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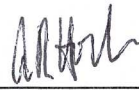
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Preface

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

The following documentation is available for Release 7.2 of NAMMU:

- NAMMU (Release 7.2) Technical Summary Document;
- NAMMU (Release 7.2) User Guide;
- NAMMU (Release 7.2) Command Reference Manual;
- NAMMU (Release 7.2) Verification Document;
- NAMMU (Release 7.2) Installation and Running Guide.

This document, the Verification Document, provides information on the verification and validation of NAMMU, which builds confidence in its flow and transport models.

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The NAMMU program makes use of the TGSL subroutine library.
All rights to the TGSL subroutine library are owned by Serco Assurance.

All documents describing the NAMMU program and TGSL subroutine library are protected by copyright and should not be reproduced in whole, or in part, without the permission of Serco Assurance.

NAMMU also makes use of the freely available LAPACK linear algebra library.

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

Capabilities of NAMMU

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

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

- Flow and transport in 3D Cartesian, 2D vertical and plan section, and 2D radial geometries;
- Deterministic and stochastic continuum modelling;
- Steady state and transient behaviour;
- Groundwater flow in saturated and unsaturated conditions;
- Saline groundwater flow with the density dependent on concentration;
- Coupled groundwater flow and heat transport with the density dependent on temperature;
- Saline groundwater flow and heat transport with the density dependent on concentration and temperature;
- Groundwater flow in a dual porosity system based on the Warren and Root model;
- Transport of contaminants, including the effects of advection, dispersion, and sorption, with solubility limitation;
- Transport of radioactive decay chains, allowing for interacting chains to be linked by solubility limitation of a common radionuclide.

NAMMU can be used to model the following features:

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

NAMMU models and results can be displayed by:

- A 3D visualisation system, GeoVisage for Nammu, that allows 3D rendering of finite-elements, rock types, permeability, fracture zones, variables, flow vectors, and pathlines;
- 2D plot and numerical output that includes:
 - Plots of the finite-element mesh and its boundaries;
 - Plots of contours of a variable on a surface;
 - Plots of contours of a variable on a 2D slice;
 - Plots of velocity arrows, showing direction and magnitude of the groundwater flow;
 - Plots of pathlines either for steady state or for transient groundwater flows;
 - Plots of backward pathlines, showing the region of influence of a borehole;
 - Graphs of variables along a line;
 - Graphs of the evolution of variables at a point;
 - Graphs of data;
 - Integrals (e.g. flux of groundwater across a plane).

NAMMU models have been used in the following applications:

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

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

NAMMU has been developed by Serco Assurance (formerly UKAEA) over a period of more than 15 years and has been verified extensively in international comparison exercises. It is developed under a rigorous quality system that conforms to the international standards ISO 9001 and TickIT.

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1 INTRODUCTION

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 the numerical model appropriately represents features of the site and processes occurring at the site that could have an important influence on flow and transport.

NAMMU is a computer program for calculating groundwater flow and solute and heat transport through porous media [1]. 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 were 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 verification 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. In section 2 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. Section 3 describes the purpose of

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modelling and its context within an assessment. Section 4 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. Section 5 describes the evidence that models of groundwater flow and radionuclide transport are fit for the purpose for which they are applied. In addition, 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.

2 VALIDATION FRAMEWORK

2.1 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.)' [2].

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 the nature of the model. If the model is a general model, for example a model of a process such as groundwater flow, the approach will be different from that for 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 e.g. [3]). 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 outside 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 the relevant 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 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 planetary movement. 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 [4]. 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 by Jackson et al. [5], can help to minimise the subjective aspects, but cannot eliminate them.

2.2 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.

2.2.1 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 possibility of great importance, as one useful outcome of a validation process may be the ability to discriminate between alternative conceptual models. This leads 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. [5]).

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 or 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 is 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.

2.2.2 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.

2.2.3 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, so will include issues related to the validation of the site-specific conceptual model, which lie outside 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 interpretation.

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' [6]) 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. [5]).

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.

2.2.4 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.

2.2.5 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 [7, 8, 9, 10], INTRAVAL [11], GEOTRAP).

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

2.2.6 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. Related fields where similar models are used include water resources engineering and oil reservoir modelling.

3 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.

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), a rock block of 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 timescale 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.

For example, 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 sources 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;

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- 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 sources 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 by Boghammar et al. [12]. 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 km² and 50 km², 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.

