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Assessment model validity document

NAMMU: A program for calculating groundwater flow and transport through porous media

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AEA Technology, Harwell, UK

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ABSTRACT

NAMMU is a computer program for modelling groundwater flow and transport through porous media. This document provides an overview of the use of the program for geosphere modelling in performance assessment calculations and gives a detailed description of the program itself. The aim of the document is to give an indication of the grounds for having confidence in NAMMU as a performance assessment tool. In order to achieve this the following topics are discussed. The basic premises of the assessment approach and the purpose of and nature of the calculations that can be undertaken using NAMMU are outlined. The concepts of the validation of models and the considerations that can lead to increased confidence in models are described. The physical processes that can be modelled using NAMMU and the mathematical models and numerical techniques that are used to represent them are discussed in some detail. Finally, the grounds that would lead one to have confidence that NAMMU is fit for purpose are summarised.

SAMMANFATTNING

NAMMU är ett datorprogram för modellering av grundvattenflöde och transport i porösa medier. Föreliggande dokument innehåller en översikt om hur NAMMU kan användas för geosfärsmodellering inom säkerhetsanalys. Vidare erbjuder dokumentet en detaljerad beskrivning av själva datorprogrammet. Dokumentets syfte är att tillhandahålla indikationer om varför man kan ha god konfidens i användandet av NAMMU som ett verktyg inom säkerhetsanalys. För att uppnå detta diskuteras följande ämnen: De grundläggande förutsättningarna över analysmetodiken presenteras. Vidare presenteras vilka olika typer av beräkningar som kan utföras med NAMMU samt dessa beräkningars syfte. Koncept för validering av modeller och de överväganden som kan leda till ökad konfidens i modeller beskrivs. Vidare diskuteras i detalj de fysikaliska processer som kan modelleras med hjälp av NAMMU samt de matematiska modeller och numeriska tekniker som används för att representera processerna. Slutligen sammanfattas de överväganden som leder till konfidens i NAMMU som lämplig för sitt syfte.

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SUMMARY AND CONCLUSIONS

One of the options being considered by several countries for the long term disposal of radioactive waste material is deep burial in stable geological formations. In Sweden it is intended that spent nuclear fuel and long-lived low- and intermediate-level wastes will be disposed in a deep repository. In order to achieve long-term safety, the repository system is designed so as to ensure that several factors contribute to the overall performance. The transport pathways and dilution and retardation mechanisms in the rocks between the repository and the biosphere, i.e. the far-field mechanisms of transport through the geosphere generally make a very important contribution to the overall performance of the repository.

Analysis and understanding of the groundwater flow and radionuclide transport in and around a site for a radioactive waste repository will therefore play important roles in a performance assessment. The radionuclides from the wastes will dissolve in the groundwater and may then be transported back to man's immediate environment by the flowing groundwater. Groundwater flows slowly, particularly in regions that are considered suitable for the location of a repository. Thus, the timescales of interest are very long and the only method available for assessing the consequences of this groundwater pathway is mathematical modelling of the physical and chemical processes involved. However, the models are often too complicated to solve analytically and so they must be incorporated into computer programs.

NAMMU is a computer program for calculating groundwater flow and solute and heat transport through porous media. It is widely used for repository performance-assessment calculations. It is very important that a high level of confidence can be placed in any computer code to be used for such work. This confidence is built up over a number of years and comes from a variety of sources. The purpose of this document is to present, in a concise form, the evidence that leads one to have a high degree of confidence in NAMMU. Essentially, the purpose of the report can be summarised as: 'to give a clear presentation of the reasons why an independent, reasonably knowledgeable person, would believe that the mathematical models that are used in NAMMU give an adequate representation of the processes that could occur in a groundwater flow system, and that the numerical algorithms used in the computer program allow reliable calculations of the consequences of the mathematical models to be made.' This means that if NAMMU is used to represent a conceptual model of a groundwater flow system, the results of the NAMMU calculations will give reliable predictions of the behaviour of the system, insofar as the conceptual model itself adequately represents the real system.

The contents of the document are therefore as follows. An overview of the role of the geosphere in a performance assessment and the physical processes that lead to the movement of groundwater and the transport of radionuclides is presented. The general approach to the validation of models is then discussed and the various sources of information that can contribute to building confidence in the models are summarised. The role of geosphere models in the performance assessment process is subsequently discussed in more detail. In particular, the results of the models that play important roles in assessment calculations and the inputs that are required by the models are identified. An account is also given of the basic premises and assumptions that it is anticipated could form the basis for the geosphere modelling performed as part of assessment calculations for the Swedish repository concept. The processes that are represented in the geosphere models are then identified and discussed in more detail. The background to the understanding of these processes is also outlined in order to help build confidence in the models that are used to represent them. A description of the mathematical models that are used to represent the processes, the numerical methods that are used in NAMMU and the important subjects of verification and quality assurance are then discussed. Finally, the application of the general approach to validation of the NAMMU models is described. It is concluded that there is a wide range of evidence that gives confidence that the models of groundwater flow and radionuclide transport implemented in NAMMU are appropriate and are fit for the purposes for which they are applied.

1 INTRODUCTION

One of the options being considered by several countries for the long term disposal of radioactive waste material is deep burial in stable geological formations. In Sweden it is intended that spent nuclear fuel and long-lived low- and intermediate-level wastes will be disposed in a deep repository. The design of the deep repository is based on the KBS-3 concept (SKBF/KBS, 1983). In this concept the repository consists of two main parts, intended to be constructed at a depth of about 500m in the Swedish crystalline bedrock. The first is a repository for high-level spent nuclear fuel. This waste is enclosed in copper canisters which are then placed one by one in deposition holes bored in the bottom of a tunnel system. Each canister is surrounded by a layer of bentonite clay. The clay holds the canisters in place and isolates them from the groundwater in the surrounding rock. The clay also retards the transport of substances to and from the canister.

The other main part of the repository concept is intended for other types of long-lived waste. These are deposited in caverns excavated in the rock. Physical and chemical barriers of concrete and bentonite are included to limit the water-borne transport of radionuclides. This component of the repository resembles the existing final repository for radioactive operational waste, SFR (Lindgren and Pers, 1994). After the wastes have been deposited, it is intended that the tunnels and other spaces are backfilled.

In order to achieve long-term safety, the repository system is designed so as to ensure that several factors contribute to the overall performance. Initial containment of the radioactive waste is achieved by encapsulating the radioactive materials in tightly sealed canisters which are deposited deep in crystalline bedrock at a selected repository site. If this containment should be breached, the repository has the added function of retaining the radionuclides and retarding their transport as a result of various physical and chemical containment mechanisms. The part of the repository system concerned with the waste form, containers and the immediate physical and chemical environment of the repository is generally referred to as the near-field. The transport pathways and dilution and retardation mechanisms in the rocks between the repository and the biosphere, i.e. the far-field mechanisms of transport through the geosphere are generally also a very important contribution to the overall performance of the repository. Finally, the distribution of radionuclides in the biosphere and the consequent exposure pathways also play an important role in an evaluation of overall performance.

At this stage in the SKB deep repository project, continuing assessments of the repository performance are required in order to provide input to the processes of repository design and selection of the disposal site. In addition, the estimated performance of a repository system can be compared with the safety targets set by the regulatory authorities. A number of performance and safety assessments for the deep repository concept will therefore be carried out by SKB during the next few years.

Analysis and understanding of the groundwater flow and radionuclide transport in and around a site for a radioactive waste repository will play important roles in a performance assessment. The radionuclides from the wastes will dissolve in the groundwater and may then be transported back to man's immediate environment by the groundwater flowing through the geological formation. Groundwater flows slowly, particularly in regions that are considered suitable for the location of a repository. Thus the timescales of interest are very long and the only method available for assessing the consequences of this groundwater pathway is mathematical modelling of the physical and chemical processes involved. However, the models are often too complicated to solve analytically and so they must be incorporated into computer programs. It is very important to ensure that features of the site and processes occurring at the site that could have an important influence on flow and transport are appropriately represented by the numerical model.

NAMMU is a computer program for calculating groundwater flow and solute and heat transport through porous media (Hartley, Jackson and Watson, 1996). It is widely used for repository performance-assessment calculations. It is very important that a high level of confidence can be placed in any computer code to be used for such work. This confidence is built up over a number of years and comes from a variety of sources. The purpose of this document is to present, in a concise form, the evidence that leads one to have a high degree of confidence in NAMMU. Essentially, the purpose of the report can be summarised as: 'to give a clear presentation of the reasons why an independent, reasonably knowledgeable person, would believe that the mathematical models that are used in NAMMU give an adequate representation of the processes that could occur in a groundwater flow system, and that the numerical algorithms used in the computer program allow reliable calculations of the consequences of the mathematical models to be made.' This means that if NAMMU is used to represent a conceptual model of a groundwater flow system, the results of the NAMMU calculations will give reliable predictions of the behaviour of the system, insofar as the conceptual model itself adequately represents the real system. In practice, there are likely to be several conceptual models of the groundwater flow system that are consistent with the available data. NAMMU can then be used to calculate the consequences that would arise if a given conceptual model was a true representation of the real system. The difference between the results from different conceptual models is one source of uncertainty in the results of assessment calculations (uncertainties in the measured data are another). The treatment of these uncertainties lies outside the scope of this report.

This document is concerned with the validation of models of groundwater flow and radionuclide transport in the geosphere that are implemented in NAMMU. Therefore, near-field and biosphere issues are not discussed further. However, it should be noted that there are important links between geosphere models and those of the other components of the system. Thus, for example, the groundwater velocities at the repository location are important inputs to many models of near-field behaviour. The radionuclide flux that is required as a basic input by many biosphere models is obtained from models of radionuclide transport through the geosphere. In addition, the radionuclide concentrations in parts of the geosphere itself may be an important input to models used to assess the consequences of human intrusion (e.g. of abstraction of water by wells). In assessing the validity of the models of geosphere transport it is important to bear in mind the uses that are to be made of the information obtained from these models in other parts of the overall performance assessment.

