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Abstract

NAMMU is a software package for modelling groundwater flow and transport in porous media. The package can be used to model steady state and time-dependent behaviour, including unsaturated flow and the transport of mass and heat. An option is available for modelling radioactive decay and the transport of chains of radionuclides. The software is based on an efficient implementation of the finite-element method that provides many options for modelling complex geological regions.

The following documentation is available for NAMMU:

- NAMMU Technical Summary Document;
- NAMMU User Guide;
- NAMMU Command Reference Manual;
- NAMMU Verification Document;
- NAMMU Installation and Running Guide.

This document, the Technical Summary Document, provides a technical overview of NAMMU, including a description of the equations solved and the numerical methods used.

Additional information about the capabilities and the potential applications of NAMMU is available on request from AMEC.

Contents

Capabilities of NAMMU

NAMMU has a wide range of facilities for specifying a model region, the properties of rocks, fluids and solutes within the region, the equations to be solved, and the output options required. In addition to the standard facilities, many options are available that allow the user to customise the functionality of NAMMU for a particular project. The advanced 3D-visualisation package, GeoVisage, is available for NAMMU.

NAMMU can be used to model the following geometries and physics:

- Flow and transport in 3D Cartesian, 2D vertical and plan section, and 2D radial geometries;
- Deterministic and stochastic continuum modelling;
- Steady state and transient behaviour;
- Groundwater flow in saturated and unsaturated conditions;
- Saline groundwater flow with the density dependent on concentration;
- Coupled groundwater flow and heat transport with the density dependent on temperature;
- Saline groundwater flow and heat transport with the density dependent on concentration and temperature;
- Groundwater flow in a dual porosity system based on the Warren and Root model;
- Transport of contaminants, including the effects of advection, dispersion, and sorption, with solubility limitation;
- Transport of radioactive decay chains, allowing for interacting chains to be linked by solubility limitation of a common radionuclide.
- Advective pathlines; specifically the paths that test particles take through the model following either the finite element velocity field or a mass conserving velocity field;

NAMMU can be used to model the following features:

- Complex distributions of lithology;
- 3D volumes of enhanced or reduced permeability;
- Conductive or semi-impermeable fracture zones;
- Stochastic models of permeability and porosity;
- Boreholes, tunnels and shafts;
- Specified value (Dirichlet) and specified flux (Neumann) boundary conditions;
- Infiltration boundary conditions for surface recharge/discharge areas;
- Hydrostatic and outflow boundary conditions for vertical boundaries;
- Time-varying boundary conditions (e.g. used to model land uplift, or time-dependent contaminant discharge);
- Sources of contaminants, salinity or heat.

NAMMU models and results can be displayed by:

- A 3D visualisation system, GeoVisage for NAMMU, that allows 3D rendering of finite-elements, rock types, permeability, fracture zones, variables, flow vectors, and pathlines;
- 2D plot and numerical output that includes:
  - Plots of the finite-element mesh and its boundaries;

- Plots of contours of a variable on a surface;
- Plots of contours of a variable on a 2D slice;
- Plots of velocity arrows, showing direction and magnitude of the groundwater flow;
- Plots of pathlines either for steady state or for transient groundwater flows;
- Plots of backward pathlines, showing the region of influence of a borehole;
- Graphs of variables along a line;
- Graphs of the evolution of variables at a point;
- Graphs of data;
- Integrals (e.g. flux of groundwater across a plane).

NAMMU models have been used in the following applications:

- Calculations in support of safety assessments for radioactive waste disposal programmes:
  - Regional groundwater flow;
  - Site investigation;
  - Pump test simulation;
  - Tracer test.
- Modelling for groundwater protection schemes:
  - Aquifer;
  - Saline intrusion.
- Modelling to design and evaluate remediation strategies;
  - Aquifer contamination;
  - Landfill site.

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

NAMMU has been developed over a period of more than 20 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.

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' [1]. This document provides a technical overview of NAMMU, including a description of the equations solved and the numerical methods used.

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 variables of interest (see subsections 2.1 and 4.2), the boundary conditions (see subsection 2.2), the processes 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;
- Binary files for use with the GeoVisage visualisation package or for subsequent NAMMU runs.

1.2 Availability

NAMMU is written in standard FORTRAN 95 and therefore is portable across a wide range of computers. NAMMU is supported on a range of computer platforms, from desktop PCs running Windows to Unix mainframes. The software is available from AMEC by contacting the support team gw.support@Amec.com or from a download at www.connectflow.com.
NAMMU also forms part of the ConnectFlow package [2], developed by AMEC, for modelling groundwater flow and transport in porous and fractured media.

1.3 The iCONNECT Club

The ***iCONNECT club*** (***i***ntegrated ***CON***tinuum and ***NE***twork approach to groundwater flow and ***C***ontaminant ***T***ransport) is AMEC's response to the desire expressed by those involved in radioactive waste management to address a range of generic and site-specific issues related to the evaluation of the geosphere as part of a safety assessment.

The purpose of the ***iCONNECT club*** is to draw like-minded organisations together into a club in order to dilute the costs of addressing modelling issues, in particular those generic issues faced by organisations wanting to evaluate the performance of the geosphere as part of a repository safety assessment. The ***iCONNECT club*** will act as a forum for the focused application and enhancement of the ConnectFlow methodology, resulting in wide-ranging benefits to all participants.
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;
- 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.;
- Agence Nationale pour la Gestion des Déchets Radioactifs (ANDRA), France;
- 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:

1. **NAMMU Technical Summary Document** (this document). This document provides a general technical overview of the software, including a description of the equations solved and the numerical methods used.
2. **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.
3. **NAMMU Command 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.
4. **ConnectFlow Verification Document**. This document includes the testing of NAMMU's capabilities.
5. **NAMMU Installation and Running Guide**. This document describes how to install and run NAMMU on the various computer platforms supported.

In addition to the references cited within the report, a bibliography is provided at the end of this report listing some of the studies that have made use of NAMMU.

2 Concepts Within the Model

2.1 Relevant Physical Processes

The aim of this section is to identify a list of physical processes relevant to groundwater flow and transport that can be investigated using NAMMU, and then to present the approach to the modelling of the phenomena that is adopted within NAMMU. Many other processes that occur in subsurface flows (e.g. those relating to transport of radionuclides in the gas phase or colloidal transport) are not considered further because these processes are not included in the models that have been implemented in NAMMU. The processes that can be explicitly modelled by NAMMU are summarised in the rest of this section. The models used in NAMMU are then discussed in the remaining sections.

The following is a list of FEPs (features, events and processes) identified by the NEA as relevant to subsurface flow in the performance assessment of a repository:

1.2.5 Hydrothermal Activity;
1.3.7 Hydrogeological response to climate
1.4.6 Groundwater extraction
2.1.6 Hydrogeological changes and response
2.1.8 Thermal changes and response
2.2.3 Hydrogeological regime
2.2.4 Hydrochemical effects
2.2.5 Groundwater flow system
2.2.6 Solute transport
2.2.10 Dilution processes
2.2.11 Heterogeneity
3.1.1 Radioactive decay and ingrowth
3.1.3 Water mediated transport (including advection, dispersion, diffusion and rock matrix diffusion.
3.1.5 Sorption / desorption processes.
3.1.10 Dilution processes
3.1.11 Transfer by human actions (drilling, mining, excavation, etc.)

In the following sections, the conceptual model to represent these processes in NAMMU is described along with the parameterisation of the models.

In each case, the theoretical and experimental justification for the treatment of the process in the NAMMU model is presented. In particular, the issue of whether the treatment is conservative or realistic is discussed.

2.2 Groundwater Movement

The soils and rocks that make up the Earth's crust generally are porous, that is they contain empty spaces which can be occupied by groundwater. This empty space is the porosity of the rock, and is defined as the fraction of the volume of the rock that is accessible to groundwater. If the spaces are interconnected then the groundwater may flow under the action of external forces [3, 4, 5, 6, 7]. Generally speaking, groundwater velocities are extremely small.

Nevertheless, flowing groundwater can transport dissolved substances over significant distances if sufficient time is available. In the context of a deep radioactive waste repository, it is important to ensure that groundwater movement does not return unacceptable quantities of radionuclides from the repository to man's environment.

The most common approach to modelling groundwater flow, and the approach used in NAMMU, is the continuum approach. The idea is to treat all the quantities of interest, such as the pressure in the groundwater, as quantities that vary continuously over space. There are two ways of defining

these continuous quantities. In the first, the notion of a Representative Elementary Volume (REV) is introduced [3]. This is a volume of rock that is very large compared to length scales characteristic of the microscopic structure of the rock, but small compared to the length scales of interest from the viewpoint of groundwater flow. The continuum quantities are defined as spatial averages over the REV's. In the second, the medium is thought of as being a realisation of a random process [6]. The quantities of interest are now defined as ensemble averages. Although the two approaches are philosophically quite different, they lead to virtually the same governing equations for groundwater flow.

In some rocks most of the groundwater actually flows through an interconnected network of fractures. This leads to a quite different approach to modelling groundwater flow known as fracture-network modelling, in which the flow through an explicitly modelled set of fracture planes is calculated [8, 9, 10, 11]. One potential use of these fracture network models is to determine the appropriate values to use for the effective permeability of a block of fractured rock, if it is to be represented appropriately in a continuum model such as NAMMU. Thus, the fact that NAMMU is based upon a continuum-porous-medium approach does not mean that the models described in this document cannot be used to represent flow and transport within a fractured rock. Provided that the scale of interest in the flow and transport calculation is larger than the length scale of the individual fractures and is large enough to include several fractures, it is reasonable to use a porous medium approach to represent flow and transport through the fracture network.

The movement of groundwater is described quantitatively by the specific discharge, $\mathbf{q}$, sometimes called the Darcy velocity. This is the volumetric rate of flow of water per unit cross-sectional area. The specific discharge, $\mathbf{q}$, is calculated in NAMMU from Darcy's law [3, 4, 5, 6],

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}\left(\nabla P^T - \rho_l \mathbf{g}\right). \tag{2.1}$$

This law is empirical. However, it can be shown that Darcy's law is basically an expression of the law of conservation of momentum for the fluid. The fundamental model for flow of a viscous fluid is embodied in the Navier-Stokes equations [12] and in principle these could be used. However, it would be impractical and inappropriate to apply these equations in the geosphere models used in performance assessments. The situation of interest is then the flow of fluid through the connected void spaces in the rock. In order to apply the Navier-Stokes equations it would be necessary to specify the geometry of the void space. This is clearly impractical. It would also be inappropriate. Such a model would provide far more detail than is actually required. The appropriate expression of the law of conservation of momentum for the fluid in these circumstances is given by Darcy's law, which can be derived from the Navier-Stokes equations of fluid flow for certain simplified models of the microscopic structure of the rock (see e.g. [13]).

Darcy's law was originally derived from experiments on flow through sand columns. It has since been demonstrated experimentally to apply over a wide range of conditions. Darcy's law also forms the basis for innumerable calculations of groundwater flow in water resources engineering and of the production of oil in oil reservoir models. It can therefore be considered to be a well-validated model, for the circumstances of interest. However, it should always be borne in mind when constructing models based on this approach that deviations from Darcy's law have been observed at very high flow rates, when the flow is not purely laminar [4, 6, 13] (which can occur close to wells, for example). Possible deviations from Darcy's law have also been suggested for very small hydraulic gradients, where in some types of materials the flow may be zero below a critical value of the hydraulic gradient [6]. Theoretical considerations suggest that under transient conditions, an additional term will appear in Darcy's law, although in practice this term will be negligible except at short times following a sudden large change in conditions [6]. The use of Darcy's law can therefore be regarded as realistic, or at worst to lead to an overprediction of the flow rate, for the types of systems of relevance to a performance assessment.

The question arises of what value to assign for the permeability of the rock, since, in practice, rock properties are rarely, if ever, homogeneous. The approach adopted will depend on the nature of the rock system, and the quality of data available, but essentially it is necessary to assign an

effective permeability to the hydrogeological unit, which will lead to the correct flow in an average sense.

In the case of highly fractured rock, it may not be possible to assign an effective property that adequately reproduces the correct average flow behaviour. In this case it may be possible to represent the system as two coexisting continua, one corresponding to the fractures, and one corresponding to the rock matrix [14]. In the steady state, this simplifies to a single continuum described by a single effective permeability, but in transient flow, pressure variations can be transmitted through the fractures more rapidly than through the matrix. This type of model is not currently supported in the standard release of NAMMU, although a specially modified version has been used to study this type of system in the past. In extreme cases, an explicit fracture-network approach may be better able to represent the groundwater movement.

The groundwater flow depends on the fluid viscosity, through Darcy's law. The viscosity will in general be a function of temperature, and can vary by as much as 50% over the range 10 - 100ºC. It may also be a function of salt concentration. In NAMMU, this can be modelled by making the viscosity an arbitrary function of temperature and salt concentration.

In unsaturated conditions, the accessible porosity is less than the saturated porosity by a factor called the saturation, S. S is a function of pressure, and in NAMMU can be modelled as an arbitrary function of pressure. The permeability is also normally reduced in the unsaturated case by a factor k_r called the relative permeability. The relative permeability can be modelled as an arbitrary function of pressure.

It should be noted that NAMMU does not treat the generation or transport of gas, which may influence the movement of groundwater. This approximation is neither realistic nor conservative, but can be addressed by the use of other models specifically designed to model the effects of gas generation and transport [15].

2.3 Groundwater Pressure

In hydrogeology, it is useful to distinguish between two different descriptions of the pressure associated with the groundwater at a given location.

