can be used, for example, to import grids generated using other programs into NAMMU.

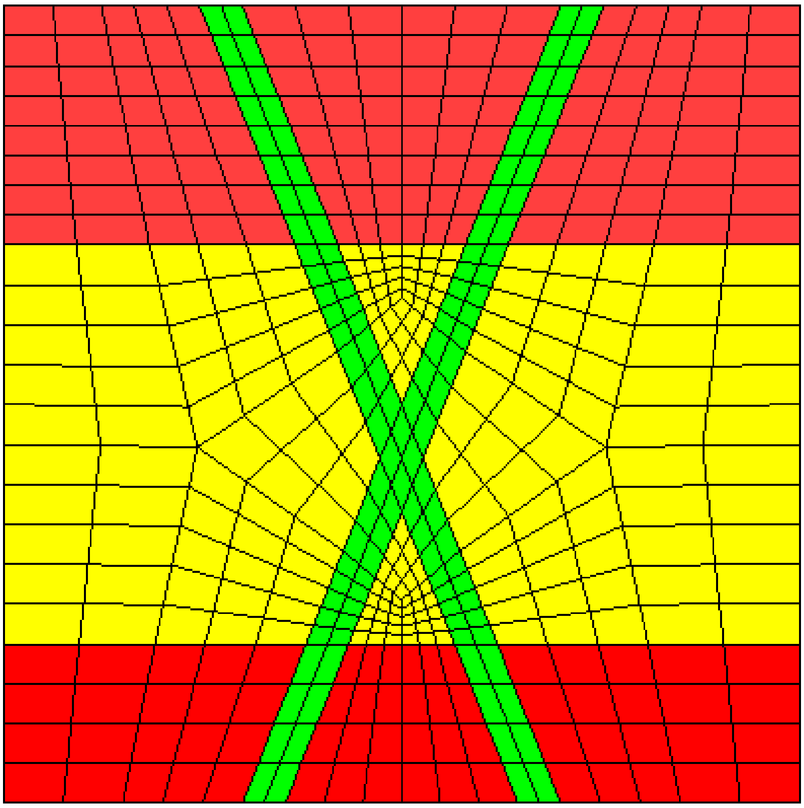

Figure 2.1: A simple 2D grid generated using polygons. The finite elements are coloured according to the rock type.

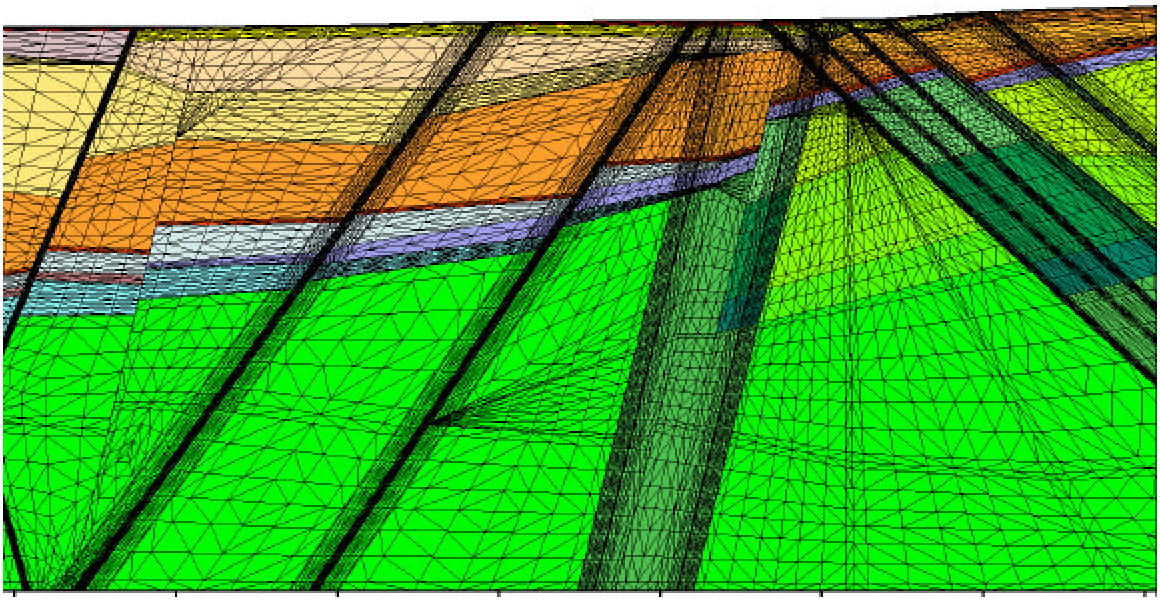

Figure 2.2: An example of part of a complex 2D grid generated using polygons. The finite elements are coloured according to the rock type.

