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NAMMU (Release 6.4) User Guide

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Abstract

NAMMU is a software package for modelling groundwater flow and transport in porous media in one, two and three dimensions. The package can be used to model steady-state and time-dependent behaviour, including unsaturated flow and the transport of heat and mass. An option is available for modelling radioactive decay and 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 strata.

This User Guide introduces the package using a number of realistic examples. It discusses the principles of modelling and gives practical advice on how best to use the package. The input language is summarized, and the output from the program is described, including the error diagnostics.

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Preface

NAMMU is a finite-element package for modelling groundwater flow and transport in porous media. This User Guide provides a general introduction to the package using a number of realistic examples.

The following documentation is available for Release 6.4 of NAMMU:

- NAMMU (Release 6.4) Technical Overview
- NAMMU (Release 6.4) User Guide
- NAMMU (Release 6.4) Installation and Running Guide
- NAMMU (Release 6.4) Reference Manual

Summary of Changes for Release 6.4

The major changes to the software are as follows:

- Supported on DEC Alpha and Silicon Graphics R10000 platforms.
- Year 2000 compliant on all platforms.
- New tetrahedral mixed elements.
- New patch types to assist in modelling "pinched-out" geological layers.
- New facility to insert boreholes into grid.
- New feature to add fault zones and quadrilateral features to a grid of polygons.
- New facility to specify initial values of variables at patch corners.
- New current value boundary condition.
- Major improvements to time-dependent boundary conditions.
- Major improvements to interpolation of solutions between models.
- New storativity formulation for salt transport and groundwater flow calculations.
- New automatic timestepping algorithm for solving non-linear equations.
- New output phase keywords to specify scalars e.g head, fluid density, saturation etc.
- New output phase keywords to specify options for vector plots.
- Appearance of graphs and contour plots improved.
- Improvements to plotting of contours on slices through 3D models.
- Supports output to the AVIZIER visualisation package.
- Archaic grid generation options removed.

The major changes to the User Guide are as follows:

- Examples updated for Release 6.4.
- NAMMU equation library now described in the Technical Overview.
- Editorial changes.

Summary of Changes for Release 6.3

The major changes to the software are as follows:

- Supported on Silicon Graphics Power Challenge and Convex platforms.
- Performance of the Solver improved.
- Maximum number of rock types increased from 100 to 500.
- Mixed-element flux variable changed from a specific discharge to a mass flux.
- Grid generation by generalised polygons supported.
- Groundwater flow coupled simultaneously with heat and salt transport supported.
- Time-dependent transport calculation with a time-dependent velocity field supported.
- Adjoint sensitivity calculation supported for mixed-element groundwater flow.
- Temperature is now defined in absolute, not relative terms.
- New output phase options to specify page layout, and to plot additional non-grid objects. For example, compass, symbols and text.
- Keywords of ≫ `SET PLOT OPTIONS` act globally; keywords of other output phase commands act locally.

The major changes to the User Guide are as follows:

- Examples updated for Release 6.3.
- Editorial changes.

Summary of Changes for Release 6.2

The major changes to the software are as follows:

- Supported on Silicon Graphics platform.
- New mixed element types: QMX2, TMX2, CBMX, PRMX.
- Salt transport equations re-formulated, transient salt calculations supported.
- Adjoint sensitivity calculations supported.
- Frontal solver improved – typically twice as fast for large models.
- New fast solver available for solving time-dependent linear equations.
- Crank Nicholson solver supports nuclide chains.
- Rocks may be defined by names.
- 1-D patch type available.
- Option to plot rock lithologies with line graph.
- Option to colour pathlines by speed, elapsed time or rock type.
- New format for pathline summaries.
- Generalized flux law boundary conditions made easier to use.
- Contour key and rock type legend added to plotting options.
- Date, time and version number printed on all output.
- Postscript output conforms to Adobe Document Structure Conventions.

The major changes to the User Guide are as follows:

- Chapters describing mixed-elements, salt transport and adjoint analysis added.
- Examples updated for Release 6.2
- Editorial changes

Summary of Changes for Release 6.1

The major changes to the software are as follows:

- Supported on Cray-YMP, SUN, IBM RS/6000 platforms.
- Solver modified to use Basic Linear Algebra Subroutine (BLAS) library. Optimized versions of the BLAS library are available on many platforms.
- Solver modified to avoid saving lower triangular matrix. This improves performance and reduces the temporary storage space required.
- New grid generation facilities:
    1. New keywords for patch sub-division.
    2. Well patch added to enable refinement of the grid in the vicinity of boreholes.
    3. New `FAULT SHIFTS` keyword to simplify the generation of grids containing fault zones.
- Shaded contour plots supported.
- Pathline calculations supported in time-dependent flow fields.

The major changes to the User Guide are as follows:

- Examples updated for Release 6.1.
- Editorial changes.

CONTENTS

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1 INTRODUCTION

This manual is the User Guide to Release 6.4 of the NAMMU finite-element package for modelling groundwater flow and transport in porous media.

The acronym **NAMMU** stands for **N**umerical **A**ssessment **M**ethod for **M**igration **U**nderground. The name has further significance:

Nammu, a Sumerian goddess whose name was expressed by the ideogram for 'sea', was described as the 'mother who gave birth to heaven and earth'. Elsewhere she was called 'mother of all gods' and more specifically, 'mother of Enki, the god who will organise the world of men'! See Figure 1.1.

NAMMU was developed by the Theory of Fluids Group of the Theoretical Physics Division[1] at Harwell Laboratory in the United Kingdom. It is based on routines from the TGSL library of subroutines for solving coupled non-linear partial differential transport equations using the finite-element method. Input to NAMMU is in the free-format TGIN language, which is supported by subroutines from the TGIN library; graphical output is handled using the THGRAPH library of post-processing subroutines. NAMMU also interfaces to the AVIZIER 3D visualisation environment. The code has been extensively tested and verified [1–6] and its use has been widely adopted throughout Europe.

NAMMU is only one of several packages that have been based on the above subroutine libraries; others include ENTWIFE, CAMLE and WAFT. NAMMU also forms part of the CONNECTFLOW package, for modelling groundwater flow and transport in porous and fractured media.

1.1 How to Use This Manual

This manual is intended to introduce the new user to NAMMU, and also to provide some guidance and hints for the more experienced user. In particular, several examples are discussed in detail. The manual should be read together with the NAMMU Reference Manual [7], which gives the definitive descriptions of all the input instructions for NAMMU.

This manual is organised as follows:

Section 1 introduces NAMMU and outlines its technical capabilities.

Section 2 is aimed at the new user of NAMMU. The syntax and structure of the input data (in the TGIN language) is explained briefly using a very simple example, and the way that the program is run is discussed.

Section 3 gives some general guidance on finite-element modelling of groundwater flow and radionuclide transport.

[1] Now the Hydrogeology Department of AEA Technology.

Sections 4 to 10 present a number of examples of the use of NAMMU. These examples illustrate many of the features of NAMMU as used in realistic case studies.

Section 11 deals with one of the more powerful facilities of NAMMU: the option to link user-specified subroutines into certain well-defined interfaces in the program. This gives the user the ability to customise, for example, material properties and output options to meet specific needs.

Section 12 discusses some of the more common error messages.

1.2 Technical Capabilities of NAMMU

NAMMU can be used to calculate:

- groundwater flow;
- coupled groundwater flow and heat transport;
- unsaturated groundwater flow;
- coupled groundwater flow and solute transport with the fluid density strongly dependent upon concentration;
- coupled groundwater flow, heat transport and solute transport with the fluid density dependent upon concentration and temperature;
- radionuclide transport (which may take place in the groundwater flow field of any of the above except coupled groundwater flow, heat transport and solute transport with the fluid density dependent upon concentration and temperature);
- the stream function in two-dimensions;
- adjoint sensitivity analysis.

The conceptual models underlying all of these processes are flow and transport in a porous medium, modelled by Darcy's law and its extensions. The radionuclide transport model includes a linear equilibrium sorption model, and chains of up to six radionuclides can be considered. A detailed presentation of the mathematical models used is given in the NAMMU Technical Overview [8].

NAMMU uses the finite-element method, which enables complicated geometries with many different rock types to be readily modelled in a straightforward fashion. Brief comments on the finite-element method and some sources of reference are given in Appendix A.

Options for transient calculations include Crank-Nicholson and Gear's method. Non-linear cases can be tackled using Newton-Raphson linearisation, supplemented with parameter

stepping. The algebraic equations resulting from linearisation in space (and time, if necessary) are solved using a very fast direct linear solver [9] from the Harwell Subroutine Library [10].

The main features of the current release are as follows:

- problems can be modelled in one-, two-, or three-dimensional Cartesian geometry or two-dimensional cylindrical geometry;
- fluid properties such as density can be specified as constants, as functions of position, or as functions of pressure, temperature and solute concentration;
- rock properties such as permeability can be specified as constants, as functions of position, or as functions of pressure, temperature and solute concentration;
- grid generation facilities make it as easy as possible for the user to generate the sort of grids needed to represent complex geological formations;
- boundary conditions of both Dirichlet (specified value) and Neumann (specified flux) type can be specified;
- generalised flux boundary conditions;
- time-dependent boundary conditions;
- more complicated boundary conditions can be specified through the use of suitable user-supplied subroutines;
- the grid can be plotted as a line diagram or shaded according to rock types;
- graphs of the variables and related scalars along lines in the domain can be drawn;
- contours of pressure, temperature, concentration and related scalars can be plotted;
- the flow field can be graphically depicted by plotting the velocity vectors or advective pathlines;
- in 3D the grid can be plotted as a wireframe picture viewed from any point in space;
- contours of the variables and related scalars can be plotted on slices through the 3D grid or on its surface;
- output options can be customised by the use of user-supplied routines;
- SI units are used throughout.

A wide selection of finite elements, which includes mixed elements, is available, and is catalogued in Appendix B.

Figures for Section 1

Figure 1.1 **A statuette of the Sumerian goddess Ur-Nammu, shown carrying a basket. From Nippur, about 2100 BC.**

2 EXAMPLE 1: GETTING STARTED

The current version of NAMMU is run in batch, using a suitable input file created using any suitable text editor or word processor. The input file describes the finite-element model to be created, that is the geometry of the grid, the boundary conditions, the physical properties of the rocks and fluid, the equations to be solved, and the output required (plots of the grid, for example). Details of how to run the program on specific platforms can be found in the NAMMU Installation and Running Guide [11].

2.1 The Input File

The input file is written in a free-format input language called TGIN. A full description of the structure and syntax of this language, and detailed specifications of the commands available, is given in the NAMMU Reference Manual [7]. An example input file is included below. The case is that of solving for the steady-state groundwater flow in a square domain with isotropic homogeneous permeability. The domain and boundary conditions are illustrated in Figure 2.1.

Here is the example input file (Example 1):

```
   /* NAMMU TEST CASE SIMPLE                                    */
   /*                                                           */
   /* DATASET 2.1 - A SIMPLE EXAMPLE                            */

   /* SPACE ALLOCATION                                          */
   /* INTEGER WORKSPACE  300000                                 */
   /* REAL WORKSPACE     120000                                 */

   /* SOURCE FILES                                              */
   /* COMPILED FILES                                            */
   /* LIBRARY FILES                                             */

   /* INPUT DATA FILES                                          */
   /* OUTPUT DATA FILES                                         */
   /* 6        nammu/output/simple.out                          */
   /* GRAPHICS nammu/output/simple.ps                           */

   /* END JOB INFORMATION                                       */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      VARIABLES  1
      END
```

```
   >> SET VARIABLES
      VARIABLE NAMES   'PRES'
      END

>> INITIAL DATA

   >> PHYSICAL PROPERTIES

      ROCK TYPE PERMEABILITIES
      ROCK NUMBER,    KXX,     KYY
           1       1.0E-16  1.0E-16

      ROCK TYPE PROPERTIES
      ROCK NUMBER,  POROSITY
           1         1.0E-4
      END

>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         PATCH SPACING IN FIRST DIRECTION
         SIZE
           2

         PATCH SPACING IN SECOND DIRECTION
         SIZE
           2

         PATCH POSITIONS
         CORNER NUMBER, COORDINATES
                1       < 0.0 0.0 >
                2       < 1.0 0.0 >
               11       < 0.0 1.0 >
               12       < 1.0 1.0 >

         PATCH TOPOLOGY
         PATCH TYPE,    CORNERS
           'SQQ9'    < 11 1 2 12 >
         END

   >> SET BOUNDARY CONDITIONS

      >> SPECIFIED  VALUE

         >> CONSTANT VALUE
            VARIABLES  'PRES'
            VALUES     1.0
            END

            >> SELECT LINE
               START POINT  1.0  0.0
```

```
            END POINT    1.0  1.0
            END

         >> CONSTANT VALUE
            VARIABLES  'PRES'
            VALUES      0.0
            END

            >> SELECT LINE
               START POINT  0.0  0.0
               END POINT    0.0  1.0
               END


>> SOLVER DATA

   >> STEADY STATE
      END

      >> GROUNDWATER FLOW
         END


>> OUTPUT DATA

   >> SET PLOT OPTIONS
      HEADING          'EXAMPLE 1'
      BOUNDARY COLOUR  'BLACK'
      GRID COLOUR      'BLACK'
      END

   >> PRINT GLOBAL FREEDOMS
      END

   >> PLOT GRID
      END

   >> PLOT CONTOURS
      VARIABLE            'PRES'
      NUMBER OF CONTOURS  11
      COLOURS             'BLACK'
      CAPTION             'Contours of Residual Pressure'
      KEY TITLE           'Residual Pressure'
      END

   >> DRAW LINE GRAPH
      VARIABLE           'PRES'
      START POINT         0.0  0.5
      END POINT           1.0  0.5
      NUMBER OF POINTS   11
      JOIN POINTS
      SYMBOL COLOUR      'BLACK'
      LINE COLOUR        'BLACK'
      X AXIS TITLE       'Distance'
```

```
      Y AXIS TITLE       'Residual pressure'
      AXES TITLES CHARACTER SIZE 0.016
      AXES LABELS CHARACTER SIZE 0.014
      CAPTION            'Residual Pressure along Y=0.5'
      END


>> STOP
```

There are two parts to this NAMMU input file. The first part, which will be referred to as the *job information*, is data for a *job submission program* that creates the necessary operating system commands to run NAMMU on the chosen computer and then submits the job. The second part is a sequence of TGIN instructions that specify the required NAMMU options.

2.2 Job Information

The data in this part are in lines, each enclosed between a /∗ and a ∗/, so that they are treated as comments by NAMMU itself when it reads the input file (see subsection 2.1). The information is divided into blocks of lines, each of which begins with a line that is a special phrase such as `SPACE ALLOCATION` or `OUTPUT DATA FILES`. Within a block there may be one or more lines that specify numerical values or files to be used by the job submission program. The format of these lines is a phrase such as `REAL WORKSPACE` or `GRAPHICS` followed by one or more numbers or file identifiers or other character strings. The format of a file identifier depends on the computer and operating system in use. For a detailed description of these identifiers, and for further information on the format of the job information section, the Installation and Running Guide [11] should be consulted.