The structure of the remainder of this document is as follows. An overview of the role of the geosphere in a performance assessment and the physical processes that lead to the movement of groundwater and the transport of radionuclides is presented in section 2. In section 3 the general approach to the validation of models is discussed and the various sources of information that can contribute to building confidence in the models are summarised. In section 4 the role of the geosphere models in the assessment process is discussed in more detail. In particular, the results of the models that play important roles in subsequent assessment calculations and the inputs required by the models are identified. Section 5 gives an account of the basic premises and assumptions that form the basis for the geosphere modelling performed as part of the assessment calculations for the repository concept outlined above. In section 6 the processes that are represented in the models are identified and discussed in more detail. The background to the understanding of these processes is also outlined in order to help build confidence in the models that are used to represent them. Section 7 contains a description of the mathematical models that are used to represent the processes. The numerical methods that are used in NAMMU as well as the important subjects of verification and quality assurance are also discussed. Finally, Section 8 describes the application of the approach to validation outlined in Section 3 to the NAMMU models.

2 COMPONENT UNDER CONSIDERATION

This Assessment Model Validity Document for NAMMU is concerned with the models of groundwater flow and radionuclide transport in the geosphere that have been implemented within the NAMMU program. The physical processes that the models represent and the mathematical formulations of the models are discussed in more detail in sections 6 and 7, respectively. The role of NAMMU within performance assessment calculations is discussed in section 4. It will be clear from that discussion that the options available within NAMMU can be used to obtain models of flow and transport that are appropriate in a very wide range of situations. The aim of the present Section is to give a brief indication of the potential role of such models within a performance assessment for a deep repository and of the type of models to be discussed in the later sections.

An understanding of flow and transport in the geosphere plays a crucial role in a performance assessment. This can be understood from a consideration of the function of the geosphere in a multi-barrier containment system which, in summary, is:

(a) for some radionuclides, to provide sufficient containment, so that the flux of these radionuclides to the biosphere is always negligible;

(b) to provide sufficient spreading in time of the discharge to the biosphere of other radionuclides so that their concentrations in near-surface groundwaters or other environmental media are acceptably low.

A more detailed discussion of these issues can be found in Baker et. al, 1995. Good geosphere performance is attained when all radionuclides that are not adequately contained in the near-field fall into one of the above categories. Effective containment occurs when the travel time for transport from the repository through the geosphere, taking account of any relevant retardation processes, is greater than the half life of the radionuclide by a sufficiently large margin. The discharge of radionuclides to the biosphere is spread in time as result of a combination of two processes. The first is a spreading in time, which is related to the timescale for the removal of the radionuclide inventory from the repository. The second is related to the spreading of the radionuclide plume during transport through the geosphere. The process of hydrodynamic dispersion is a major contributor to the second process.

In many cases, the rate of groundwater flow at the repository location will be an important control on the rate of radionuclide removal from the repository and will be an important input to models of near-field behaviour (the precise role played by the groundwater flow rate in determining the rate of radionuclide release will depend on the repository design and the chemical behaviour of the individual radionuclides). An understanding of the factors that control the groundwater flow rate at the repository location is therefore an important component of a performance assessment and models that can provide this information are required.

The timescale for the transport of radionuclides from the repository to the biosphere and the amount of dilution and dispersion that occurs along the transport pathway from the repository to the biosphere will also be important factors that play a role in determining the overall performance of the repository. These quantities will depend upon the rate of groundwater flow along the transport pathway as well as the amount of spreading of the plume and retardation of the radionuclides relative to the groundwater movement that are produced by transport processes such as dispersion and sorption. Thus, models of the flow and transport processes along the transport pathway are required.

The rate of radionuclide transfer to the biosphere is an important input to the biosphere models that are used to assess the doses to exposed groups that form the basis for the evaluation of the overall performance of the repository. Thus, models that can be used to assess the radionuclide fluxes from the geosphere to the biosphere are required.

In summary, in order to perform a performance assessment it is necessary to have an understanding of the processes of groundwater flow and radionuclide transport at the repository location and along the transport pathways from the repository to the biosphere. In practice, this will require an understanding of the groundwater flow system, including the driving forces for groundwater flow in the region of interest. However, radionuclides are not simply advected with the groundwater flow, their migration is affected by additional processes such as sorption and dispersion. An understanding of these processes and models of their effects will also be required.

In the remainder of this section a brief outline is given of the processes that are treated in the flow and transport models and of the general status of the models of these processes. A more detailed discussion of these issues is given in section 6. The processes that are described are those that can be represented using NAMMU. Other processes (e.g. colloidal transport) can be envisaged but are not relevant for the purposes of this model validity document. It would be important to ensure that any such processes that are considered to be potentially important are included in the overall suite of calculations that are performed for a performance assessment.

First, consider the model for groundwater movement. Basically a model that describes the conservation of momentum of the fluid is required. An appropriate expression of this principle in the circumstances of interest is given by Darcy's law (see subsection 6.2), according to which the groundwater velocity is related to the pressure gradient and the groundwater density and is proportional to a tensor coefficient that characterises the resistance to flow offered by the rock. As explained in section 6.3, combination of Darcy's law with the principle of conservation of mass gives an equation that can be solved for the pressure distribution. Darcy's law is an empirical relationship, originally derived from experiments on flow through sand columns. It has since been demonstrated experimentally to apply over a wide range of conditions. In addition, it is possible to derive Darcy's law from more fundamental principles. 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. All of this gives considerable confidence in the validity of the model.

The groundwater velocity is influenced by the groundwater density which, in general, depends on temperature and on the groundwater chemistry. The presence of solutes, especially salt, can significantly affect the density. 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, buoyancy effects can have a substantial influence on the pattern of groundwater flow. It is then necessary to couple the solution of the groundwater flow problem to that of the heat or salt transport problem.

In some rocks, most of the groundwater actually flows through an interconnected network of fractures, rather than through the porous rock matrix. Such cases can be treated using 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. However, the equation that is used to give the flow rate in an individual fracture in such models has the same form as Darcy's law, in that the flow rate is proportional to the pressure gradient along the fracture. In addition, Darcy's law can be used to represent flow within a fractured rock on a larger scale. Provided that the scale of interest in the flow calculation is larger than the length scale of the individual fractures and is large enough to include several fractures, it is then reasonable to use a porous medium approach and Darcy's law can be used to give the effective flow rate through a block of fractured rock.

The movement of the groundwater will result in the transport of dissolved radionuclides. However, there are many additional processes that should be taken into account in models of radionuclide migration, such as diffusion, hydrodynamic dispersion, rock-matrix diffusion, sorption, anion exclusion and radioactive decay and ingrowth (see section 6). These processes can be treated using the models of radionuclide transport that are implemented in NAMMU and are briefly discussed in the following paragraphs.

The process of molecular diffusion will lead to the migration of radionuclides through the porewater even when there is no significant groundwater flow. Molecular diffusion in free water is a well understood process and is modelled according to Fick's law, which 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.

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'. Qualitatively, dispersion acts in a similar way to diffusion. 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. 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 process of rock-matrix diffusion is potentially significant in many fractured rocks. 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.

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. 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.

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 effect can be represented using a simple exclusion factor, which is equivalent to the fraction of the porosity that is accessed.

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. This can be represented by multiplying the sorption distribution coefficient that would be considered appropriate in the absence of organic complexants by a sorption reduction factor.

Radioactive concentrations are also affected by the processes of radioactive decay and ingrowth from parent radionuclides. Models of these processes have the status of widely accepted physical laws.

3 VALIDATION FRAMEWORK

3.1 THE CONCEPT OF VALIDATION

This section sets out the framework for the process of model validation. A number of definitions of the term 'validation' have appeared in the literature concerned with the performance assessment of radioactive waste repositories. Perhaps the most appropriate for the purpose of this document is that given by the IAEA:

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

In general terms, validation can be described as the process of building confidence in the fitness for purpose of models that are used in a performance assessment and hence in the results obtained from the models. The concept of fitness for purpose is important. The aim of validation in the context of performance assessment should be to demonstrate that the model is adequate for the purpose for which it is intended. It may not be necessary that a model be extremely accurate, just that it should be appropriate for its intended purpose. This issue is particularly relevant because of the very long times over which the models will be used to make predictions of the behaviour of the system. Consider, for example, the advective movement of a particle of groundwater from the repository to the biosphere at some site for which an assessment is performed. It would clearly be unrealistic to suggest that a model of groundwater flow for the site could be used to accurately predict the date and time of day at which the particle reaches the biosphere. However, this impractical level of accuracy is not required. The model will be adequate for the purposes of performance assessment if it can be used to produce an estimate of the travel time and, most importantly, a characterisation of the uncertainty in the travel time. Even in cases in which the uncertainties in the calculated travel times span ranges of tens of thousands or even hundreds of thousands of years the model may still be adequate.

The nature of the validation process (i.e. the approach to building confidence in the model) will be slightly different, depending on whether the model is a general model, for example of a process such as groundwater flow, or a specific model, for example an attempt to model the behaviour observed in a particular experiment or at a particular site. Validation can therefore take place on several levels. This is perhaps best illustrated by an example. The models in NAMMU for treating coupled groundwater flow and salt transport can be regarded as an acceptable approach to treating the phenomena in question. In this general and wide sense they can be regarded as validated. However, in order to apply these models successfully to an assessment of a particular site, a conceptual model of the site needs to be developed. This conceptual model would include a description of the relevant geology and assignment of the hydrogeological properties and boundary conditions (see, for example, Porter et. al, 1995). The conceptual model of the site can, of course, be subject to the validation procedure and confidence can be built in the model over a period of time as information is gathered and comparisons are made between observations and predictions. By its nature, the validation of this conceptual model is specific to the site and is outwith the scope of the NAMMU Assessment Model Validity document. However, examples of successful applications are included in the document, as they can help to build confidence in the generic model of coupled groundwater flow and salt transport in NAMMU, as discussed in the next subsection. The development and validation of site-specific conceptual models is part of the overall performance assessment process.

An important aspect of the validation of a general model is its use and wide acceptance within the scientific community. The wide use of the model will mean that it is, in effect, constantly being subjected to the scrutiny of many individuals with relevant technical knowledge. A specific model, by its very nature, is unlikely to be so widely used and examined. Thus, for a specific model this aspect of validation would consist of establishing a scientific justification or case for the model. The case should be such that it would be reasonable to expect that individuals with relevant technical knowledge, who were not involved in the establishment of the case, would conclude that the model was acceptable, if the case were presented to them.

It can be seen from the last example that validation involves more than comparing the predictions of a model with observations, although, as indicated by the IAEA definition, this can be an important part of the process. Validation also implies a need to establish whether or not the model is an acceptable representation of the physical phenomenon. As such, it will also include checking that the model is internally consistent and examining the model for consistency with principles that are generally accepted in the scientific community. Thus, for example, a valid model of the process of coupled groundwater flow and salt transport that was referred to above should predict that mass is conserved. This example also illustrates another aspect of the way in which a model should be fit for purpose and need not be extremely accurate. Strictly speaking, the scientific principle that the model should satisfy is conservation of total mass-energy. However, circumstances in which the equivalence of mass and energy need to be taken into account (e.g. at the very high energies associated with velocities near the speed of light) are not relevant for the situations of interest in performance assessment. Thus, the 'approximate' model of conservation of mass is adequate for the purpose.