The first description is in terms of the total pressure, P^T, which is the pressure commonly used in other branches of physical sciences and which would be measured using a device such as a manometer. It is measured in units of Pascals. The second description involves the "residual pressure", P^R, (also referred to as the "non-hydrostatic pressure"). The residual pressure is defined with respect to the selected reference elevation (with respect to which all vertical positions are defined). It is often the case in groundwater studies that the reference elevation lies above the location where the total pressure is measured (because the reference elevation is defined with respect to sea level or a convenient ground surface elevation). The residual pressure, P^R, is then the pressure that is obtained after subtraction from the total pressure of the hydrostatic pressure due to a freshwater column that extends vertically from to the location where the total pressure is measured to the reference elevation (see section 3.3.1). This explains the name. The residual pressure is also measured in units of Pascals. If the reference elevation lies below the point at which the total pressure is measured then the residual pressure would actually be the total pressure augmented by that of a freshwater column of the appropriate length. The residual pressure is a useful concept, because, according to Darcy's law, groundwater flow is proportional to the gradient in the residual pressure (see section 3.3.1).

The familiar concept of groundwater or hydraulic "head" [4] is a quantity closely related to the residual pressure. Hydraulic head is the residual pressure divided by the specific weight of the groundwater (see section 3.3.1). Hydraulic head is therefore measured in metres. Hydraulic head is useful for two reasons: firstly, Darcy's law can be conveniently formulated in terms of hydraulic head and hydraulic conductivity (the latter being a quantity depending on properties of both rock and fluid), and, secondly, hydraulic head is very easily measured in the field. For a well that is only open to the formation at a particular level, the height to which water rises in the well is equivalent to

the groundwater head at the level of the opening. However, a more general formulation in terms of pressures is more convenient when it is necessary to treat cases in which variations in the groundwater density (e.g. due to variations in groundwater temperature or salinity) have to be taken into account.

The total groundwater pressure, P^T, can be calculated from Darcy's law (Equation (2.1)), together with the equation of conservation of mass,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0\,. \tag{2.2}$$

These two equations lead to a single second-order equation for the total pressure,

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.\left(\rho_l \frac{\mathbf{k}}{\mu}\left(\nabla P^T - \rho_l \mathbf{g}\right)\right) = 0\,. \tag{2.3}$$

This is the basic equation that is solved by NAMMU. It is straightforward to formulate the pressure equation in terms of total pressure, residual pressure, or pressure head, and all three formulations are supported by NAMMU.

In general, the density and viscosity of the water depend on temperature and on the groundwater chemistry, in particular the presence of solutes, especially salt. Temperature and salt are in turn transported by the groundwater. When the variations in temperature or salt concentration are large enough to produce significant changes in density or viscosity, it is necessary to couple the solution of the groundwater flow problem to that of the heat or salt transport problem. This is discussed in sections 2.4 and 2.5.

2.4 Groundwater Chemistry

Groundwater chemistry can affect groundwater movement by changing the density or the viscosity of the groundwater. These changes are likely to be dominated by the presence of dissolved salt. This is because salt is the only mineral normally present in rocks in sufficient quantities and with a sufficient solubility to be found in groundwater in concentrations significant enough to affect its physical properties. Salt is therefore normally the only dissolved mineral modelled by NAMMU. This approximation is not necessarily conservative, but is likely to be realistic in all cases of interest.

In NAMMU the density of the groundwater is generally modelled using a mass-fraction formulation:

$$\frac{1}{\rho_l} = \frac{c}{\rho_{c0}} + \frac{1-c}{\rho_0}\,. \tag{2.4}$$

However, the user can specify the relationship between the groundwater density and the concentration of total dissolved solids, in order to reflect conditions appropriate to a particular site.

In the current release of NAMMU, the viscosity of the fluid is generally assumed to be independent of the salt concentration. However, there is no fundamental difficulty in taking account of this effect. Cases in which this has been done have been treated in the past.
The model of the transport of salt by groundwater takes account of the same processes as that for radionuclide transport, i.e. advection, diffusion, hydrodynamic dispersion and anion exclusion. In the conditions prevailing at depth, sorption of the salt ions is not usually considered to be a significant effect.

In principle, the groundwater chemistry can affect the transport of radionuclides by modifying the solubility limit of the radionuclides, and by increasing or decreasing the amount of sorption that they undergo. These effects can be taken into account in a NAMMU model as follows.

For some radionuclides it can be anticipated that the concentration in the repository will be maintained at the solubility limit until sufficient radionuclide has been removed to allow the concentration to fall below the solubility limit, whence the repository concentration becomes inventory limited. The period of solubility limitation can be estimated, based on the groundwater flow rate through the repository (which can be estimated from the NAMMU model of the site), the repository volume accessible to the radionuclide and the radionuclide inventory. The migration of the radionuclide from the repository, taking account of solubility limitation can then be modelled in a two-stage NAMMU radionuclide transport calculation. In the first stage, which covers the time period of solubility limitation, the radionuclide concentration at the repository is maintained at the solubility limit. The second calculation then uses the results of the first as an initial condition.
In NAMMU, sorption is modelled by a linear equilibrium model, as described in section 2.6.5.

This simple model is effectively characterised by a parameter K_d, the sorption distribution coefficient. In the current release of NAMMU, K_d is simply specified as a constant for each hydrogeological unit and is not explicitly related to the calculated groundwater chemistry in the unit. However, if appropriate values of K_d are used, that take into account the prevailing groundwater chemistry in different rock units, then the effect of groundwater chemistry on sorption can be modelled fairly realistically.

2.5 Temperature / Heat

The principle effect of changes in temperature in the far field is to cause changes to the groundwater density and viscosity, which leads to changes in the groundwater movement. Changes in density as a result of temperature changes are usually no more than a few percent, for any temperature normally encountered in groundwater. The model used in NAMMU to simulate this change is to make the change in density equal to the product of the change in temperature and a constant called the coefficient of thermal expansion. This model may not be valid for large changes in temperature, but the resultant changes in fluid density are sufficiently small for this to be of little significance to the resulting groundwater movement and pressure.
Changes to the viscosity of the groundwater as a result of temperature changes are usually of more importance.

It is also possible that changes in temperature may affect the solubility and sorption of radionuclides. These effects are not modelled in the current release of NAMMU.

Temperature variations within the far field arise as a consequence of heat sources, and the transport of heat. Various sources of heat are potentially relevant, such as the natural radioactivity of the rock and the radiogenic heating of the repository itself. There are several ways in which these sources of heat can be represented in a NAMMU model. Regions of specified temperature or specified heat flux can be identified or distributed heat sources can be specified. The processes that result in the transport of heat are the same as or analogous to those that lead to the migration of radionuclides. However, one important difference is that heat energy can be conducted through the solid rock. In many low permeability environments, where the water velocities are low, conduction of heat through the solid rock is the most significant heat transport mechanism.

2.6 Radionuclide Transport

In the following subsections, the processes that can result in transport of dissolved radionuclides by groundwater are described in more detail. These processes can all be treated by NAMMU, albeit to different degrees of accuracy.

2.6.1 Advection

Advection is the process by which the dissolved radionuclides are transported simply by the displacement of the groundwater in rock pores or fractures. The advective flux, $\mathbf{F}_A$, of a radionuclide is related to the specific discharge, $\mathbf{q}$, (Equation (2.1)) by

$$\mathbf{F}_{\mathrm{A}} = \mathbf{q} N_{\alpha} . \tag{2.5}$$

Although $\mathbf{q}$ has units of velocity, the actual water velocity in the pores is rather larger because the flow only takes place in the pores rather than over the whole area of the porous medium. The average water velocity in the pores is

$$\mathbf{v} = \frac{\mathbf{q}}{\phi} . \tag{2.6}$$

In some rocks, some water is mobile and some water is immobile, and only the mobile water is directly considered in transport, so ϕ is the proportion of the rock volume taken up by mobile water, and is called the 'transport' or 'flowing' porosity. In fractured rocks, for example, it is often the case that the water in the fractures is mobile and water in the intact rock matrix is much less mobile.

2.6.2 Molecular Diffusion

Even when the driving forces are not sufficient for significant groundwater flow to occur, radionuclides will still migrate through the porewater as a result of molecular diffusion. The flux will be smaller than in free water, both because of the restricted area in the porous medium over which diffusion occurs and because of the tortuous nature of the pores. Fick's Law,

$$\mathbf{F}_{\mathrm{D}} = -D_i \nabla N_{\alpha} . \tag{2.7}$$

links the flux per unit surface area of porous medium, $\mathbf{F}_{\mathrm{D}}$, to the concentration gradient [16]. Here, the intrinsic diffusion coefficient, D_i, is less than the free water diffusion coefficient and is related to the latter by a scaling factor that depends on the porosity and tortuosity of the rock.
Molecular diffusion in free water is a well-understood process and Fick's law is generally accepted in the scientific community as a valid model of the process. Models of diffusion in the presence of a porous medium are generally based on the application of scaling factors to the fluxes obtained from Fick's law for diffusion in free water. The scaling factors represent the effects of the presence of the solid material and of the tortuous nature of the void spaces. The values of the scaling factors are based on the measurements of the migration of radionuclides in laboratory experiments.

2.6.3 Hydrodynamic Dispersion

Transport of a dissolved species through a porous medium does not simply involve movement along a single well-defined path in the direction of the local velocity. Various processes act to spread the radionuclide about such a path and these processes are collectively termed 'hydrodynamic dispersion'. The hydrogeological properties of the rocks at any site will exhibit variability on all length scales. As a result of this variability, different paths through the medium will have different path lengths and different travel times. This variability in the transport paths is what gives rise to the processes of hydrodynamic dispersion. Qualitatively, dispersion acts in a similar way to diffusion.

Detailed, explicit modelling of the heterogeneity of the rocks at all length scales and of the resulting dispersion of radionuclides is not always practicable. Effective parameters are therefore often used to represent this aspect of the behaviour of the system. In such cases, dispersion is usually represented by a diffusion-like term in the transport equation, with the dispersive flux taken to be proportional to the concentration gradient, by analogy with Fick's law [4]. Different amounts of dispersion are generally observed parallel to and perpendicular to the flow, and the dispersion coefficient is taken to be a tensor. It is usually modelled by a 'geometrical dispersivity', where the coefficient is the product of the velocity and a dispersion length [4]. The dispersion length is generally larger in the direction of flow than transverse to it. Using detailed models of heterogeneity, the dispersion lengths can be shown to be related to the length scale of heterogeneities in the medium [17, 18, 19].

Hydrodynamic dispersion is a very complex process, and the Fickian model is an approximation. In general, very careful choices of the parameters that are used in the Fickian model will be necessary in order to ensure that the model is fit for purpose, or at least conservative. The validity of the model for a particular case depends on the nature of the variability in the rock properties and the relationship between the distance travelled by the radionuclides and the length scale of the variability.

One case that has been extensively studied is that in which the variability in the logarithm of the permeability can be represented by a Gaussian model with a well-defined length scale. In this model the travel distance of interest ranges from values smaller than the length scale of the variability to values greater than the length scale of the variability. Several analytical studies of the dispersive behaviour to be expected in such cases have been performed [17, 18, 19]. The analyses are only valid for cases in which the variance of the log-permeability field is small (less than 1) and for the conditions of uniform mean flow in an infinite domain. Nevertheless, the analytical studies provide useful insights into the dispersion that is produced by the heterogeneity in the permeability field.

It is found that the dispersive flux is proportional to the concentration gradient, but that the dispersion coefficients are not constant, as assumed in the Fickian model, but depend on the distance travelled. The longitudinal dispersion coefficient, which characterises the dispersive spreading parallel to the mean flow direction, tends to a constant value, which for practical purposes is attained at distances equal to a few tens of the length scale of the variability itself. The length scale of the heterogeneity and the variance of the log-permeability determine the asymptotic value of the longitudinal dispersion coefficient. The transverse dispersion coefficients, which characterise the dispersive spreading transverse to the flow direction, tend to zero, so that, asymptotically, the transverse dispersion is not controlled by the heterogeneity but by the spreading process on a smaller scale than is represented in the Gaussian model, such as molecular diffusion.

In most cases the variance of the log-permeability values for real rocks is greater than 1, so that the approximations made in the analytical studies are not strictly valid. In order to investigate the dispersion produced by the heterogeneity in such cases, numerical Monte-Carlo studies are performed. This means that numerical realisations of spatially correlated random fields are generated to represent the rock properties (generally the log-permeability). Numerical calculations of groundwater flow and particle transport are then performed in each realisation and the results for the particle movements are analysed in order to assess the dispersion produced by the heterogeneity in the permeability.

It is important to ensure that the random fields that are generated have the intended statistical structure. A detailed discussion of this issue lies outside the scope of this document but it is noted that this requires a very careful choice of the parameters in the method that is used to generate the random field (see e.g. [20]). If the permeability field is not generated with sufficient accuracy, then the dispersive behaviour that is obtained from calculations of flow and transport through the field will also be inaccurate. This was demonstrated in a Monte-Carlo study [21] in which many realisations of a permeability field with a relatively small variance were generated.

Calculations of groundwater flow and particle transport through the realisations of the permeability field were performed using NAMMU. The variance of the permeability field had been chosen to be small and the conditions of the flow and transport calculations were set so that the analytical solution for the dispersive spreading of the particles [17, 18] was valid. The results from the NAMMU calculations were compared with the analytical solution in order to assess the accuracy of the numerical calculations. It was found that the results of the Monte-Carlo study were very sensitive to the choice of the parameters used in the method used to generate the random fields. With an appropriate choice of parameters, good agreement could be obtained between the numerical and analytical results. This builds confidence in the numerical method and its use in circumstances in which the analytical approximations are not valid.

It should be noted that this study also provides a useful and quite stringent test of the groundwater flow and particle transport algorithms used in NAMMU. The fact that good agreement could be obtained between the analytical and numerical results for the dispersion of the particles indicates

that NAMMU had provided an accurate solution for the groundwater velocities in a case with a heterogeneous permeability field. This case therefore also builds confidence in the validity of NAMMU.

NAMMU has also been used to perform a Monte-Carlo study of flow and transport in a heterogeneous permeability field at a real potential repository site [22]. In that case, the statistics of the transmissivity field for the heterogeneous formation were inferred from borehole data at the site. The variance of the log-transmissivity was much greater than 1. The calculations were used to investigate a number of issues associated with the heterogeneity, for example, the impact of different levels of site investigation on the uncertainties in the calculated travel times from the repository.