4 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 judgements or assumptions underlying the development of the modelling approach. In the present context, these are basically judgements about the type of model that will give a good representation of the behaviour of the hydrogeological system or about 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. The second category consists of the assumptions that underlie the basic models of the physical processes that are implemented in NAMMU.

Assumptions of the assessment approach 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, relevant to assessments performed by SKB [13]. 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 3.

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The second category of assumptions, those that underlie the basic models of the physical processes that are implemented in NAMMU, would include assumptions of the validity of 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.

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.

5 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 set out in section 2.2. 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.

5.1 Model Development

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.

5.2 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, to check that the models form an adequate representation of the relevant physical phenomena.

5.2.1 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 project [7, 8, 9, 10] 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 [14];
- Steady-state flow in a region containing highly permeable faults [15];
- Transient coupled groundwater flow and heat transport [16];
- Groundwater flow through a hypothetical shallow disposal facility [14];

- Coupled groundwater flow and solute transport with the fluid density strongly dependent upon solute concentration [17].

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

A verification exercise for NAMMU has recently been performed for ANDRA [18]. Cases covering a range of groundwater flow and radionuclide transport problems were investigated. The exercise included cases that were diffusion dominated, cases that were advection and dispersion dominated, cases in two- and three-dimensions, and cases with permeability contrasts between regions of the models such that the dominant flow and transport processes differed between the regions. With appropriate choices of the grid, the initial and boundary conditions, and the time-stepping scheme, NAMMU was found to accurately reproduce the analytic solutions given for all cases considered.

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 [19], 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 [20]. 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.

The results of a Monte-Carlo study of dispersion in a heterogeneous porous medium [21] 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 provided an accurate solution for the groundwater flow in a heterogeneous permeability field. 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 [22, 23, 24]. 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.

5.2.2 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 maintained.

This includes establishing procedures for reporting and fixing program errors and defining a system for testing and issuing new releases of the program that 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 [25] by the Environmental Management Department within Serco Assurance. The QA Programme conforms to the international standard BS EN ISO 9001 (1994) and to the TickIT Guidelines. The Concurrent Versions System (CVS) version management system 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, Serco Assurance 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 70 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 the summary of data sets given in Appendix A).

5.3 Comparison with Observations

As indicated in section 2, 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. 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 Limited as part of the Nirex 97 assessment [26], which gives increased confidence in NAMMU.

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. 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. [27]. 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 [28]. 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. Therefore, a 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. It was reasonable to expect that a better match to the observations could be obtained from further calibration work, as indeed was achieved in work performed as part of the Nirex 97 assessment [26].

The groundwater flow modelling that was performed with NAMMU for the Nirex 97 assessment [26] 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- 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 [29]. 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 [30] 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 was 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.

5.4 Validation of Submodels

When an overall system model can be considered to be made up of individual submodels, then, to help to build confidence in the system model, it is valuable, where possible, to validate the individual submodels. 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 describing the physical process that are implemented in NAMMU (given in the Technical Summary Document [31]) corresponds to a set of routines in NAMMU. These submodels can be considered validated in the sense that 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.

5.5 Peer Review

The various aspects of peer review that are relevant in assessing the validity of a model have been outlined in section 2.2.5. The peer review provided for NAMMU by the existence of the NAMMU User Group is discussed in section 5.5.1. Aspects of peer review related to publications involving NAMMU are then discussed in section 5.5.2.

5.5.1 NAMMU User Group

Using a large program such as NAMMU is a task that requires a high level of technical expertise. Serco Assurance recognises this fact and, accordingly, runs training courses to help new users become familiar with the program and its use. In addition Serco Assurance 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. Serco Assurance 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 that have used NAMMU:

- **United Kingdom Nirex Limited, UK;**
- **Department of the Environment, UK;**
- **British Nuclear Fuels Limited (BNFL), UK;**
- **RM Consultants, UK;**
- **British Geological Survey (BGS) Keyworth, UK;**
- **Golder Associates, UK;**
- **Entec, UK;**
- **University of Bath, UK;**

- **University of Birmingham, UK;**
- **Gesellschaft fur Reaktorsicherheit (GRS), Germany;**
- **Federal Office for Radiation Protection (BfS), Germany;**
- **Federal Institute of Geosciences, Germany;**
- **Swedish Nuclear Fuel and Waste Management Company (SKB), Sweden;**
- **Swedish Nuclear Power Inspectorate (SKI), Sweden;**
- **Kemakta Consultants, Sweden;**
- **Conterra AB, Sweden;**
- **Agence Nationale pour la Gestion des Déchets Radioactifs (ANDRA), France;**
- **National 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;**
- **Georgia Institute of Technology, USA.**

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 support to users provided by Serco Assurance to members of the User Group means that any difficulties or problems that are found will be quickly reported to Serco Assurance for resolution. Thus, in effect, the program is undergoing continuous review and testing.