Comment lines can be placed at the beginning of the job information section, as shown in the example. It is strongly recommended that the user should take advantage of this facility to identify each input file. When NAMMU is run, a number of output files will be produced. Normally these will consist of a text file, containing information related to the running of the program and execution of the selected TGIN instructions, and a graphics file of output generated by the post-processing options that have been selected by the user. In order that output files can be readily associated with their corresponding input file, it is advised that a sensible naming convention be used. Suitable naming conventions will depend on the particular computer and operating system in use. However, some suggestions are given in the Installation and Running Guide [11].

2.3 Input Language: Syntax

The input data for the NAMMU program itself comes after the job information. It is written in the structured free-format input language TGIN. Data in TGIN can be classified into three categories, namely comments, commands and keywords.

Comments are enclosed by a '/∗' and a '∗/'. These comment characters may be used either to make notes in the data or to comment out TGIN instructions.

Commands consist of the command marker '>> ' followed by a phrase, and sometimes followed by qualifying data. For example:

```
>> NAMMU
```

is a command. The phrase may consist of one or more words separated by blanks. Each command should be the only TGIN instruction (other than comments) on its line.

The order in which commands are specified is important. For instance, the user may wish to set up part of the model, then produce various plots of the model generated so far, before modifying the model by adding further elements to the grid and replotting it. In this case, there is a clear sequence of events and this must be reflected in the order in which the commands to create the grid, produce the output and modify the model are specified.

The TGIN commands are organised into a hierarchy in which each command may have several subcommands associated with it. Detailed descriptions of the commands may be found in the NAMMU Reference Manual [7].

Each command may have a number of keywords associated with it. These are used to specify additional information for a chosen option. The format of a keyword consists of a phrase which is often followed by one or more values (numbers or character strings). For example,

```
VARIABLES    1
```

is a keyword that specifies that only a single variable will be used in the model. The keywords available for each command are described in detail in the NAMMU Reference Manual [7].

In some instances, it is convenient to provide keyword data in the form of tables. A table keyword is used to declare the table and other keywords are used to define the columns, each separated by a comma. For example,

```
PATCH POSITIONS
  CORNER NUMBER,    COORDINATES
        1            < 0.0 0.0 >
        2            < 1.0 0.0 >
       11            < 0.0 1.0 >
       12            < 1.0 1.0 >
```

Here, the angle brackets denote a list. Tables are used to input data for several keywords where the values for the different keywords are in one-to-one correspondence.

2.4 Input Language: Structure

When constructing an input file, it is important that the user should have an understanding of the sequence in which events take place during the execution of the NAMMU program. There are five main phases. First, the user selects the package by the command ≫ NAMMU. The next two phases involve a definition of the model, in which material properties and the finite-element model of the problem are specified. This is followed by a calculation phase. Finally, the required output is generated. Execution of the program is terminated by the command ≫ STOP.

Thus at the highest level, a NAMMU input file will consist of the options:

```
>> NAMMU
>> INITIAL DATA
>> MODEL DATA
>> SOLVER DATA
>> OUTPUT DATA
>> STOP
```

A brief explanation of the five major options and some of their more important sub-options is given in the following sections using Example 1 as an illustration. The definitive description of each option and its sub-options, and the associated commands and keywords, is given in the NAMMU Reference Manual, which should be consulted when creating input for a NAMMU run.

2.5 Invoking NAMMU (≫ NAMMU)

After any job information that may be required by a particular system, for which the user is referred to the Installation and Running Guide [11], the command ≫ NAMMU is the first TGIN instruction that appears in an input file. Its purpose is to invoke the NAMMU package.

The subcommands of ≫ NAMMU are concerned with:

1. defining the geometry of the problem;
2. selecting the coordinate system to be used;
3. choosing the variables to be solved for;
4. setting limits on the size of the problem.

The NAMMU package has been designed to be user-friendly. To this end, defaults have been set up with the solution of groundwater flow and radionuclide transport problems specifically in mind. The most important defaults for ≫ NAMMU are:

- The variables, which are:

a pressure variable with the name	'PRES',
a temperature variable with the name	'TEMP',
the horizontal Darcy velocity with the name	'UVEL',
the vertical Darcy velocity with the name	'VVEL',
a streamfunction variable with the name	'STFN',
a nuclide concentration variable with the name	'NUC1'.

- The default upper limits on the size of the problem that can be tackled in NAMMU, which are:

MAXIMUM NUMBER OF ELEMENTS	500,
MAXIMUM NUMBER OF NODES	4500,
MAXIMUM NUMBER OF FREEDOMS	27000,
BOUNDARY CONDITION INTEGER WORKSPACE	1000,
BOUNDARY CONDITION REAL WORKSPACE	200,
VARIABLES	6,
SPACE DIMENSIONS	2.

The defaults may be changed by using appropriate commands. For illustration, in the simple example the defaults relating to the variables are overwritten by the instructions:

```
>> SET LIMITS
   VARIABLES    1
   END

>> SET VARIABLES
   VARIABLE NAMES   'PRES'
   END
```

This limits the program to storing only a single variable, namely pressure. Further examples of how to set the variables are given in Sections 4–10.

The most common instance in which it becomes necessary to change the defaults is when the model size becomes too large. In this case, the user should increase the limits on the size of the model by including the command ≫ `SET LIMITS` and the appropriate keywords. Exact definitions of each of the limits that may be set are given in the NAMMU Reference Manual [7]. Note that the limits do not have to be exact. The use of excessively large limits incurs a penalty in computer memory.

2.6 Specifying Material Properties (≫ `INITIAL DATA`)

The command ≫ `INITIAL DATA` is used to specify data to be used throughout a run, such as the material properties. These are specified using the ≫ `PHYSICAL PROPERTIES` sub-command. Material properties may be constant throughout the domain, or the domain may

be sub-divided into several regions each with a different rock type. In Example 1, the physical properties are those appropriate to groundwater flow through granite. The permeability is taken to be $1 \times 10^{-16}\mathrm{m}^2$, and the porosity is set to 1×10^{-4}. In more complicated situations, each element may be assigned an appropriate set of material properties.

It is also possible to specify the behaviour of the material properties more generally by using the NAMMU interfaces to user-supplied routines. For example, the user may wish to model the flow of a fluid that in which the density does not vary according to the standard expression coded in NAMMU (see the NAMMU Technical Overview [8]). The way in which NAMMU interfaces with user-supplied FORTRAN routines is described in Section 11. The NAMMU Reference Manual [7] describes all the available user routines.

Note: all quantities should be given in S.I. units (kg, m, s).

2.7 Defining the Domain and Boundary Conditions (≫ `MODEL DATA`)

The command ≫ `MODEL DATA` is used to specify details of the finite-element model, such as the grid and boundary conditions. To create a finite-element grid, the subcommand ≫ `CREATE GRID` is used. The basic approach to grid generation using TGIN is to generate sub-regions of simple topology such as quadrilaterals, triangles and three-dimensional blocks.

The standard method for creating a finite-element grid is to create a grid composed of patches or polygons (polygons are restricted to two-dimensional problems). In two dimensions, the terms patch and polygon are used to mean a region bounded by straight sides, which is subdivided into elements. These methods of grid generation are ideally suited to generating the sort of grids needed to model complex geological formations. In Example 1, a patch consisting of a 2×2 grid of square elements is used to represent a square domain as shown in Figure 2.2. More complicated domains can be modelled using the same approach. A full list of the elements that are available in the TGSL element library is included in Appendix B.

There is no unique way of constructing a grid to model a particular region, and the resulting distribution of elements in the region will depend on how it has been sub-divided. Some guidelines on sensible techniques for modelling complicated domains are presented in Sections 3 and 4. Further guidance on grid generation may be found in 'A Guide to Finite-Element Grid Generation Using the TGIN Language' [12].

The boundary conditions are set using the command ≫ `SET BOUNDARY CONDITIONS`. Several types of boundary conditions may be specified by appropriate subcommands. In Example 1 the pressure has Dirichlet or specified value boundary conditions along the left and right hand sides. The boundary conditions along the top and bottom default to zero flux normal to the boundary.

Finally, the model is completed by setting initial values for the variables. The values may be required as an initial guess for Newton-Raphson solution of the equations to be solved,

or as an initial profile for a time-dependent calculation. The default is to set each variable to zero throughout the domain, except where a Dirichlet type boundary condition has been set. However, for non-linear problems it is strongly suggested that if any approximate solution is available then it should be used as an initial guess. This guess can be supplied to NAMMU through user routines. For the example discussed in this Section, the default initial condition is adequate.

Detailed definitions of each of the subcommands of ≫ `MODEL DATA` appear in the NAMMU Reference Manual [7].

2.8 Specifying the Equations to be Solved (≫ `SOLVER DATA`)

The command ≫ `SOLVER DATA` is used to specify the way in which the problem is to be solved.

The options available within NAMMU include:

- the solution of steady-state problems using ≫ `STEADY STATE`;
- an option for solving time-dependent problems with constant timestepping or automatic timestepping using ≫ `CRANK NICHOLSON`;
- an option for solving time-dependent problems with variable timestep sizes using ≫ `TRANSIENT`;
- an option for solving linear time-dependent problems using ≫ `FAST LINEAR TRANSIENT`.

The subcommands of these main options are used to specify the particular equations of interest and the variables for which they are to be solved. A full list of the equations that may be solved using NAMMU is given in the NAMMU Technical Overview [8]. In the example, options suitable for solving steady-state groundwater flow in a porous medium are selected.

Details of the options within ≫ `SOLVER DATA` are given in the NAMMU Reference Manual [7].

2.9 Specifying the Required Output (≫ `OUTPUT DATA`)

The command ≫ `OUTPUT DATA` is used to determine the type of output required.

Some of the more useful options are to:

- plot the grid;
- plot the boundary of the grid;

- plot the grid with different rock types shaded;
- plot contours of any variable or related scalar;
- plot line profiles of any variable or related scalar;
- plot advective pathlines;
- plot a vector representation of the flow field;
- print out the global freedoms vector (i.e. the values of all variables at the nodes of the finite-element grid).

In Example 1, the graphical output consists of plots of the grid, contours of the residual pressure field and a section through the residual pressure field, as reproduced in Figures 2.2, 2.3 and 2.4 respectively. The global freedoms vector is also written to the output file. Note that successive plots can be superimposed, for instance a plot of velocity vectors may be superimposed on contours of residual pressure.

The various output options are catalogued in the NAMMU Reference Manual [7].

2.10 Results

When NAMMU is run, various forms of output will be produced. A text file will always be generated, as well as graphics files or other types of output specified by the user. The text output from NAMMU will normally consist of an echo of the input data, interspersed with a title page, information on the model, information on the solver, and information on the output options.

Certain information concerning the grid and boundary conditions is automatically printed during the ≫ `MODEL DATA` phase, without being specifically requested, as follows:

- the number of elements of each type that were used, the number of variables, nodes and global freedoms present.
- for each element, the element number and type are printed, followed by the node numbers on that element;
- for each node, the node number, the number of global freedoms up to and including that node, the x and y coordinates, and the freedoms at that node are printed;
- information is printed out for each node at which a boundary condition has been set, including the type of condition, the variable, the node and the value.

Information is also automatically printed out during the ≫ `SOLVER DATA` phase. This information includes, for each iteration of the frontal solver, the total time spent assembling

the equations, the total time in the frontal solver, information on the change in the solution during the iteration. The information printed out as part of the ≫ `OUTPUT DATA` phase is a mixture of output specifically requested and that which is printed automatically. For example:

- The global freedoms can be printed using the command ≫ `PRINT GLOBAL FREEDOMS`. For each node, the node number and the values of the global freedoms at that node are printed out.
- When a line graph is plotted using ≫ `DRAW LINE GRAPH`, the value of the dependent variable is printed out for each value of the independent variable.

The total time spent in each of these phases is given in seconds at the end of the relevant phase. Finally, a message stating the amount of unused workspace is printed.

A detailed explanation of the output information generated by Example 1 is given in Appendix C.

The linear pressure profile shown in Figure 2.4 comes as no surprise, since this problem has the simple analytic solution

$$P^{\mathrm{R}} = x$$

For this analytic solution the Darcy velocity is simply

$$\mathbf{q} = (-10^{-13}, 0)\,\mathrm{ms}^{-1}.$$

2.11 Comments

When creating a NAMMU input file it is not necessary to select all the main options from the outset. For instance, when setting up a finite-element model, it is **strongly recommended** that, before any attempt to solve a problem is made, the grid be plotted to check that it is correct and sensible. When selecting commands and keywords it is **important** that the exact purpose and description be checked in the NAMMU Reference Manual.

Figures for Section 2

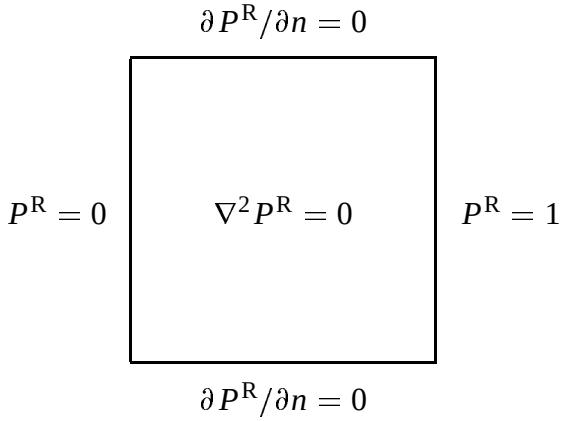


Figure 2.1 **A simple groundwater flow problem. The equation to be solved and the boundary conditions are expressed in terms of the residual pressure, P^{R}.**

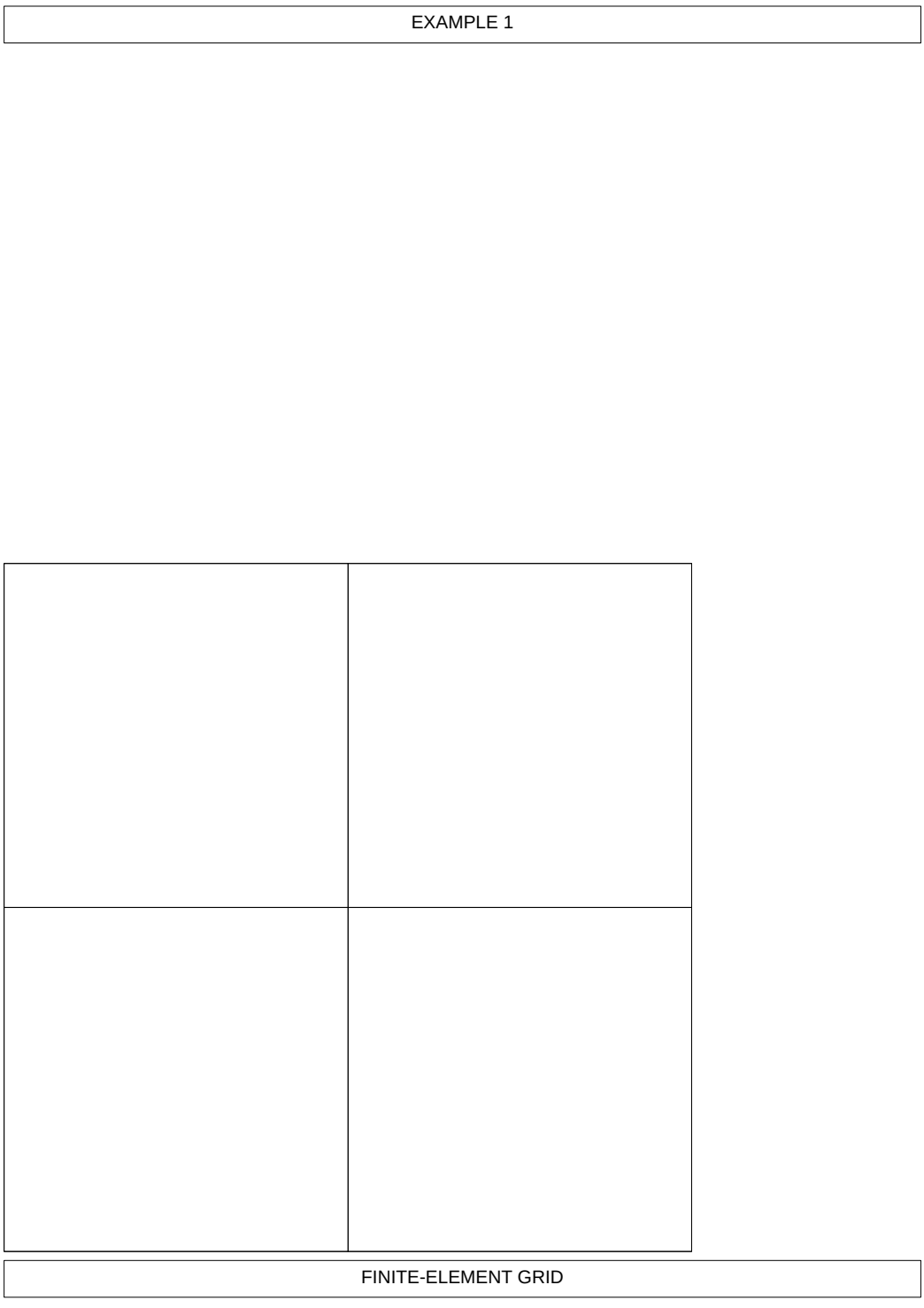


Figure 2.2 A simple grid generated using patches in Example 1.