The last example also raises the issue of the validation of general physical laws (such as conservation of mass). This is really part of the normal progress of science. A general physical law is taken to be validated when it is widely accepted within the scientific community that it provides a good representation of physical phenomena. Usually a physical law is not validated through study of a single physical system, which can only provide supporting evidence for the law. Rather, wide acceptance of the law within the scientific community is achieved by demonstrating to the scientific community that for many specific systems, models based upon the law provide good descriptions of the system. To take a specific example, the validity of Newton's theory of universal gravitation became more and more widely accepted as it was shown that, as well as for the motion of bodies near to the surface of the earth, it provided a good model for the movement of the moon around the earth, of the planets around the sun, of tides and of other phenomena. Of course the degree of accuracy required is again a factor. As part of the normal progress of science the validity of the Newtonian model came into question at the turn of the century, not least because the predictions of the model were not in sufficient agreement with the observed motion of the planet Mercury. Thus, although adequate for most terrestrial purposes the model would not now be considered valid for many astronomical calculations.

It is also important to appreciate that, in practice, as implied by the IAEA definition, there is always a subjective element in validation, since different people may have different ideas about what is considered acceptable. This can also be illustrated by an example from the history of science (Koestler, 1975). At the time of Kepler, the Ptolemaic model of the planetary motions was generally regarded as appropriate and was considered to give good enough agreement with the observations. However, Kepler eventually rejected the Ptolemaic system essentially because of a very small discrepancy between its predictions for the motion of the planet Mars and the observations of Tycho Brahe. Many others at the time would have judged that the discrepancy was not sufficient to justify the rejection of the old system. The use of a formal framework for the validation process, for example of the type outlined in Jackson, Lever and Sumner, 1991, can help to minimise the subjective aspects, but cannot eliminate them.

3.2 CONFIDENCE BUILDING

Drawing on the ideas discussed in the last subsection, a number of considerations that are relevant to building confidence in the models of groundwater flow and radionuclide transport can be identified. These are discussed in the following paragraphs. The application of these ideas to the models of flow and transport that have been implemented in NAMMU is discussed in section 8.

3.2.1 Model development

It is important that the process of the derivation and development of the model is clearly presented and documented. This will include a discussion of such issues as the identification of the process or system of interest, the assumptions and approximations that are part of the model and a review of other models that might be relevant. The latter is potentially of great importance as one useful outcome of a validation process may be the ability to discriminate between alternative conceptual models, leading to the conclusion that one or more models that were originally considered plausible are not acceptable representations of the process or system of interest (see e.g. Jackson, Lever and Sumner, 1991).

Of course the amount of detailed documentation of the model development that is required will depend upon the nature of the model. For a model that is widely accepted in the scientific community (e.g. Darcy's law, models of radioactive decay), reference to a standard textbook where the model is explained could be considered to be sufficient documentation. For a model that it not so widely known a fuller justification may be appropriate. In such a case it will be important to demonstrate that the model is built upon existing scientific knowledge. Reference should be made to supporting research programmes and to any similar work carried out by organisations in other countries. As noted in the last section, the aim is to make the case to individuals with relevant technical knowledge that the model is acceptable.

3.2.2 Verification

In order to test a model it is necessary to be able to quantify the implications of the model for particular cases. This can sometimes be achieved analytically but more often requires a numerical implementation of the model in a code such as NAMMU. In either case it is important to verify that the method used to obtain the results is mathematically and numerically correct and that any errors introduced by the solution process (e.g. by a numerical approximation) are quantified and taken into account when the results are compared with measurements. It is important to distinguish between verification and validation. Verification, for a program such as NAMMU, is the process of establishing a high degree of confidence that the computer program correctly solves the equations of the mathematical models which it encapsulates. Validation is the process of building confidence in the models themselves and their applicability to the physical situation under consideration.

3.2.3 Comparison with observations

It is clear from the IAEA definition of validation that comparison of the results of a model with independent field observations and experimental measurements is an important component of the validation process. By its nature, this aspect of validation is specific to a particular site and so, as discussed in subsection 3.1, will include issues related to the validation of the site-specific conceptual model, which lie outwith the scope of this NAMMU Assessment Model Validity document. However, examples of successful applications are included in the document, as they can help to build confidence in the generic model of the physical processes that are implemented in NAMMU. There are a number of issues that it is important to bear in mind when performing such comparisons.

It is only possible to perform a meaningful comparison if the uncertainties in both the predictions and the measurements are quantified. Only then is it possible to establish the extent to which a match can be expected. In estimating the uncertainties in the data it is important to bear in mind that many 'observations' are not raw data but are the result of the interpretation of raw data in terms of some model of the system ('measured' environmental pressures in boreholes, for example, are the result of the extrapolation of an observed response to an imposed pressure pulse).

In most cases a model will be capable of producing a wide range of results, depending on the values that are assigned to the parameters of the model. It will generally be necessary to calibrate the model, that is to obtain values for the parameters so that the model provides a good description for at least some of the data. The quality of the fit that can be obtained gives some indication of the confidence that can be placed in the model. The level of confidence that can be placed in a model is greatly increased if it can then be used to make adequate predictions of the values of quantities that are independent of those that were used to calibrate the model.

When assessing the acceptability of the agreement between model predictions and data it is important to take into account the length scales (technically the 'support scale', Journel & Huijbregts, 1978) of the information. For example, it may be that the measurements have been performed at a scale that is smaller than the resolution of the mesh used in the numerical representation of the model. In such a case the model would not be capable of reproducing the detailed variability of the measurements, but should be able to give an acceptable representation of any overall larger-scale trends.

Many different types of data can play a role in the validation of models of groundwater flow and radionuclide transport. Each type has its own advantages and disadvantages. Laboratory experiments play an important role in the development of models of processes that can be considered to be significant at the pore scale, such as rock-matrix diffusion and anion exclusion. The experiments serve both to provide parameter values for the models and to test the validity of different models (e.g. Jackson, Lever and Sumner, 1991).

Field experiments within and between boreholes have the advantages that the disturbances that are induced to the natural system are relatively well controlled so that the appropriate inputs to be used in models of the experiments are reasonably clear. The degree of agreement that can be expected between the measurements and the model predictions is therefore fairly well defined. However, at locations that are considered suitable for a repository the groundwater velocities are likely to be relatively small. The volume of the rock that can be tested within a reasonable experimental timescale will therefore be a small fraction of the volumes of interest in an assessment calculation.

Natural analogue studies provide data that arise from processes that occur on timescales similar to those of interest in an assessment. They therefore provide a means to assess the ability of the models to predict the behaviour of the system over relatively large length scales and long timescales. However, the initial conditions of the system are very uncertain and these uncertainties must be taken into account in assessing the acceptability of the model.

3.2.4 Validation of submodels

When an overall system model can be considered to be made up of individual submodels, it is valuable, where possible, to validate the individual submodels as well as the overall system model. This helps to build confidence in the system model. The following example illustrates the principle. Models of radionuclide transport contain a term that depends on the groundwater velocity and simply describes advection of radionuclides by the groundwater. The values of the groundwater velocities will be obtained from an underlying model of the groundwater flow. Before attempting to validate the overall model of radionuclide transport it would be valuable to ensure that the underlying groundwater flow model is valid.

3.2.5 Peer review

Peer review is, of course, an important part of the scientific enterprise. In practice, it can take many forms including:

- peer review of journal articles and conference papers that are based on the use of the model;
- use of the model by organisations other than that by which it was originally developed;
- formal external review of all or part of an assessment or other modelling study by a recognised scientific body;
- involvement in international model testing and collaborative projects (e.g. HYDROCOIN (1988, 1990, 1991, 1992), INTRAVAL (1990), GEOTRAP).

In all of these cases, independent external assessment of the models helps build confidence that they are fit for the purposes for which they are being applied.

3.2.6 Work in related fields

Additional confidence in the models of groundwater flow and radionuclide transport can be obtained from the fact that identical or very similar models are used in related fields. Many of the models of groundwater flow and radionuclide transport processes were developed and are still applied in water resources engineering (Bear, 1979, de Marsily, 1986). Very similar models of fluid movement in porous media are used in models of oil reservoirs (e.g. Pinder, 1983). In both of these cases the timescales of interest are much shorter than in repository performance assessment calculations and the results of the models can be evaluated by comparison with the observed response of the system. The continued (indeed increasing) application of the models in these fields testifies to their usefulness and to the confidence that can legitimately be placed in them.

4 PURPOSE OF MODEL AND CONTEXT

The validity of a model only needs to be demonstrated for that part of the assessment process to which it will be applied. It is therefore necessary to consider the overall purpose of the model and the context in which it will be used. In practice, even within the restricted context of performance assessment calculations, many uses can be envisaged for a software package with the flexibility of NAMMU. Examples of the sort of calculations relevant to a performance assessment that could be performed with NAMMU are:

- the calculation of the effective permeabilities of blocks of rock a few hundred metres across (the sub-block scale variability in the permeability is explicitly represented in a NAMMU model of the block);
- two-dimensional regional-scale calculations of coupled groundwater flow and salt transport (or groundwater flow coupled to the transport of salt and heat) in a vertical cross section;
- three-dimensional regional-scale calculations of groundwater flow coupled to the transport of salt and heat;
- two-dimensional calculations of groundwater flow in a sub-horizontal transmissive layer;
- two-dimensional regional-scale calculations of radionuclide transport in a vertical cross section;
- three-dimensional calculations of the effects of a well with a large abstraction rate on the groundwater flow in the vicinity of a potential repository;
- three-dimensional calculations to investigate the effect of shafts and drifts on the performance of a repository system;
- calculations to estimate repository resaturation times;
- calculations to investigate the effect of the extent of container failure on the flux of radionuclides leaving a waste stack.

This list is purely illustrative and is not intended to be comprehensive. Many other potential uses of NAMMU can easily be envisaged (for example, calculations of flow and transport in the unsaturated zone, calculations with a detailed representation of the heterogeneity in rock properties, etc.). It is clearly impractical to anticipate all of the potential applications of NAMMU in the course of a performance assessment. However, the type of information that is abstracted from calculations of the type listed above for subsequent use in other parts of the performance assessment falls into four general categories:

- groundwater velocities in the domain of interest and across the boundaries of the domain;
- groundwater travel times along advective pathlines;
- radionuclide concentrations in the domain;

- radionuclide fluxes within the domain and across the boundaries of the domain.