5.5.2 Documentation and Publications

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

- **NAMMU (Release 7.2) Technical Summary Document;**
- **NAMMU (Release 7.2) User Guide;**
- **NAMMU (Release 7.2) Command Reference Manual;**
- **NAMMU (Release 7.2) Verification Document (this document);**
- **NAMMU (Release 7.2) Installation and Running Guide.**

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 Serco Assurance and other NAMMU users in international model testing and collaborative projects such as HYDROCOIN [7, 8, 9, 10], INTRAVAL [11], 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. [17, 32, 33, 34, 35]). A bibliography of reports relating to projects that have used NAMMU is given at the end of this document.

5.6 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 [36, 37]. Very similar models of fluid movement in porous media are used in models of oil reservoirs (e.g. [38]). 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 (and indeed increasing) application of the models in these fields testifies to their usefulness and to the confidence that is placed in them.

5.7 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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Appendix A The NAMMU Test Library

The NAMMU library of test data sets is designed to test the functionality of the program on all supported platforms. In particular:

- New developments are verified using test cases specific to the changes being made, and then the test library is used to check that the changes do not affect the program in any unexpected way;
- The test library is used to confirm that the program has been installed correctly, and therefore is an important part of Quality Assurance;
- The test library is used as a set of templates for creating new models.

This appendix lists all the data sets in the NAMMU test library. The test cases are listed in Tables A.1-A.8. The tables record the following information for each test case:

- Dimension and geometry (rectangular or cylindrical);
- Type of finite-elements used and other grid related options;
- Boundary condition types;
- Physics and type of solver;
- Output;
- Purpose of the test.

Abbreviations for the test data

GWF = Groundwater Flow

GWFH = Groundwater Flow and Heat Transport

NCT = Nuclide Chain Transport

NT = Nuclide Transport

PCCG = Preconditioned Conjugate Gradients

S-S = Steady-State

ST = Salt Transport

UGWF = Unsaturated Groundwater Flow

Table A.1 Test Data Sets 1.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
4n3_rad_1d	2D Cylindrical	QAD9	Generalised flux Time varying input flux	Crank Nicholson Transient NCT	Plot time evolution	4n3 chain – U235
bblocks	3D	CB08 IFZ Modify region			Plot grid slice Plot grid surface	Large 3D regional model to IFZ
bigwell	3D	CB08	Specified value Specified flux	S-S GWF PCCG Crank-Nicholson GWF	Select time Draw line graph Plot time evolution	Test geometric time-stepping
bigwell2	3D	CB08	Specified value Point sink	S-S GWF PCCG	Plot contours on slice Plot vectors	Test point sink to represent abstraction
block_comparison_nammu	3D	CB08	Specified value	S-S GWF PCCG Crank Nicholson GWF	Pathlines Draw line graph Select time	For comparison with NAPSAC model of matrix in steady and transient flow
borehole	3D	CB27 Borehole shell	Specified value	S-S GWF	Plot grid slice Plot vectors	Test grid refinement around a shaft
chain	2D	QAD9	Specified value	S-S GWF Fast linear transient NCT Crank Nicholson NCT	Select time Draw line graph	Transient nuclide chains test of two different time-stepping methods
dporos	3D	CB27 Well patch	Specified value Specified flux	Dual-porosity GWF Transient	Plot time evolution Draw data graph	Dual-porosity based Warren-Root test on analytical solution
fault2d	2D	QAD9 Fault shifts			Set rock styles Plot grid	Tests 2D fault generation