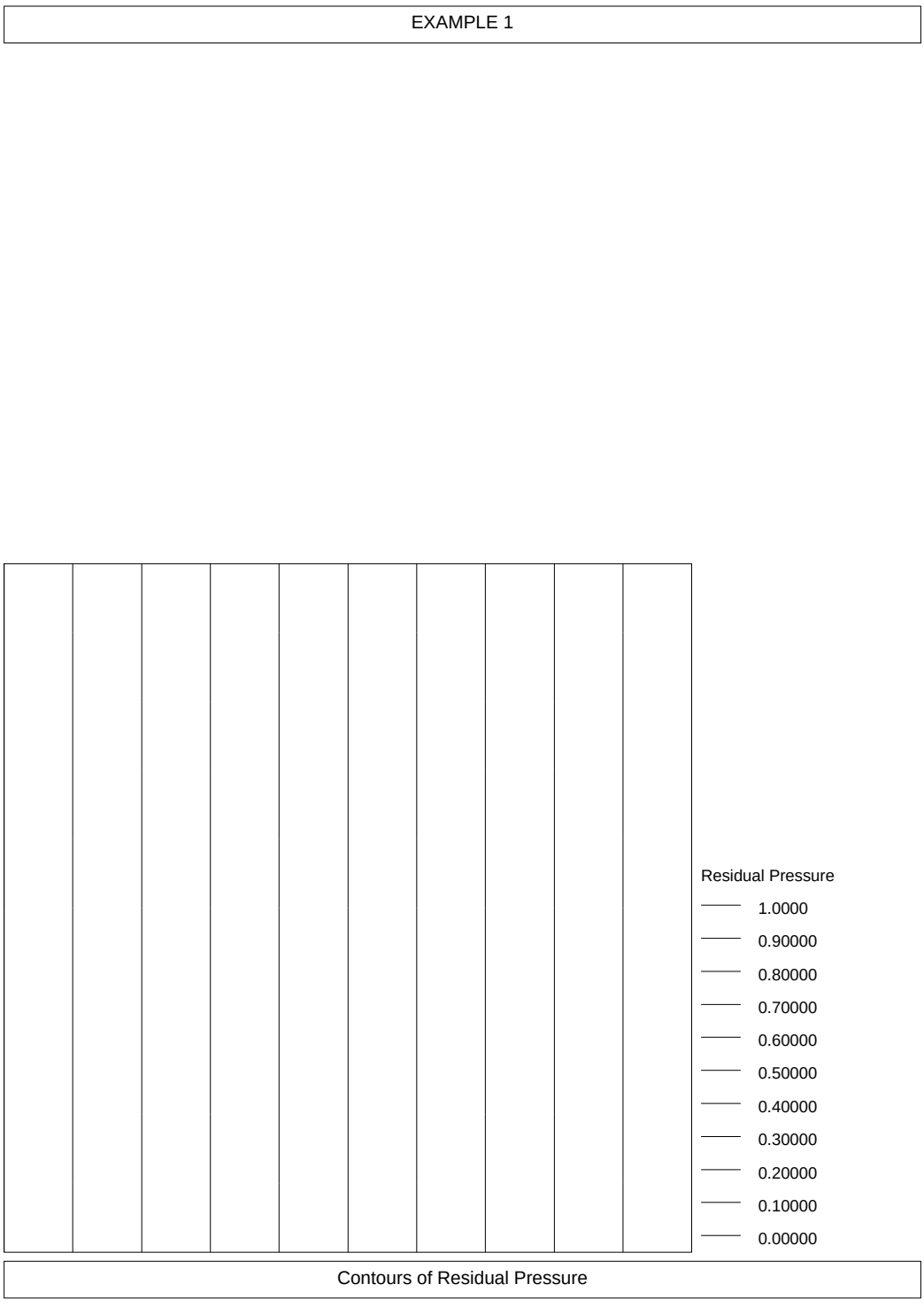


Figure 2.3 **Contours of the residual pressure field for Example 1. Eleven contours are plotted at equally spaced residual pressures in the range varying from $0\,\mathrm{Nm}^{-2}$ at $x = 0$ to $1\,\mathrm{Nm}^{-2}$ at $x = 1$.**

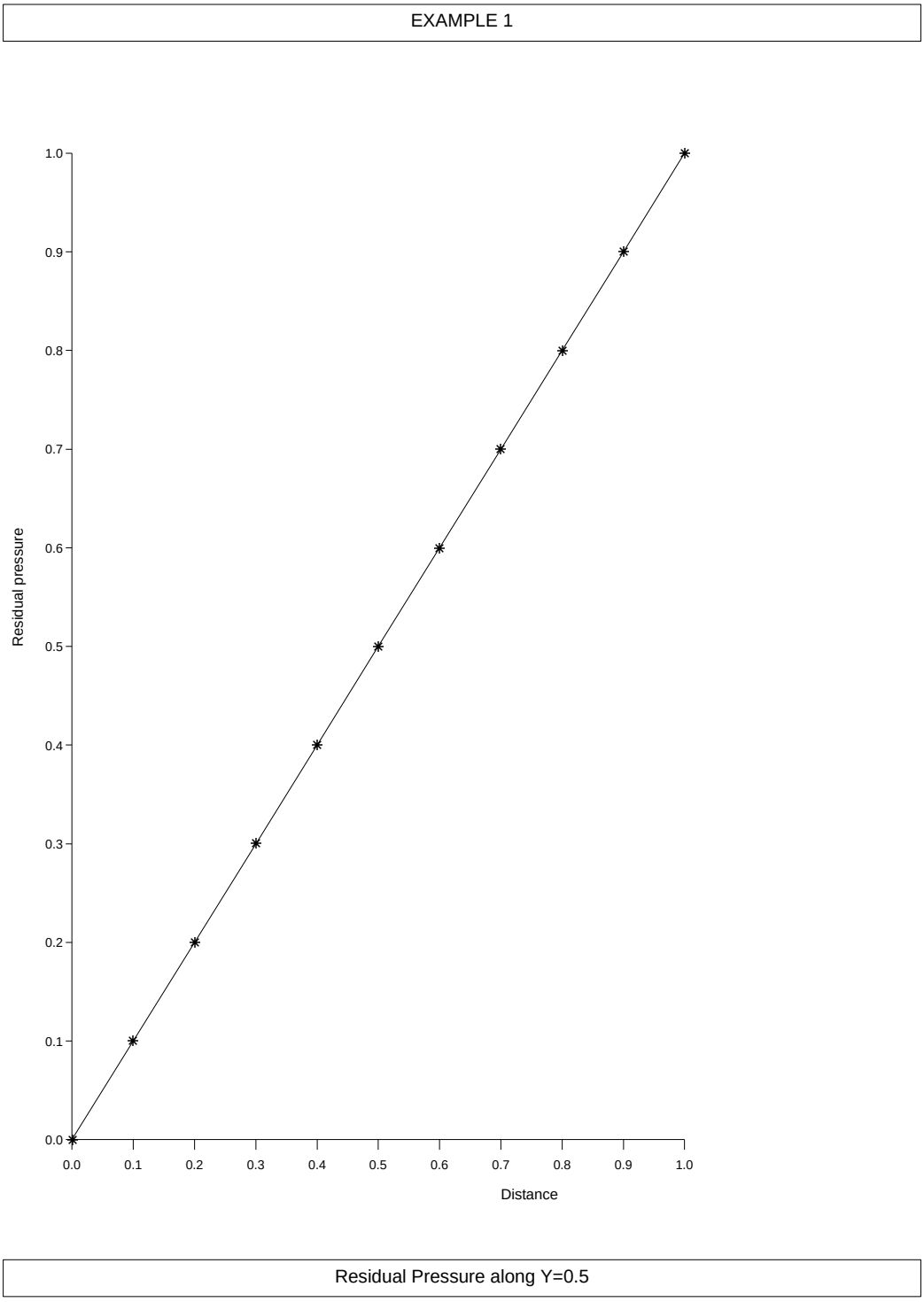


Figure 2.4 The residual pressure profile across the grid at $y = 0.5$.

3 MODELLING

This Section gives guidelines on finite-element modelling using NAMMU. A few of the topics discussed relate specifically to NAMMU, but most of the discussion addresses groundwater flow and transport modelling in general, and is equally applicable to other finite-element programs or to finite-difference programs.

The main points and recommendations of this Section are as follows:

- The aim of the modeller is to set up a representation of the system that is sufficiently accurate, but at the same time to keep the costs of setting up and running the model sufficiently low;
- An iterative approach is strongly recommended, starting from a simple model and refining or modifying it;
- If time and budget allow, the sequence of calculations should be a water-balance calculation, followed by two-dimensional areal calculations of the flow in the major aquifers, followed by calculations for one or more two-dimensional vertical cross sections, and only then should three-dimensional modelling be undertaken;
- The grid should reflect the material properties and the solution. It may need to be refined near boundaries and near changes in material properties;
- The need to modify and refine the grid should be anticipated when designing the model;
- Refinement tends to propagate through the grid. Before the input data set is created, the effect of refinement on the grid should be considered;
- Adjacent finite-elements must match (unless the constraints facility in NAMMU is used);
- Avoid the use of highly distorted finite-elements;
- Element sides should be nearly horizontal and vertical where possible;
- The topology of the grid should be kept rectangular in so far as possible. Number the patches or polygons systematically;
- In the first instance, faults should be represented as narrow bands of elements through which the formations continue and are displaced;
- Check the model. Plot the grid and the material property types;
- Make sure that convergence has been achieved for non-linear problems. For NAMMU, this is checked by monitoring the values of the variable RSTEP reported for each Newton-Raphson iteration.

These points are discussed below. The recommendations given are based on many years' modelling experience, and although there will undoubtedly be exceptions to specific points, the suggestions should not be ignored without due reason.

3.1 Goals of Modelling

Modelling is a skill that can be learned. The primary objective is to set up a model of the system of interest that represents all the relevant features sufficiently well that the predictions of the model are of acceptable accuracy, that is match the actual behaviour of the system sufficiently closely. A poor model may give inaccurate, or even completely wrong results, particularly for a non-linear system. However, the cost of setting up the model and of running it must be acceptable. The skill in modelling lies in setting up a model that gives adequate accuracy for acceptable cost. It should be stressed that there is no unique model of any system.

3.2 Adequate Representation

The size of the error, or difference between the model and the behaviour of the system, that is acceptable depends on the application. Two parts to this error can be identified. First, there is a component due to the approximations made in representing the system by the underlying mathematical model, including the choice of parameters. It is not possible to give any guidance on the size of this, as it depends on the physical system and the information that is available. Experience is the best guide here. The judgement of the analyst can be supported by calculations to quantify the sensitivity of the model to changes in the model or parameters. The uncertainty in the results resulting from the uncertainty in the model or the parameters can then be assessed.

The second component of the error is the numerical discretisation error resulting from the use of the finite-element model. The shape, size and orientation of the elements should be chosen so that the finite-element representations of all the relevant quantities are good approximations.

Usually, on a single finite element a quantity is represented by a low-order polynomial. Typically, the material properties are represented by constants (zero-order polynomials) on each element, and the unknown fields that the model is being solved for (for example, head in a groundwater flow model) are represented by first- or second-order polynomials (see Appendix A and Reference [13]). Therefore, in general, a single finite element will not be a good representation of a quantity that oscillates several times over the region of the element, or varies very rapidly (see Figure 3.1(a)). In order to represent such a quantity well, it is necessary to use several finite elements, chosen so that the variation of the quantity over each element can be well-approximated by the appropriate polynomials on the element (see Figure 3.1(b)).

Similarly, a single finite element will not in general give a good approximation to a quantity that varies discontinuously, or has discontinuous derivatives (see Figure 3.1(c)). In order

to represent such a quantity well, it is best to try to place the element boundaries approximately along the lines (in two dimensions) or surfaces (in three dimensions) where the discontinuities occur (see Figure 3.1(d)), as the constant polynomials on each element are discontinuous there and the first- and second-order polynomial have discontinuous derivatives there.

In general, for a consistent numerical discretisation, the discretisation error is reduced if the grid is refined and more, smaller elements are used. For example, the discretisation error in the groundwater head calculated from a finite-element model using quadratic finite-elements ultimately decreases proportionally to the cube of the size of the elements as this is reduced; if linear finite-elements are used the discretisation error in the groundwater head ultimately decreases proportionally to the square of the size of the elements. Therefore, in principle, the discretisation error can be quantified by the use of calculations on highly refined models, if these are practicable.

The number of elements required to obtain a given accuracy is much greater in three dimensions than in two. For example, a $10 \times 10 \times 10$ grid of quadratic finite-elements in three dimensions has 1000 elements and about 8000 pressure degrees of freedom. A 10×10 grid of quadratic finite-elements that would give a similar level of accuracy in two dimensions would only have 100 elements and about 400 degrees of freedom.

In general, numerical models give more accurate results for the primary quantities that are calculated using the model, such as the groundwater head in a groundwater flow calculation, than for secondary quantities, such as the velocity, which are calculated from derivatives of the head. As a very rough rule of thumb, the best that can be expected in practice with a suitably refined grid is to be able to obtain groundwater heads accurate to 1% say, whereas the groundwater velocities will probably be accurate to only 10% using the same grid. These figures should be treated with caution. For simple two-dimensional problems, it may be possible to obtain rather greater accuracy on practical grids, but for complicated three-dimensional problems, it may not be possible to obtain even this level of accuracy for grids that have sufficiently few unknowns for calculations to be practicable.