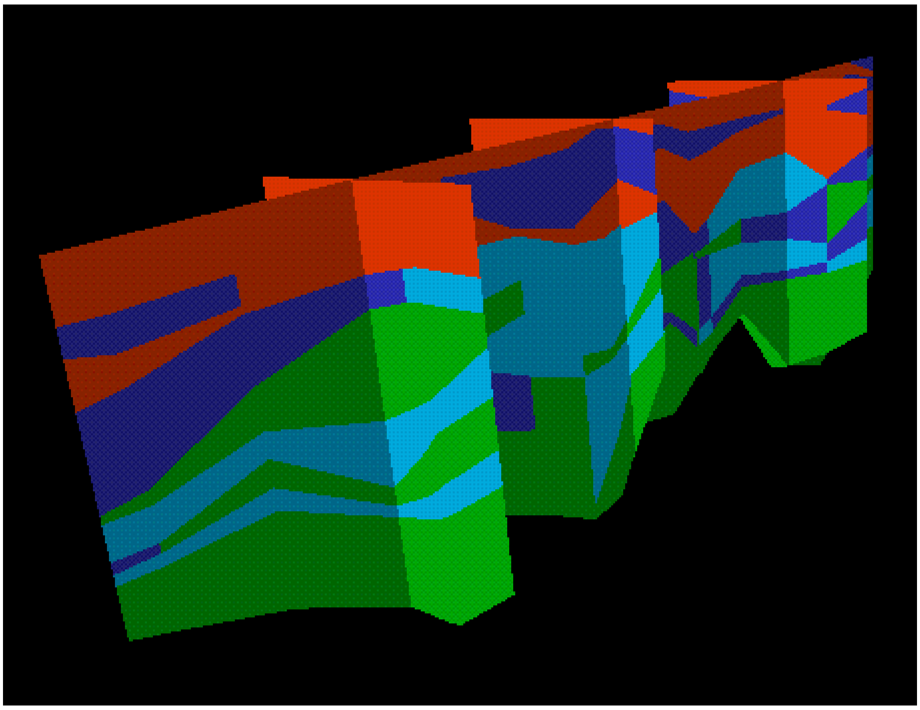

Figure 2.3: Slices coloured according to rock type through a 3D grid. The individual elements are not shown in this picture. This picture was produced using Avizier.

4.2 Rock and Fluid Properties

Most of the parameters used to specify the properties of the rocks and the fluids represented in the NAMMU model can be specified in one or more of the following ways:

- to have a constant value throughout the model;
- to have a constant value for a particular rock unit and/or solute species;
- to vary as a function of the variables, for example, the pressure, and certain pre-defined parameters, for example, the fluid compressibility. These relationships are built into NAMMU;
- to vary (subject to certain limitations) as a function of the standard parameters, the variables and user-defined parameters in an arbitrary manner specified by the user through a set of FORTRAN subroutines, which have standard, well-defined interfaces.

Some of the key parameters are discussed in the following subsections. A description of all of the parameters used to specify the rock and fluid properties is given in the NAMMU User Guide and NAMMU Reference Manual. A list of symbols and the units for each parameter is given in the Nomenclature and Units Section.

4.2.1 Fluid properties

In calculations of the transport of a dense solute (equations (1), (3), (5) and (8)), the fluid density, r_l, is given by

$$\frac{1}{r_l} = \frac{1-C}{r_0(1+a(P^T - P_0^T))} + \frac{C}{r_{ls}(1+a_s(P^T - P_0^T))}, \tag{18}$$

where

r_0 is the density of fresh water ($C = 0$);
r_{ls} is the density of saturated salt solution ($C = 1$);
a is the compressibility of fresh water;
a_s is the compressibility of saturated salt solution;
P^T is the total pressure;
P_0^T is the reference pressure.

By default, the dense solute is taken to be salt.

For heat transport calculations (equations (1-5) and (10)), the fluid density is given by

$$r_l = r_0(1+a(P^T\text{-}P_0^T)\text{-}b(T\text{-}T_0)), \tag{19}$$

where

b is the coefficient of volumetric expansion of fresh water;
T is the temperature;
T_0 is the reference temperature.