These results obtained from NAMMU can play many roles in other calculations that contribute to the performance assessment. Again, it is not possible to give a comprehensive list, but the following examples will serve as illustrations:

- groundwater velocities can be used as inputs to models of near-field behaviour and can be used in assessing how well the model agrees with the available data on the overall water balance at a site;
- travel times can be used to parameterise simplified (e.g. one-dimensional) models of radionuclide transport and to assess the performance of the model relative to the available site data on groundwater ages;
- radionuclide concentrations can be used in some types of assessment calculations (e.g. those considering the radiological impact of water supply wells);
- radionuclide fluxes can be used as inputs to models of radiological exposure in the biosphere.

It will be clear that the models implemented in NAMMU can be applied over a wide range of length- and time-scales. The length scales of interest include that relevant to a single waste canister (a few metres), that of a block of rock a few tens or hundreds of metres in extent and that of regional-scale groundwater flow models (a few tens of kilometres). Models of the regional groundwater flow system are required because the transport pathways and the controls on groundwater flow may be on this scale. Similarly, the timescales of interest range from a few tens or hundreds of years (the possible timescales for some near-field processes or repository resaturation) to tens of millions of years (the possible timescales for the transport of strongly-sorbed long-lived radionuclides).

The inputs required by the models will depend on the type of system that the model is intended to represent. In general, it will be necessary to specify the geometry of the domain of interest and the distribution of hydrogeological properties within the domain. In many cases the distribution of properties will be related to the distribution of sub-regions that can be identified on other grounds (e.g. lithostratigraphic units) and represented as units within the model. It is also necessary to specify sufficient boundary conditions for each of the variables of interest to make the problem mathematically well posed. Initial conditions will also be required for transient calculations.

As an illustration of the types of information that would be required in a typical case, suppose that the aim is to calculate the migration of radionuclides from the repository to the biosphere in a domain in which the groundwater flow is influenced by the effect of dissolved salt on the density of the water. The first stage in such a calculation would be to compute the groundwater flow, taking account of the coupling between the flow and the transport of salinity. Assuming that a steady-state calculation is appropriate, the following information would have to be specified:

- the geometry of the domain;
- the distribution of permeability within the domain;
- the relationship between salt concentration and the density of the water;
- either the residual pressure or the groundwater flux at all points on the boundary of the domain;
- either the concentration of salt or the flux of salt at all points on the boundary of the domain;
- any internal source or sinks of salt (e.g. from dissolution of halite-bearing rocks).

The output from the above calculation could then be used as an input to a calculation of radionuclide transport. The information that would have to be specified for that calculation is then:

- the geometry of the domain;
- the distributions of porosity, sorption coefficients, dispersion coefficients and effective diffusion coefficients in the domain;
- the initial concentration of radionuclide in the domain (presumably significant in the repository and zero elsewhere);
- either the concentration of radionuclide or the flux of radionuclide at all points on the boundary of the domain;
- any internal source or sinks of radionuclide (e.g. from decay or ingrowth).

A similar pattern of requirements would apply to most calculations of interest.

A specific example of the use of NAMMU in an assessment performed by SKB is provided by the work described in Boghammar, Grundfelt and Hartley, 1997). In this case, NAMMU was used to calculate the large-scale groundwater flow at the 'Ceberg' example site. Three-dimensional groundwater flow calculations were performed for models at two different length scales, covering areas of approximately 300 km^2 and 50 km^2, respectively. The models were used to calculate the groundwater velocities in the domain and, in particular, to investigate the locations of areas of significant groundwater recharge and discharge. Advective pathlines were used to investigate groundwater velocities at a hypothetical repository location and to calculate travel times from that location. Pathlines were also used to help identify locations of groundwater recharge and discharge. The models were used to investigate the sensitivity of the calculated groundwater flow patterns and travel times to the boundary conditions applied to the model and to the hydrogeological properties of the rock units that were included in the model. It was also anticipated that the smaller of the two models would be used to supply boundary conditions for an even smaller, local-scale groundwater flow model in which the heterogeneity of the permeability would be explicitly represented using a geostatistical approach.

5 BASIC PREMISES OF THE ASSESSMENT APPROACH

Inevitably, there are various aspects of the modelling work carried out as part of a performance assessment that are simply basic judgments or assumptions underlying the development of the modelling approach. In the present context, these are basically judgments of the type of model that will give a good representation of the behaviour of the hydrogeological system or of the likely evolution of the repository system after closure. The assumptions can usefully be divided into two categories. The first category consists of basic assumptions of the assessment approach. These are not specific to any particular model of the system (or parts of the system) but are general assumptions that would need to be taken into account in any model of the system. Indeed, given that in any performance assessment many modelling tools will be used, it is important to ensure that these assumptions are identified and applied consistently in all of the calculations that are performed. The following are examples of the type of assumptions in the first category that are relevant to assessments performed by SKB (SR 95, 1995). This is not an extensive list, but is sufficient to give an indication of the type of assumptions in this category. It is assumed, for example, that:

- the rock where the waste is deposited remains basically stable;
- the part of the rock that is affected by the construction of the repository belongs chiefly to the near field;
- radionuclides will be accessible for transport into the far-field, which implies some container damage;
- the repository is closed and backfilled;
- the transient nature of the groundwater flow induced by processes associated with climate change may be significant and should be taken into account.

Assumptions in this category are too broad to warrant inclusion in a general model validity document such as this. These assumptions relate to the overall assessment strategy, rather than to the individual model under consideration. However, when the overall strategy is developed, it will be important to ensure that the models that are to be used are capable of adequately representing the phenomena that are required by the assessment strategy. An example may help to illustrate this point. As noted above, it is expected that it will be necessary for the assessment to take account of the transient groundwater flow associated with climate change. Thus, a groundwater flow model that can deal with transient flow will be required. In practice, this will involve calculations of coupled, transient, groundwater flow and salt transport, because one result of climate change will be the movement of the boundaries of the Baltic Sea. In this sense, NAMMU will be a valid model to use, as it can represent this process. However, the detailed validity of any particular model of flow and transport at the site depends upon the validity of the climate sequence that is constructed to provide boundary conditions for the NAMMU model and of the initial conditions supplied to the NAMMU model. These are not issues of the validity of the model of flow and transport processes that has been implemented in NAMMU, but of the inputs to NAMMU. These issues lie outside the scope of the present document which need only consider the general validity of the model of flow and transport that is implemented in NAMMU.

It should also be borne in mind that a complete performance assessment will make use of a wide range of analytical and numerical models and it is not necessary for all models to be able to represent all of the processes of interest. Various uses that could be made of NAMMU were summarised in section 4.

The second category of assumptions are those that underlie the basic models of the physical processes that are implemented in NAMMU. These have been outlined in section 2 and are discussed in more detail in section 6. This category would include the assumptions that representations such as:

- the continuum porous medium approach (for both groundwater flow and radionuclide transport);
- Darcy's law;
- the Fickian model of diffusion;
- the Fickian model of dispersion;
- the linear equilibrium model of sorption;
- the treatment of anion exclusion;

are valid.

In many of these cases, the model is not universally valid, but is fit for purpose in most situations of interest. It is important to ensure that any model is only applied within its domain of validity.

6 TREATMENT OF PHENOMENA WITHIN THE MODEL

6.1 IDENTIFICATION OF RELEVANT FEPS

The aim of this section is to identify a list of Features, Events and Processes (FEPs) relevant to the performance assessment of a repository that can be investigated using NAMMU, and then to present the approach to the modelling of the FEPs that is adopted within NAMMU. In the past few years a number of studies have been performed with the aim of compiling lists of FEPs that should be considered in a performance assessment. Three examples that are perhaps most relevant to the present document are:

- the NEA international FEP list, compiled by the OECD/NEA (NEA, 1995);
- the Process Influence Diagram that was produced as part of the SKI Site-94 Deep Repository Performance Assessment Project (SKI, 1996);
- the interaction matrix for the far field produced for the Rock Engineering System (RES) approach by SKB (see e.g. SR 95).

The RES approach has been used to identify the key parameters that are of relevance in characterising the far-field Process System (Skagius, Ström and Wiborgh, 1995), and to list the interactions between them. All of these sources of information can be used to identify FEPs that are relevant when modelling groundwater flow and radionuclide transport. In each case, many other FEPs (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 FEPs from each of the information sources that can be explicitly modelled by NAMMU are summarised in the rest of this subsection. The models used in NAMMU are then discussed in the remaining subsections.

The relevant FEPs from the NEA FEP list are:

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.)

The relevant FEPs that can be identified from the Site-94 PID include:

- Groundwater flow;
- temperature;
- matrix diffusion;
- dispersion;
- anion exclusion;
- diffusion;
- radioactive decay,
- groundwater chemistry;
- sorption.

These processes were identified as relevant in both the near and far field. Additional relevant FEPs that were more specifically identified as either far field or near field were:

- resaturation;
- deep saline water intrusion
- distribution and release of radionuclides from the geosphere;
- transport and release of radionuclides, near field;

The relevant parameters identified in the RES approach that are modelled explicitly by NAMMU are as follows:

- groundwater movement
- groundwater pressure
- groundwater chemistry
- temperature/heat
- transport of radionuclides

The remaining far field parameters in the interaction matrix are represented implicitly in a NAMMU model. For example, the biosphere parameter is modelled in terms of its effects on the boundary conditions that would be applied to a NAMMU model. Similarly the effects of the repository source term parameter can be modelled as source terms for radionuclides and heat that are included in the NAMMU model.

It can be seen that there is a broad similarity between the three lists, the differences essentially being in the amount of detail that any individual list includes for a particular process. The list obtained from the RES analysis could be considered to be a useful summary of the 'top level' processes that should be considered. The other lists give more detail, for example on the individual processes that contribute to radionuclide transport (and these can also be found in the full interaction matrix from the RES approach). In the following subsections, the list from the RES approach will be used to give a framework for a description of the way in which NAMMU models the parameters in the list, and the interactions of these parameters on others (both explicit and implicit). Together, this forms a complete description of how NAMMU treats each of the FEPs identified by SKB as being of relevance to the far field.

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

It should be noted that this approach to describing the models used in NAMMU is essentially phenomenological. That is, it describes the models in terms of the FEPs that have been identified by experts as being important, rather than describing the fundamental phenomena that might be expected on theoretical grounds (the traditional textbook approach).