The validity of the Fickian model of dispersion and the investigation of alternative approaches, including models in which the heterogeneity is modelled explicitly are very active areas of research in many national programmes (e.g. [23, 24, 25]). An appropriate and consistent treatment of heterogeneity on all length scales is an important aspect of performance assessment calculations (e.g. [26]).

2.6.4 Rock-Matrix Diffusion

The process of rock-matrix diffusion is potentially significant in many fractured rocks [6, 27]. In such cases, most of the groundwater flow takes place through a network of interconnected fractures, which comprise the 'flowing porosity'. In addition to the flowing porosity, the rock matrix is itself porous. Radionuclides can be transported from the pore water in the flowing porosity into the relatively immobile water in the low permeability rock matrix by diffusion. This process retards the progress of radionuclides. For non-sorbed radionuclides, it is a retardation mechanism, because they would otherwise be transported at a velocity determined by the water velocity and the accessible flowing porosity. For sorbed radionuclides, rock-matrix diffusion also gives access to additional sorption sites away from fractures. Thus rock-matrix diffusion increases radionuclide travel times; it also acts as an additional dispersive process, since radionuclides that have diffused into the rock matrix can diffuse back out over a period of time, increasing the spread of travel times between early and late arrivals.

Understanding of the process of rock-matrix diffusion is developed both by a programme of laboratory experimental work [23] and by studies of rock-matrix diffusion in natural systems. A number of approaches exist which allow this effect to be modelled realistically, including the MATDIF module of NAMMU [28].

2.6.5 Sorption

The migration of radionuclides through the geosphere is retarded by a number of geochemical processes, some of which are grouped together under the label 'sorption'. 'Sorption' is defined as a set of processes, excluding the formation of a discrete phase, by which radionuclides are partitioned between the solution and a solid surface. Of these processes, ion exchange and surface complexation appear to be the dominant processes of relevance in the geosphere. Both of these processes are observed in natural geochemical systems [23]. Both ion exchange and surface complexation are rapid processes, with equilibrium being established in a timescale accessible through laboratory experiments. In both cases, a relationship exists between the equilibrium concentration of radionuclide in solution and the concentration adsorbed on the mineral surface. At its simplest, and especially at the very low aqueous concentrations that are relevant for radionuclide transport calculations, it can be assumed that the ratio of 'adsorbed' to 'dissolved' radionuclide is constant and independent of the concentration of radionuclide in the system. This concept is termed 'linear sorption' and is a widely used model of these processes. Radionuclides can also be removed from solution by the incorporation of the radionuclide in the mineral structure.

In the model implemented in NAMMU, the geochemical retardation of radionuclides in the geosphere is represented as a simple linear sorption process characterised by a sorption distribution coefficient, K_d. The extent of sorption is measured in laboratory experiments that are carried out over timescales of the order of months or years in which equilibrium conditions are

attained. It is therefore reasonable to assume that a similar equilibrium will be attained during the longer timescales of radionuclide transport through the geosphere. The assumption of equilibrium will be reasonable provided that the timescale of any transients associated with the sorption process is much less than the timescale for radionuclide transport by advection and dispersion.

The linear K_d approach to representing sorption is a simplification, since, for example, the experimentally measured sorption distribution coefficients are commonly observed to decrease at higher aqueous radionuclide concentrations. However, K_d values may be appropriately chosen so that the extent of sorption is adequately approximated over the concentration range of interest. Research in the Nirex Safety Assessment Research Programme (NSARP) is directed at confirming and increasing confidence that the linear K_d approach is an appropriate representation for the radionuclides of interest [23].

2.6.6 Anion Exclusion

Experimental observations indicate that the porosity of the rock matrix that is accessible by diffusion to some anionic species is less than that accessible to neutral species or to cations. This is believed to be the result of charge effects. Anions are excluded from a portion of the porosity owing to the effect of negatively charged mineral surfaces [23]. This effect can be represented in NAMMU models by using a simple exclusion factor, which is equivalent to the fraction of the porosity that is accessed.

2.6.7 Effect of Organic Complexants

Organic complexants may be present in the geosphere around the repository, although their concentrations will be diluted within the geosphere and they may undergo microbial degradation. The effect of the presence of organic complexants is to reduce sorption. A programme of work in the NSARP has been undertaken to address the impact of such organic complexants [23]. The effect of organic complexants can be represented in a NAMMU model by multiplying the sorption distribution coefficient that would be considered appropriate in the absence of organic complexants by a sorption reduction factor.

2.6.8 Radioactive Decay and Ingrowth

The processes of radioactive decay and ingrowth from parent radionuclides also affect radionuclide concentrations. Models of these processes have the status of widely accepted physical laws. Representations of radioactive decay are easily implemented as a sink term in NAMMU models of radionuclide transport. Accurate representation of the processes of decay and ingrowth for several members of a decay chain may require the simultaneous solution of models of radionuclide transport for several radionuclides. NAMMU can treat chains with up to 48 members (depending on the options selected) in this way.

3 Mathematical Representation of Physical Processes

3.1 Conceptual Models

In this section we describe the conceptual models used in NAMMU. Before describing the various models, it is necessary to consider what a conceptual model means. For the purposes of this report we will use the definition put forward by Olsson et al. [29]. According to these authors the ingredients that make up a conceptual model are: the processes modelled, the geometric framework, the parameters required by the model, the method of spatial assignment of the parameters and the boundary and initial conditions required by the model.

NAMMU is a very flexible and powerful tool that can be used to model a wide range of flow and transport phenomena in porous media. Any model of a system that is constructed using NAMMU will contain all of the elements of a conceptual model identified by Olsson et al. [29]. However, it is useful to present these ingredients of the conceptual model in two parts. This is because one of the powerful features of the NAMMU program is the way in which the full flexibility of the geometric framework and the method of spatial assignment of the parameters are available to all of the models of physical processes that are implemented in NAMMU. This means, for example, that many different types of finite-element discretisation can be used to represent the different physical processes that can be modelled with NAMMU. Thus, for example, if it were appropriate, different element types could be used in the solution of the groundwater flow and the radionuclide transport equations for a particular system.

In section 3.2, the geometric framework, the method of spatial assignment of the parameters and some general features of the boundary conditions are described. In section 3.3 the physical processes that can be represented, the parameters that must be specified and the initial and boundary conditions required for each model available in NAMMU are presented. The mathematical description of the processes is presented in terms of the governing equations. The scientific basis for these conceptual models has been described in section 2. The numerical techniques used in NAMMU are summarised in section 4.3.

3.2 Common Features

3.2.1 Geometric Framework

The spatial region represented in a NAMMU model is discretised using the finite-element method. The finite-element mesh used is specified either by importing a mesh from a file or defined explicitly by a patch grid. A patch is a simple region bounded by points in one dimension, straight sides in two dimensions, or planar surfaces in three dimensions. One-dimensional patches are lines, two-dimensional patches may be triangles or quadrilaterals and three-dimensional patches may be triangular prisms, hexahedra or tetrahedra. Patches of different dimensions can be mixed within a single model, for example to represent features such as boreholes by one-dimensional patches within a two- or three-dimensional model. Patches are subdivided into elements and can have different numbers of elements in each direction. The size of the elements within a patch may be constant, or may be assigned arbitrarily. All elements within a single patch are of the same rock type.

The geometric parameters required to define a grid of patches are the co-ordinates of the corners of each patch, the topology of the patches, and the number of elements and their relative sizes within each patch. The rock type of each patch must also be specified.

Fault zones are also represented either explicitly by patches, with rock types specified in the same way as for ordinary patches, or implicitly by using the Implicit Fracture Zone (IFZ) method to modify the properties of finite-elements intersected by one or more fracture zones. In the explicit case, the fault zones may be defined by specifying a fault line or plane and a fault width vector. In the IFZ

case 3D fault zones are defined by a polygon of coplanar points together with a width and properties for the rock within the fracture zone. Both facilities enable the position and thickness of a fault zone to be modified with the minimum of effort.

If required, meshes comprising elements with curved sides in two dimensions, or curved faces in three dimensions can be generated. The curved elements are derived from planar elements by use of a polynomial mapping function. Grids comprising curved elements may be defined by specifying the co-ordinates of the corners of each element, its mapping function, and its rock type.

3.2.2 Spatial Assignment of Parameters

Physical parameters of the geological regions in the NAMMU model can be specified as constants, or more usually as constants for a given rock type. Stochastic modelling can be performed by defining permeability as a heterogeneous variable in terms of an exponential variogram with specified mean and standard deviation for each rock type. In this case, and in the case where IFZ is used to model fracture zones, permeability and porosity are calculated for each finite-element and stored in a file. It is also possible for these parameters to be specified as arbitrary functions of space, and sometimes as functions of other parameters, or of variables such as pressure and temperature. This is done through the use of user-supplied FORTRAN subroutines, which can be interfaced to the program at appropriate places.

In summary, 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, according to relationships 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.

3.2.3 Boundary Conditions

The basic types of boundary conditions available in NAMMU consist of specified value and specified flux conditions for the variables. The boundary conditions may be constant, or spatially varying. Specified value conditions may be constant in time, or can be varying in time for transient calculations. More complex boundary conditions that are non-linear, in that variables or fluxes depend on variables themselves are possible. One example of such a boundary condition is the Recharge-Discharge condition that is a generalised flux condition with the magnitude and direction of flux depending on the difference between the height of the watertable and the topographic height. The default (i.e. if nothing is set explicitly) boundary condition for each variable is zero flux. The following section describes the types of boundary conditions that are available for each physical model in NAMMU. In addition to the conditions described here, more generalised boundary conditions can be specified through user-supplied FORTRAN subroutines. These allow the value of a variable or its flux to be specified as a function of position and the values of other variables at the boundary.

3.3 Specific Features

The following subsections describe the physical processes, the parameters required, and the initial and boundary conditions for the various equations solved for each model available in NAMMU. Also, the flux term for each equation used is given. This flux is the quantity that is specified by imposing a specified-flux type of boundary condition.

3.3.1 Groundwater Flow

3.3.1.1 Physical Processes

Groundwater flow in a porous medium is modelled in terms of Darcy's law (see section 2.2),

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}\nabla P^{\mathrm{R}}, \tag{3.1}$$

and the equation of continuity,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0. \tag{3.2}$$

These are combined to form a single second-order equation for the residual pressure,

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.\left(\rho_l \frac{\mathbf{k}}{\mu}\nabla P^{\mathrm{R}}\right) = 0, \tag{3.3}$$

and the flux for this pressure equation is

$$F_P = \rho_l \mathbf{q}.\mathbf{n}. \tag{3.4}$$

The residual pressure, P^R, is related to the total pressure, P^T, by the expression

$$P^R = P^T + \rho_0 g(z - z_0). \tag{3.5}$$

The hydraulic head, h, is related to the residual pressure by

$$h = \frac{P^R}{\rho_0 g}. \tag{3.6}$$

3.3.1.2 Parameters Required

The parameters required are as follows:

Parameter	Symbol/definition	Comments
Permeability	$\mathbf{k}$	A symmetric tensor. Can be constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic.
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position and pressure.
Fluid density	$\rho_l = \rho_0\left(1 + \alpha\left(P^T - P_0^T\right)\right)$	α and P_0^T are constants.
Fluid viscosity	μ	A constant.

3.3.1.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed pressure.

The following boundary conditions can be specified:

- Prescribed pressure;
- Prescribed flux of fluid;
- Non-linear recharge-discharge (see below);
- Hydrostatic for vertical sides (see below);
- Point sinks for abstraction/injection at boreholes.

For the non-linear recharge-discharge condition the discharge of groundwater varies in magnitude and sign as the difference between the watertable, head, and the topographic height, z, such that

$$F_P = \begin{cases} \rho_l I\,(h - z)/L, & h > z - L \\ -\rho_l I, & h \le z - L \end{cases}, \tag{3.7}$$

for a maximum potential infiltration I. The arbitrary transition thickness, L, is usually set to the soil thickness.

The hydrostatic boundary condition is zero vertical flow:

$$q_z = 0\,. \tag{3.8}$$

3.3.1.4 2D Areal Groundwater Flow

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 (3.2). The resulting equation is

$$\nabla.(b\rho_l \mathbf{q}) = Q\,. \tag{3.9}$$

Here, the effective thickness of the aquifer, b, is given by

$$b = \begin{cases} z_t - z_b, & \dfrac{P^R}{\rho_l g} \geq z_t \ \text{(confined aquifer)} \\ \dfrac{P^R}{\rho_l g} - z_b, & \dfrac{P^R}{\rho_l g} < z_t \ \text{(unconfined aquifer)} \end{cases}. \tag{3.10}$$

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

$$Q = \frac{\rho_l k_v}{\mu}\left(\frac{\rho_l g z_s - P^R}{z_s - z_t}\right). \tag{3.11}$$

3.3.2 Groundwater Flow and Heat Transport

3.3.2.1 Physical Processes

NAMMU can calculate the non-linear flow due to coupled groundwater flow and heat transport, where the fluid density is dependent upon the temperature. This is modelled using Darcy's law,

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}\left(\nabla P^R - (\rho_l - \rho_0)\mathbf{g}\right), \tag{3.12}$$

the continuity equation,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0\,, \tag{3.13}$$

and the heat transport equation [3],

$$(\rho c)_a \frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q}.\nabla T - \Gamma_a \nabla^2 T = H\,. \tag{3.14}$$

The first two of these equations are combined to form a single second-order equation for the residual pressure,

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.\left(\rho_l \frac{\mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right)\right) = 0\,. \tag{3.15}$$

The fluxes for the pressure and temperature equations are

$$F_P = \rho_l \mathbf{q}.\mathbf{n}\,, \tag{3.16}$$

$$F_T = -\Gamma_a \nabla T.\mathbf{n}\,. \tag{3.17}$$

3.3.2.2 Parameters Required

The parameters required are as follows:

Parameter	Symbol/definition	Comments
Permeability	$\mathbf{k}$	A symmetric tensor. Can be constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic.
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position, pressure and temperature.
Fluid density	$\rho_l = \rho_0\left(1 + \alpha\left(P^T - P_0^T\right) - \beta\left(T - T_0\right)\right)$	α, β, P_0^T and T_0 are constants.
Fluid viscosity	$\mu = \mu_0 \mathrm{e}^{-\delta_1 (T - T_0)}$	T_0, μ_0 and δ_1 are constants.
Average thermal conductivity of the rock and fluid	$\Gamma_a = \phi\Gamma_l + (1-\phi)\Gamma_s$	Approximated by the thermal conductivity of the rock, Γ_s. Can be constant, or constant for a given rock type.
Average heat capacity of the rock and fluid	$(\rho c)_a = \phi\rho_l c_l + (1-\phi)\rho_s c_s$	Approximated by the heat capacity of the rock, $\rho_s c_s$. c_l is a constant. ρ_s can be constant, or constant for a given rock type. c_s can be constant, or constant for a given rock type.