For calculations of the transport of heat and a dense solute (equations (1), (3), (5), (8) and (11)), the fluid density is given by

$$\frac{1}{r_l} = \frac{1-C}{r_0(1+a(P^T - P_0^T) - b(T-T_0)} + \frac{C}{r_{ls}(1+a_s(P^T - P_0^T) - b_s(T-T_0)}, \tag{20}$$

where b_s is the coefficient of volumetric expansion of saturated salt solution.

The default variation of fluid viscosity with temperature, m, is given by

$$m = m_0 e^{-d_1(T-T_0)}, \tag{21}$$

where m_0 is the viscosity at the reference temperature and d_1 is a parameter that is sometimes called the viscosibility.

4.2.2 Rock properties

The permeability is a symmetric tensor, **k**. The full tensor representation of the permeability is implemented in NAMMU so by entering the appropriate components of this tensor, (3 components in two dimensions and 6 components in three dimensions), the user may specify any orientation or degree of anisotropy.

For calculations of unsaturated groundwater flow (equations (2) and (4)), the way in which the permeability varies with the saturation, S, must be specified. In NAMMU, this is specified using the relative permeability, k_r.

$$k_r = \begin{cases} \dfrac{AKR}{BKR + (-P^T)^{SKR}} & P^T < 0 \\ 1 & P^T \geq 0 \end{cases} . \tag{22}$$

S is calculated from the capillary pressure curve. The default form used in NAMMU is

$$S = \begin{cases} \dfrac{APC}{BPC + (-P^T)^{SPC}} & P^T < 0 \\ 1 & P^T \geq 0 \end{cases} . \tag{23}$$

AKR, *BKR*, *SKR*, *APC*, *BPC* and *SPC* are constants for a rock unit.

4.2.3 Dispersion

The standard transport equations included in NAMMU contain representations of both diffusion and hydrodynamic dispersion. The default form of the dispersion tensor for each of the transport equations is given below.

For the advection-dispersion equation for solute transport where the fluid density depends on the solute concentration (equation (8)), the dispersion tensor, **D**, is given by

$$\mathbf{D} = \frac{D_m}{t} d_{ij} + a_T v d_{ij} + (a_L - a_T)\frac{v_i v_j}{v} , \tag{24}$$

where

D_m	is the molecular diffusion coefficient for the solute;
t	is the tortuosity;
a_L	is the longitudinal dispersion length;
a_T	is the transverse dispersion length;
$\mathbf{v}$	is the porewater velocity, $\mathbf{v} = \mathbf{q}/f$ (with components v_i).

For the heat transport equation (equation (11)), the heat dispersion tensor, $\mathbf{D}'$ is given by

$$\mathbf{D}' = G_a d_{ij} + b_T v d_{ij} + (b_L - b_T)\frac{v_i v_j}{v} , \tag{25}$$

where

G_a	is the average thermal conductivity of rock and fluid;
b_L	is given by $r_l f c_l a'_L$;
b_T	is given by $r_l f c_l a'_T$;
a'_L	is the longitudinal dispersion length for temperature;
a'_T	is the transverse dispersion length for temperature;
c_l	is the specific heat capacity of the fluid.

It should be noted that the full heat dispersion tensor is currently only implemented for coupled transport of a dense solute and heat.

For the solute transport equations (equations (12) and (13))), the dispersion tensor, $\mathbf{D}_a$ is given by

$$\mathbf{D}_a = \frac{D_{ma}}{t} d_{ij} + a_{Ta} v d_{ij} + (a_{La} - a_{Ta}) \frac{v_i v_j}{v}, \qquad (26)$$

where D_{ma} are the molecular diffusion coefficients for each solute and a_{Ta} and a_{La} are the longitudinal and transverse dispersion lengths for each solute.

4.2.4 Chemical properties

It is possible to represent up to 6 different passive solutes, each with different chemical properties, within a NAMMU calculation. The contaminant transport models represented in NAMMU include the effects of decay. Decay constants, l_a, may be entered for each solute. If more than one solute is represented in a calculation, they are assumed to form a radioactive decay chain.

The interaction between a solute and a rock is represented using a retardation factor, R_a, to represent the effects of linear equilibrium sorption. The relationship used in NAMMU is

$$R_a = 1 + \frac{(1-f)}{f} K_{da}. \qquad (27)$$

In the case of unsaturated contaminant transport, it is assumed that K_{da} scales linearly with the saturation, S. It should be noted that, in NAMMU, the quantity referred to as K_{da} differs from the quantity for which this notation is usually adopted (although it is related).