6.2 GROUNDWATER MOVEMENT

The soils and rocks which make up the Earth's crust are generally porous, that is they contain empty spaces which can be occupied by groundwater. This empty space is called 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 (Bear 1972, Bear 1979, Freeze and Cherry 1979, de Marsily 1985, Ward 1975). 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 (Bear 1972). 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 (de Marsily 1985). 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 (Herbert 1991, Herbert and Spawski 1990, Robinson 1984, Stratford et al. 1990). 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 (Bear 1972, Bear 1979, Freeze and Cherry 1979, de Marsily 1985),

$$\mathbf{q} = -\frac{k}{\mu}(\nabla P^T - \rho_l \mathbf{g}) \qquad 6\text{-}1$$

where P^T is the groundwater pressure (specifically the total pressure - see section 6.1.2),
ρ_l is the groundwater density,
$\mathbf{g}$ is the gravitational acceleration,
μ is the viscosity of the groundwater, and
k is the permeability of the rock, a measure of its ability to permit flow

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 (Batchelor, 1967) 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. Scheidegger, 1974).

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 (Scheidegger 1974, Bear 1979, de Marsily, 1986) (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 (de Marsily, 1986). 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 (de Marsily, 1986). 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 which 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 (Warren and Root, 1963). 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 - 100 degrees Celsius. 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 (Agg et. al 1996).

6.3 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 subsection 7.3.1). 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 subsection 7.3.1).

The familiar concept of groundwater or hydraulic “head” (Bear, 1979) is a quantity closely related to the residual pressure. Hydraulic head is the residual pressure divided by the specific weight of the groundwater (see subsection 7.3.1). 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,

$$\mathbf{q} = -\frac{k}{\mu}(\nabla P^T - \rho_l \mathbf{g}) \qquad 6\text{-}2$$

together with the equation of conservation of mass,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0 \qquad 6\text{-}3$$

where ϕ is the porosity and the other symbols are as defined previously. These two equations lead to a single second-order equation for the total pressure,

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.(\rho_l \frac{k}{\mu}(\nabla P^T - \rho_l g)) = 0 \qquad 6\text{-}4$$

This is the basic equation which 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 of the water depends 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, it is necessary to couple the solution of the groundwater flow problem to that of the heat or salt transport problem.

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. The model for the change in density associated with the presence of dissolved salt is discussed in the next section.

6.4 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 the following relationship:

$$\frac{1}{\rho_l} = \frac{c}{\rho_s} + \frac{1-c}{\rho_0}, \qquad 6\text{-}5$$

where c is the concentration of dissolved salt, ρ_l is the density of the saline groundwater, ρ_s is the density of saturated brine, and ρ_0 is the density of freshwater (i.e. at a concentration of $c = 0$). However, the relationship between the groundwater density and the concentration of total dissolved solids can be specified by the user, 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 and 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. As noted in the last section, if the concentration of salt is sufficiently large, then the density of the fluid will depend on the salt concentration and this leads to a coupling between the groundwater flow and salt transport processes.

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 subsection 6.6.5. 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.

6.5 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. These changes are discussed in subsections 6.2 and 6.3.

It is 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.

6.6 RADIONUCLIDE TRANSPORT

The processes that can result in transport of dissolved radionuclides by groundwater were outlined in section 2. In the following subsections, the processes are described in more detail. These processes can all be treated by NAMMU, albeit to different degrees of accuracy.

6.6.1 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, F_A, of a radionuclide is related to the specific discharge, $\mathbf{q}$, (equation 6-1) by

$$F_A = \mathbf{q}\, c_n / \phi\,, \qquad 6\text{–}6$$

where c_n is the local concentration of mobile radionuclide per unit volume of flowing porewater and ϕ is the porosity. 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

$$\mathbf{u} = \mathbf{q} / \phi\,, \qquad 6\text{-}7$$

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.

6.6.2 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. The flux per unit surface area of porous medium, $\mathbf{F}$, is linked to the concentration gradient by Fick's Law (Jost, 1960),

$$\mathbf{F} = -D_\mathrm{i}\, \nabla c_n\,, \qquad 6\text{-}8$$

where D_i is termed the intrinsic or effective diffusion coefficient, which is less than the free water diffusion coefficient and is related to the latter by a scaling factor which 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.

6.6.3 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 (Bear, 1979). 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 (Bear 1979). 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 (Dagan 1988,1989, Gelhar and Axness, 1983).

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 and 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 (Dagan, 1988,1989, Gelhar and Axness, 1983). 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 asymptotic value of the longitudinal dispersion coefficient is determined by the length scale of the heterogeneity and the variance of the log-permeability. 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 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. Morris, Porter and Jackson, 1997a). 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 (Morris, Porter and Jackson, 1997b) 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 (Dagan, 1988, 1989) 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 and the particle movements in a case with a heterogeneous permeability field, that is in which there was significant element to element variation in the permeability values. 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 (Cliffe and Jackson, 1993). 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. Baker and Jefferies 1997, SKI 1996, Norman 1992). An appropriate and consistent treatment of heterogeneity on all length scales is an important aspect of performance assessment calculations (e.g. Jackson and Watson, 1997).

6.6.4 Rock-matrix diffusion

The process of rock-matrix diffusion is potentially significant in many fractured rocks (de Marsily 1986, Neretniekes 1980). 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 (Baker and Jefferies, 1997) 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 (Cliffe and Herbert 1990).

6.6.5 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 (Baker and Jefferies 1997). 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. Such processes cannot be represented by the same simple models as linear sorption.

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 NSARP is directed at confirming and increasing confidence that the linear approach K_d is an appropriate representation for the radionuclides of interest (Baker and Jefferies 1997).

6.6.6 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 (Baker and Jefferies 1997). 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.

6.6.7 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 (Baker and Jefferies 1997). 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.

6.6.8 Radioactive decay and ingrowth

Radioactive concentrations are also affected by the processes of radioactive decay and ingrowth from parent radionuclides. 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 five members in this way.

7 MATHEMATICAL FORMULATION AND SOLUTION TECHNIQUES

7.1 CONCEPTUAL MODELS

In this section we describe the conceptual models used in NAMMU. Before describing the various models, it is necessary to consider what is meant by a conceptual model. For the purposes of this report we will use the definition put forward by Olsson, Bäckblom, Gustafson, Rhén, Stanfors and Wikberg, 1994. 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 it constructed using NAMMU will contain all of the elements of a conceptual model identified by Olsson et. al. 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 is 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 7.2, the geometric framework and the method of spatial assignment of the parameters is described. In section 7.3 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 is described in section 6. The numerical techniques used in NAMMU are summarised in section 7.4.

7.2 COMMON FEATURES

7.2.1 Geometric framework

The spatial region represented in a NAMMU model is discretised using the finite-element method. The finite-element mesh used is composed of patches. 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 coordinates 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 by patches, with rock types specified in the same way as for ordinary patches. The fault zones may be defined by specifying a fault line or plane and a fault width vector. This facility enables 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 coordinates of the corners of each element, its mapping function, and its rock type.

7.2.2 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. 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.

7.2.3 Boundary conditions

The basic types of boundary conditions available in NAMMU consist of specified value and specified flux conditions for the variables. These may be constant, or spatially-varying. Specified value conditions may be constant in time, or can be varying in time for transient calculations. The default 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.

7.3 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.

7.3.1 Groundwater flow

Physical processes

Groundwater flow in a porous medium is modelled in terms of Darcy's law (see section 6.2),

$$\mathbf{q} = -\frac{k}{\mu}.\nabla P^{R} , \qquad 7\text{-}1$$

and the equation of continuity,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l\mathbf{q}) = 0 . \qquad 7\text{-}2$$

where $\mathbf{q}$ is the Darcy velocity,
k is the permeability,
μ is the fluid viscosity,
P^R is the residual pressure (see below),
ϕ is the porosity, and
ρ_l is the fluid density.

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

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.(\rho_l\frac{k}{\mu}.\nabla P^{R}) = 0, \qquad 7\text{-}3$$

and the flux for this pressure equation is

$$F_P = \rho_l\mathbf{q}.\mathbf{n} , \qquad 7\text{-}4$$

where **n** is the outward normal to the boundary across which the flux is specified.

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

$$P^R = P^T + \rho_0 g(z - z_0),$$

where ρ_0 is a reference density, g is gravitational acceleration, z is height, and z_0 is a reference elevation.

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

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

Parameters required

The parameters required are as follows:

Permeability, k, is constant, or constant for a given rock type, or can be an arbitrary function of position, and can be an anisotropic tensor,

Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant, and ϕ_0 and $\frac{d\phi}{dP^T}$ are constant, or constant for a given rock type, or can be arbitrary functions of position and of pressure,

Fluid density, ρ_l, is a constant,

Fluid viscosity, μ, is a constant.

Initial and boundary conditions

Initial conditions - prescribed pressure.

Boundary conditions - prescribed flux of fluid, prescribed pressure.

7.3.2 Groundwater flow and heat transport

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,

$$\mathbf{q} = -\frac{k}{\mu}(\nabla P^R - (\rho_l - \rho_0)\mathbf{g}), \qquad 7\text{-}5$$

the continuity equation,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l\mathbf{q}) = 0, \qquad 7\text{-}6$$

and the heat transport equation (Bear 1972),

$$(\rho c)_a\frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q}.\nabla T - \Gamma_a \nabla^2 T = H, \qquad 7\text{-}7$$

where T is the temperature, $(\rho c)_a$ is the average heat capacity of the rock and liquid, c_l is the specific heat capacity of the liquid, Γ_a is the average thermal capacity of the rock and liquid, and H is a heat source.

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

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.(\rho_l \frac{k}{\mu}.(\nabla P^R - (\rho_l - \rho_0)g)) = 0, \qquad 7\text{-}8$$

The fluxes for the pressure and temperature equations are

$$\begin{aligned} F_P &= \rho_l \mathbf{q}.\mathbf{n}, \\ F_T &= -\Gamma_a \nabla T.\mathbf{n} \end{aligned} \qquad 7\text{-}9$$

where $\mathbf{n}$ is the outward normal to the boundary across which the flux is specified.