3.3.2.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed pressure;
- Prescribed temperature.

The following boundary conditions can be specified:

- Prescribed pressure;
- Prescribed flux of fluid;
- Hydrostatic for vertical sides (see section 3.3.1);
- Point sinks for abstraction/injection at boreholes;
- Prescribed temperature;
- Prescribed heat flux.

3.3.3 Unsaturated Groundwater Flow

3.3.3.1 Physical Processes

This is modelled in terms of a modified version of Darcy's law (see section 2.2),

$$\mathbf{q} = -\frac{k_r \mathbf{k}}{\mu} \nabla P^{\mathrm{R}}, \tag{3.18}$$

and the equation of continuity,

$$\frac{\partial}{\partial t}(\phi S \rho_l) + \nabla.(\rho_l \mathbf{q}) = 0. \tag{3.19}$$

These are combined to form a single second-order equation for the residual pressure,

$$\frac{\partial}{\partial t}(\phi S \rho_l) - \nabla.\left(\rho_l \frac{k_r \mathbf{k}}{\mu} \nabla P^{\mathrm{R}}\right) = 0, \tag{3.20}$$

and the flux for this pressure equation is given by

$$F_P = \rho_l \mathbf{q}.\mathbf{n}. \tag{3.21}$$

3.3.3.2 Parameters Required

The parameters required are as follows:

Parameter	Symbol/definition	Comments
Permeability	$\mathbf{k}$	A symmetric tensor. Can be constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic.
Relative permeability	k_r	An arbitrary function of saturation, which is related to the total pressure through a specified capillary pressure curve (see below).
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position and pressure.

Parameter	Symbol/definition	Comments
Fluid density	$\rho_l = \rho_0\left(1+\alpha\left(P^T - P_0^T\right)\right)$	α and P_0^T are constants.
Fluid viscosity	μ	A constant.

In NAMMU, the way in which the permeability varies with the saturation, S, is specified using various empirical models for the relative permeability, k_r, and saturation, S.
The Brooks and Corey model is

$$k_r = \left(\frac{S - S_{res}}{1 - S_{res}}\right)^{(2+3\gamma)/\gamma}, \tag{3.22}$$

$$S = S_{res} + (1 - S_{res})\left(\frac{P_E}{-P^T}\right)^{\gamma}. \tag{3.23}$$

The Van Genuchten model is

$$k_r = \sqrt{S_\alpha}\left[1 - \left(1 - S_\alpha{}^{\gamma/(\gamma-1)}\right)^{(\gamma-1)/\gamma}\right]^2, \tag{3.24}$$

$$S = S_{res} + (1 - S_{res})\left(\frac{1}{1 + \left(-P^T/P_E\right)^{\gamma}}\right)^{(\gamma-1)/\gamma}, \tag{3.25}$$

where S_α is given by

$$S_\alpha = \frac{S - S_{res}}{1 - S_{res}}. \tag{3.26}$$

The NAMMU default model for k_r is

$$k_r = \begin{cases} \dfrac{A_{KR}}{B_{KR} + (-P^T)^{S_{KR}}}, & P^T < 0 \\ 1, & P^T \geq 0 \end{cases}. \tag{3.27}$$

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

$$S = \begin{cases} \dfrac{A_{PC}}{B_{PC} + (-P^T)^{S_{PC}}}, & P^T < 0 \\ 1, & P^T \geq 0 \end{cases}. \tag{3.28}$$

A_{KR}, B_{KR}, S_{KR}, A_{PC}, B_{PC} and S_{PC} are constant for a given rock type.

3.3.3.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed pressure.

The following boundary conditions can be specified:

- Prescribed pressure;
- Prescribed flux of fluid;
- Non-linear recharge-discharge (see section 3.3.1);
- Hydrostatic for vertical sides (see section 3.3.1);
- Point sinks for abstraction/injection at boreholes.

3.3.4 Unsaturated Groundwater Flow and Heat Transport

3.3.4.1 Physical Processes

This is modelled using a modified version of Darcy's law,

$$\mathbf{q} = -\frac{k_r \mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right), \tag{3.29}$$

the equation of continuity,

$$\frac{\partial}{\partial t}(\phi S \rho_l) + \nabla.(\rho_l \mathbf{q}) = 0\,, \tag{3.30}$$

and the heat transport equation,

$$(\rho c)_a \frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q}.\nabla T - \Gamma_a \nabla^2 T = H\,. \tag{3.31}$$

The first two of these equations are combined to form a single second-order equation for the residual pressure,

$$\frac{\partial}{\partial t}(\phi S \rho_l) - \nabla.\left(\rho_l \frac{k_r \mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right)\right) = 0\,. \tag{3.32}$$

The fluxes for the pressure and temperature equations are

$$F_P = \rho_l \mathbf{q}.\mathbf{n}\,, \tag{3.33}$$

$$F_T = -\Gamma_a \nabla T.\mathbf{n}\,. \tag{3.34}$$

3.3.4.2 Parameters Required

The parameters required are as follows:

Parameter	Symbol/definition	Comments
Permeability	$\mathbf{k}$	A symmetric tensor. Can be constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic.
Relative permeability	k_r	An arbitrary function of saturation, which is related to the total pressure through a specified capillary pressure curve (see section 3.3.3).
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position, pressure and temperature.
Fluid density	$\rho_l = \rho_0\left(1 + \alpha\left(P^T - P_0^T\right) - \beta\left(T - T_0\right)\right)$	α, β, P_0^T and T_0 are constants.
Fluid viscosity	$\mu = \mu_0 \mathrm{e}^{-\delta_1(T-T_0)}$	T_0, μ_0 and δ_1 are constants.
Average thermal conductivity of the rock and fluid	$\Gamma_a = \phi\Gamma_l + (1-\phi)\Gamma_s$	Approximated by the thermal conductivity of the rock, Γ_s. Can be constant, or constant for a given rock type.
Average heat capacity of the rock and fluid	$(\rho c)_a = \phi\rho_l c_l + (1-\phi)\rho_s c_s$	Approximated by the heat capacity of the rock, $\rho_s c_s$. c_l is a constant. ρ_s can be constant, or constant for a given rock type. c_s can be constant, or constant for a given rock type.

3.3.4.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed pressure;
- Prescribed temperature.

The following boundary conditions can be specified:

- Prescribed pressure;
- Prescribed flux of fluid;
- Hydrostatic for vertical sides (see section 3.3.1);
- Point sinks for abstraction/injection at boreholes;
- Prescribed temperature;
- Prescribed heat flux.

3.3.5 Radionuclide Transport

3.3.5.1 Physical Processes

This is modelled using the following equation [3, 4, 5, 6],

$$\frac{\partial}{\partial t}(\phi R_\alpha N_\alpha) + \mathbf{q}.\nabla N_\alpha - \nabla.(\phi \mathbf{D}_\alpha \nabla N_\alpha) = -\lambda_\alpha \phi R_\alpha N_\alpha + \lambda_{\alpha-1}\phi R_{\alpha-1} N_{\alpha-1} + \phi f_\alpha . \quad (3.35)$$

Here, the subscript $\alpha-1$ is used to indicate the parent nuclide of nuclide α.

Normally, since the groundwater flow is not coupled to the radionuclide transport, $\mathbf{q}$ will be calculated from an initial groundwater flow calculation.

The flux for the nuclide equation is

$$F_{N_\alpha} = (\mathbf{q} N_\alpha - \phi \mathbf{D}_\alpha \nabla N_\alpha).\mathbf{n} . \quad (3.36)$$

3.3.5.2 Parameters Required

The parameters required are as follows:

Parameter	Symbol/definition	Comments
Porosity	$\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position and pressure.
Darcy velocity	$\mathbf{q}$	Obtained from a previous NAMMU calculation.
Retardation factors for each nuclide	$R_\alpha = 1 + \frac{(1-\phi)}{\phi} K_{d,\alpha}$	$K_{d,\alpha}$ is constant for a given rock type and nuclide. (Note Nammu's definition of K_d differs from the literature definition: i.e. Nammu K_d = rock density multiplied by literature K_d)
Decay constants for each nuclide	λ_α	A constant for each nuclide.
Dispersion tensor for each nuclide	$\mathbf{D}_\alpha = \frac{D_{m\alpha}}{\tau}\delta_{ij} + \alpha_{T\alpha} v \delta_{ij} + (\alpha_{L\alpha} - \alpha_{T\alpha})\frac{v_i v_j}{v}$	$D_{m\alpha}$ is constant for each nuclide. τ is constant for a given rock type. $\alpha_{L\alpha}$ and $\alpha_{T\alpha}$ are constant for a given rock type. v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \mathbf{q}/\phi$.
Source term for each nuclide	f_α	A function of position and time.

3.3.5.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed concentration of each nuclide.

The following boundary conditions can be specified:

- Prescribed concentration of each nuclide;
- Prescribed flux of each nuclide;
- Zero dispersive flux for each nuclide (see below).

The zero dispersive flux condition is basically an outflow condition

$$F_{N_\alpha} = N_\alpha \mathbf{q}.\mathbf{n}\,. \tag{3.37}$$

This condition is realistic for surfaces where flow is known to be discharging from the model. Where there is a mixture of recharge and discharge then the boundary condition can be generalised to

$$F_{N_\alpha} = \begin{cases} (N_\alpha - N_{\alpha 0})\mathbf{q}.\mathbf{n}/\varepsilon, & \mathbf{q}.\mathbf{n} \le 0 \\ N_\alpha \mathbf{q}.\mathbf{n}, & \mathbf{q}.\mathbf{n} > 0 \end{cases}. \tag{3.38}$$

This is effectively a mixed boundary condition such that $N_\alpha = N_{\alpha 0}$ at inflows and an outflow condition is applied elsewhere.

3.3.6 Radionuclide Transport in Unsaturated Flow

3.3.6.1 Physical Processes

This is modelled using the following equation [3, 4, 5, 6],

$$\frac{\partial}{\partial t}(\phi S R_\alpha N_\alpha) + \mathbf{q}.\nabla N_\alpha - \nabla.(\phi S \mathbf{D}_\alpha \nabla N_\alpha) = -\lambda_\alpha \phi S R_\alpha N_\alpha + \lambda_{\alpha-1}\phi S R_{\alpha-1} N_{\alpha-1} + \phi S f_\alpha\,. \tag{3.39}$$

Here, the subscript $\alpha-1$ is used to indicate the parent nuclide of nuclide α.

Normally, since the groundwater flow is not coupled to the radionuclide transport, $\mathbf{q}$ will be calculated from an initial unsaturated groundwater flow calculation.

The flux for the nuclide equation is

$$F_{N_\alpha} = (\mathbf{q}N_\alpha - \phi S \mathbf{D}_\alpha \nabla N_\alpha).\mathbf{n}\,. \tag{3.40}$$

3.3.6.2 Parameters Required

The parameters required are as follows:

Parameter	Symbol/definition	Comments
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position and pressure.
Darcy velocity	$\boldsymbol{q}$	Obtained from a previous NAMMU calculation.
Retardation factors for each nuclide	$R_\alpha = S + \frac{(1-\phi)}{\phi} K_{d,\alpha}$	$K_{d,\alpha}$ is constant for a given rock type and nuclide. (Note Nammu's definition of K_d differs from the literature definition: i.e. Nammu K_d = rock density multiplied by literature K_d)
Decay constants for each nuclide	λ_α	A constant for each nuclide.
Dispersion tensor for each nuclide	$\mathbf{D}_\alpha = \frac{D_{m\alpha}}{\tau}\delta_{ij} + \alpha_{T\alpha} v \delta_{ij} + (\alpha_{L\alpha} - \alpha_{T\alpha})\frac{v_i v_j}{v}$	$D_{m\alpha}$ is constant for each nuclide. τ is constant for a given rock type. $\alpha_{L\alpha}$ and $\alpha_{T\alpha}$ are constant for a given rock type. v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \mathbf{q}/\phi$.
Source term for each nuclide	f_α	A function of position and time.

3.3.6.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed concentration of each nuclide.

The following boundary conditions can be specified:

- Prescribed concentration of each nuclide;
- Prescribed flux of each nuclide;
- Zero dispersive flux for each nuclide (see section 3.3.5).

3.3.7 Coupled Groundwater Flow and Solute Transport

3.3.7.1 Physical Processes

NAMMU can calculate the non-linear flow due to coupled groundwater flow and solute transport, where the fluid density is strongly dependent upon the concentration of the solute. This is modelled using Darcy's law,

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right), \tag{3.41}$$

the continuity equation,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0\,, \tag{3.42}$$

and the advection-dispersion equation,

$$\frac{\partial}{\partial t}(\phi\rho_l c) + \nabla.(\rho_l \mathbf{q} c) = \nabla.(\phi\rho_l \mathbf{D}\nabla c)\,. \tag{3.43}$$

The first two of these equations are combined to form a single second-order equation for the residual pressure,

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.\left(\rho_l \frac{\mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right)\right) = 0\,. \tag{3.44}$$

The fluxes for the pressure and concentration equations are

$$F_P = \rho_l \mathbf{q}.\mathbf{n}\,, \tag{3.45}$$

$$F_C = (\rho_l \mathbf{q} c - \phi\rho_l \mathbf{D}\nabla c).\mathbf{n}\,. \tag{3.46}$$

3.3.7.2 Parameters Required

The parameters required in this case are as follows:

Parameter	Symbol/definition	Comments
Permeability	$\mathbf{k}$	A symmetric tensor. Can be constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic.
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\frac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position and pressure.
Dispersion tensor	$\mathbf{D} = \frac{D_m}{\tau}\delta_{ij} + \alpha_T v\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{v}$	D_m is constant. τ is constant for a given rock type. α_L and α_T are constant for a given rock type. v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \mathbf{q}/\phi$.
Fluid density	ρ_l (defined below)	α, α_c, ρ_0, ρ_{c0}, and P_0^T are constants.
Fluid viscosity	μ	A constant.