5. OUTPUT

A wide variety of output options are available within NAMMU. These include:

- plots of the finite-element grid;
- plots of the grid with elements shaded according to rock type;
- plots showing planar slices through three-dimensional grids;
- plots showing the grid surface or certain internal surfaces for three-dimensional grids;
- plots of the grid boundary;
- shaded plots or contour lines of scalar functions of the variables;
- plots of vector quantities;
- one-dimensional line graphs of scalar functions of the variables along a line;
- one-dimensional line graphs of scalar functions of the variables as a function of time;
- plots of advective pathlines;
- calculation of capture zones;
- mass balance calculations;
- plotted quantities can be coloured in many ways, for example, according to the values of the variables, scalar functions of the variables and user defined functions of the variables;
- plots may be superimposed to build up complex images;
- user-defined text and lines can be added to plots.

The finite-element model and its results can also be visualised using the AVIZIER graphics package. This is a fully interactive tool with the capability of displaying and manipulating images of the NAMMU model on the screen. The AVIZIER package has been customised to enable it to display faithfully the results of the NAMMU model. Thus, the finite-element grid is displayed without any re-sampling of grid points, and scalar and vector quantities are plotted using the same interpolation method used by NAMMU in the original calculation. These features make AVIZIER a unique and powerful tool for the NAMMU modeller.

The following figures illustrate some of the types of pictures that can be produced using NAMMU and Avizier.

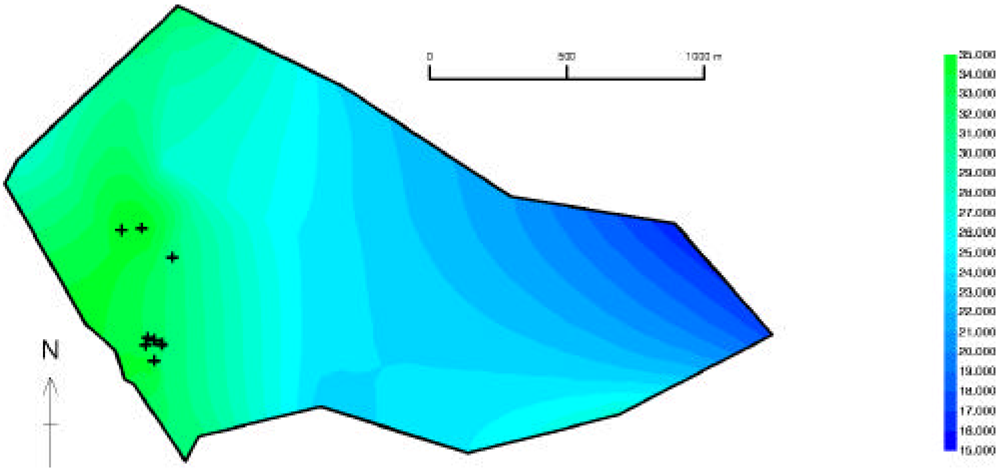

Figure 5.1: Shaded contour plot of groundwater head.

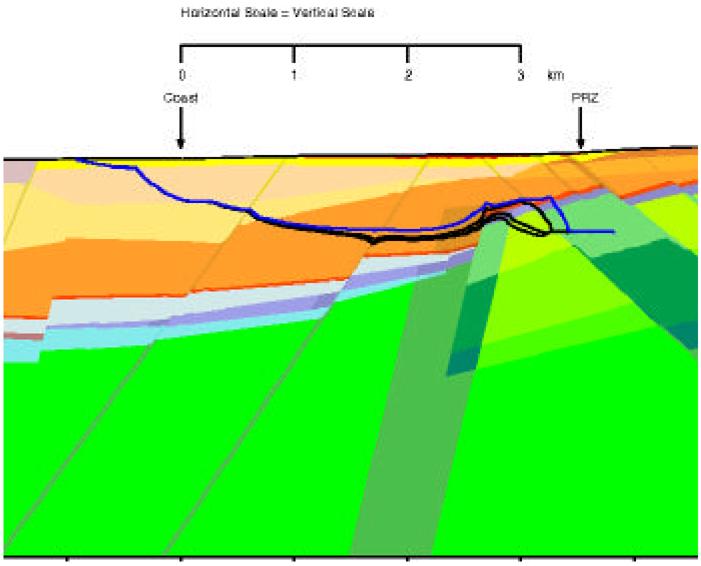

Figure 5.2: Pathlines for a model based on the grid shown in Figure 4.2.