The use of refined models reduces the numerical discretisation error, but considerable computational resources are required to undertake calculations with a highly refined model with many finite elements. The resources required typically grow faster than linearly with the size of the model. For example, finite-element calculations in two dimensions using a direct frontal solver, as used in NAMMU, require in-core storage that is asymptotically proportional to the number of elements, and the CPU time is asymptotically proportional to the square of the number of elements; in three dimensions the in-core storage required is asymptotically proportional to the 4/3 power of the number of elements and the CPU time is asymptotically proportional to the 7/3 power of the number of elements. Bearing in mind that the number of elements required to obtain a given accuracy is much greater in three dimensions than in two dimensions, the computational resources required for three-dimensional models may be very considerable. Part of the skill in modelling lies in choosing a grid that is refined in only the regions where this is necessary. This enables accurate calculations to

be undertaken but keeps the cost down.

Similar remarks hold for discretisation in time. Most time-stepping schemes are equivalent to adopting a polynomial approximation to the variation in the solution at a point over several time steps. Over a single element or time step, the solution is being approximated in a simple fashion, the element, grid block or time step should be sufficiently small for this to be a good approximation. For example, in transient calculations of advection-dominated solute transport, it would not be advisable to choose time steps such that a solute front passes over more than one element in a single time step. This corresponds to a limit on the time step that is equal to the Courant stability limit for a simple upwind finite-difference scheme. Although longer time steps might be possible with a suitably stable implicit scheme, the accuracy of the solution is likely to be low, unless little is changing in the elements in question over the time step.

3.3 Iterative Approach

An iterative approach to modelling is strongly recommended. One should not attempt to 'dive straight in at the deep end' and try to set up a complicated model with many finite elements as soon as a modelling task is presented. Rather one should proceed with caution, starting from simple models, and gradually building up understanding of the behaviour of the system using more and more complicated models. At each step, the experience gained at previous steps should be used in setting up an improved model.

Experience has shown that once a model has been set up and preliminary calculations undertaken, it is nearly always necessary to modify or refine the model. Modifications may be required because the behaviour of the solution was not anticipated precisely. (Of course, if one could anticipate the results precisely it would hardly be necessary to undertake the modelling.) Modifications may also be required because the requirements of the modelling task are changed once the preliminary results have been examined.

3.4 Sequence of Calculations

As emphasised above a step-by-step approach should be adopted, gradually building up the complexity of the model. If time and budget allow, probably the best approach is to begin by undertaking a water-balance calculation taking into account the major aquifers in the region of interest. Then two-dimensional areal or vertically integrated calculations of the flow in the major aquifers should be made. Next, calculations should be made for one or more carefully chosen two-dimensional vertical cross sections. Only then, when the behaviour of the system is well understood, should calculations be made for three-dimensional models, as these take much longer to set up, and require much greater computer resources.

The areal calculations will provide support for the choice of vertical cross sections, as the flow in the aquifers will control to some extent the flow in the low-permeability formations. However, it may be possible to estimate the flow in the aquifers, and so areal calculations may not be necessary. Vertical cross-section models enable travel times from depth to the

surface to be computed, so they are probably the most useful groundwater flow calculations for repository performance assessments.

It is recommended that steady-state calculations are undertaken before any transient calculations are attempted. Before carrying out a transient solute transport calculation, it is often useful to carry out a simple steady-state solute transport calculation, which is cheaper than the transient calculation. In combination with the pathline calculations in the flow field, the steady-state transport calculation provides guidance on the regions that solute reaches at significant concentration; and it can also be useful for initial grid-refinement studies.

3.5 Data

The first step in modelling should be to review all the available data. This may come from many sources. Information on the geological structure may come from geological maps, from information from boreholes, or from seismic or other surveys. Data on the hydrogeological properties may come from borehole measurements, or it may be necessary to base the modelling on generic data appropriate to the types of rock in question. For example, Table 3.1 (taken from Reference [14]) gives typical values of permeability.

$\log_{10}(k(\mathrm{m}^2))$	-20	-19	-18	-17	-16	-15	-14	-13	-12	-11	-10	-9	-8	-7
$\log_{10}(K(\mathrm{m\,s}^{-1}))$	-13	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0
$\log_{10}(K(\mathrm{cm\,s}^{-1}))$	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1	0	1	2
$\log_{10}(k(\mathrm{cm}^2))$	-16	-15	-14	-13	-12	-11	-10	-9	-8	-7	-6	-5	-4	-3
$\log_{10}(\mathrm{md})$	-5	-4	-3	-2	-1	0	1	2	3	4	5	6	7	8
Aquifer	None					Poor				Good				
Soils						Very fine sand, silt loess, loam, solonetz				Clean sand or sand or gravel			Clean gravel	
	Unweathered clay					Stratified clay			Peat					
Rocks	Breccia, granite			Good limestone, dolomite		Sandstone		Oil rocks						

Table 3.1 Typical values of hydraulic conductivity (K) and permeability (k) (from Reference [14]). (The millidarcy (md) is a permeability unit much used in the oil industry.)

The next step is to decide on the important features that should be included in the model. In particular, the aquifers (high-permeability formations) and the aquitards (low-permeability formations) should be identified. The extent of the region to be modelled should also be determined. It may be necessary to model a much larger region than that of direct interest in order to have a region for which appropriate boundary conditions can be defined.

It is also necessary to decide whether it is necessary to model coupled groundwater flow and the transport of salinity or heat, or whether it is sufficient to model freshwater flow alone. This can only be decided after consideration of the available data.

If there are many different formations in the region of interest it may be possible to simplify

the model by combining formations into effective units. For example, a series of horizontal layers as shown in Figure 3.2 can be combined into a single unit with an effective horizontal permeability given by the arithmetic average of the horizontal permeability of the layers and an effective vertical permeability given by the harmonic average of the vertical permeability of the layers. It is recommended that in the first instance this approach is only used to combine aquifers and aquitards separately.

In initial studies, the top surface of the model should be taken as the position of the water table, and the boundary condition on the top surface should be taken as a fixed-head condition (at the value corresponding to the elevation of the water table). In most cases in the UK, there is sufficient rainfall to ensure that the water table is near to the ground surface, except under the peaks of hills. It is therefore recommended that the top surface of the model be taken at an elevation slightly less than the ground surface, except under the peaks of hills, where the top surface should be taken rather deeper below the ground surface. If the boundary condition is a specified flux then it is necessary to ensure that the value used is appropriate to recharge the deep groundwater system, otherwise groundwater heads greater than those observed may be calculated. A high-permeability layer of surface soils and rocks can be included and the properties of this calibrated to ensure that the heads in the model are physical, that is the heads in the surface layer are below ground surface.

3.6 Initial Choice of Grid

It is necessary to choose the grid so that it gives an adequate representation of both material properties (such as permeability in groundwater flow calculations) and the unknown quantities of interest (such as groundwater head in groundwater flow calculations). It is usually fairly straightforward to choose the grid to represent material properties such as permeability, the variation of which is known before the model has been set up and calculations made. The grid should be chosen to have many small elements in regions where the properties are varying rapidly, and to have element boundaries at interfaces across which the material properties change discontinuously.

In principle, exactly the same approach should be adopted to ensure that the grid can adequately represent the unknown quantities of interest. The difficulty is that because these quantities are unknown, the regions of rapid variation or discontinuities are not known before the calculations are undertaken, but to undertake the calculations requires the grid to have been set up. It is therefore necessary to set up an initial grid using one's best judgement as to the regions that need refinement and then to modify the grid iteratively until it gives acceptable results.

It is usually possible to make a reasonably good initial guess at the regions where the solution is changing rapidly. For an equation similar to the steady-state equation for groundwater head (which, in technical terms, is elliptic), these regions are likely to be near the boundaries of the domain, near rapid variations in the material properties and near discontinuities in material properties. Thus these are the regions where many elements are expected to be necessary, and the regions where the grid should be refined in the initial version of the model.

For an equation such as the heat transport equation, which is likely to be predominantly a diffusion equation (in technical terms a parabolic equation), the regions needing refinement are likely to be around any sources of heat, such as a repository for radioactive waste.

However, for an equation such as the equation for transport of a solute (for example, radionuclides or salinity) the behaviour of the system is likely to involve the movement of a plume of the solute through the system; and the regions needing a fine grid are likely to be around the front of the plume. This is likely to mean that the grid has to be refined over all of the region through which the plume moves. One possible approach to try to minimise the number of elements is to use more than one grid, starting with a grid that is refined only in a region near the source of the solute, and following the motion of the plume until it starts to go beyond the region of refinement, when the grid is changed to one that is refined in the region that the plume is about to move through, but is coarse in the region that the plume has already traversed.

If several different processes are being modelled simultaneously, then the grid has to be refined appropriately to represent all of the processes adequately. However, if one (or more) of the processes is not affected by the other processes of interest it may be possible to undertake calculations for that process (or processes) on one grid, and then undertake calculations for the remaining processes on a different grid. For example, radionuclide transport does not affect the groundwater flow because the concentrations of radionuclides are very low and do not affect the density of the groundwater. Thus it is possible to calculate the groundwater flow using a grid that is suitably refined to represent adequately the groundwater head (or pressure). Once the flow has been determined then the radionuclide transport can be calculated using a grid that covers only the region where the concentration of radionuclide is significant. This is likely to be much smaller than the region required to model the groundwater flow, which will extend to locations where boundary conditions for the flow can be sensibly assigned.

However, the radionuclide transport calculation will probably require a grid with much smaller elements than the grid for the flow calculation, as it will have to represent the transient motion of the radionuclide plume. Thus the cost of the radionuclide transport calculations may well be comparable or even larger than the cost of the flow calculations. However, the combined cost will be considerably less than the cost of undertaking calculations on a grid that was fine enough to represent the motion of the radionuclide plume and covered a large enough region to model the flow.

3.7 Elements Must Match

One very important point that must be noted is that in general the elements must match along their common boundary, that is the corners of one element must be at the same positions as the corners of the other element and any other nodes along the sides must also match, as shown in Figure 3.3. It is not generally sensible to build a model in which the elements do not match. (NAMMU does include a facility, the ‘constraint’ facility, that can be used to interface between grids that do not match. However, this facility is not part of the

standard release and should be used with extreme caution, preferably after consultation with AEA Technology. It should not be used to try to make a bad grid into a good grid. Rather its purpose is to enable unnecessary refinement to be avoided by allowing localised regions of refinement to be matched into a coarser grid.) Similarly it is not generally sensible to build a model in which there are gaps between the elements as shown in Figure 3.3 (c), or some regions are covered by more than one element as shown in Figure 3.3(d), although regions having effectively zero permeability can be omitted from the model.

3.8 The 'Patch Grid' Facility

The 'patch grid' input facility (and the closely related polygon grid input facility) in NAMMU (NAMMU Reference Manual [7]) is designed to make it as easy as possible to refine a model of a complicated geology with many different formations. Once a basic model of the geological structure has been set up, it can be refined simply by changing a few parameters that describe the refinement required in large blocks or 'patches' of finite-elements. However, it is necessary to anticipate the possible need for refinement to exploit this facility properly.

The basic idea of the 'patch grid' facility is that the complicated geometry of the domain of interest is built up from 'patches' that are bounded by straight lines and subdivided into elements, with all the elements in a patch having the same material properties. In the current release, triangular and quadrilateral patches are available for modelling in two dimensions, and prism and hexahedral patches are available for modelling in three dimensions, some of which are shown in Figure 3.4. The patches in a particular model are effectively just mappings of the patches in their standard form shown in Figure 3.4 to their position, shape and orientation in the model. For example, Figure 3.5(a) shows a very simple two-dimensional geological structure with three layers, and Figure 3.5(b) shows a possible discretisation of this into patches, and Figure 3.5(c) shows a possible refined grid of elements generated from the basic patch grid. The quadrilateral patches in two dimensions are subdivided into elements by lines parallel to the coordinate axes in the standard orientation of the patch. Triangular patches are subdivided into elements by lines that where possible are parallel to the coordinate axes in the standard form. The hexahedral and prism patches in three dimensions are similarly subdivided by surfaces that where possible are parallel to the coordinate planes. Hence the subdivision of a patch is specified by the subdivisions in the directions of the coordinate axes in the standard form of the patch. These are identified by 'refinement indices' for the patch that specify the refinement pattern from a list of possible patterns used in the model. Therefore by changing a few parameters that define the refinement pattern, the refinement can be changed for all the patches whose indices specify that pattern. Indeed, this is precisely why the subdivision is specified by a refinement index.

In order to exploit the power of the patch grid facility, some rules must be followed. First, the corners of patches that have a side in common must match. Secondly, the patterns of refinement along the common side must match. This ensures that the elements match along common sides, as discussed above. Of course, it is possible, through careful choice of the refinement patterns, to build a grid in which the elements match, although the patches do

not. However, if the patches were set up in this way it would not be possible to define the refinement patterns arbitrarily and changing the refinement would require care, whereas if the rules are followed the refinement patterns can be arbitrarily changed. The second requirement can be readily achieved by simply making the refinement indices for the corresponding directions along the matching sides the same.

Because of the way patches are refined, the refinement on the top side of a quadrilateral patch in standard orientation is the same as that on the bottom side. Similarly the refinement on the left and right sides is the same, but may be different to the refinement of the top and bottom sides, of course. If there is another quadrilateral patch on top of the first, then its top side will have the same refinement as the bottom, which is the same refinement as the top side of the first patch, which in turn has the same refinement as the bottom side of the first patch. Hence the refinement propagates through the patches.

For triangular patches, two of the sides have the same refinement and the third side is subdivided into fewer elements. In some types of triangular patch, the refinement of the most refined sides is propagated through the patch, although it may be converted from a refinement in the horizontal direction to a refinement in the vertical direction. Unless this change of refinement direction is specifically desired for some reason, it is best avoided. In addition, if the relative values of the two different refinements assigned to such a patch change, the refinement that is propagated through the third side may change. For other types of triangular patch, the refinement in one direction passes directly through the patch and the refinement in the other direction 'pinches out'.

It is strongly recommended that before an input data file is set up the independent refinement indices for all the patches are determined as shown in Figure 3.5(b). This will enable one to decide if refinement would be propagated into unnecessary regions of the model because of an unfortunate choice of the patch topology. If necessary the topology could then be modified.

It should be noted that because triangular patches may effectively have six orientations it is necessary to be careful about which sides correspond to the coordinate axes in the standard form so that the patch is refined as required. It should also be noted that it may be necessary to have refinement patterns that are essentially the mirror image of one another to specify the refinement of both a triangle in standard orientation and its mirror image as shown in Figure 3.6.

Rectangular patches may have essentially two orientations. It is recommended that in the input data all the rectangular patches are described in the same manner, such that the first coordinate in the standard form corresponds to the horizontal x-axis. This avoids possible confusion. Therefore the description in the patch topology table should begin with the lower left corner and proceed anticlockwise around the patch.

Corresponding remarks hold for the hexahedral and prism patches in three dimensions.