Table A.2 Test Data Sets 2.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
fault3d	3D	CB27			Plot boundary Plot grid slice	Tests fault shifts in 3D
femgvg1	3D	CB08 FEMGV import			Save avizier data	Tests import from FEMGV
g1	2D	QAD9	Specified value Zero dispersive flux	S-S GWF S-S NT	Plot contours Draw line graph	Tests zero dispersive flux
g1a	2D	QAD9	Specified value	S-S GWF S-S NT	Plot contours Draw line graph	Comparison with g1
g1mix	2D	QMX2	Specified value Zero dispersive flux	S-S GWF S-S NT	Plot contours Draw line graph	Tests mixed elements
g1-12	2D	QAD9	Specified value Zero dispersive flux	S-S GWF S-S NCT	Plot contours Draw line graph	Tests having 12 variables
gorleben	3D	CB27	Specified value	S-S GWF	Save avizier data Plot grid slice	Tests complex 3D patch grids
henry1	2D	Q9/1	Specified value (linear) Specified flux Zero dispersive flux	S-S ST Transient	Plot contours Calculate line integral	Standard Henry test case for salt transport
henry2	2D	Q9/1	Specified value (linear) Specified flux (using subroutine BNDVAL) Zero dispersive flux	S-S ST Transient	Plot contours Calculate line integral	Standard Henry test case for salt transport with boundary pressure set

Table A.3 Test Data Sets 3.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
henry3dmtc	3D	TTMX	Specified value (linear) Specified flux	S-S ST (mixed-elements)	Plot contors Plot contours on slice	Standard Henry test case for salt transport with mixed-elements
hill	2D	QAD9	Specified value	S-S GWF	Plot vectors Pathlines	2D flow for a hill
hillside	2D	QAD9	Specified value Recharge discharge	S-S GWF	Plot contours	Test recharge discharge bc
hydro2.alt	2D	QAD9 Many patches			Plot grid	Complex patch grid with fractures
hydro2.coarse	2D	QAD9	Specified value	S-S GWF	Pathlines Draw line graph	Hydrocoin testcase 2 (coarse)
hydro2.fine	2D	QAD9	Specified value	S-S GWF	Pathlines Draw line graph	Hydrocoin testcase 2 (fine)
hydro2.medium	2D	QAD9	Specified value	S-S GWF	Pathlines Draw line graph	Hydrocoin testcase 2 (medium)
hydro4	2D	QAD9, TRT6	Specified value	GWFH Transient	Plot time evolution Draw line graph Pathlines	Hydrocoin testcase 4 couple heat and flow
l2c1	2D	QAD9	Specified value Specified flux Heat source	S-S GWFH	Draw line graph	Hydrocoin level 2 case 1

Table A.4 Test Data Sets 4.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
l3c2	2D	QAD9	Specified value Specified flux	S-S GWF S-S UGWF	Draw line graph	Hydrocoin level 3 case 3
mix2d.tdbcs	2D	QMX2	Specified value for mixed-elements	S-S GWF (mixed-elements) Crank-Nicholson GWF	Output data for step Plot vectors	Tests time dependent boundary conditions for mixed elements
nd1	2D	QAD9	Specified value Zero dispersive flux Nuclide source	S-S GWF S-S NT	Plot contours Plot vectors Draw line graph	Tests dispersion of nuclide
nd2	2D	QAD9	Specified value Zero dispersive flux Nuclide source	S-S GWF S-S NT	Plot contours Plot vectors Draw line graph	Tests dispersion of nuclide
pacoma.coarse	2D	QAD9, TRT6	Specified value	S-S GWF, stream-function	Plot contours	Pacoma test case GWF on coarse mesh
pacoma.fine	2D	QAD9, TRT6	Specified value	S-S GWF, stream-function	Plot contours Plot vectors	Pacoma test case GWF on fine mesh
pacoma.nuc1	2D	QAD9, TRT6	Specified value	Fast linear transient NT	Plot contours Calculate line integral	Pacoma test case NT in chalk
pacoma.nuc2	2D	QAD9, TRT6	Specified value	Fast linear transient NT	Plot contours Calculate line integral	Pacoma test case NT in chalk
pacoma.nuc3	2D	QAD9, TRT6	Zero dispersive flux	Fast linear transient NT	Plot contours Calculate line integral	Pacoma test case NT in clay