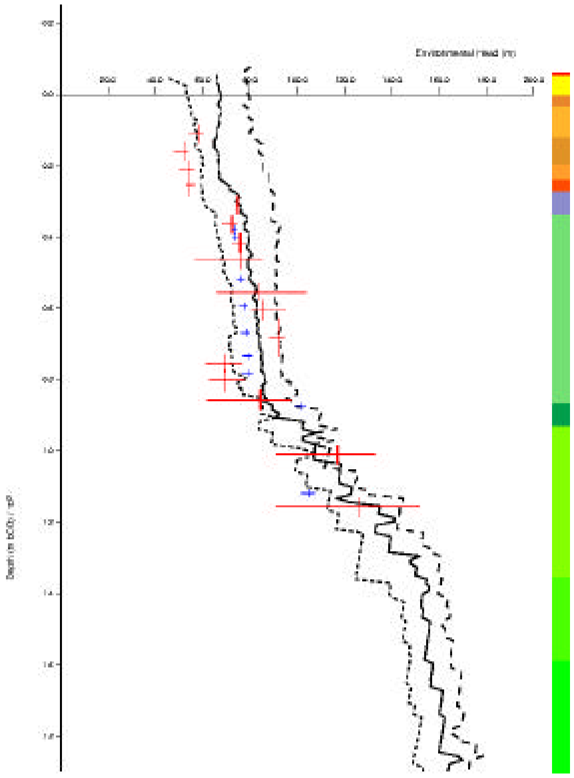

Figure 5.3: Line graph showing variation of environmental head with depth and the observations from the site along a vertical line through the model shown in Figure 5.2.

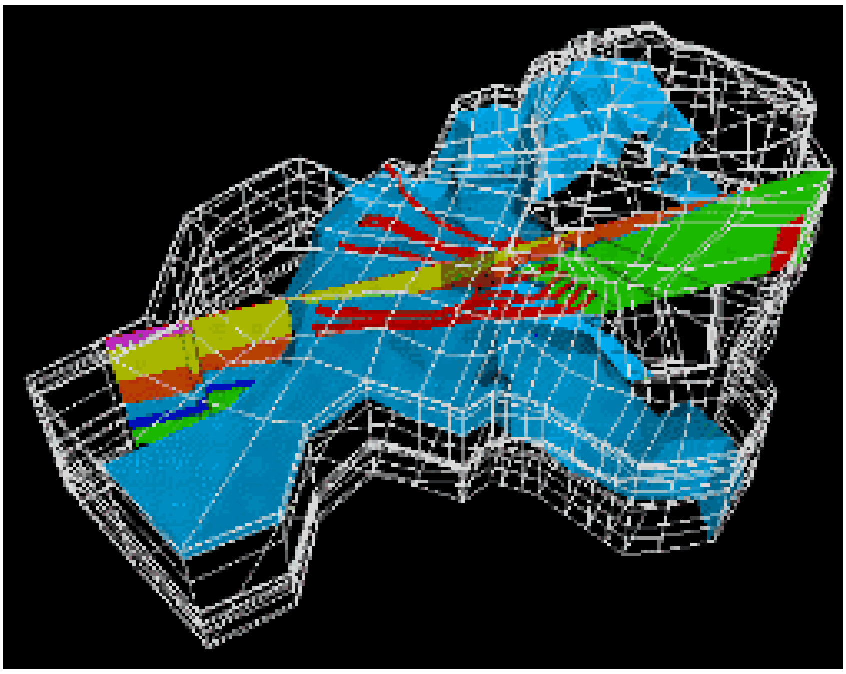

Figure 5.4: Complex image showing (i) slice through the grid, (ii) surface of constant salinity and (iii) pathlines for a 3D version of the model shown in Figures 4.2, 5.2 and 5.3. This figure was produced using Avizier.