The fluid density in the above table is given by

$$\frac{1}{\rho_l} = \frac{1-c}{\rho_0\left(1+\alpha\left(P^T - P_0^T\right)\right)} + \frac{c}{\rho_{c0}\left(1+\alpha_c\left(P^T - P_0^T\right)\right)}, \tag{3.47}$$

3.3.7.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed pressure;
- Prescribed concentration of solute.

The following boundary conditions can be specified:

- Prescribed pressure;
- Prescribed flux of fluid;
- Non-linear recharge-discharge (see section 3.3.1);
- Hydrostatic for vertical sides (see section 3.3.1);
- Point sinks for abstraction/injection at boreholes;
- Prescribed concentration of solute;
- Prescribed flux of solute;
- Zero dispersive flux for solute (see below).

The zero dispersive flux condition is basically an outflow condition

$$F_C = \rho_l c \mathbf{q}.\mathbf{n}\,. \tag{3.48}$$

This condition is realistic for surfaces where flow is known to be discharging from the model. Where there is a mixture of recharge and discharge then the boundary condition can be generalised to

$$F_C = \begin{cases} \rho_l (c - c_0)\mathbf{q}.\mathbf{n}/\varepsilon, & \mathbf{q}.\mathbf{n} \le 0 \\ \rho_l c \mathbf{q}.\mathbf{n}, & \mathbf{q}.\mathbf{n} > 0 \end{cases}, \tag{3.49}$$

This is effectively a mixed boundary condition such that $c = c_0$ at inflows and an outflow condition is applied elsewhere.

3.3.8 Coupled Groundwater Flow, Solute Transport and Heat Transport

3.3.8.1 Physical Processes

NAMMU can calculate the non-linear flow due to coupled groundwater flow, solute transport and heat transport, where the fluid density is strongly dependent upon the concentration of the solute and upon the temperature. This is modelled using Darcy's law,

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right), \tag{3.50}$$

the continuity equation,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0\,, \tag{3.51}$$

the advection-dispersion equation,

$$\frac{\partial}{\partial t}(\phi\rho_l c) + \nabla.(\rho_l \mathbf{q}\mathrm{c}) = \nabla.(\phi\rho_l \mathbf{D}\nabla c), \tag{3.52}$$

and the heat transport equation [3],

$$(\rho c)_a \frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q}.\nabla T - \nabla.(\mathbf{D}'\nabla T) = H\,. \tag{3.53}$$

The first two of these equations are combined to form a single second-order equation for the residual pressure,

$$\frac{\partial}{\partial \mathrm{t}}(\phi\rho_l) - \nabla.\left(\rho_l \frac{\mathbf{k}}{\mu}\left(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}\right)\right) = 0\,. \tag{3.54}$$

The fluxes for the pressure, concentration and temperature equations are

$$F_P = \rho_l \mathbf{q}.\mathbf{n}\,, \tag{3.55}$$

$$F_C = \left(\rho_l \mathbf{q} c - \phi \rho_l \mathbf{D} \nabla c\right).\mathbf{n}\,, \tag{3.56}$$

$$F_T = -\mathbf{D}' \nabla T.\mathbf{n}\,. \tag{3.57}$$

3.3.8.2 Parameters Required

The parameters required in this case are as follows:

Parameter	Symbol/definition	Comments
Permeability	$\mathbf{k}$	A symmetric tensor. Can be constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic.
Porosity	$\phi = \phi_0 + \left(P^T - P_0^T\right)\dfrac{d\phi}{dP^T}$	P_0^T is a constant. ϕ_0 and $d\phi/dP^T$ can be constant, or constant for a given rock type, or can be arbitrary functions of position, pressure and temperature.
Dispersion tensor	$\mathbf{D} = \dfrac{D_m}{\tau}\delta_{ij} + \alpha_T v \delta_{ij} + (\alpha_L - \alpha_T)\dfrac{v_i v_j}{v}$	D_m is constant. τ is constant for a given rock type. α_L and α_T are constant for a given rock type. v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \mathbf{q}/\phi$.
Fluid density	ρ_l (defined below)	α, α_c, β, β_c, ρ_0, ρ_{c0}, P_0^T, and T_0 are constants.
Fluid viscosity	$\mu = \mu_0 \mathrm{e}^{-\delta_1 (T - T_0)}$	T_0, μ_0 and δ_1 are constants.
Heat dispersion tensor	$\mathbf{D}' = \Gamma_a \delta_{ij} + \phi\rho_l c_l \alpha_T' v \delta_{ij} + \phi\rho_l c_l (\alpha_L' - \alpha_T')\dfrac{v_i v_j}{v}$	α_L' and α_T' are constant for a given rock type. c_l is a constant. v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \mathbf{q}/\phi$.
Average thermal conductivity of the rock and fluid	$\Gamma_a = \phi\Gamma_l + (1-\phi)\Gamma_s$	Approximated by the thermal conductivity of the rock, Γ_s. Can be constant, or constant for a given rock type.
Average heat capacity of the rock and fluid	$(\rho c)_a = \phi\rho_l c_l + (1-\phi)\rho_s c_s$	Approximated by the heat capacity of the rock, $\rho_s c_s$. c_l is a constant. ρ_s can be constant, or constant for a given rock type. c_s can be constant, or constant for a given rock type.

The fluid density in the above table is given by

$$\frac{1}{\rho_l} = \frac{1-c}{\rho_0\left(1+\alpha\left(P^T - P_0^T\right) - \beta\left(T - T_0\right)\right)} + \frac{c}{\rho_{c0}\left(1+\alpha_c\left(P^T - P_0^T\right) - \beta_c\left(T - T_0\right)\right)}, \tag{3.58}$$

3.3.8.3 Initial and Boundary Conditions

The following initial conditions are required:

- Prescribed pressure;
- Prescribed concentration of solute;
- Prescribed temperature.

The following boundary conditions can be specified:

- Prescribed pressure;
- Prescribed flux of fluid;
- Hydrostatic for vertical sides (see section 3.3.1);
- Point sinks for abstraction/injection at boreholes;
- Prescribed concentration of solute;
- Prescribed flux of solute;
- Zero dispersive flux for solute (see section 3.3.7);
- Prescribed temperature;
- Prescribed heat flux.

4 Numerical Methods

4.1 Spatial Discretisation

4.1.1 Approach

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 domains that represent geological structures with several lithological units or 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 irregular shaped grids provides much more flexibility in accurately representing the subsurface flow capture area than is possible using the regular blocks of a simple finite-difference method. In particular triangular and tetrahedral elements allow unstructured meshes to be created.

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 in 2D;
- Bi-linear and bi-quadratic quadrilaterals in 2D;
- Linear and quadratic tetrahedra in 3D;
- Tri-linear and tri-quadratic prisms in 3D; and
- Tri-linear and tri-quadratic cuboids in 3D.

The library also includes variants of the so-called 'mixed elements' (see section 4.1.3). This provides considerable flexibility in representing the domain.

4.1.2 Grid Generation

Various facilities have been implemented in NAMMU to try to make generation of grids of finite elements as simple as possible. Grids can be created within NAMMU itself or imported from other packages via a formatted file. An interface to the grid generator FEMGEN (FEMGV) is supported. The principal approach used for generating grids within NAMMU is based on the concept of 'patches', which can be subdivided into a number of finite 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. 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. Figure 4-1, Figure 4-2 and Figure 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.

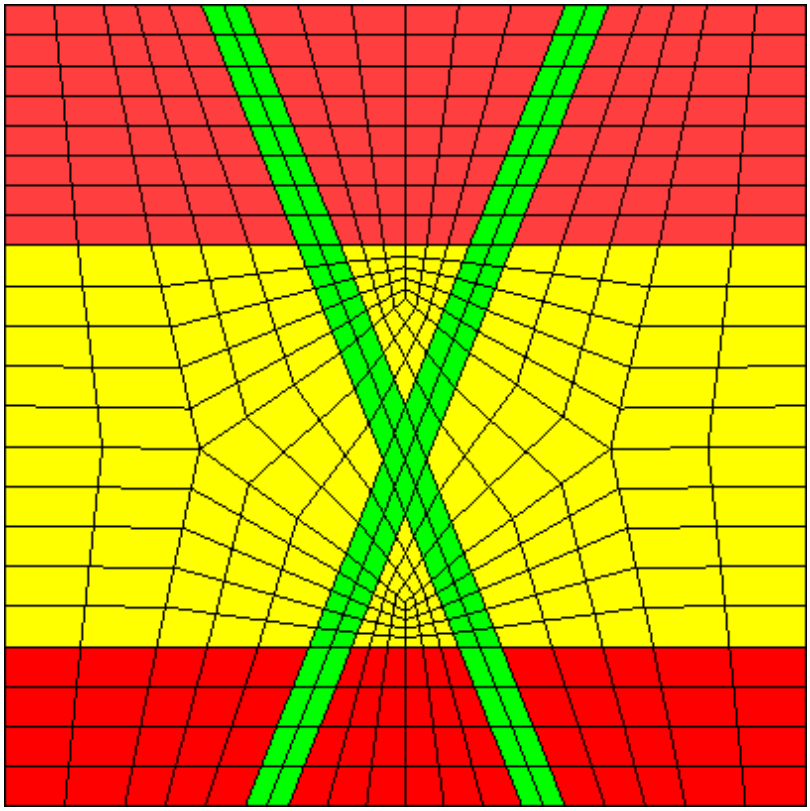

Figure 4-1 A simple 2D grid generated using polygons. The finite elements are coloured according to the rock type.

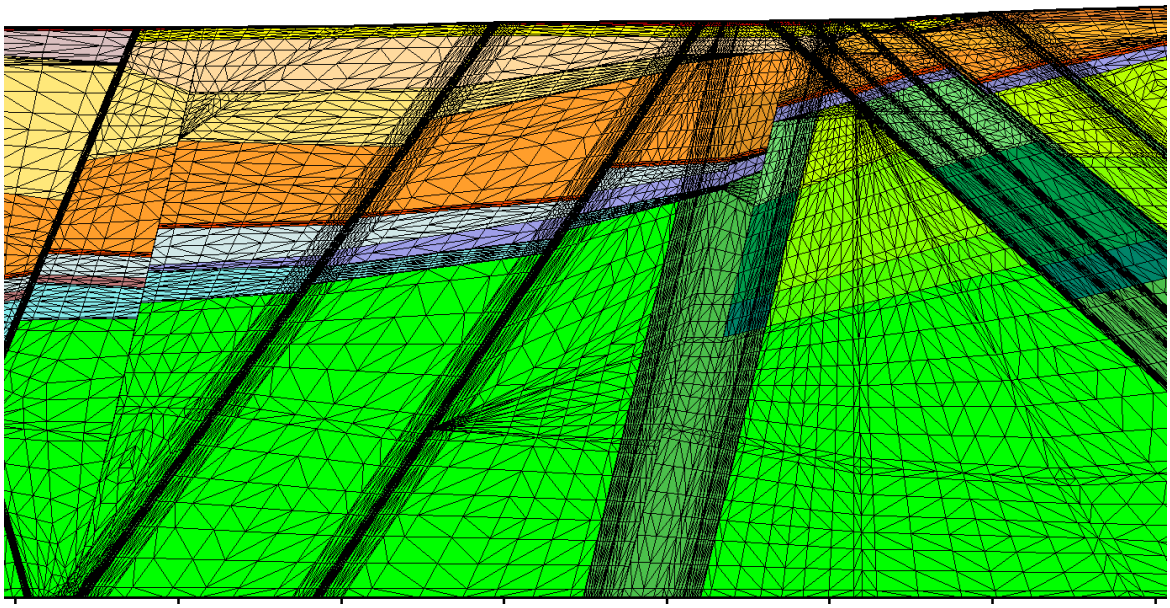

Figure 4-2 An example of part of a complex 2D grid generated using polygons. The finite elements are coloured according to the rock type.

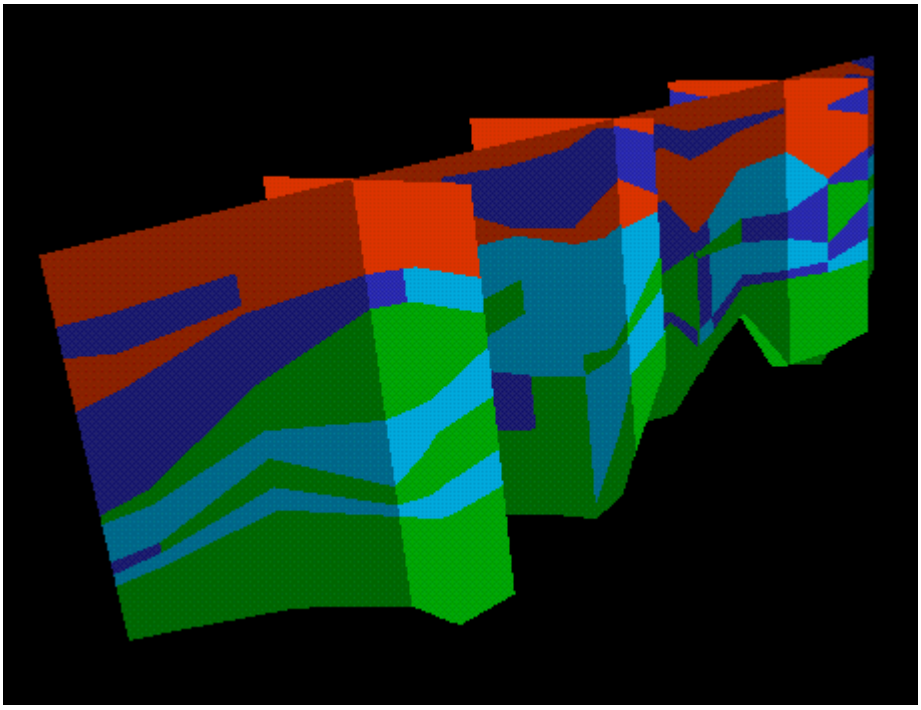

Figure 4-3 Slices through a 3D grid coloured according to rock type. The individual elements are not shown in this picture.