Table A.5 Test Data Sets 5.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
pacoma.nuc4	2D	QAD9, TRT6	Specified value	S-S GWF, S-S NT Adjoint sensitivity	Plot contours Calculate line integral	Pacoma test case NT in 3 layers
pacoma.nuc.adj	2D	QAD9	Specified value Specified flux	S-S GWF S-S UGWF	Plot contours Sensitivities	Adjoint sensitivity analysis of NT
pacoma.patch	2D	QAD9			Plot text	
pacoma3d	3D	CB27	Specified value	S-S GWF	Pathlines Contours on surface	3D version of Pacoma
pacoma_trt	2D	QAD9	Specified value	S-S GWF GWF adjoint sensitivity	Pathline sensitivity	GWF adjoint sensitivity for pathlines
pacoma_trt1	2D	QAD9	Specified value	S-S GWF GWF adjoint sensitivity	Pathline sensitivity	GWF adjoint sensitivity for pathlines
pacoma_trt2	2D	QAD9	Specified value	S-S GWF GWF adjoint sensitivity	Pathline sensitivity	GWF adjoint sensitivity for pathlines
patch1	2D	QAD9, TRT6	Specified value	S-S GWF, Velocity field stream-function	Plot contours	Velocity field calculation and streamfunction
pccgtest	3D	CB27	Specified value	S-S GWF PCCG S-S GWF		Tests PCCG versus Frontal solver
pccgtest1	3D	CB08	Specified value	S-S GWF PCCG S-S GWF		Tests PCCG versus Frontal solver

Table A.6 Test Data Sets 6.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
polygon2	2D	QAD9 Fault shifts Polygon topology			Plot grid	Tests polygon method of grid generation
pressure	2D	QAD9, TRT6	Specified value	S-S GWF (residual pressure, total pressure, head)		Tests different formulations of flow variables
simp_mod	3D	CB08 Permeability values	Specified value	S-S GWF	Plot grid surface Plot grid slice	Test elementwise permeabilities - change values in a block
simple	2D	QAD9	Specified value	S-S GWF	Plot contours	Simple GWF case
simple12	2D	QAD9	Specified value	S-S GWF	Plot contours	Case with 12 variables
sol_lim	2D	QAND	Specified value	Crank-Nicholson NTC with solubility limitation	Draw line graph	Test solubility limitation on a chain
stan2d.tdbcs	2D	Q9/1	Specified value for nodes	S-S GWF Crank-Nicholson GWF	Pathline sensitivity	Test time-dependent boundary conditions
stfn	2D	QAD9	Specified value	S-S GWF Streamfunction	Plot contours	GWF and streamfunction
tcbmx	3D	CBMX	Specified value	S-S GWF (mixed elements)	Draw line graph	Tests 3D mixed elements
testa	2D	QAD9	Specified value	S-S GWF	Plot contours Plot node numbers	Tests zoom option in output
testblk1	3D	CB08	Specified value	S-S GWF		Tests domain decomposition solver

Table A.7 Test Data Sets 7.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
testblk1d	3D	CB08	Specified value	S-S GWF (domain decomposition)		Tests domain decomposition solver
testifz1	3D	CB08 Stochastic, IFZ	Specified value	S-S GWF (3 realisations)	Plot grid slice Pathlines	Tests IFZ and stochastic models
testifz2	3D	CB08 IFZ (2 models)	Specified value	S-S GWF PCCG	Plot grid slice Pathlines (2 alternatives)	Tests IFZ and two alternatives for calculating pathlines
testk	2D	QAD9	Specified value Specified flux	S-S GWF Transient NT	Draw line graph Plot time evolution	Test transient GWF
testl	2D	QAD9	Specified value	S-S GWF Streamfunction		Test streamfunction
testm	2D	QAD9	Specified value Specified flux	Transient unsaturated NT	Draw line graph Plot time evolution	Test transient unsaturated NT
testnuc1d	1D	L3/2	Specified value	S-S GWF S-S NT (adjoint sensitivity)	Draw line graph Calculate sensitivity coefficients	Test adjoint sensitivities for nculide concentration
testp	3D	CB08	Specified value	S-S GWF Crank-Nicholson GWF		Test 3D GWF
testq1	1D	L3/2	Specified value	S-S GWF (adjoint sensitivity)	Draw line graph Calculate sensitivity coefficients	Test adjoint sensitivities for velocity

Table A.8 Test Data Sets 8.

Data set	Geometry	Mesh/element	Boundary conditions	Solve/physics	Output	Comments
testrot	2D	QAD9 Permeability rotations	Specified value	S-S GWF	Plot vectors Plot tensors	Tests permeability rotations
tqmx2	2D	QMX2	Specified value	S-S GWF (mixed elements)	Draw line graph	Tests 2D mixed elements quadrilaterals
ttxmx2	2D	TMX2	Specified value	S-S GWF (mixed elements)	Draw line graph	Tests 2D mixed elements triangles
unsat	2D	QAD4	Specified value	S-S UGWF	Plot contours	Tests 2D unsaturated flow
well3d	3D	CB27 Borehole shell	Specified value Specified flux	S-S GWF Velocity field	Plot vectors Pathlines	Tests 3D borehole

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