Parameters required

The parameters required are as follows:

Permeability, k, is constant, or constant for a given rock type, or can be an arbitrary function of position, Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant and ϕ_0 and $\frac{d\phi}{dP^T}$ are constant, or constant for a given rock type, or can be arbitrary functions of position, pressure, and temperature,

Fluid density, ρ_l is a function of pressure and temperature,

Fluid viscosity, μ, is a function of temperature,

Average thermal conductivity of rock, $\Gamma_a = \phi\Gamma_l + (1-\phi)\Gamma_s$ is approximated by the thermal conductivity of the rock, Γ_s, and is constant, or constant for a given rock type,

The average heat capacity of the rock and liquid, $(\rho c)_a = \phi\rho_l c_l + (1-\phi)\rho_s c_s$, is approximated by the heat capacity of the rock, $\rho_s c_s$, where c_l is the specific heat capacity of the liquid and is a constant, ρ_s is the density of the solid and is constant, or is constant for a given rock type, and c_s is the specific heat capacity of the solid and is constant, or is constant for a given rock type.

Initial and boundary conditions

Initial conditions - prescribed pressure, prescribed temperature.

Boundary conditions - prescribed flux of fluid, prescribed pressure, prescribed temperature, prescribed heat flux.

7.3.3 Unsaturated groundwater flow

Physical processes

This is modelled in terms of a modified version of Darcy's law (see section 6.2),

$$\mathbf{q} = -\frac{k_r k}{\mu}.\nabla P^R , \tag{7-10}$$

and the equation of continuity,

$$\frac{\partial}{\partial t}(\phi S \rho) + \nabla.(\rho_l \mathbf{q}) = 0, \tag{7-11}$$

where k_r is the relative permeability, and
S is the saturation,

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

$$\frac{\partial}{\partial t}(\phi S \rho_l) - \nabla.(\rho_l \frac{k_r k}{\mu}.\nabla P^R) = 0, \qquad 7\text{-}12$$

and the flux for this pressure equation is given by

$$F_P = \rho_l \mathbf{q}.\mathbf{n}. \qquad 7\text{-}13$$

where $\mathbf{n}$ is the outward normal to the boundary across which the flux is specified.

Parameters required

The parameters required are as follows:

Permeability, k, is constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic,

Relative permeability, k_r, is an arbitrary function of saturation, S, where S is related to the total pressure through a specified capillary pressure curve.

Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant and ϕ_0 and $\frac{d\phi}{dP^T}$ are constant, or constant for a given rock type, or can be arbitrary functions of position and of pressure,

Fluid density, ρ_l is a constant,

Fluid viscosity, μ, is a constant.

Initial and boundary conditions

Initial conditions - prescribed pressure.

Boundary conditions - prescribed flux of fluid, prescribed pressure.

7.3.4 Unsaturated groundwater flow and heat transport

Physical processes

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

$$\mathbf{q} = -\frac{k_r k}{\mu}(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}), \tag{7-14}$$

the equation of continuity,

$$\frac{\partial}{\partial t}(\phi S \rho_l) + \nabla.(\rho_l \mathbf{q}) = 0, \tag{7-15}$$

and the heat transport equation,

$$(\rho c)_a \frac{\partial T}{\partial t} + \rho_l c_l \mathbf{q}.\nabla T - \Gamma_a \nabla^2 T = H, \tag{7-16}$$

where T is the temperature and H is a heat source.

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

$$\frac{\partial}{\partial t}(\phi S \rho_l) - \nabla.(\rho_l \frac{k_r k}{\mu}.(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g})) = 0, \tag{7-17}$$

The fluxes for the pressure and temperature equations are

$$\begin{aligned} F_P &= \rho_l \mathbf{q}.\mathbf{n}, \\ F_T &= -\Gamma_a \nabla T.\mathbf{n}' \end{aligned} \tag{7-18}$$

where $\mathbf{n}$ is the outward normal to the boundary across which the flux is specified.

Parameters required

The parameters required are as follows:

Permeability, k, is constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic,

Relative permeability, k_r, is an arbitrary function of saturation, S, where S is related to the total pressure through a specified capillary pressure curve.

Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant and ϕ_0 and $\frac{d\phi}{dP^T}$ are constant, or constant for a given rock type, or can be arbitrary functions of position pressure, and temperature,

Fluid viscosity, μ, is a function of temperature, Fluid density, ρ_l is a function of pressure and temperature,

Average thermal conductivity of rock, $\Gamma_a = \phi\Gamma_l + (1-\phi)\Gamma_s$ is approximated by the thermal conductivity of the rock, Γ_s, and is constant, or constant for a given rock type,

The average heat capacity of the rock and liquid, $(\rho c)_a = \phi\rho_l c_l + (1-\phi)\rho_s c_s$, is approximated by the heat capacity of the rock, $\rho_s c_s$, where c_l is the specific heat capacity of the liquid and is a constant, ρ_s is the density of the solid and is constant, or is constant for a given rock type, and c_s is the specific heat capacity of the solid and is constant, or is constant for a given rock type.

Initial and boundary conditions

Initial conditions - prescribed pressure, prescribed temperature.

Boundary conditions - prescribed flux of fluid, prescribed pressure, prescribed temperature, prescribed heat flux.

7.3.5 Radionuclide transport

Physical processes

This is modelled using the following equation (Bear 1972, Bear 1979, Freeze and Cherry 1979, de Marsily 1985),

$$\frac{\partial}{\partial t}(\phi R_\alpha N_\alpha) + \mathbf{q}.\nabla N_\alpha - \nabla.(\phi\mathbf{D}_\alpha.\nabla N_\alpha) = -\lambda_\alpha \phi R_\alpha N_\alpha + \lambda_{\alpha-1}\phi R_{\alpha-1} N_{\alpha-1} + \phi f_\alpha \qquad 7\text{-}19$$

where N_α is the concentration of nuclide α, R_α is the retardation factor for nuclide α, D_α is the dispersion tensor for nuclide α, λ_α is the decay constant for nuclide α and f_α is the source term for nuclide α.

Normally $\mathbf{q}$ will be calculated from an initial groundwater flow calculation.

The flux for the nuclide equation is

$$F_{N_\alpha} = (\mathbf{q}N_\alpha - \phi\mathbf{D}_\alpha \nabla N_\alpha).\mathbf{n} \qquad 7.20$$

where $\mathbf{n}$ is the outward normal to the boundary across which the flux is specified.

Parameters required

The parameters required are as follows:

Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant and ϕ_0 and $\frac{d\phi}{dP^T}$ are 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, R_α, for each nuclide, are defined in terms of the sorption coefficients, $K_{d,\alpha}$, which are constant for a given rock type and nuclide, by $R_\alpha = 1 + \frac{(1+\phi)}{\phi}K_{d,a}$.

Decay constants, λ_α, for each nuclide, are constant,

Dispersion tensor, $\mathbf{D}_\alpha$ is given by

$$\mathbf{D}_\alpha = \frac{D_{p\alpha}}{\tau}\delta_{ij} + \alpha_{T\alpha} v \delta_{ij} + (\alpha_{L\alpha} - \alpha_{T\alpha})\frac{v_i v_j}{v},$$

where $D_{p\alpha}$ are the molecular diffusion coefficients for each nuclide and are constant, τ is the tortuosity which is constant for a given rock type, $\alpha_{T\alpha}$ and $\alpha_{L\alpha}$ are the longitudinal and transverse dispersion lengths for each nuclide, and are constant, or constant for a given rock type, or can be arbitrary functions of position, saturation and velocity, and v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \frac{\mathbf{q}}{\phi}$,

Source term, f_α for each nuclide is a function of position and time.

Initial and boundary conditions

Initial condition - prescribed concentration.

Boundary conditions - prescribed concentration or prescribed flux of radionuclide or zero dispersive flux.

7.3.6 Radionuclide transport in unsaturated flow

Physical processes

This is modelled using the following equation (Bear 1972, Bear 1979, Freeze and Cherry 1979, de Marsily 1985),

$$\frac{\partial}{\partial t}(\phi S R_\alpha N_\alpha) + \mathbf{q}.\nabla N_\alpha - \nabla.(\phi S \mathbf{D}_\alpha.\nabla N_\alpha) = -\lambda_\alpha \phi S R_\alpha N_\alpha + \lambda_{\alpha-1}\phi S R_{\alpha-1} N_{\alpha-1} + \phi S f_\alpha \qquad 7\text{-}21$$

where N_α is the concentration of nuclide α, R_α is the retardation factor for nuclide α, D_α is the dispersion tensor for nuclide α, λ_α is the decay constant for nuclide α and f_α is the source term for nuclide α.

Normally $\mathbf{q}$ will be calculated from an initial unsaturated groundwater flow calculation.

The flux for the nuclide equation is

$$F_{N_\alpha} = (\mathbf{q}N_\alpha - \phi S \mathbf{D}_\alpha \nabla N_\alpha).\mathbf{n} \qquad 7\text{-}22$$

where $\mathbf{n}$ is the outward normal to the boundary across which the flux is specified.

Parameters required

The parameters required are as follows:

Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant and ϕ_0 and $\frac{d\phi}{dP^T}$ are 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, R_α, for each nuclide, are defined in terms of the sorption coefficients, $K_{d,\alpha}$, which are constant for a given rock type and nuclide, by $R_\alpha = S + \frac{(1+\phi)}{\phi}K_{d,\alpha}$.

Decay constants, λ_α, for each nuclide, are constant,

Dispersion tensor, $\mathbf{D}_\alpha$ is given by

$$\mathbf{D}_\alpha = \frac{D_{p\alpha}}{\tau}\delta_{ij} + \alpha_{T\alpha} v \delta_{ij} + (\alpha_{L\alpha} - \alpha_{T\alpha})\frac{v_i v_j}{v},$$

where $D_{p\alpha}$ are the molecular diffusion coefficients for each nuclide and are constant, τ is the tortuosity which is constant for a given rock type, $\alpha_{T\alpha}$ and

$\alpha_{L\alpha}$ are the longitudinal and transverse dispersion lengths for each nuclide, and are constant, or constant for a given rock type, or can be arbitrary functions of position, saturation and velocity, and v_i are the components of the porewater velocity, which is given by $\mathbf{v} = \dfrac{\mathbf{q}}{\phi}$,

Source term, f_α for each nuclide is a function of position and time.

Initial and boundary conditions

Initial condition - prescribed concentration.

Boundary conditions - prescribed concentration or prescribed flux of radionuclide or zero dispersive flux.