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 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.

4.1.3 Formulation of the Equations

There are several approaches to the finite-element method, which all lead to similar equations. In NAMMU, the Galerkin finite-element method [30, 31, 32] is used to carry out the spatial discretisation of the equations (see [33] for a brief NAMMU-specific discussion). The finite-element method starts from an integral form of the equations.

The dependent variables in the problem are 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 e.g. [31]). Temporal discretisation of the equations in NAMMU is described in section 4.2. The equations are solved using the methods described in section 4.3.

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 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 sometimes the case that numerically calculated pathlines could 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 upwinding, 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 [34].

If numerical instabilities appear, the user has two alternatives: either to refine the mesh in the regions of high gradients so that the instabilities disappear or are reduced to an acceptable level, or to increase the physical dispersion lengths to stabilise the calculation.

4.1.4 Use of Constraints

It is often necessary to consider a variety of scales in groundwater flow modelling. For example, a large regional-scale model to understand boundary conditions affecting flow at depth, and a more detailed (or site-) scale around contaminant sources. In NAMMU it is possible to nest meshes constructed from elements of different scales using constraints.

An example of how meshes can be nested is illustrated in Figure 4-4. Here a refined (35m element-size) site-scale model is joined to a coarser (105m) regional-scale model. The model is 3D, although only a plan view is shown. Hence, at the interface between the two scales, one element in the regional-scale is adjacent to nine elements in the site-scale, and only every third node in the site-scale mesh is coincident with a node in the regional-scale, the other two nodes being ‘pinch’ nodes.

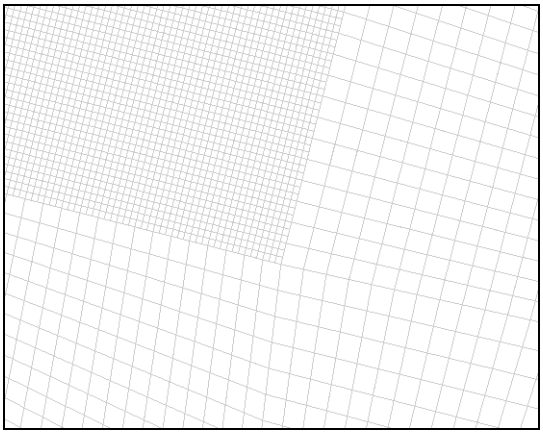

Figure 4-4 Part of a finite-element mesh showing the constraint boundary between a refined site-scale model and a coarse regional-scale model.

To ensure that the physics of groundwater flow is maintained at the interface between meshes, the finite-element equations for elements on the interface are modified using constraint equations. For pinch nodes in a site-scale element on the interface, the pressure is interpolated from the pressures at the nodes in the adjacent regional-scale element, to ensure continuity in the discrete system. The numerical implementation of this constraint in NAMMU is

$$P^R{}_{s,i} = \sum_j \psi_{r,ij} P^R{}_{r,j} \ . \qquad (4.1)$$

For a regional-scale element on the interface, the flux across the interface is balanced with the sum of the fluxes across the interface for the adjoining site-scale elements, to ensure conservation of mass. The numerical representation of this constraint in NAMMU is included implicitly.

Similar principles can be applied to more complex processes, such as salt transport.

4.2 Temporal Discretisation

In NAMMU, the spatial discretisation is carried out using the Galerkin finite-element method (see section 4.1). For time-dependent problems, the application of this method leads to a set of coupled, possibly non-linear, ordinary differential equations in time. There are two basic methods available in NAMMU for integrating these ordinary differential equations:

- The Crank-Nicholson method;
- Gear's method (see e.g. [35]).

The Crank-Nicholson method contains a parameter, θ, that controls the degree of implicitness of the method. The scheme is implicit for all values of θ 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 $\theta = 1$ (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 ($\theta = 0$) and the second-order accurate scheme ($\theta = 0.5$) 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 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 '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.

4.3 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, both direct and iterative methods are available for solving these systems. The direct method is an efficient implementation of the Frontal Method [36, 37, 38] 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.

However, a direct method can be prohibitively slow for large 3D models, in which case an iterative method may be more appropriate. Two implementations of the Preconditioned Conjugate Gradient (PCCG) are incorporated in NAMMU. These are the Generalised Minimum Residual (GMRES) and Biconjugate Stabilised (BicStab) methods. GMRES is suited to non-symmetric systems (e.g. coupled flow and salt transport) and is generally more robust, while BicStab requires less memory.

4.4 Mass Conserving Particle Tracking

Existing methods for calculating pathlines in Nammu can lead to stuck particles and inaccurate pathlines. One cause of this is due to the lack of mass balance between elements when using the finite element method. In their paper [39] Cordes and Kinzelbach propose a method for achieving mass balance between cubic elements by sub-dividing them into tetrahedra and calculating a velocity for each tetrahedron such that mass balance is achieved. Once this is done more robust pathlines can be calculated.

The mass conserving method divides a cubic finite element into eight sub cubes (or hexahedra in the case of a deformed finite element in the general case). These are then further subdivided into five sub-tetrahedra (Figure 4-5). There are 40 sub-tetrahedra per element, Velocities are calculated for each sub-tetrahedra so that mass balance is achieved between elements. This has the effect of a better specified velocity vector field in a given element such that particles do not disappear. The velocity is constant within each tetrahedron.

To calculate the velocities in each tetrahedron first consider a corner node on the element in Figure 4-5. Assume this node is surrounded by eight other tetrahedra, one from the element shown and seven more from other elements adjacent to the node. The first step is to calculate the fluxes in these 8 tetrahedra surrounding a node (see Figure 4-6). The tetrahedra form an octahedron and the fluxes through the 8 outer surfaces are assumed to be equal to the corresponding “nodal fluxes.”

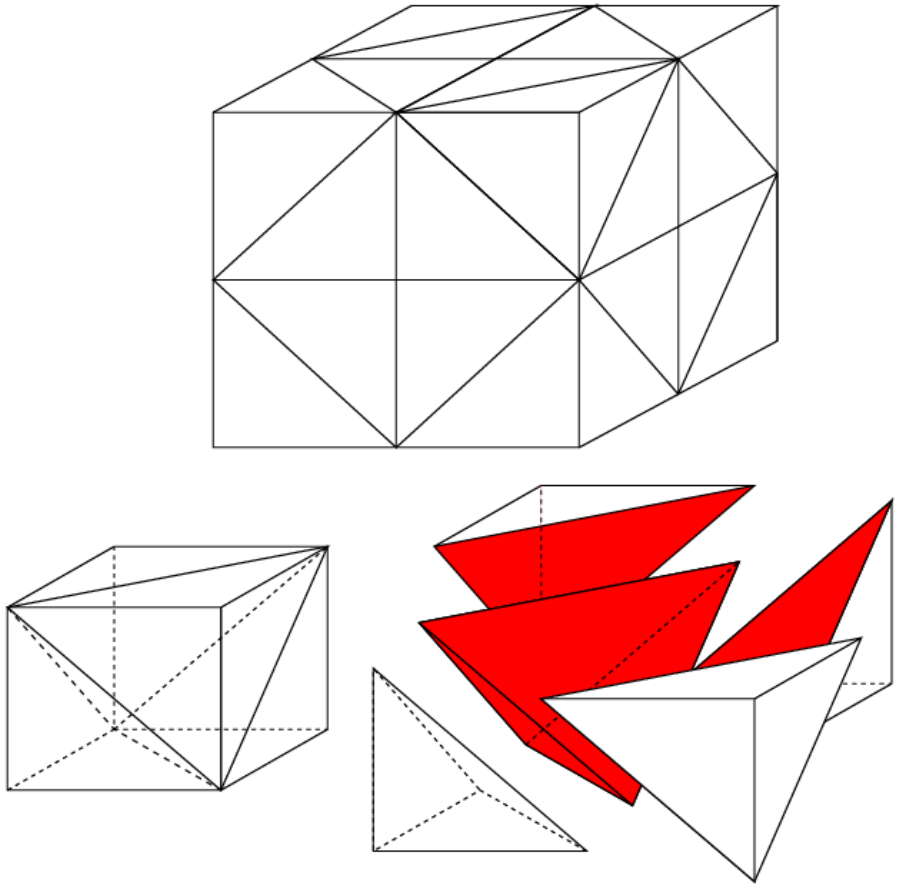

Figure 4-5: A finite element is divided into 8 sub-elements and then further sub-divided into 5 sub-tetrahedra.

The nodal fluxes in finite element theory are conceptually the fluxes from an element *E* towards the nodes *I* on that element. They are derived using Galerkin's method (the reader is pointed to Cordes and Kinselbach for the derivation of a similar equation for square finite elements) and have the important property that they always sum to zero around a node with no sources or sinks. The nodal flux towards node *I* on element *E* is given by:

$$Q_{IE}^{N} = -\frac{1}{2\mu_E}\int_{V_E} dx \nabla \psi_{IE}(x).\left(K_E.\nabla P^R(x)\right) \qquad (1)$$

where K_E is the permeability for element *E*, μ_E is the fluid viscosity inside the element, P^R is the residual pressure, ψ_{IE} is the basis function associated with node *I* on element *E* (there are 8 basis functions, one for each node, which are defined such that the pressure inside the element is given by $P^R(x) = \sum_I P_I^R \psi_{IE}(x)$ where the P_I^R are the residual pressures at the nodes) and the integration is over the volume V_E of element *E*. The factor of -1/2 at the beginning is obtained from a simple example for which the solution is known.

Note that the pressure gradient can be rewritten in the form $\nabla P^R(x) = \sum_J P_J^R \nabla \psi_{JE}(x)$ which gives:

$$Q_{IE}^{N} = -\frac{1}{2\mu_E}\int_{V_E} dx \nabla \psi_{IE}(x).\left(K_E . \sum_J P_J \nabla \psi_{JE}(x) \right)$$

This integral is evaluated using a Gaussian scheme.

The other fluxes in the 8 tetrahedra are calculated using zero-vorticity constraints and mass balance constraints. Once this is accomplished for each of the 8 nodes around an element, the fluxes are then calculated for the tetrahedra in the element not adjacent to a node. This is also accomplished using zero-vorticity and mass balance constraints. Once the fluxes have all been obtained, the flow velocity for each tetrahedron is calculated.

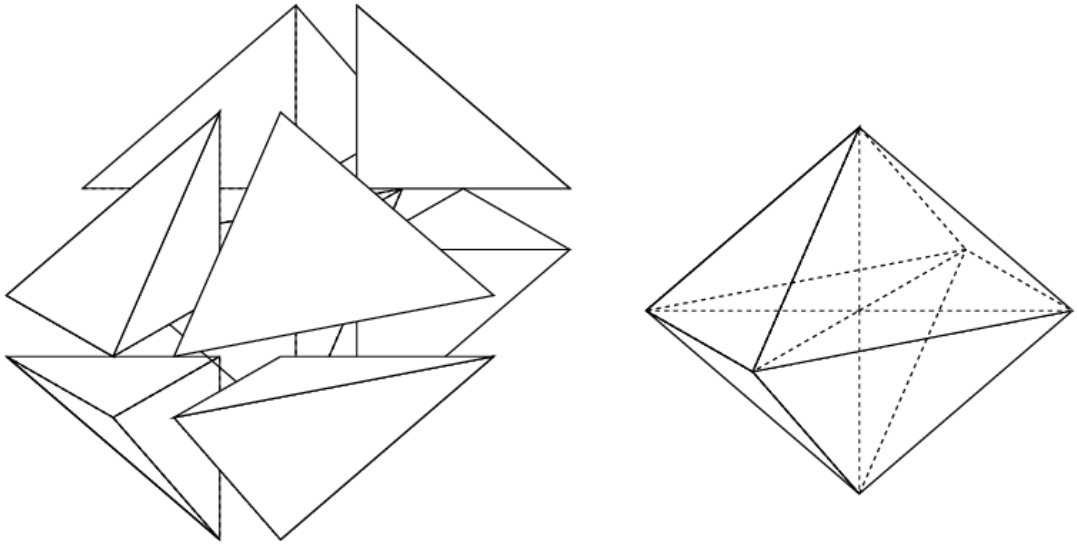

Figure 4-6: The first step of the calculation is finding the fluxes in the eight tetrahedra surrounding each node (which form an octahedron). The fluxes through the 8 outer surfaces are calculated using Galerkin's method, the others are solved using mass conservation & zero vorticity constraints.

The flow velocities are then used to track particles across an element from a start point to an end point. Due to the constant velocity in each tetrahedron, this leads to piecewise pathlines. However, the non-vorticity and mass-balance constraints used in the calculation of the velocity field mean the pathlines rarely get stuck, if at all (some pathlines occasionally still get stuck for numerical reasons).

Mass conserving pathlines are available in the following Nammu models:

- Fully saturated or unsaturated groundwater flow
- Fixed or variable density models
- Hexahedral CB08 or CB81 finite elements (which can be distorted)
- Models with or without nodal quadrature
- Models with regular hexahedral meshes (this means no more than 8 elements per node)
- Models with or without variable mesh refinement (constraint boundaries)

A mass conserving method is already available in the NAPSAC package. This has been coupled to the mass conserving pathline capability in NAMMU to provide mass conserving particle tracking in the CONNECTFLOW package for combined DFN-CPM models.