3.9 Triangles and Prisms

In principle, the use of triangle elements in two dimensions and prism elements in three dimensions can make it easy to generate grids to represent complicated geometries as shown in Figure 3.5. However, there is some evidence to suggest that triangle elements are less accurate than quadrilateral elements [15]. The use of triangles (for some of the available triangular patches) and prisms can lead to difficulties in refinement. For the prism patches and for some of the triangular patches used in the current release of NAMMU, the refinement propagates through a triangle, in the sense that one of the other sides must have the same refinement as the most refined side. This may mean that refinement in one direction is converted into refinement in the other direction and then propagates throughout the whole grid. Further, the use of triangle elements means that the grid no longer has a simple rectangular topology. This may make it more difficult to set up and check the model. It is therefore recommended that the use of triangle and prism elements is kept to a minimum.

A case such as that shown in Figure 3.5, in which a particular formation 'pinches out', might seem an obvious candidate for the use of a triangle element, but it can be readily modelled using a quadrilateral element with one very short side as shown in Figure 3.7, so that the grid has a rectangular topology. This approximates the supposed geological structure, but might actually be more realistic than a sharp pinch out. It is not necessary for the elements that are the continuation of the layer that pinched out to remain thin: their thickness can be chosen as convenient away from the pinch out. Alternatively, one of the triangular patches that pinches out could be used.

In three dimensions there are also potential difficulties with the use of prisms in that a prism cannot simply be used locally, as the triangular face effectively propagates through the model (see Figure 3.8). It should be noted that it is not advisable for example to put two prisms together and try to match the resulting hexahedral shape to a standard hexahedral element, as shown in Figure 3.9. At the interface the elements do not match. Thus although it may be very convenient to set up a grid that mainly comprises hexahedral elements in a rectangular topology, and then replace selected hexahedra by the combinations of two prisms, this propagates along a line of hexahedra throughout the grid as shown in Figure 3.10, if the elements are to match properly.

If prisms are used in a three-dimensional model then as noted above the triangular faces will propagate throughout the grid. If prisms are used then it is recommended that they are only used with the triangular faces in one of the coordinate planes. If this is not done then care must be taken to avoid lines of prisms propagating in different coordinate directions meeting, since at such meetings there are likely to be considerable difficulties in refining the grid.

3.10 Orientation

In general the horizontal dimensions of aquifers are much greater than their vertical dimensions. This means that the head in an aquifer is usually nearly constant in a vertical direction

and varies predominantly in the horizontal direction. Therefore it is recommended that for two-dimensional cross-sectional models, two opposite sides of quadrilateral elements are vertical in an aquifer, and similarly one side of a triangle element is vertical, unless there is some other reason for a non-vertical orientation, such as the need to model a fault, or other change in material properties, along a line that is not vertical.

Using the patch grid facility in NAMMU, this is achieved by making two sides of a quadrilateral patch vertical. It is probably best for the other patch sides to lie along the tops and bottoms of the various formations being modelled. Similar remarks hold in three dimensions.

There is another benefit to making the patch sides vertical where possible, in that it simplifies entry of the coordinates of the patch corners in NAMMU, as then the horizontal coordinates of groups of corners are the same.

One should expect that it will be necessary to refine an aquifer in the horizontal direction in order to obtain an adequate representation, but a single element in the vertical direction may be adequate.

The use of highly distorted elements should be avoided as the accuracy of the solution may be low in their vicinity.

3.11 Faults

It is to be expected that there will be faults in the region of interest. The rock in the vicinity of faults may have a wide range of hydrogeological properties, depending on the nature of the rock and its history. For example there may be greatly enhanced fracturing, leading to enhanced permeability compared to the rock away from the fault. At the opposite extreme clay minerals may have been formed along the fault, leading to greatly reduced permeability.

Unless there is information to suggest an alternative model, it is recommended that the rock in the immediate vicinity of faults be modelled as a zone through which the formations continue, but are displaced as shown in Figure 3.11(b). This provides maximum flexibility for possible future grid refinement, and the two extreme possibilities for the properties of the rocks in the vicinity of the fault can be catered for by appropriate choice of the properties of the elements in the fault zone. However, it may be necessary to modify the grid in the fault zone as shown in Figure 3.11(d) in order to cater for the possibility of the fault acting as a simple geometrical feature that brings different aquifers into hydrogeological contact.

3.12 Checking

The importance of checking the model carefully cannot be stressed enough. The model should be checked carefully before any calculations are undertaken. It is recommended that the input data file, other than the geometry of the model, be checked by someone other than its author. It is very difficult to check the geometry from the tables of input data:

the best check of the geometry is by visual comparison of plots with the maps and other diagrams, such as cross sections, that define the domain of interest. In two dimensions this is straightforward: the grid should be plotted and compared with the domain. The grid should also be plotted with the elements shaded according to material property type. If the grid has been generated using the patch-grid facility in NAMMU, the cost of this type of plot can be reduced by shading the patches with only a single element per patch. The boundary of the domain should be plotted, as this is a sensitive check on any possible element mismatches, which show up as isolated internal sections of boundary. Any regions where the elements are very small, such as in the vicinity of faults should be zoomed in on.

In three dimensions it is more difficult to check the geometry of the model. The surface of the model should be plotted from different viewpoints, both with the element boundaries marked, and with the elements shaded according to material property type. It is also recommended that the elements and the material property types be plotted on a series of slices parallel to the coordinate directions or to major directions of the model, both in perspective plots and as a series of individual plots. If it is available, it is recommended that Avizier is used to check the model.

Given a satisfactory grid, calculations can be undertaken. The results of these calculations should be checked for obvious problems, and to see if the grid is sufficiently refined. The best indications of an inadequate grid are oscillations of the solution on the scale of the elements. (This is related to the error-measure suggested in Reference [16]). It is therefore recommended that profiles of the velocities along horizontal and vertical lines are plotted. Pathlines also provide a sensitive measure of the adequacy of the grid. If the grid is insufficiently refined then the pathlines will oscillate or may even stop in an element in the middle of the domain.

If the equations solved are non-linear (e.g. the equations for salt transport) then it is essential to check that the solution has converged. In NAMMU this is done by considering the behaviour of the quantity called RSTEP. This is a measure of the magnitude of the largest change in one of the unknown nodal values (degrees of freedom) over an iteration. The exact definition of RSTEP depends on the basis functions being used. RSTEP is calculated for each Newton-Raphson iteration. Once the iterations are sufficiently close to the solution they converge quadratically and RSTEP correspondingly decreases quadratically. However, RSTEP (and the convergence) is ultimately limited by round-off. The smallest value of RSTEP that can reasonably be expected is about 10^3 times the computer precision, but this may be slightly larger for large problems whose solution involves many arithmetic operations. For example, on the Silicon Graphics Power Challenge computer, real numbers normally have about 15 significant figures and so one cannot expect to achieve a value of RSTEP smaller than about 10^{-12} or 10^{-11}.

In practice, it is not necessary to converge a problem to this level. Once the iterations are starting to converge properly they converge quadratically. Thus once RSTEP has decreased to about 10^{-6} the next iteration should give a much smaller RSTEP, indicating that the change in the solution would be very small. Thus it is not really necessary to undertake the

iteration.

Although the first iteration for a linear problem gives the answer to sufficient accuracy, the value of RSTEP will be large as it measures the change in the solution from the initial guess for the solution. If the problem is known to be linear, for example a simple groundwater flow problem, then it is not necessary to undertake further iterations, even though the only value of RSTEP is large. However, it is a useful check when testing the program to undertake several Newton-Raphson iterations for a supposedly linear problem. The second value of RSTEP should then be much smaller than the first.

Finally, whatever the problem being addressed, it should be checked that the results calculated numerically are sensible physically, perhaps by comparing with the results of hand calculations for simplified models. Mass balance for various regions should also be checked.

3.13 Solvers

In simple groundwater flow calculations the discretised approximation to the head or pressure is determined as the solution to a linear matrix equation. NAMMU includes a very robust direct frontal solver that is more or less guaranteed to solve such an equation provided that there is sufficient computer storage available and sufficient time is allowed. Iterative solvers or semi-iterative preconditioned conjugate gradient solvers could also be used. If the details of the methods are examined it can be seen that the direct solver used in NAMMU is likely to be as fast as, for example, preconditioned conjugate gradient solvers for all practical problems in two dimensions. However, in three dimensions preconditioned conjugate gradient solvers are likely to be faster than direct solvers for moderately large grids.

The direct frontal method is a variant of Gaussian elimination that uses only a small in-core working matrix (called the frontal matrix). The elements are processed in sequence. Contributions from successive elements to the overall matrix are assembled and then added to the in-core frontal matrix. As the assembly proceeds, entries in the matrix become 'fully-summed', in that there will be no further contributions to the entries in question from any of the remaining elements. Once all the entries in a row of the matrix are fully summed, Gaussian elimination is carried out for that row. In this way the in-core matrix needs to be only as large as the 'frontwidth', which is the largest number of freedoms that are not fully summed at any stage in the process. The computational cost of solving any particular problem can be minimised by ordering the elements to minimise the frontwidth. A good approximation to this can usually be achieved by ordering the elements sequentially starting with the direction in which there are the least number of elements, as shown in Figure 3.12(a).

NAMMU has a facility for renumbering elements automatically using the command `>> RENUMBER ELEMENTS`, and it is strongly recommended that this is used for any grid containing more than a single patch.

3.14 Non-linear Calculations

Simple groundwater flow calculations are linear, and can be solved using the matrix solution technique described above. However, in some cases it is necessary to use non-linear equations to represent the processes of interest. For example, coupled groundwater flow and transport of salinity, or coupled groundwater flow and heat transport are both non-linear because the salinity (or temperature) affects the groundwater density, which in turn affects the groundwater flow, and the salinity (or heat) can be transported by the flow. The other case of solute transport that is of particular interest, namely radionuclide transport, is not really non-linear, as the concentrations of radionuclide are expected to be so small that they have negligible effect on the groundwater density and hence on the flow.

Non-linear equations can be much more difficult to solve than linear equations. NAMMU includes some very powerful facilities for the solution of non-linear equations. Generally, the Newton-Raphson iteration technique is used. Provided that the initial guess is sufficiently close to the solution this converges quadratically. However, it can be hard to find an initial guess sufficiently close to the solution for difficult non-linear cases. In this case the technique of parameter stepping is recommended. The basic idea of this is very simple. The solution to the problem of interest is obtained by considering a series of problems related through the variation of a parameter such that the first problem is easy to solve and the last is the problem of interest and intermediate problems are progressively more difficult to solve. At each step the solution to the previous problem is used as the initial guess for the next problem. This technique can be used to obtain the solution (and indeed to explore the nature of the solution as a function of the parameter, that is the bifurcation structure of the problem). Parameter stepping can be carried out in an ad hoc way by hand, and in most cases this is probably best. NAMMU also includes automatic parameter-stepping algorithms, but the use of these is probably best left until one has some experience with parameter-stepping by hand.

Figures for Section 3

Figure 3.1 **Illustrations of poor and more acceptable finite-element representations of quantities (in one dimension for convenience). (a) a poor representation of a quantity that is varying several times over a single element, (b) a much better representation of the quantity shown in (a) obtained by refining the grid and using several elements, (c) a poor representation using a single element for a quantity that is varying discontinuously, (d) a much better representation of the quantity shown in (c) using two elements chosen to locate the discontinuity on the boundary between the elements.**

Figure 3.2 Effective properties for a combination of layers.

Figure 3.3 **Illustration of acceptable and (generally) unacceptable ways of joining finite-elements. (a) an acceptable grid with adjacent elements matching, (b) an unacceptable grid with a mismatch between the elements along the line AB, (c) an unacceptable grid with a hole, (d) an unacceptable grid with some regions covered by more than one element.**

Figure 3.4 **Some of the available patches: (a) quadrilateral in two dimensions, (b) triangle in two dimensions, (c) hexahedron in three dimensions, (d) prism in three dimensions.**

Figure 3.5 **An illustration of the use of patches. (a) a simple domain, (b) a representation of the domain using patches (patch corners are numbered in a logical ordered fashion, with gaps to maintain the relation of numbers to layers, and refinement indices are given in brackets, with the refinement indices for the triangle patch flagged as a warning to take care for this patch), (c) a refined finite-element grid for the domain.**

Figure 3.6 **Illustration why two refinement patterns may be necessary if triangle patches are included in the grid. The lower triangle is refined near a vertex, whereas the upper triangle has the same refinement near a side in order to match.**

Figure 3.7 **Illustration of the way in which triangle patches can be avoided through the use of quadrilateral patches with one very short side. The Figure presents an alternative grid for the example shown in Figure 3.5.**

Figure 3.8 **Illustration of the way that triangular faces of prisms propagate through the grid in three dimensions.**

Figure 3.9 The mismatch between two prisms and a hexahedron.

Figure 3.10 Illustration of the way a hexahedron formed from two prisms propagates through the grid in three dimensions.

Figure 3.11 **Possible ways to grid a fault. (a) the geological structure with a fault, (b) a possible grid that is appropriate if the fault has high transmissivity, which is modelled by taking the elements in the fault zone to have high permeability (note that if the fault is purely geometric and its only effect is to bring the thicker layers (which are aquifers) into hydraulic contact this can be achieved by taking all elements in the fault zone to have a permeability corresponding to an aquifer), (c) another geological structure, (d) a possible grid designed to ensure hydraulic contact between the aquifer layers.**

Figure 3.12 **Possible numbering schemes for a finite-element grid: (a) a sensible numbering designed to give a low frontwidth. For example the frontwidth after elements 1 to 10 have been assembled is given by all the freedoms on the thick line. (b) a numbering that is not sensible. The frontwidth after elements 1 to 10 have been assembled is given by all the freedoms on the thick line and is over three times as large as the corresponding frontwidth in (a).**

4 EXAMPLE 2: STEADY GROUNDWATER FLOW IN A COMPLICATED DOMAIN (HYDROCOIN LEVEL 1 TEST CASE 2)

This second example of a groundwater flow problem solved using the NAMMU package is more realistic than the previous one. The example is taken from Level 1 of the international HYDROCOIN project for verification of groundwater flow codes [15]. It concerns steady-state flow in a two-dimensional vertical slice of fractured rock, there being two inclined fractures which intersect one another at depth, and have a higher permeability than the surrounding rock. The full definition of the case study is provided in Appendix D.

4.1 Generation of a Finite-Element Grid Using Patches

The difficulty with producing a satisfactory model for this problem arises from the complicated geometry of the domain, which involves internal interfaces. The first step in creating a NAMMU grid is to decide on a sensible sub-division of the domain into regions of simple geometry. The easiest way to do this is to split the domain into a number of patches that fit the prominent geological features as closely as possible. The domain could also have been divided into a number of polygons.

A patch is a simple region bounded by straight sides in two dimensions or planar surfaces in three dimensions. It is sub-divided into elements. The patch can have different numbers of elements in each direction. There are several different types of patches available within NAMMU: for two-dimensions one can use either quadrilateral or triangular patches; in three-dimensions a grid can be generated from brick and prism-like patches.

Figure 4.1 demonstrates two examples of how the domain shown in Figure D.1 may be divided into patches. In the Figure 4.1(a) only quadrilateral patches are used, while in Figure 4.1(b) a combination of both triangular and quadrilateral patches are used. Both of these have advantages and disadvantages. The first example will be the simpler for which to create the appropriate input data. Its drawbacks are that the patches adjacent to the fractures are not uniformly refined around the important fracture regions, and so any solution obtained on this grid would be correspondingly non-uniformly resolved. Furthermore, a number of the patches are quite severely distorted away from the optimum square patch. The second example has much better refinement of the area around the fractures, with a set of patches positioned adjacent and almost parallel to each fracture, and triangles are used to avoid having any distorted patches. However, the use of triangular patches introduces other problems: they are often less accurate than quadrilaterals, and require greater consideration when refining the grid. A grid of patches with features somewhere between these two examples is probably optimal.