7.3.7 Coupled groundwater flow and solute transport

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,

$$\mathbf{q} = -\frac{k}{\mu}(\nabla \mathrm{P}^{\mathrm{R}} - (\rho_l - \rho_0)\mathbf{g}), \qquad 7\text{-}23$$

the continuity equation,

$$\frac{\partial}{\partial t}(\phi\rho_l) + \nabla.(\rho_l \mathbf{q}) = 0, \qquad 7\text{-}24$$

and the advection-dispersion equation,

$$\frac{\partial}{\partial t}(\phi\rho_l c) + \nabla(\rho_l \mathbf{q} c) = \nabla.(\phi\rho\mathbf{D}.\nabla c). \qquad 7\text{-}23$$

where c is the concentration of solute as a mass fraction of the reference concentration, and ρ_l is the liquid density.

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

$$\frac{\partial}{\partial t}(\phi\rho_l) - \nabla.(\rho_l \frac{k}{\mu}.(\nabla P^R - (\rho_l - \rho_0)g)) = 0, \qquad 7\text{-}24$$

The fluxes for the pressure and concentration equations are

$$F_P = \rho_l \mathbf{q}.\mathbf{n},$$
$$F_c = (\rho_l \mathbf{q} c - \phi\rho_l \mathbf{D}.\nabla c).\mathbf{n} \qquad 7\text{-}25$$

Parameters required

The parameters required in this case are as follows:

Permeability, k, is constant, or constant for a given rock type, or can be an arbitrary function of position, and can be anisotropic,

Porosity, ϕ, is given by $\phi = \phi_0 + (P^T - P_0^T)\frac{d\phi}{dP^T}$, where P_0^T is a constant and ϕ_0 and $\frac{d\phi}{dP^T}$ are constant, or constant for a given rock type, or can be arbitrary functions of position and pressure,

Dispersion tensor, $\mathbf{D}$ is given by $\mathbf{D} = \frac{D_m}{\tau}\delta_{ij} + \alpha_T v\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{v}$, where D_m is the molecular diffusion coefficient and is constant, τ is the tortuosity and is constant for a given rock type, α_T and α_L are the longitudinal and transverse dispersion lengths, and are constant, or constant for a given rock type, or can be arbitrary functions of position, saturation and velocity, and the porewater velocity is given by $\mathbf{v} = \frac{\mathbf{q}}{\phi}$,

The liquid density, ρ_l is given by $\frac{1}{\rho_l} = \frac{1-c}{\rho_0} + \frac{c}{\rho_s}$, where ρ_0 and ρ_s are constants.

Fluid viscosity, μ, is a constant.

Initial and boundary conditions

Initial condition - prescribed pressure and concentration.

Boundary conditions - prescribed flux of fluid, prescribed pressure, prescribed concentration or prescribed flux of solute or zero dispersive flux.

7.4 NUMERICAL METHODS

7.4.1 Spatial discretisation

In NAMMU the Galerkin finite-element method (Ciarlet 1978, Mitchell and Wait 1977, Zienkeiwicz 1977) is used to carry out the spatial discretisation of the equations presented in section 7.3. The starting point for the Galerkin finite element method is the weak form of the basic equations (Herbert et al 1994). The weak from is a generalisation of the partial differential equation in that any solution of the partial differential equation that satisfies the appropriate boundary conditions also satisfies the weak form. In addition the weak form may have solutions that are not sufficiently smooth to be solutions of the partial differential equation.

The region to be modelled is divided up into elements which have a simple geometric shape. NAMMU uses triangles and quadrilaterals in two dimensions and tetrahedra, triangular prisms and hexahedra in three dimensions. The dependent variables in the problem are approximated by functions which have a simple polynomial behaviour on each of the elements. The discretisations lead to equations for the coefficients of these polynomials as described in Mitchell and Wait, 1977 for example. The equations are coupled algebraic equations for steady-state problems, and coupled ordinary differential equations for transient problems.

A remark must be made about the treatment of advection in NAMMU. Many authors recommend the use of some form of upwind differencing for finite-difference discretisations of the equations or its equivalent in the finite-element context, namely upstream weighting. 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 in that upwinding introduces a numerical dispersion effect which amounts to dispersion with a dispersion length closely related to the mesh spacing. This is generally unsatisfactory and so a consistent Galerkin approach is used for the advective terms (Gresho and Lee, 1981). If numerical instabilities appear the user has two alternatives: either refine the mesh in the regions of high gradients so that the instabilities disappear or are reduced to an acceptable level, or increase the physical dispersion lengths to stabilise the calculation. The latter approach has an effect which is very similar to upwinding but has the virtue of making the amount of dispersion in the calculation explicit.

7.4.2 Temporal discretisation

In NAMMU the spatial discretisation is carried out using the Galerkin finite-element method as indicated in section 7.4.1. For time dependent problems the application of this method leads to a set of coupled, possibly non-linear, ordinary differential equations for the parameters determining the finite-element approximation of the dependent variables. There are two basic methods available in NAMMU for integrating these ordinary differential equations, namely the Crank-Nicolson method and Gear's method (Byrne and Hindmarsh, 1975).

The Crank-Nicolson method uses a constant timestep size, and is appropriate for problems with a single time scale such as radionuclide transport in advection dominated flows. It contains a parameter, θ, that controls the degree of implicitness of the method. The scheme is implicit for all values of θ except 0, and first order accurate for all values except 0.5 when it is second order accurate. For $\theta = 1$ the method is fully-implicit and reduces to the backward Euler scheme. The backward Euler scheme has the merit of being very robust but is not particularly accurate. A fast version of the Crank-Nicolson method is available for the special case of linear problems.

Gear's method is a variable timestep size scheme. It is an implicit time-stepping scheme and so has good stability properties. It uses high order differencing and so it is also a very accurate method. In fact the algorithm incorporated into NAMMU chooses the size of the time step and the order of the difference scheme to minimise the computation time whilst meeting a specified accuracy criterion. Because it is capable of taking increasingly large timesteps once the rapidly changing components have decayed from the solution, it is an efficient method for problems with large-time diffusive behaviour.

7.4.3 Solution methods

The methods described in sections 7.4.1 and 7.4.2 give rise to large, non-linear, coupled algebraic systems of equations. In NAMMU the non-linearities are treated using the Newton-Raphson iterative method. This is a powerful technique for solving non-linear equations and converges very rapidly provided the initial guess is sufficiently close to the solution of the equations. For transient problems this is nearly always the case since one does not want the solution to change too much over a single time step for reasons of accuracy. For steady state problems one cannot always be sure of finding a sufficiently good initial guess. In this case it is sometimes possible to approach the solution of the desired problem by varying one or more parameters and so solving a sequence of progressively more non-linear problems.

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 which is determined by the underlying finite-element discretisation. In NAMMU an efficient implementation of the Frontal Method (Duff 1981, Duff 1983, Duff and Scott 1993, Hood 1976, Irons 1975) is used to solve linear systems. The Frontal method has several very nice features: it uses a predetermined amount of memory, it recognises the fact that the linear systems arise from a finite-element discretisation, and it is very robust.

8 CONFIDENCE IN THE MODEL

The purpose of this section is to present the evidence that the models of groundwater flow and radionuclide transport that are implemented in NAMMU are an adequate representation of these processes and are fit for the purposes for which they are applied. The discussion is organised in terms of the considerations relevant to building confidence in models of groundwater flow and radionuclide transport that were identified in section 3. It is recognised that evidence in all of these categories will not necessarily be available for all of the programs used in a performance assessment calculation. However, as indicated in the following subsections, some evidence is available in all of these categories for NAMMU, which leads to greater confidence in the validity of the models available in NAMMU.

8.1 MODEL DEVELOPMENT

This topic has already been covered in the discussions in sections 6 and 7, from which it will be clear that the models implemented in NAMMU have been based on widely accepted scientific principles and on conceptual models of individual processes that are frequently used and accepted within the scientific community. Darcy's law, for example, is a generally accepted and well tested empirical relationship which can be shown to be a consequence of even more fundamental scientific principles. In some other cases (e.g. the Fickian model of dispersion) although the model is widely used it is recognised that it has some limitations, which must be taken into account when it is used. The mathematical representations of the processes that are used in NAMMU are the standard forms that are applied and accepted throughout the scientific community. The numerical methods that are used to discretise and solve the equations are among those that are generally accepted as appropriate and sufficiently accurate for these types of problems.

8.2 VERIFICATION

Verification, as applied to a computer program such as NAMMU, is the process of checking that the program correctly represents the mathematical models on which it is based. A verified program can then be used to help validate the mathematical models, that is to check that the models form an adequate representation of the relevant physical phenomena.

8.2.1 Verification of NAMMU

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

The HYDROCOIN project included test cases intended to verify transient groundwater flow from a borehole penetrating a confined aquifer (Herbert 1985b); steady-state flow in a region containing highly permeable faults (Herbert 1985a); transient coupled flow groundwater flow and heat transport (Cherrill and Herbert, 1985); and coupled groundwater flow through a hypothetical shallow disposal facility (Herbert 1985b). In each case, the results obtained from NAMMU were in excellent agreement with the analytic solution, where one was available, or with the agreed results from other groundwater flow modelling programs used within the project, in cases where an analytic solution was not available.

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

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

As noted in subsection 6.6.3, the results of a Monte-Carlo study of dispersion in a heterogeneous porous medium (Morris, Porter and Jackson, 1997b) 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 and the particle movements in a case with a heterogeneous permeability field, that is in which there was significant element to element variation in the permeability values. This case therefore also builds confidence in the correctness of NAMMU.

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

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

All this experience provides considerable confidence in the mathematical correctness and general applicability of NAMMU.

8.2.2 The role of QA in verification

A Quality Assurance (QA) programme defines a set of procedures for carrying out a particular type of work in such a way as to maintain the quality of the work. A well designed QA programme plays an important role in verification by ensuring that high standards of coding are adhered to, that there are procedures for reporting and fixing program errors and that there is a system for testing and issuing new releases of the program which ensures that the new program gives the correct results for a standard set of test cases. NAMMU is maintained and developed under an appropriate QA programme (Morris and Webster, 1997) by the Hydrogeology Department of the Waste Environmental Group within AEA Technology. The QA program conforms to the international standard ISO 9000. The UNIX Source Code Control System (SCCS) is used to store all source code and test data for NAMMU. This automatically logs the author and date of each change to the system, and enables previous versions of the code to be accessed and recreated if necessary. All changes are thoroughly tested, and must be approved by the Software Manager before they are accepted. Through the NAMMU QA programme, AEA Technology seeks to continually improve the quality and reliability of the program.