4.5 Using the Mass Conserving Method to Create a Particle Tracking Library

An alternative approach (still using the mass conserving method) is to discretise the pathlines or in other words, limit the points a particle can pass through (say 24 per element). By doing so it is possible to create a "library" file which stores information on all possible particle tracks for a given model. This can then be used to reconstruct any desired particle track the user may wish to consider.

The benefits of this "discrete" scheme are as follows:

1. The library file can easily be used by software other than Connectflow/Nammu to produce particle tracks. It is very convenient to produce particle tracks in Geovisage since they can be instantly visualised and quickly modified if necessary.
2. The library file is slow to calculate, but once it has been produced, particle tracking is much faster to accomplish.
3. The library can be constructed in a probabilistic manner so that the particles can take different routes dependent on random numbers generated during the particle tracking.

To understand how the discretisation works, consider a hexahedral finite element. In the mass conserving method this is broken down into 40 tetrahedra, and a constant Darcy velocity is calculated for each. Particles can then be tracked across the finite element using those velocities. In the continuous scheme particles are free to enter and exit the element at any point. In the discrete scheme, the entry and exit points are limited to a few fixed points on the element, known as transport nodes. Consider Figure 4-7 this shows 4 and 16 transport nodes arranged evenly on each surface of the element. The number can be increased to 36 or more if required. In general the number of transport nodes per surface is given by $m=4n^2$, where n is a positive integer chosen by the user.

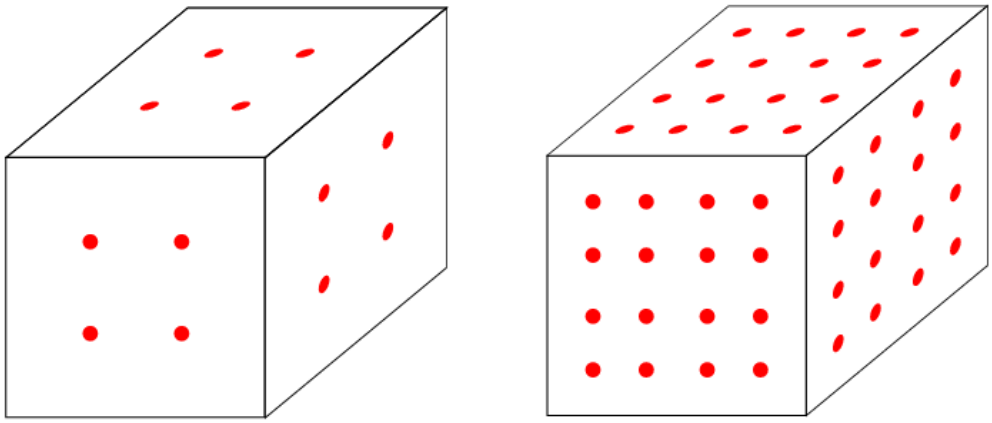

Figure 4-7: Transport nodes are arranged on the surface of each element. The number of nodes per element (m) is given by $m=4n^2$ where n is an integer chosen by the user

Transport nodes are assigned for every element. When two elements share a surface the transport nodes on that surface are only stored once, so there are never two transport nodes at exactly the same position (an exception to this is on constraint boundaries which are discussed later).

Particle tracks are calculated starting from each transport node using the mass conserving method. These are followed until they leave the element(s) the transport node is located on. The positions the tracks leave the elements are used to select "destination" nodes which are stored in a file. This file then forms a library of the links between transport nodes, and can be used by Connectflow or Geovisage to produce particle tracks for a CPM region.

To make the calculation probabilistic, four paths are calculated from each transport node. The start points for each are offset a small distance from the location of the transport node, so that they produce different destinations. There is also a slight offset away from the surface towards the inside of the element. To describe this offset requires a third local coordinate *t* of range [-1,1]. In that coordinate the offset is 0.002. (This helps when particles skim along the CPM-DFN boundary in Connectflow models).

A particle is tracked from each of the four start points to the element boundary. The surface quadrants associated with these exit point are used to determine the destination nodes (see Figure 4-8).

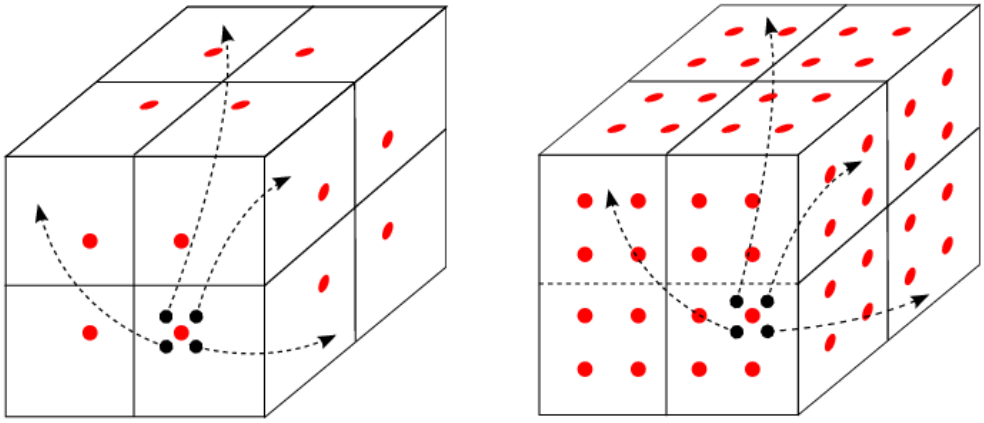

Figure 4-8: The destination nodes are chosen from the surface quadrant the particle leaves from. If m=4 (left) then there is only one node on each quadrant but if m=16 (right) there are four. In the latter case the four possibilities are assigned probabilities according to how far they are from the exit point.

When m=4, the destination node for each start point is the single transport node on the surface quadrant the particle arrives at (note that the flux is constant over the quadrants of a hexahedral surface in the mass conserving method.) Since there are four start points per destination node and one possible destination for each there are potentially four destination nodes for each transport node. Typically each is assigned a 25% probability, however, if two paths go to the same transport node then that destination has a 50% probability, also if the destination node is on the same surface quadrant as the start node then the probability is set to zero for that destination (this also applies if m>4). The “good” destinations would then be re-weighted to make sure the total probability was equal to 100%.

Pathline libraries can be calculated for any model appropriate for mass conserving pathlines (see previous section).

Pathline calculations begin by specifying the starting coordinates for each pathline. The library contains the coordinates of each transport node which are used to find the node closest to each pathline starting point. Each particle is then tracked in the following manner. After the first transport node is determined all of the possible destination nodes are obtained and a random number between 0 and 1 is calculated and used to select the destination nodes whose total probability should always sum to one. Once the destination node is selected the destination nodes for that node are obtained and so on until the particle gets to the boundary and the algorithm stops. Due to this probabilistic approach 2 particles starting from identical positions can take increasingly different paths the greater the number of steps they take.

5 Model

5.1 Stochastic Modelling

NAMMU has the capability to efficiently perform stochastic simulations for both linear systems (e.g. constant-density groundwater flow) and non-linear systems (e.g. coupled variable-density flow and salt transport). For this purpose the generation of stochastic permeability fields in NAMMU has been implemented based on pre-existing methods used in the TBCODE software.

This is based on the Turning Bands method. TBCODE has been used and tested extensively as part of the GEONAM module that was used in comparisons with HYDRASTAR [40] and on the WIPP2 test case [22]. The stochastic continuum approach requires that calculations be performed on tens or hundreds of Monte-Carlo realisations of essentially the same hydrogeological system. Therefore, care has been taken to ensure that the stochastic continuum method was implemented efficiently.

The methodology allows a good deal of flexibility in the stochastic modelling. The rock mass and individual fracture zone domains can have independent statistical parameters, and the domains can be defined as stochastic or deterministic independently. By treating the rock mass and fracture zones as independent domains this method contrasts to HYDRASTAR where the spatial process is continuous and 'trends' (scaling of the local conductivity) are used to represent the fracture zones. Currently, simulations are unconditioned. Conditioning of the rock mass or fracture domains would be straightforward to implement numerically, but careful consideration needs to be given to how the data is defined. For example, on what rock volume the data is defined and whether it is associated with a particular zone or just a borehole interval. The stochastic methods for the rock mass are described in the remainder of this section. The stochastic methods for the fracture zones are described in section 5.2.

For the current release, unconditioned realisations of the rock mass are based on an exponential variogram, and can be combined with deterministic fracture zone properties using IFZ (see section 5.2). It may be desired to have different statistical parameters in different parts of the model. For example, a median permeability that decreases with depth. Another important possibility is to have different statistics for the regional- and site-scale domains, since different values will be obtained for upscaling to the different mesh sizes. Generally, the larger the grid size, the higher the median and the smaller the variance until a REV is reached. These requirements are met by having a continuous spatial process in terms of the underlying variogram, but such that the mean and standard deviation can vary spatially by rock type. This approach is therefore appropriate for models whose statistical properties are generally associated with trends rather than absolute discontinuities at lithological boundaries.

The approach is to use a single Gaussian spatial process with a uniform correlation length, and normalised to have zero mean and variance 1.0. This generated normalised field is then rescaled by the mean and variance parameters for the discrete parts of the model. Thus, different upscaled mean and variance parameters can be applied to an embedded regional- and site-scale model, but in a way such that a high permeability in the regional-scale would generally be adjacent to a high permeability in the site-scale near the interface. This avoids having artificial barriers to flow around the boundary of the site-scale model due to discontinuities in the spatial process.

NAMMU also allows anisotropic permeabilities to be defined. For the stochastic case, this is implemented by scaling the normalised spatial process by different factors for the different components of the permeability tensor. Different degrees of anisotropy can be defined for different domains.

5.2 Implicit Representation of Tabular Features (Fracture Zones) Using IFZ

A new method for calculating the effective permeability of a grid block in a model for groundwater flow in a domain containing tabular features has been implemented in NAMMU. The method was based on the IFZ approach [41], but represents a significant enhancement in the range of structures it can represent, how it handles fracture intersections, and its efficiency. The permeability of the background rock and the features may have arbitrary orientation, and the features may be more or less permeable than the surrounding rock. The approach is simple to implement and has low computational cost.

There are various approaches to modelling groundwater flow in domains containing tabular features. If the features are much more permeable, or more transmissive, than the background rock, the modelling can be undertaken using discrete fracture-network models (see e.g. [42]) in which each feature is represented by a planar 'fracture', and the background rock is not represented. Such models are easy to set up, and it is easy to change the numbers, positions and properties of the features. However, the features may not be that much more permeable or more transmissive than the background rock, or some features may act as barriers to flow across them, or some features may have a more complicated behaviour in that they act as barriers to flow across them, but in the directions along their larger extents are more transmissive than the surrounding rock. It may, therefore, be necessary to model the flow through the background rock as well as through the features. This can be done using fracture-network models, but it may be necessary to approximate the background rock in some way in terms of 'fractures'.

Another approach to the modelling is to use continuum porous medium models in which each tabular feature is represented by a group of finite elements chosen so that the boundaries of the feature lie along element boundaries. There are variants of this approach in which, for example, the features are approximated using two-dimensional elements in a grid of three-dimensional elements. All of these approaches represent the flow in both the features and the surrounding rock, and can handle the various types of features discussed above.

However, it is very difficult and time-consuming to set up the grids for such a model in three dimensions, and in general it is very difficult to automate the process of setting up the grid. This is particularly important if one wants to address the uncertainties, which will always exist, in the number and position of the features. This would be done by undertaking Monte-Carlo simulations. Realisations of the features would be generated numerically based on the available information about the features and then the flow would be calculated for each realisation. In this way, the uncertainty about the flow resulting from the uncertainties about the features could be quantified. However, if it were necessary to manually set up the grid for the numerical flow calculation for each realisation, it would only be practicable to undertake calculations for a very small number of realisations, which would limit the usefulness of the Monte-Carlo technique.

An alternative approach to modelling flow in a domain containing tabular features using continuum porous medium models is as follows. The finite-element (or finite-difference) grid is set up independently of the features. Typically, a simple cubic grid might be used. Then for each element, or grid block, a suitable effective permeability would be determined, appropriate to represent the background rock and all the features crossing the element, or grid block. This approach is often used in finite-difference calculations, because many finite-difference programs can only handle simple cubic grids. Variants of this approach have been proposed by, for example, Svensson [43] and Lee et al. [44]. In fact, the approach is better suited to implementation in finite-element models as they allow an arbitrary direction of hydraulic anisotropy in the effective permeability to be specified. This is important since, in the general case, the principal directions of the permeability tensor will differ from element to element according to the alignment of features that cross them. Another motivation for using simple cubic grids is in undertaking stochastic calculations to address the effects of heterogeneity in the background rock, because the statistical parameterisation may require that all elements or grid blocks have similar sizes.

The approach is particularly flexible. It can be readily automated, which makes it straightforward to undertake Monte-Carlo simulations to address the uncertainties in the number and position of the

features. However, for a particular level of grid refinement, the flow calculated for an individual realisation would not be quite as accurate as that calculated using a grid chosen so that each feature is represented accurately by a number of finite elements, although this can be addressed by grid refinement.

6 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;
- A number of options for colouring plotted quantities, for example, according to the values of the variables, scalar functions of the variables and user defined functions of the variables;
- Superimposing any combination of plots, and addition of user-defined text and lines to build up complex images.

The finite-element model and the modelled results can also be visualised using the GeoVisage graphics package. This is a fully interactive tool with the capability of displaying and manipulating images of the NAMMU model on the screen. The GeoVisage 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. These features make GeoVisage 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 GeoVisage.