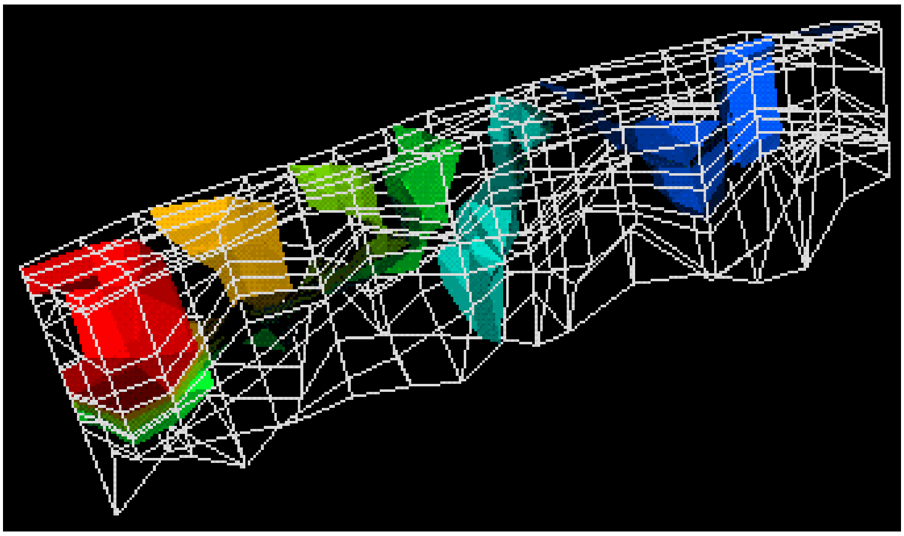

Figure 5.5: Isosurfaces of pressure for the model shown in Figure 4.3. This figure was produced using Avizier.

6. VERIFICATION AND VALIDATION

Confidence in NAMMU has been built up over a number of years and comes from a variety of sources. It is important to distinguish between verification and validation. Verification, as applied to a computer program such as NAMMU, is the process of checking that the program correctly represents the mathematical models on which it is based. A verified program can then be used to help validate the mathematical models, that is to check that the mathematical models form an adequate representation of the relevant physical phenomena and that they are applicable to the situation under consideration.

6.1 Verification of NAMMU

Verification can be addressed by comparing the results of numerical calculations with analytic solutions when such solutions are known, and by intercomparison with calculations from independently written codes for more complicated examples. NAMMU has been extensively verified in this way. A number of international projects addressing the verification and validation of groundwater flow and radionuclide transport models for repository performance assessments have been organised in recent years. The HYDROCOIN (1988, 1990, 1991, 1992) project is perhaps the most important of these. HYDROCOIN was organised around various test cases addressing particular issues of concern. NAMMU was used, with considerable success, on a number of the test cases in the HYDROCOIN project.

The HYDROCOIN project included test cases intended to verify

- transient groundwater flow from a borehole penetrating a confined aquifer (Herbert 1985b);
- steady-state flow in a region containing highly permeable faults (Herbert 1985a);
- transient coupled groundwater flow and heat transport (Cherrill and Herbert, 1985);
- groundwater flow through a hypothetical shallow disposal facility (Herbert 1985b);
- coupled groundwater flow and solute transport with the fluid density strongly dependent upon concentration (Herbert et al, 1988).

In each case, the results obtained with NAMMU were in excellent agreement with the analytic solution, where one was available, or with the results from other groundwater flow modelling programs, in cases where an analytic solution was not available.

NAMMU has also been used in two reviews of repository assessments. These reviews compared the results obtained using different programs for the same finite-element model. In a review of the Swedish KBS-3 study (Atkinson et al 1984), the groundwater heads obtained using NAMMU were compared with those obtained using the program GWHRT, for several different cases. In every case, the results agreed to at least six significant figures (the number of figures listed for the output from GWHRT). This gives great confidence that both programs were coded correctly.

Results obtained using NAMMU were also compared with results obtained using the FEM301 program for the Swiss Project Gewähr (Robinson et al 1986). Initially, the results obtained using NAMMU differed slightly from those obtained using FEM301. These differences were traced to discrepancies between the FEM301 program and its documentation and differences between NAMMU and FEM301 in the treatment of highly distorted elements. When an appropriate temporary modification was made to NAMMU to enable it to mimic the behaviour of FEM301, the results obtained agreed to within five significant figures with those obtained from FEM301. It should be stressed that the initial differences were not due to any problems with NAMMU.

More confidence in the correctness of NAMMU is provided by the results of verification exercises for other finite-element programs such as ENTWIFE that use the same numerical techniques, finite-element solvers and post-processing routines from the TGSL subroutine library as are used in NAMMU. Indeed, since these programs use very different conceptual models, with different numbers of variables and so on, the testing provided in this way for the numerical techniques, the solver and post-processing routines is more severe than testing only for groundwater flow and transport problems.