The complete list of patch types available in two dimensions is as follows:

1. SQQ9 – a four-sided patch built from quadrilateral elements;
2. SQTR – a four-sided patch built from triangular elements;

3. TRT6 – a three-sided patch built from triangular elements in which both refinement directions propagate through the patch;

4. TR69 – a three-sided patch built from quadrilateral and triangular elements in which both refinement directions propagate through the patch;

5. TRPQ – a three-sided patch built from quadrilateral and triangular elements in which the refinement pinches out in one direction;

6. TRPT – a three-sided patch built from triangular elements in which the refinement pinches out in one direction.

The input data required to specify a grid of patches has been minimised to make this option relatively straightforward to use. This is done by identifying the corner of each patch by numbers. The coordinates of each of the corners are input, and then the patches are specified by giving the corner numbers in sequence round the patch. The corner numbers should always be specified in an anticlockwise sequence around the patch.

Once the distribution of patches has been decided upon, the next task is to define a consistent numbering system for the corners of each patch, in which each patch can be easily identified. A logical way of doing this is to number corners by row and column. For instance, starting at the top left-hand corner, the corners could be numbered consecutively along the top boundary and prefixed with the number '1.' There are thirteen patch corners along this boundary, so these would be numbered 11 to 113. Moving down the grid to the next row of patch corners, these corners would be numbered from left to right between 21 and 213; and so on for the next row of corners being prefixed by a '3.' This is simple enough for rows of patches running roughly horizontally across the domain, but a little more thought is required in the 'diamond' shaped sub-region around the intersection of the fractures. For example, the very small patch where the two fractures intersect could be numbered 46, 59, 510, 47, where 46 corresponds to farthest left corner and the others follow in an anticlockwise sense; the additional patch corners around the bottom of the diamond might be numbered 66, 67, 68, 69, 610 from left to right. Numbering the patch corners on the bottom boundary from 71 to 713 would complete a system in which each patch could be quickly located.

This numbering system is used in the Dataset 4.1, which represents an example of a NAMMU input file for solving this test case on a refined version of the grid shown in Figure 4.1(b). In order to highlight some general features of the patch grid generation facility, we will discuss an abbreviated form of this dataset. Consider the following MODEL DATA phase instructions:

```
>> CREATE GRID
  >> GENERATE A GRID OF PATCHES
     PATCH SPACING IN FIRST DIRECTION
     SIZE
      1
```

```
      PATCH SPACING IN SECOND DIRECTION
      SIZE
       1

>> PATCH POSITIONS
   CORNER NUMBER, COORDINATES
        11         < 0.0 150.0 >
        12         < 10.0 150.0 >
        .               .
        .               .
        .               .
       113         < 1600.0 150.0 >
        .               .
        .               .
        .               .
       713        <  1600.0 1000.0 >

  PATCH TOPOLOGY
  PATCH TYPE, CORNERS,        INDICES,  ROCK NAME
     'SQQ9' < 11 21 22 12 >   < 1 1 >   'ROCK'
               .                 .
               .                 .
               .                 .
     'TR69' < 23 24 13 >      < 1 1 >   'ROCK'
               .                 .
               .                 .
               .                 .
     'SQQ9' < 35 66 46 36 >   < 1 1 >   'ROCK'
     'SQQ9' < 36 46 47 37 >   < 1 1 >   'FRACTURE'
     'SQQ9' < 37 47 39 38 >   < 1 1 >   'ROCK'
               .                 .
               .                 .
               .                 .
     'SQQ9' < 312 712 713 313 > < 1 1 > 'ROCK'
```

In this, the subcommand ≫ `GENERATE A GRID OF PATCHES` is the relevant MODEL DATA option when using patches. The `PATCH SPACING` keywords that follow concern the sub-division of the patches into elements, which will be dealt with in subsection 4.2. Next, the coordinates of the corners of each patch are input through the table keyword `PATCH POSITIONS`. Finally, the types of patches and the sequence of the corners are supplied through the table keyword `PATCH TOPOLOGY`. The data given in the last two columns of this table concern refinement and rock types, which will be explained later in subsections 4.2 and 4.3 respectively. For example, the middle three rows of this table define the sequence of corners in the patches near to the fracture intersection and positioned immediately below the fracture running top-left to bottom-right. The patch type appropriate to quadrilaterals is `'SQQ9'`, while we have chosen the `'TR69'` patch type for the triangles.

Once the grid has been created it may be checked for any inconsistencies, such as nodes that do not match on the sides of adjacent elements, using the output options discussed in subsection 4.5.

4.2 Grid Refinement

As they stand, the MODEL DATA commands above will generate the coarse grid of patches shown in Figure 4.1(b). Having created an initial grid such as this, it is good practice to check it thoroughly and then try to obtain solutions using this model. Although it is unlikely to produce satisfactory results with such poor refinement, it should give an indication of where the grid needs to be refined.

In order that the user may refine a grid of patches without having to specify every single element, a number of convenient options have been provided in the MODEL DATA phase. The user specifies the degree of refinement required through the table keywords concerning PATCH SPACING. These tables are distinguished by a direction which identifies the different local patch coordinate directions. In two dimensions these directions are referred to as the first and second directions. These local directions for a patch are determined by the order in which the corners of the patch are input in the CORNERS column of the PATCH TOPOLOGY table. The first direction is aligned from the first corner specified to the second, while the second direction is aligned from the first to the fourth corner for quadrilateral patches, and from the first to the third corner for triangular patches. Thus, it is possible to sub-divide patches in different ways in the different directions.

The SIZE columns in the PATCH SPACING tables specify the number of elements that the patch is sub-divided into, in the appropriate local direction. The choice of value for each patch is conveyed to NAMMU by specifying the row of this table in the INDICES column of the PATCH TOPOLOGY table. In the above example, only a single row was specified in the PATCH SPACING tables, the value '1' in the SIZE column specifies that none of the patches are to be sub-divided.

Suppose it were desired to sub-divide each of the patches immediately to the left of the fracture running from top-right to bottom-left into four elements in the direction normal to the fracture. To do this, an extra row is added to the PATCH SPACING columns as follows:

```
PATCH SPACING IN FIRST DIRECTION
      SIZE
       1
       4

PATCH SPACING IN SECOND DIRECTION
      SIZE
       1
       4
```

To specify which patches are to be refined and in which local patch direction, some of the entries in the INDICES column of the PATCH TOPOLOGY table need to be changed, as follows:

```
PATCH TOPOLOGY
```

```
PATCH TYPE,   CORNERS,      INDICES,   ROCK NAME
  'SQQ9'  < 18 28 29 19 >   < 1 2 >     'ROCK'
  'SQQ9'  < 28 38 39 29 >   < 1 2 >     'ROCK'
  'SQQ9'  < 35 66 46 36 >   < 2 1 >     'ROCK'
  'SQQ9'  < 36 46 47 37 >   < 2 1 >     'FRACTURE'
  'SQQ9'  < 37 47 39 38 >   < 2 1 >     'ROCK'
  'SQQ9'  < 68 79 710 69 >  < 1 2 >     'ROCK'
```

where only the rows that were actually changed are listed, corresponding to the six patches of interest. The index '2' corresponds to the second row in the PATCH SPACING table. This example also demonstrates that, when refining adjacent patches, the rows in the appropriate PATCH SPACING tables used to discretise the adjoining edges must be identical. In the above, the first and second directions of the patches near the fracture intersection were orientated differently to the other patches, and so the refinement had to be associated with a different local direction for these patches.

It is also possible to discretise a patch into elements in a non-uniform distribution using the GRADE POWERS column in the PATCH SPACING table. By specifying a higher grading for the right edge of a patch than for the left edge, elements will be concentrated near the right edge. For instance, if the PATCH SPACING columns in the above example were changed to:

```
SIZE,   GRADE POWERS
 1       < 1.0 1.0 >
 4       < 1.0 2.0 >
```

and similarly for the second direction, then the refinement would be finer toward the fracture. The default for the PATCH SPACING table is that the entry in the SIZE column is 1 and the entry in the GRADE POWERS column is `< 1.0 1.0 >`

Note:

1. the process of refinement can be made simpler by using a sensible numbering system for the patch corners;
2. refinement should be a gradual process;
3. for the first iteration of grid refinement it is a good idea to refine all the patches in a single direction (say horizontally), and check for mismatches between element sides by plotting the boundary;
4. consecutive refinements of the grid can be used as a check of convergence with respect to spatial resolution.

The stages in the refinement of the example grid are shown in Figures 4.1b and 4.2. The finest grid is that generated by the Dataset 4.1.

4.3 Specifying Multiple Rock Types

Different rock types may be defined for each patch by the use of the ROCK NAME column in the PATCH TOPOLOGY table. A rock name is entered in this column corresponding to the appropriate rows in the material property tables of the ≫ PHYSICAL PROPERTIES command. For this example there are two different rock types, having different permeabilities, k, but the same flowing porosity, ϕ. To input this information into the data file, the following tables are included in the INITIAL DATA phase:

```
>> PHYSICAL PROPERTIES
   ROCK TYPE PERMEABILITIES
   ROCK NAME,    KXX,    KYY,    KXY
   'ROCK'      1.0E-15  1.0E-15  0.0
   'FRACTURE'  1.0E-13  1.0E-13  0.0

   ROCK TYPE PROPERTIES
   ROCK NAME,  POROSITY
   'ROCK'        0.03
   'FRACTURE'    0.03
   END
```

Here the permeabilities have been obtained by multiplying the hydraulic conductivities given in Appendix D by the factor $\mu/\rho g$.

All the patches in the fracture zones must then have the rock name 'FRACTURE' placed in the ROCK NAME column of PATCH TOPOLOGY table to associate them with the higher permeabilities. For example the very small patch where the two fractures intersect will be specified by the row:

```
PATCH TYPE,  CORNERS,      INDICES,   ROCK NAME
 'SQQ9'   < 46 59 510 47 >  < 1 1 >    'FRACTURE'
```

4.4 Specifying the Boundary Conditions

The other important stage in setting up a finite-element model is to specify the conditions on the boundary of the grid. For this example, there are no-flow conditions at the vertical boundaries and on the bottom boundary. Since natural boundary conditions are the default for NAMMU, these require no specification. For the top boundary it is required that

$$P^{\mathrm{R}}(x,\ y) = \rho g \times y,$$

where P^{R} is the residual pressure, and y is the height of the ground surface. This boundary condition is set using the command ≫ SET BOUNDARY CONDITIONS, and the subcommand appropriate for Dirichlet type conditions, which is ≫ SPECIFIED VALUE. This section of the input file is as follows:

```
>> SET BOUNDARY CONDITIONS

  >> SPECIFIED VALUE

    >> VALUE VARYING LINEARLY WITH POSITION
       VARIABLES   'PRES'
       BASE VALUES  0.0
       Y FACTORS    9733.5
       END

    >> SELECT BOUNDARY SEGMENT
       START POINT  0.0     150.0
       MID POINT    800.0   150.0
       END POINT    1600.0  150.0
       PRECISION    1.0E-1
       END
```

The command ≫ VALUE VARYING LINEARLY WITH POSITION is designed specifically for boundary conditions that are given as a simple linear function of position. The keyword data for this command specifies the coefficients of this linear function. Here, the keyword Y FACTORS has been set to ρg and the keyword X FACTORS defaults to zero. The ≫ SELECT BOUNDARY SEGMENT subcommand defines a segment of the boundary for which the condition is to be set. Simply supplying the coordinates of the two end points, together with any mid point uniquely defines the boundary segment required, avoiding the necessity of setting a condition individually for each patch with an edge on the boundary.

4.5 Output Options

There are a number of output options available within the OUTPUT DATA phase of NAMMU to help the user develop a finite-element model for groundwater flow problems. They provide useful diagnostic tools for locating any errors that may have occurred during the input of the data. Some of the more useful OUTPUT DATA commands of relevance to Example 2 are discussed below.

4.5.1 Plotting the Grid and Boundary

Two very useful subcommands of ≫ OUTPUT DATA when setting up a grid of patches are ≫ PLOT GRID and ≫ PLOT BOUNDARY. Plotting the boundary gives a quick and simple test for the presence of irregularities in the grid, and any breaks in the boundary or sections of boundary internal to the model. Figure 4.3 is an example of a boundary plot for a correctly defined grid.

The grid can be checked in more detail using the command ≫ PLOT GRID. Using this option, the discretisation of patches into elements can be examined for any unmatched nodes on the adjoining edges of patches. Also, it is possible to verify that the different material properties have been input correctly by shading regions according to their property types. For instance, the patches specified in Example 2 may be shaded differently for each rock

type using the following commands in the OUTPUT DATA phase of the input file:

```
>> SET ROCK STYLES
   ROCK STYLES
   ROCK NAME, COLOUR
   'ROCK'      'YELLOW'
   'FRACTURE'  'RED'
   END

>> PLOT GRID
   SHADE
   CAPTION  'ROCK TYPES'
   END
```

The keyword SHADE by default shades according to rock types. In Example 2 there are only two distinct rock types, as shown in the shaded plot reproduced in Figure 4.4. Other criteria for shading regions may be specified by including further keywords. As an example, the keyword POROSITIES causes patches to be shaded using the values of porosity.

Another option for checking the grid is invoked by the command ≫ CHECK GRID. This checks the grid for any highly distorted or long thin elements, and prints appropriate warnings in the output file.

4.5.2 Plotting Contours

Once the user is satisfied that the finite-element grid is correct, solutions can be obtained for the current model by invoking the solver. To view this solution, contours of the variables may be plotted in any given region using the command ≫ PLOT CONTOURS. The default is to plot contours for the whole domain, which is probably the best option when viewing a solution for the first time (see Figure 4.5). However, if the user is mainly interested in the behaviour of the solution in a sub-region of the domain, then LIMITS OF ZOOM may be specified to focus on that region. Here is an example of how contours are plotted close to the intersection of the two fractures:

```
>> PLOT GRID
   SHADE
   X LIMITS OF ZOOM    1000.0 1200.0
   Y LIMITS OF ZOOM    -500.0 -700.0

>> PLOT CONTOURS
   VARIABLE            'PRES'
   NUMBER OF CONTOURS  30
   COLOURS             'BLUE' 'GREEN'
   X LIMITS OF ZOOM    1000.0 1200.0
   Y LIMITS OF ZOOM    -500.0 -700.0
   USE LOCAL EXTREMA
   KEY TITLE           'RESIDUAL PRESSURE'
```

```
   CAPTION              'RESIDUAL PRESSURE CONTOURS'
   SUPERIMPOSE
   END
```

In this example (see Figure 4.6), 30 contours are plotted at equally spaced contour values between the minimum and maximum. Alternatively, the user could specify the contour values using the keyword `CONTOUR VALUES`. The contours are superimposed on a shaded plot of the grid. The keyword `USE LOCAL EXTREMA` indicates that the maximum and minimum values of the variable within the zoomed region are to be used when calculating the contour values.

The `LIMITS OF ZOOM` keywords can also be used in other output options. It could be used when plotting the grid to examine highly refined regions.