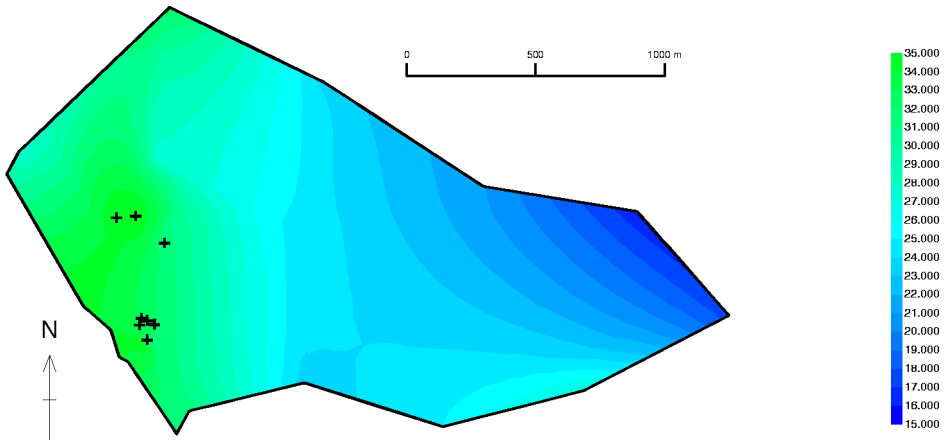

Figure 6-1 Shaded contour plot of groundwater head.

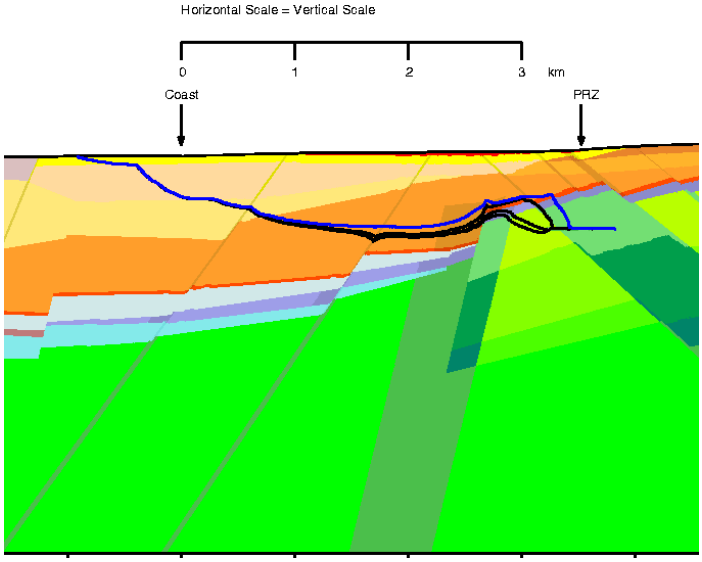

Figure 6-2 Pathlines for a model based on the grid shown in Figure 4-2.

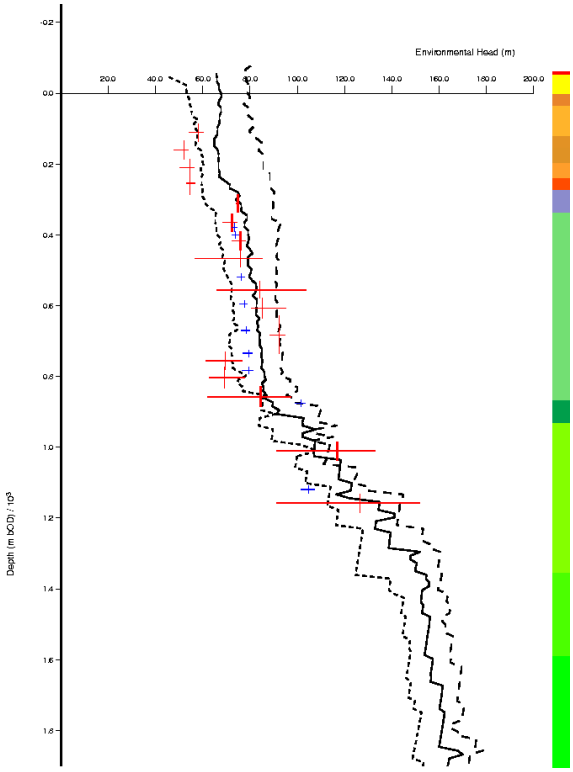

Figure 6-3 Line graph showing variation of environmental head with depth and the observations from the site along a vertical line through the model shown in Figure 4-2.

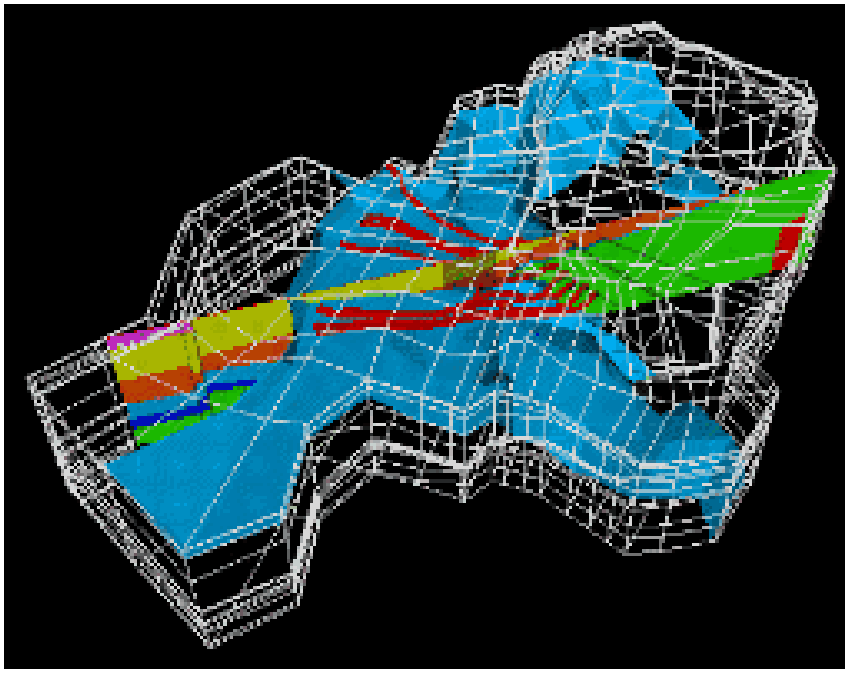

Figure 6-4 Complex image for a 3D version of the model shown in Figure 4-3, showing (i) a slice through the grid, (ii) a surface of constant salinity and (iii) a number of pathlines.

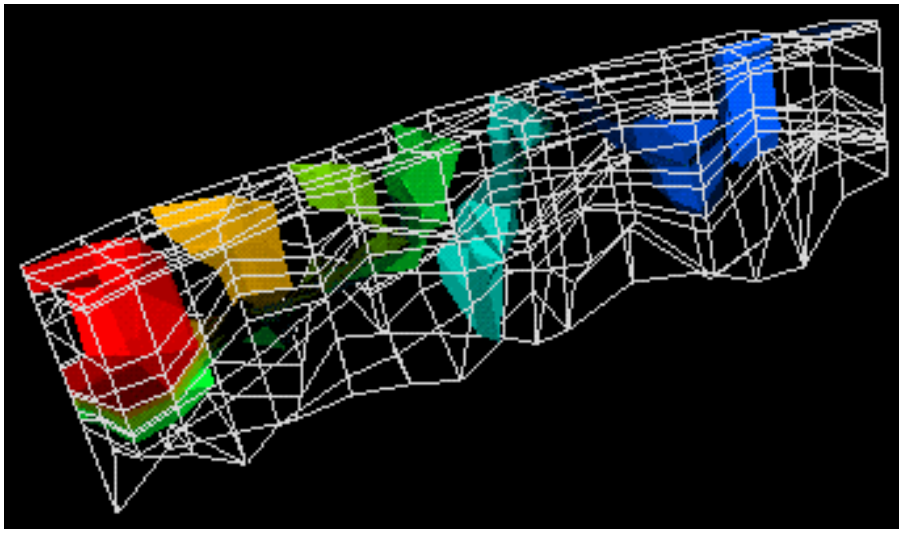

Figure 6-5 Isosurfaces of pressure for the model shown in Figure 4-3.

7 Nomenclature and Units

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

Symbol	Definition	Units
A_{KR}	constant in NAMMU default relative permeability model	Pa $^{S_{KR}}$
A_{PC}	constant in NAMMU default capillary pressure model	Pa $^{S_{PC}}$
B_{KR}	constant in NAMMU default relative permeability model	Pa $^{S_{KR}}$
B_{PC}	constant in NAMMU default capillary pressure model	Pa $^{S_{PC}}$
b	effective aquifer thickness (see Equation (3.10))	m
c	concentration (or mass fraction) of dissolved solute (normally salt)	–
c_0	specified inflow concentration for solute (normally salt)	–
c_l	specific heat capacity of the fluid	J $kg^{-1}K^{-1}$
c_s	specific heat capacity of the rock solids	J $kg^{-1}K^{-1}$
$\mathbf{D}$	dispersion tensor for solute (normally salt)	m^2s^{-1}
$\mathbf{D}'$	dispersion tensor for heat	W $m^{-1}K^{-1}$
D_i	intrinsic (or effective) diffusion coefficient	m^2s^{-1}
D_m	molecular diffusion coefficient for solute (normally salt)	m^2s^{-1}
$D_{m\alpha}$	molecular diffusion coefficient for nuclide α	m^2s^{-1}
$\mathbf{D}_\alpha$	dispersion tensor for nuclide α	m^2s^{-1}
$\mathbf{F}_\mathrm{A}$	advective radionuclide flux	mol $m^{-2}s^{-1}$
F_C	flux of solute (normally salt)	kg $m^{-2}s^{-1}$
$\mathbf{F}_\mathrm{D}$	diffusive radionuclide flux	mol $m^{-2}s^{-1}$
F_{N_α}	flux of nuclide α	mol $m^{-2}s^{-1}$
F_P	fluid flux	kg $m^{-2}s^{-1}$
F_T	heat flux	W m^{-2}
f_α	Source term for nuclide α	mol $m^{-3}s^{-1}$
$\mathbf{g}$	gravitational acceleration	m s^{-2}
g	magnitude of gravitational acceleration	m s^{-2}
H	heat source	W m^{-3}
h	hydraulic head	m
I	maximum potential infiltration rate	m s^{-1}
K_d	sorption distribution coefficient	–
$K_{d,\alpha}$	sorption distribution coefficient for nuclide α	–
$\mathbf{k}$	rock permeability tensor	m^2
k_r	Relative permeability (see section 3.3.3)	–
k_v	vertical permeability of semi-permeable layer	m^2
L	arbitrary transition thickness	m

N_α	concentration of nuclide α	mol m^{-3}
$N_{\alpha 0}$	specified inflow concentration for nuclide α	mol m^{-3}
$\mathbf{n}$	outward normal to a specified boundary	–
P_E	capillary entry pressure	Pa
P^R	residual fluid pressure	Pa
$P^R_{r,i}$	residual fluid pressure at node i of an element on the interface of a regional-scale mesh	Pa
$P^R_{s,i}$	residual fluid pressure at node i of an element on the interface of a site-scale mesh	Pa
P^T	total fluid pressure	Pa
P^T_0	reference total fluid pressure	Pa
Q	Source term (in 2D areal model of groundwater flow, see section 3.3.1)	kg $m^{-2}s^{-1}$
$\mathbf{q}$	specific discharge (or Darcy velocity)	m s^{-1}
q_z	vertical component of specific discharge	m s^{-1}
R_α	retardation factor for nuclide α	–
S	saturation	–
S_{KR}	constant in NAMMU default relative permeability model	–
S_{PC}	constant in NAMMU default capillary pressure model	–
S_{res}	residual saturation	–
S_α	function of saturation used in Van Genuchten relative permeability model (see Equation (3.26))	–
T	temperature	K
T_0	reference temperature	K
t	Time	s
$\mathbf{v}$	average porewater velocity	m s^{-1}
v	magnitude of porewater velocity	m s^{-1}
v_i	i-component of porewater velocity	m s^{-1}
z	elevation	m
z_0	reference elevation	m
z_b	elevation of bottom of aquifer	m
z_s	elevation of ground surface	m
z_t	elevation of top of aquifer	m
α	compressibility of freshwater	Pa^{-1}
α_L	longitudinal dispersion length for solute (normally salt)	m
α'_L	longitudinal dispersion length for heat	m
$\alpha_{L\alpha}$	longitudinal dispersion length for nuclide α	m
α_T	transverse dispersion length for solute (normally salt)	m
α'_L	transverse dispersion length for heat	m

$\alpha_{T\alpha}$	transverse dispersion length for nuclide α	m
α_c	compressibility of saturated fluid (normally brine)	Pa^{-1}
β	coefficient of volumetric expansion of freshwater	K^{-1}
β_c	coefficient of volumetric expansion of saturated fluid (normally brine)	K^{-1}
Γ_a	average thermal conductivity of the rock and fluid	W $m^{-1}K^{-1}$
Γ_l	thermal conductivity of the fluid	W $m^{-1}K^{-1}$
Γ_s	thermal conductivity of the rock	W $m^{-1}K^{-1}$
γ	constant in relative permeability models	–
δ_1	viscosibility	K^{-1}
δ_{ij}	Kronecker delta	–
ε	Penalty weight (0.01)	–
ϕ	porosity	–
ϕ_0	reference porosity	–
λ_α	decay constant for nuclide α	s^{-1}
μ	fluid viscosity	Pa s
μ_0	reference fluid viscosity	Pa s
ρ_0	reference (freshwater) fluid density	kg m^{-3}
ρ_{c0}	Density of solute-saturated fluid (normally saturated brine)	kg m^{-3}
ρ_l	fluid density	kg m^{-3}
ρ_s	Density of the rock solids	kg m^{-3}
$(\rho c)_a$	average heat capacity of the rock and liquid	J $m^{-3}K^{-1}$
τ	tortuosity	–
θ	Degree of implicitness of Crack-Nicholson solution method	–
$\psi_{r,ij}$	finite element basis function evaluated for node j of an element on the interface of a regional-scale mesh at the position of node i of an adjoining element in a site-scale mesh	–

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