The free convection program ENTWIFE has been used in a number of verification exercises (de Vahl Davis and Jones 1983, Smith and Hutton 1986, Napolitano and Orlandi 1985). In all cases, the results obtained using ENTWIFE were among the best obtained. ENTWIFE has also been used in comparisons with analytical solutions.

All this experience provides considerable confidence in the mathematical correctness and general applicability of NAMMU. The full set of verification exercises, which are used to test NAMMU at each release, currently consists of approximately 50 test cases. These include some of the HYDROCOIN test cases, as well as other test cases for which an analytic solution is available. The test cases include examples of groundwater flow in isotropic and anisotropic media under both steady-state and transient conditions, coupled groundwater flow and salt transport, coupled groundwater flow and heat transport, unsaturated flow, and radionuclide transport. The full set of test cases, together with the corresponding output, is supplied to all NAMMU users.

6.2 The Role of QA in Verification

A Quality Assurance (QA) programme defines a set of procedures for carrying out a particular type of work in such a way as to maintain the quality of the work. A well designed QA programme plays an important role in verification by ensuring that high standards of coding are adhered to, that there are procedures for reporting and fixing program errors and that there is a system for testing and issuing new releases of the program which ensures that the new program gives the correct results for a standard set of test cases. NAMMU is maintained and developed under an appropriate QA programme that conforms to the international standard ISO 9000 and to TickIT. Through the NAMMU QA programme, AEA Technology seeks to continually improve the quality and reliability of the program.

6.3 The Concept of Validation

A number of definitions of the term ‘validation’ have appeared in the literature. Perhaps the most appropriate for the purpose of this document is that given by the IAEA:

‘Validation is a process carried out by comparison of model predictions with independent field observations and experiment measurements. A model cannot be considered validated until sufficient testing has been performed to ensure an acceptable level of predictive accuracy over the range of conditions over which the model may be applied. (Note that the acceptable level of accuracy is judgmental and will vary depending on the specific problem or question to be addressed by the model.)’ (IAEA, 1989).

Validation involves more than comparing the predictions of a model with observations, although, as indicated by the IAEA definition, this can be an important part of the process. Validation also implies a need to establish whether or not the model is an acceptable representation of the physical phenomenon. As such, it will also include checking that the model is internally consistent and examining the model for consistency with principles that are generally accepted in the scientific community.

It is also important to appreciate that, in practice, as implied by the IAEA definition, there is always a subjective element in validation, since different people may have different ideas about what is considered acceptable. The nature of the validation process (i.e. the approach to building confidence in the model) will be slightly different, depending on whether the model is a general model, for example of a process such as groundwater flow, or a specific model, for example an attempt to model the behaviour observed in a particular experiment or at a particular site. Validation can therefore take place on several levels.

6.4 Validation of NAMMU

It is clear from the IAEA definition of validation that comparison of the results of a model with independent field observations and experimental measurements is an important component of the validation process. By its nature, this aspect of validation is specific to a particular site and so will include issues related to the validation of the site-specific conceptual model, which lie outside the scope of this document. However, examples of successful applications are included, as they can help to build confidence in the generic model of the physical processes that are implemented in NAMMU. There are a number of issues that it is important to bear in mind when performing such comparisons.

- The uncertainties in both the predictions and the measurements should be quantified.
- It will generally be necessary to calibrate the model. The level of confidence that can be placed in a model is greatly increased if it can then be used to make adequate predictions of the values of quantities that are independent of those that were used in the calibration.
- Length scales must be taken into account in the comparison. For example, the measurements may have been performed at a scale that is smaller than the resolution of the mesh used in the numerical representation of the model. In such a case, the model would not be expected to reproducing the detailed variability of the measurements, but should be able to give an acceptable representation of any overall larger-scale trends.

Validation of NAMMU models of specific sites has been attempted in a number of cases. A major obstacle to more extensive validation has been the relative lack of field data. Work to validate NAMMU models has been carried out at several sites including:

- predictive estimates of drawdowns in boreholes at Aspo (Grundfelt et al 1990);
- simulations of the LPT2 pump test and Tunnel Drawdown Experiment at Aspo (Holton and Milický, 1997);
- comparisons of predicted and observed flows at the Harwell site (Brightman and Noy, 1984);
- predictions and post-test modelling of the RCF3 Pump Test at Sellafield (UK Nirex Limited, 1998);
- comparisons of predicted and observed heads and distributions of salinity and temperature for two and three dimensional models of Sellafield (UK Nirex Limited, 1997).