4.5.3 Plotting Profiles

The variables can also be plotted as a function of position along a line through the domain using the option >> `DRAW LINE GRAPH`. The line is specified by providing values for the keywords `START POINT` and `END POINT`. If it is required that the profile be presented as a continuous line then the keyword `JOIN POINTS` should be included. A plot of the distribution of pressure along the horizontal line $y = -200$m is shown in Figure 4.7.

4.5.4 Pathlines

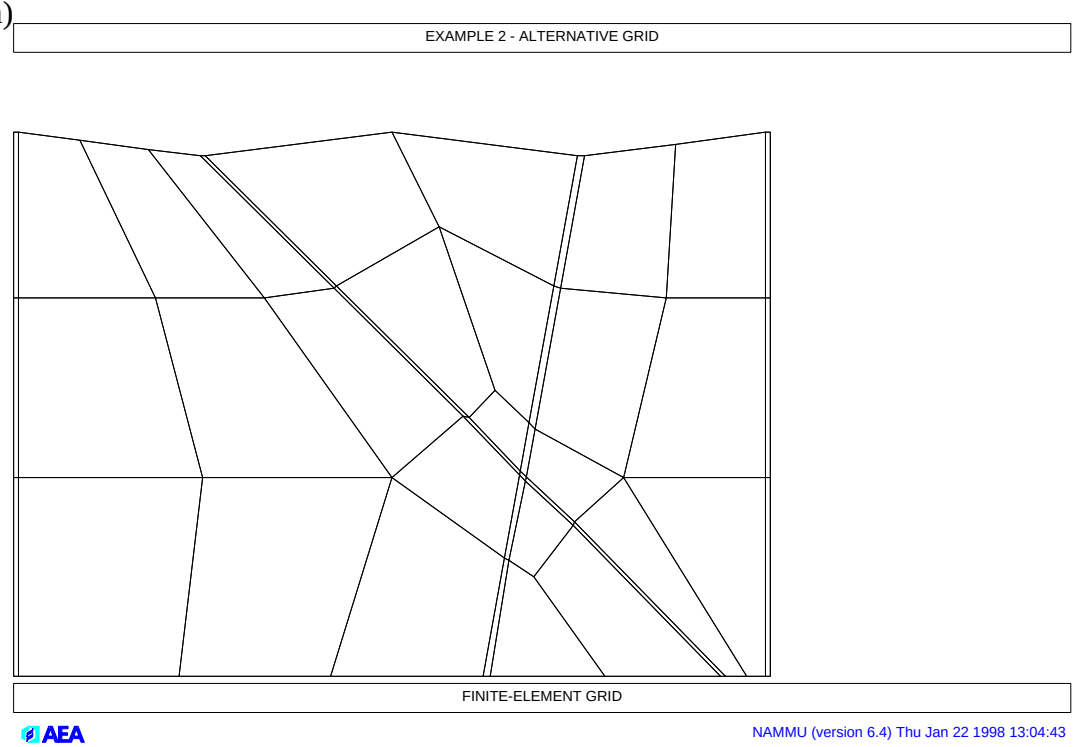
As an aid to visualising the groundwater flow field, NAMMU has a facility for plotting the advective paths traced out by fluid particles. An example of how this option is used is given below.

```
>> PATHLINES
   NUMBER OF PATHS                4
   X COORDINATES OF PATHS       100.0   100.0  1500.0  1500.0
   Y COORDINATES OF PATHS         0.0  -200.0     0.0  -450.0
   TIMES IN YEARS
   MAXIMUM NUMBER OF TIMESTEPS  2000
   ACCURACY PARAMETER             0.5
   NO KEY
   CAPTION                    'PATHLINES'
   END
```

The coordinates specified here are the start points for the pathline calculations. Here, four points have been specified corresponding to the pathlines requested in the specification [15]. Figures 4.8 represent pathlines as calculated on the grids shown in Figures 4.1b and 4.2b. Note the difference in these paths as the grid is refined. This output option is in fact a very useful facility, since it can also be used to calculate groundwater return times. The default is for these times to be in seconds. The keyword `TIMES IN YEARS` causes NAMMU to output all times in years.

Figures for Section 4

(a)



(b)

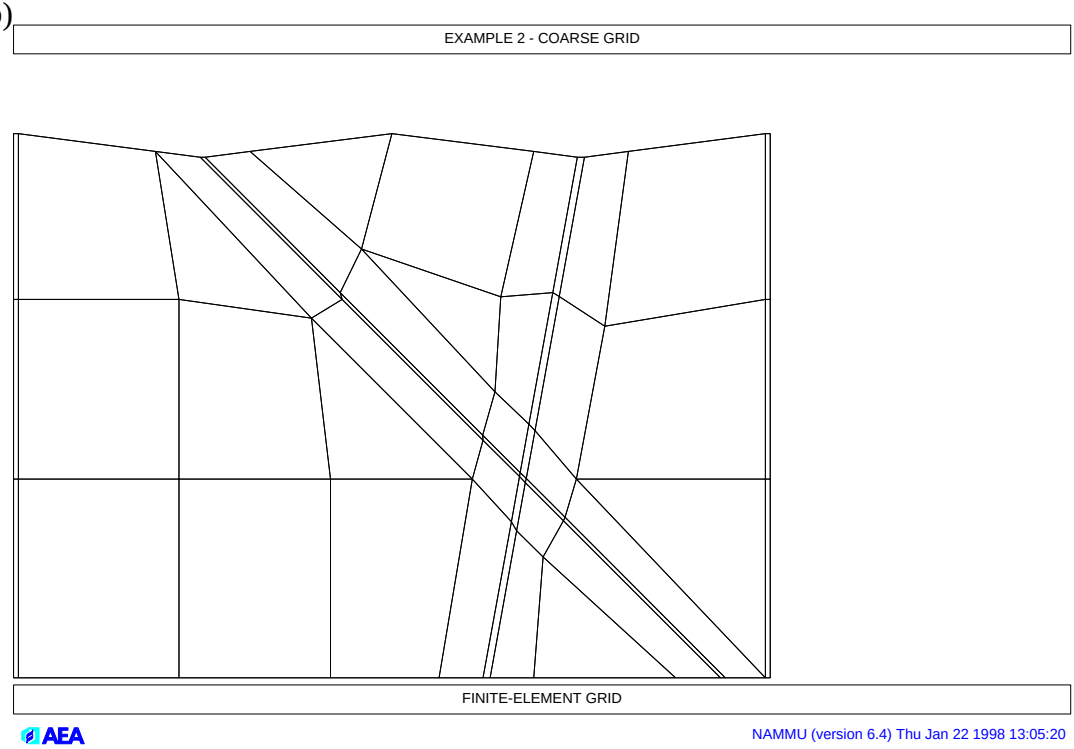
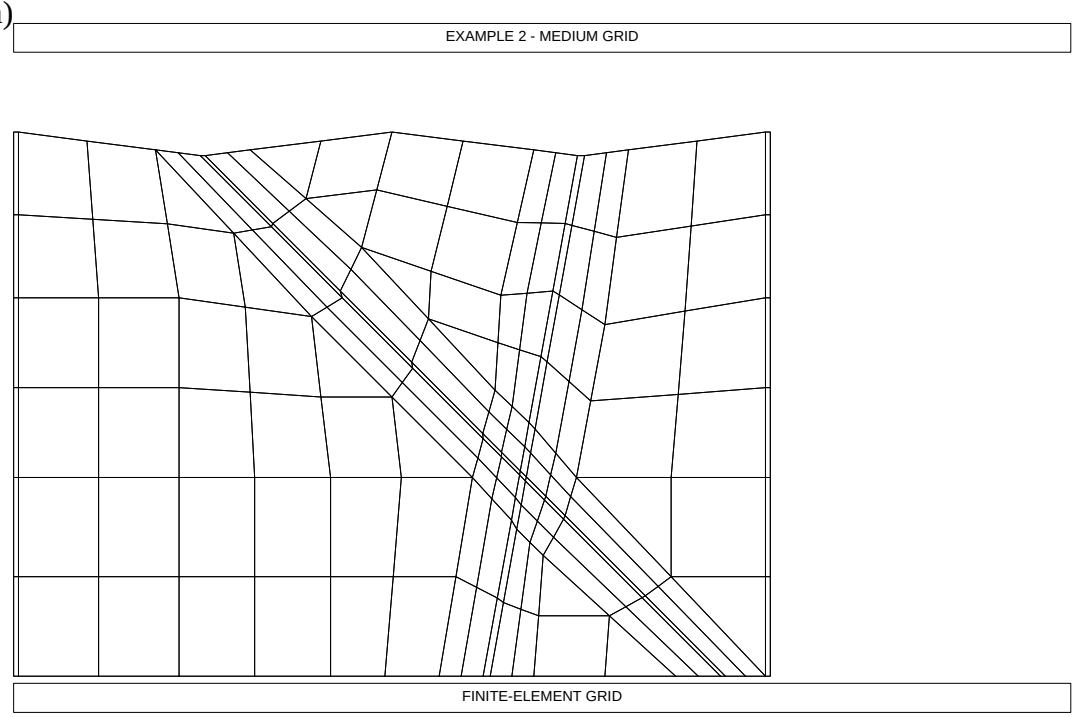


Figure 4.1 **Two possible coarse mesh designs: (a) Using only quadrilaterals [15]; (b) Using triangles and quadrilaterals [2].**

(a)



(b)

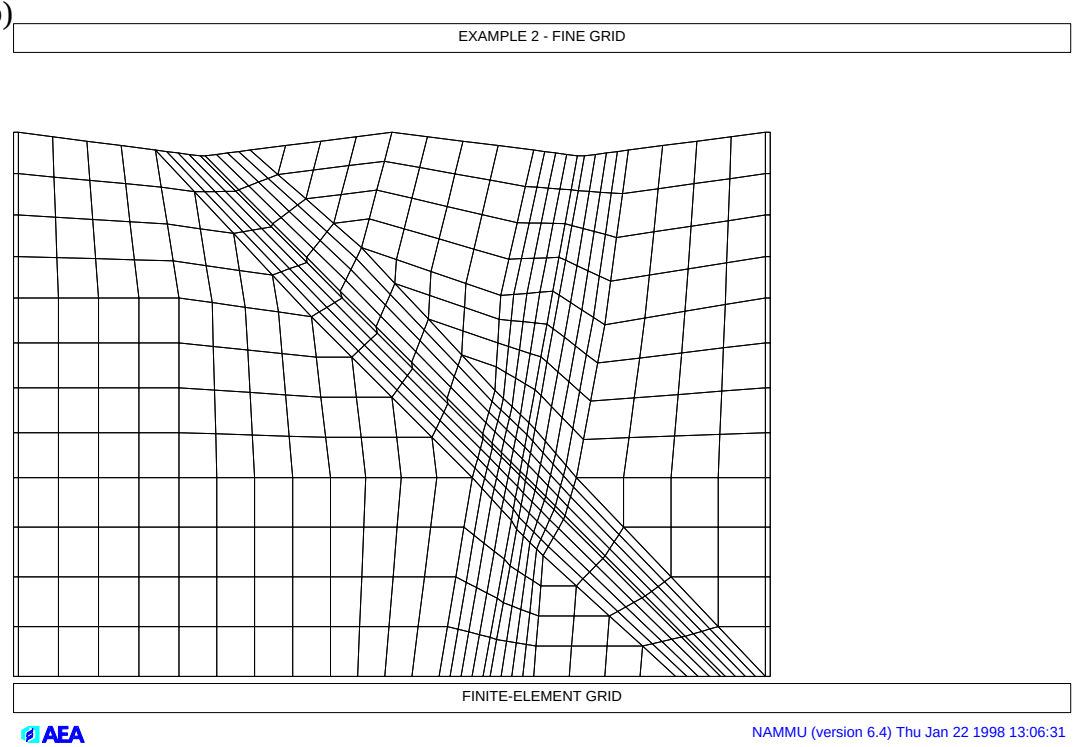


Figure 4.2 Two stages in the refinement of the grid shown in Figure 4.1(b).

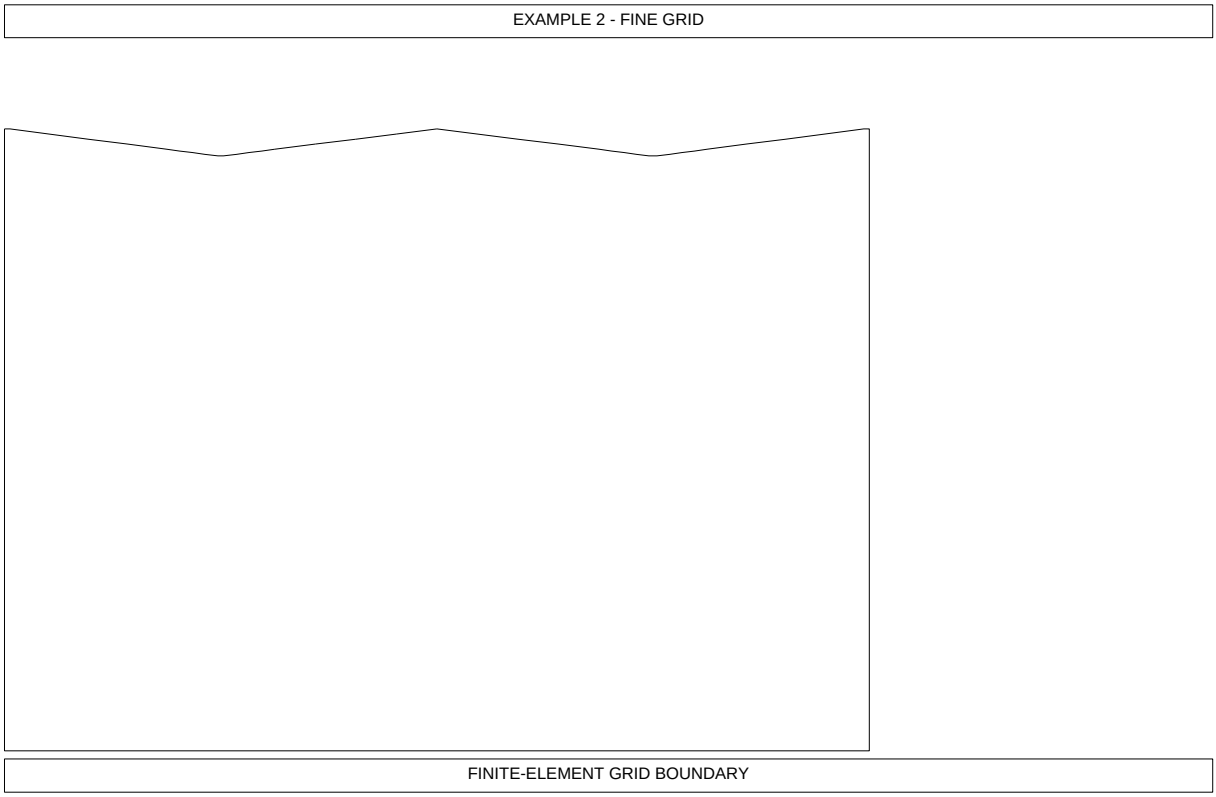


Figure 4.3 The boundary of the finite-element mesh.