The full set of verification exercises which are used to test NAMMU at each release consist of approximately 40 test cases. These include some of the HYDROCOIN test cases, as well as other test cases for which an analytic solution is available. The test cases include examples of groundwater flow in isotropic and anisotropic media under both steady-state and transient conditions, coupled groundwater flow and salt transport, coupled groundwater flow and heat transport, unsaturated flow, and radionuclide transport. The full set of test cases, together with the corresponding output is supplied to all NAMMU users (see subsection 8.5.1).

8.3 COMPARISON WITH OBSERVATIONS

It is clear from the IAEA definition of validation that comparison of the results of a model with independent field observations and experimental measurements is an important component of the validation process. Validation of NAMMU models of specific sites has been attempted in a number of cases. A major obstacle to more extensive validation has been the relative lack of field data. This situation is improving as more detailed field observations are made at specific sites, for example at the Swedish Hard Rock Laboratory at Äspö and the Sellafield site in the United Kingdom. Better calibration of the groundwater flow models used in performance assessments is a proper objective that builds confidence in the ability of the underlying numerical and mathematical models to correctly represent the processes of flow and transport. This objective has been achieved in work undertaken for United Kingdom Nirex Ltd as part of the Nirex 97 assessment (Jackson and Watson, 1997), which gives increased confidence in NAMMU.

As discussed in section 6 and subsection 8.2, there is considerable confidence that the models of the physical processes that are adopted in NAMMU and their implementation in the program, are correct, when applied to appropriate situations. The models are widely used and accepted. When comparing model results with observations from a particular site, it is vital that the validity of the site-specific conceptual model is taken into account. As discussed in subsection 3.1, this is an additional factor, which is not related to the validity of the models within NAMMU itself. Despite the additional uncertainties that are thus introduced, it is valuable to consider a few examples in which a broad comparison can be made between the results from a site-specific NAMMU model and observations. The successful application of NAMMU to new circumstances and the confirmation that the predicted behaviour is generally reasonable can contribute to increasing confidence in NAMMU. The following paragraphs therefore give a few examples from the many cases in which NAMMU has been used to represent features of a real site.

An attempt to make predictive estimates of the drawdown in a number of boreholes at Äspö was carried out by Grundfelt et al. (1990). Prior to the prediction, the boundary conditions and hydraulic conductivities used in the NAMMU model were calibrated by comparing the predicted pressure values with field observations based on short duration pumping tests in three boreholes. The drawdowns predicted by the calibrated model matched the field observations in a qualitative sense, but were found to be unrealistically high, being over-estimated by between 0.5m and 8m. This discrepancy was believed to be due to the pumping tests used to calibrate the model not having reached steady-state, leading to inappropriate parameter values being supplied to the NAMMU model.

Several models of the groundwater flow at the Sellafield site were created as part of the Nirex 95 performance assessment (Baker et. al 1995). All of these models included a source of high salinity brine and involved calculations of groundwater flow fully coupled to the transport of salinity. A detailed calibration of the models was not carried out as part of the assessment and so the match between the observed distributions of salinity and environmental heads and the results obtained from the model were not fully acceptable. These discrepancies were related to the conceptual model of the site. It was demonstrated that some improvement in the predicted heads at depth could be obtained by including additional geological features in the models. In general, the results suggested that the NAMMU model was behaving in a physically reasonable fashion and that it was reasonable to expect that a better match to the observations could be obtained from further calibration work, as has indeed was achieved in work performed as part of the Nirex 97 assessment (Jackson and Watson, 1997).

The groundwater flow modelling that was performed with NAMMU for the Nirex 97 assessment (Jackson and Watson, 1997) was a significant advance on that carried out for Nirex 95. The NAMMU models used in Nirex 97 represented coupled groundwater flow, transport of salinity and transport of heat, whereas the models used for Nirex 95 only represented coupled groundwater flow and transport of salinity. This means that the models used in Nirex 97 better represent the physical processes known to be operative at Sellafield and are more realistic. Two- and three-dimensional NAMMU models were developed for Nirex 97. Another significant advance on the modelling that was performed for Nirex 95 was that the NAMMU models used in Nirex 97 were calibrated. That is, parameter values were determined for which the models gave a good match to the observations that are independent of the data used to initially develop the model. This means that the models used in Nirex 97 are based on more observations and are more realistic than was the case for Nirex 95. The data used to calibrate the two-dimensional and three-dimensional regional-scale groundwater flow models used in Nirex 97 were:

- the observed temperatures and temperature gradients in the Nirex deep boreholes;
- the observed groundwater salinities (strictly, chloride concentrations) in the Nirex deep boreholes;
- the observed environmental heads in the Nirex deep boreholes;
- the observed freshwater heads in the Nirex deep boreholes;
- the distributions of recharge and discharge for the near-surface sandstone aquifer.

An important aspect of the calibration for Nirex 97 was that it was attempted to simultaneously match to all of the calibration data for all the boreholes. The final match to the calibration data that was obtained was considered to be good. That it was possible to achieve a good match to several different types of data from 27 deep boreholes builds confidence in the ability of the underlying numerical and mathematical models in NAMMU to correctly represent the processes of flow and transport.

NAMMU has been used to construct a model of the groundwater flow in a deep sedimentary basin in Russia (Hoek et. al 1997). The model took account of the presence of the very saline waters that were observed at depth. It was not practicable in the time available for the study to make a detailed comparison between the observations and the results of the model. However, the results obtained from the model appeared physically reasonable and it was noted that the NAMMU model did correctly predict the existence of the artesian conditions observed at the site.

Brightman and Noy (1984) attempted to validate a two-dimensional NAMMU model of the Harwell site by comparing the model predictions with various field observations. The overall predicted flow patterns agreed qualitatively with the observed flows and the predicted groundwater head in the underlying Corallian aquifer were found to match the measured values well. However, the near-surface flow showed an unrealistic pattern of recharge and discharge cells along the top aquifer layer. The overall recharge rate was too small by about an order of magnitude, although the discharge rate in to the river Thames was consistent with observation. The shortcomings of the model were attributed to the application of an unrealistic surface boundary condition to the model and the fact that the model was only two-dimensional.

NAMMU has been used to model groundwater flow coupled to the transport of salt at a coastal low-level waste disposal site. Although a detailed calibration of the model was not practical in the time available for the study, the model did reproduce the overall pattern of groundwater flow observed at the site.

8.4 VALIDATION OF SUBMODELS

When an overall system model can be considered to be made up of individual submodels, it is valuable, where possible, to validate the individual submodels as well as the overall system model. This helps to build confidence in the system model. There are a number of ways in which the concept of submodels could be interpreted for a program such as NAMMU. Perhaps the most useful is to note that each of the equations described in section 7 corresponds to a set of routines in NAMMU which implement the required model of the physical processes. These submodels can be considered validated in the sense that, as discussed in section 8.1, the mathematical models have been derived from accepted scientific principles and that each of the sets of routines has been, and continues to be, subject to verification procedures.

8.5 PEER REVIEW

The various aspects of peer review that are relevant in assessing the validity of a model were outlined in section 3. The peer review provided for NAMMU by the existence of the NAMMU User Group is discussed in subsection 8.5.1. Aspects of peer review related to publications involving NAMMU are then discussed in subsection 8.5.2.

8.5.1 NAMMU User Group

Using a large program such as NAMMU is a task that requires a high level of technical expertise. AEA Technology recognises this fact and, accordingly, runs training courses to help new users become familiar with the program and its use. In addition AEA Technology has set up the NAMMU User Group. Members of the User Group receive updates to the software, code and documentation corrections, telephone and e-mail support for technical problems and a newsletter. AEA Technology also organises regular User Group meetings which act as a forum for users to discuss applications of the program, to provide feedback for future program developments and to hear about new developments.

NAMMU is used by a significant number of organisations with an interest in radioactive waste disposal. There are representatives of both the regulatory bodies and the nuclear utilities. The following is a list of organisations using NAMMU:

United Kingdom Nirex Ltd, U.K.

BNFL, U.K.

RM Consultants, U.K.

BGS Keyworth, U.K.

Golder Associates, U.K.

Entec, U.K.

GRS, Germany.

Federal Office for Radiation Protection (BfS), Germany.

Federal Institute of Geosciences, Germany.

Swedish Nuclear Fuel and Waste Management Company (SKB), Sweden.

Swedish Nuclear Power Inspectorate (SKI), Sweden.

Kemakta Consultants, Sweden.

Conterra AB, Sweden.

National Cooperative 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), Republic of Korea.

Korea Electric Power Corporation , Republic of Korea.

Hyundai Engineering and Construction Company, Republic of Korea.

The wide use of NAMMU by the membership of the user group and the participation of these organisations in training courses and user group meetings is a very effective form of external peer review. The program is being applied by a wide range of organisations to a diverse set of problems. The support to users provided by AEA Technology to members of the user group means that any difficulties or problems that are found will be quickly reported to AEA Technology for resolution. Thus, in effect, the program is undergoing continuous review and testing.

8.5.2 Documentation and Publications

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

NAMMU Technical Overview;

NAMMU User Guide;

NAMMU Installation Manuals;

Quality Assurance for NAMMU;

TGIN Language Reference Manual: NAMMU Commands

TGIN Language Reference Manual: MODEL DATA Commands

TGIN Language Reference Manual: OUTPUT DATA Commands

These documents are extensively reviewed before publication and are widely used by members of the User Group. This is another feature of the peer review provided by the Group.

Some review of NAMMU is also provided through the involvement of AEA Technology and other NAMMU users in international model testing and collaborative projects such as HYDROCOIN, INTRAVAL, and GEOTRAP.

Another aspect of peer review is that of journal articles and conference papers that are based on the use of the model (e.g. Herbert et. al 1988, Cliffe and Jackson 1993, Jackson and Porter 1990, Porter and Jackson 1990, Jackson et. al 1989). A bibliography of reports relating to projects that have used NAMMU is given at the end of this report.

8.6 WORK IN RELATED FIELDS

Additional confidence in the models of groundwater flow and radionuclide transport used in NAMMU can be obtained from the fact that they are identical or very similar to models that are used in related fields of work. Many of the models of groundwater flow and solute transport processes were developed and are still applied in water resources engineering. Very similar models of fluid movement in porous media are used in models of oil reservoirs. In both of these cases, the timescales of interest are much shorter than in repository performance assessment calculations and the results of the models can be evaluated by comparison with the observed response of the system. The continued (indeed increasing) application of the models in these fields testifies to their usefulness and to the confidence that is placed in them.

8.7 SUMMARY

It can be seen that there is a wide range of evidence that gives confidence that the models of groundwater flow and radionuclide transport implemented in NAMMU are appropriate and are fit for the purposes for which they are applied.

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