As discussed above, there is considerable confidence that the models of the physical processes that are adopted in NAMMU and their implementation in the program, are correct, when applied to appropriate situations. When comparing model results with observations from a particular site, it is vital that the validity of the site-specific conceptual model is taken into account. This is an additional factor, which is not related to the validity of the models within NAMMU itself.

NOMENCLATURE AND UNITS

By default, NAMMU uses SI units, but any internally consistent set of units could be used.

Symbol	**Definition**	**Units**
a_L	longitudinal dispersion length for dense solute	m
a_T	transverse dispersion length for dense solute	m
a_{La}	longitudinal dispersion length for contaminant species	m
a_{Ta}	transverse dispersion length for contaminant species	m
a'_L	longitudinal dispersion length for temperature	m
a'_T	transverse dispersion length for temperature	m
AKR	constant in relative permeability expression	-
APC	constant in capillary pressure expression	-
b	aquifer thickness	m
BKR	constant in relative permeability expression	-
BPC	constant in capillary pressure expression	-
C	solute concentration	-
c_l	specific heat capacity of fluid	J kg^{-1}K^{-1}
$\mathbf{D}$	solute dispersion tensor	m^{2}s^{-1}
$\mathbf{D}'$	heat dispersion tensor	W m^{-1}K^{-1}
$\mathbf{D}_a$	contaminant species dispersion tensor	m^{2}s^{-1}
D_m	molecular diffusion coefficient	m^{2}s^{-1}
D_{ma}	molecular diffusion coefficient of solute	m^{2}s^{-1}
f_a	contaminant species source into porewater	mol m^{-3}s^{-1}
$\mathbf{g}$	gravitational acceleration	m s^{-2}
H	heat source	W m^{-3}
h	hydraulic head	m
I	infiltration rate into areal aquifer	kg m^{-2}s^{-1}
K_{da}	sorption coefficient for passive solute	-
$\mathbf{k}$	permeability tensor	m^2
k_r	relative permeability	-
k_v	vertical permeability of semi-permeable layer	m^2
N_a	concentration of contaminant species	mol m^{-3}
P^R	residual pressure	N m^{-2}
P^T	total pressure	N m^{-2}
$P_0{}^T$	reference total pressure	N m^{-2}
$\mathbf{q}$	Darcy velocity / specific discharge	m s^{-1}
Q	Source term for mass inflow into aquifer	kg m^{-2}s^{-1}
R_a	retardation factor for passive solute	-
S	saturation	-
s	specific storage	m^{-1}
SKR	constant in relative permeability expression	-
SPC	constant in capillary pressure expression	-
t	time	s

Symbol	**Definition**	**Units**
T	temperature	K
T_0	reference temperature	K
$\mathbf{v}$	average porewater velocity	$m\ s^{-1}$
v	magnitude of average porewater velocity	$m\ s^{-1}$
z	elevation	m
z_b	elevation of base of aquifer	m
z_s	elevation of ground surface	m
z_t	elevation of top of aquifer	m
z_0	reference elevation	M
a	fluid compressibility (fresh water)	$N^{-1}m^2$
a_s	fluid compressibility of saturated salt solution	$N^{-1}m^2$
b	coefficient of volumetric expansion (fresh water)	K^{-1}
b_s	coefficient of volumetric expansion of saturated salt solution	K^{-1}
b_L	parameter appearing in heat dispersion equation	$J\ m^{-2}K^{-1}$
b_T	parameter appearing in heat dispersion equation	$J\ m^{-2}K^{-1}$
G_a	average thermal conductivity of rock and fluid	$W\ m^{-1}K^{-1}$
d_{ij}	Kronecker delta	-
d_1	viscosibility	K^{-1}
l_a	decay constant for contaminant species	s^{-1}
m	fluid viscosity	$kg\ m^{-1}s^{-1}$
m_0	reference fluid viscosity	$kg\ m^{-1}s^{-1}$
r_l	fluid density	$kg\ m^{-3}$
r_{ls}	density of saturated salt solution	$kg\ m^{-3}$
r_0	reference fluid density	$kg\ m^{-3}$
$(rc)_a$	average heat capacity of fluid and rock	$J\ m^{-3}K^{-1}$
t	tortuosity	-
f	porosity	-

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