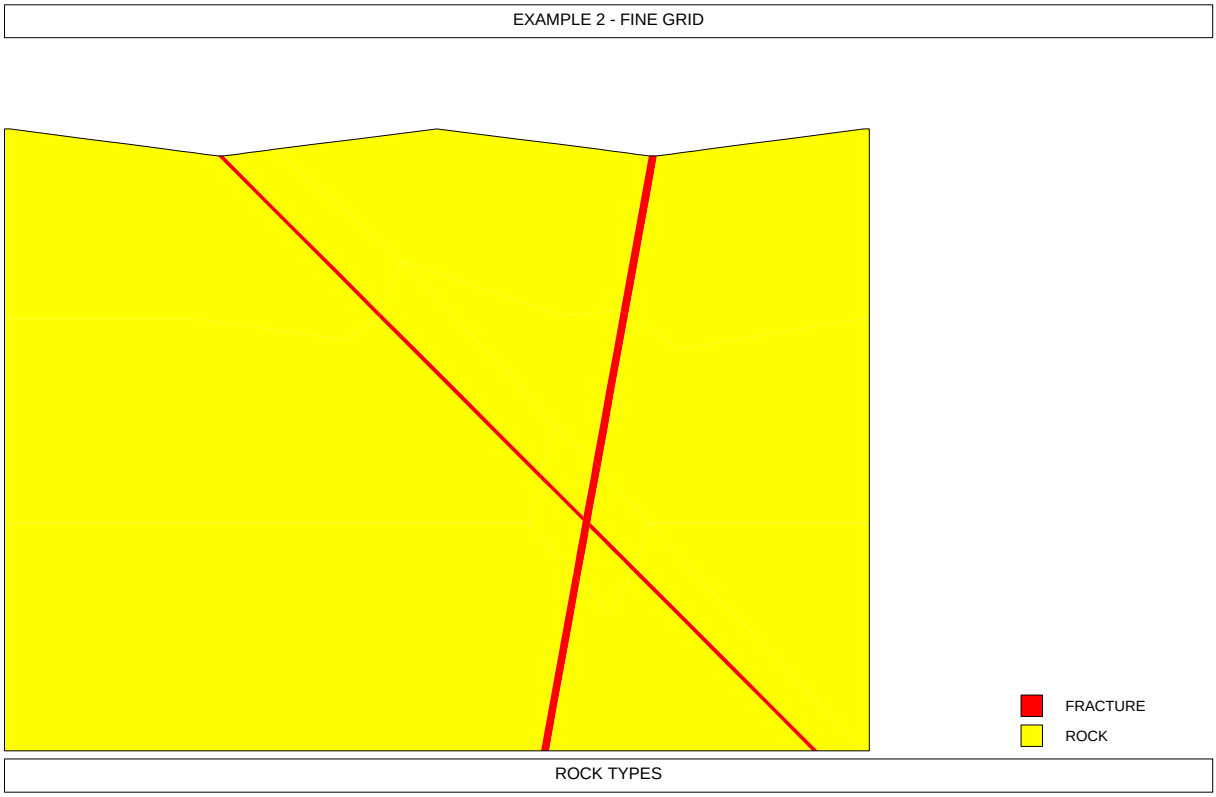


Figure 4.4 **A grid of patches shaded according to rock types. The darker shading corresponds to fracture zones of higher permeability.**

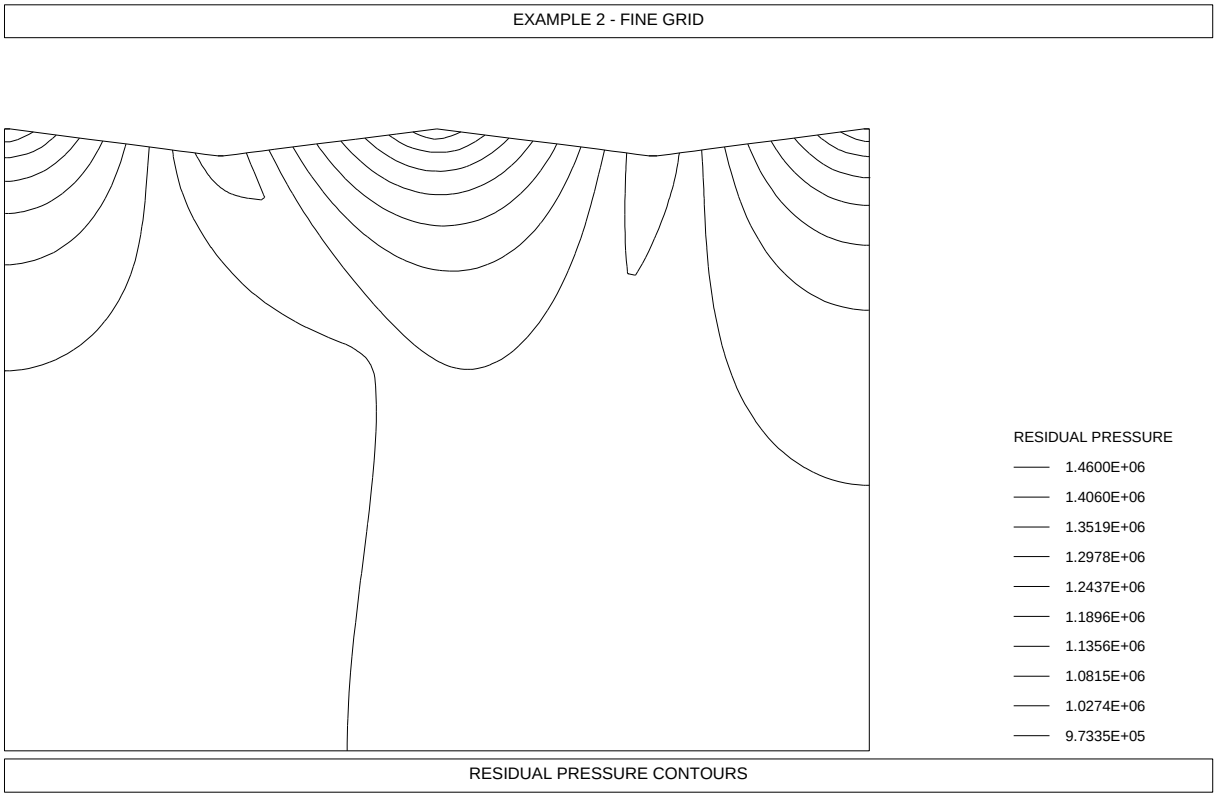


Figure 4.5 Contours of residual pressure for the fine grid.

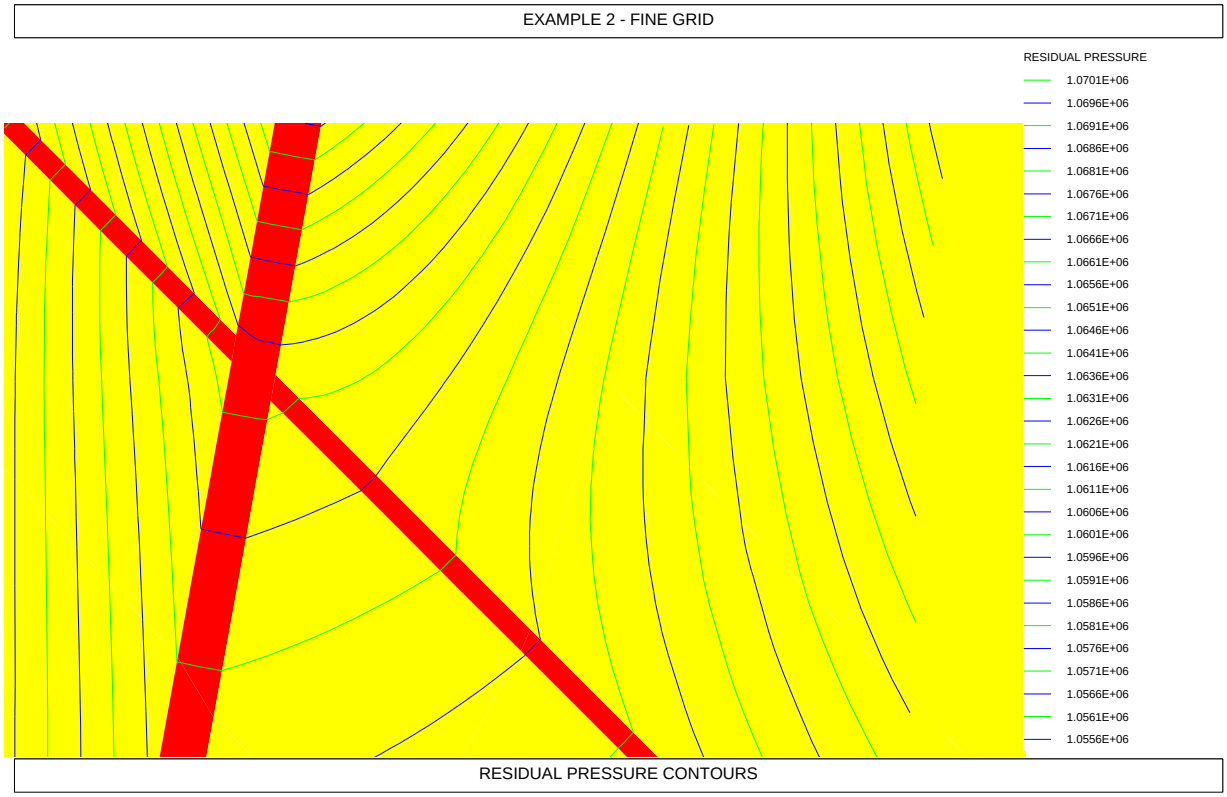


Figure 4.6 **Contours of residual pressure in the region close to the intersection of the two fractures for the fine grid. The contours are superimposed on a plot of the grid shaded according to rock type.**

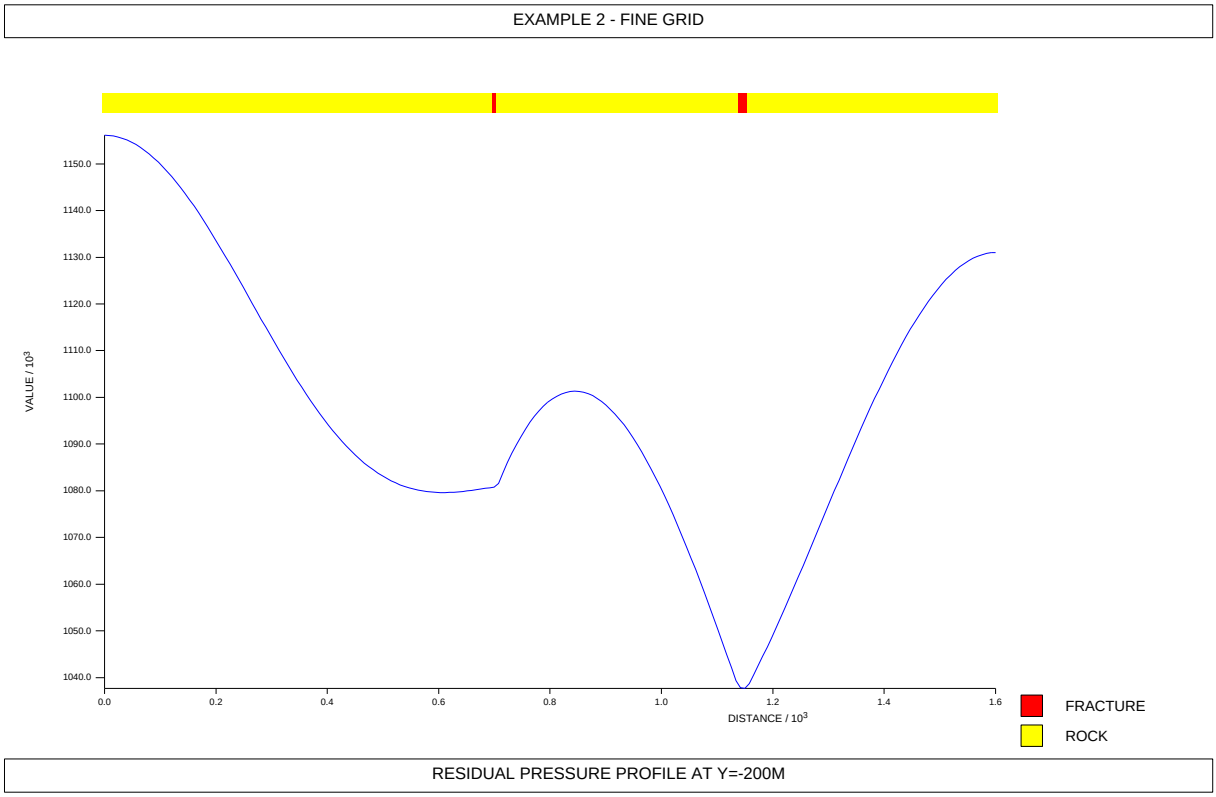
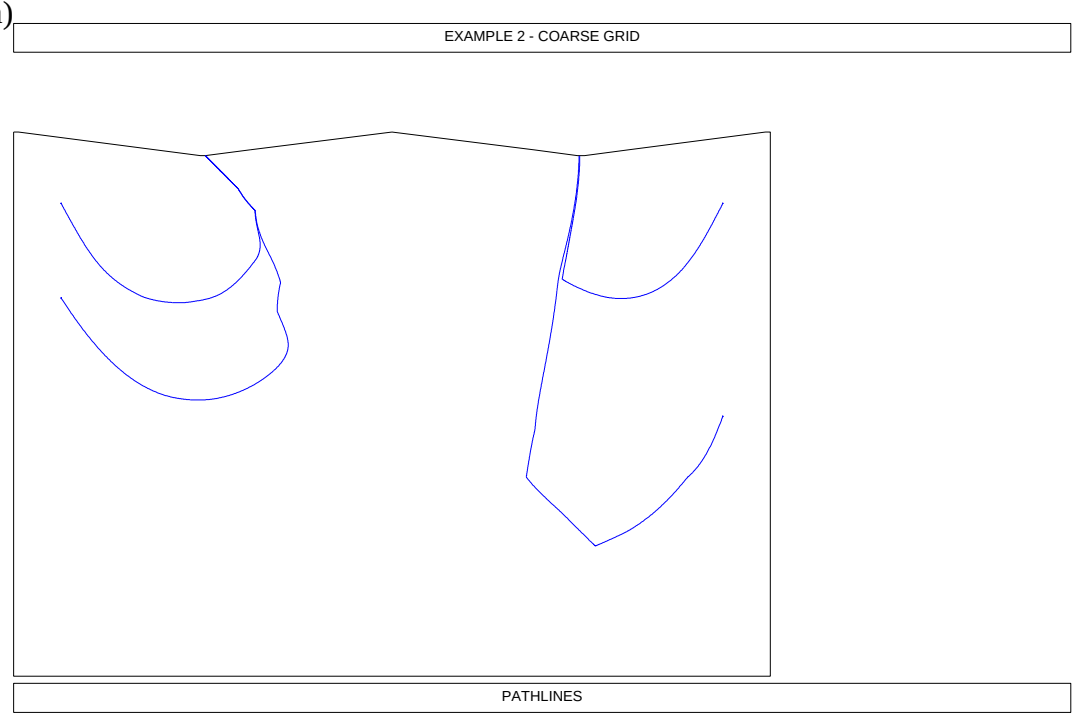


Figure 4.7 **Distribution of residual pressure at a level of $y = -200\mathrm{m}$ for the fine grid.**

(a)



(b)

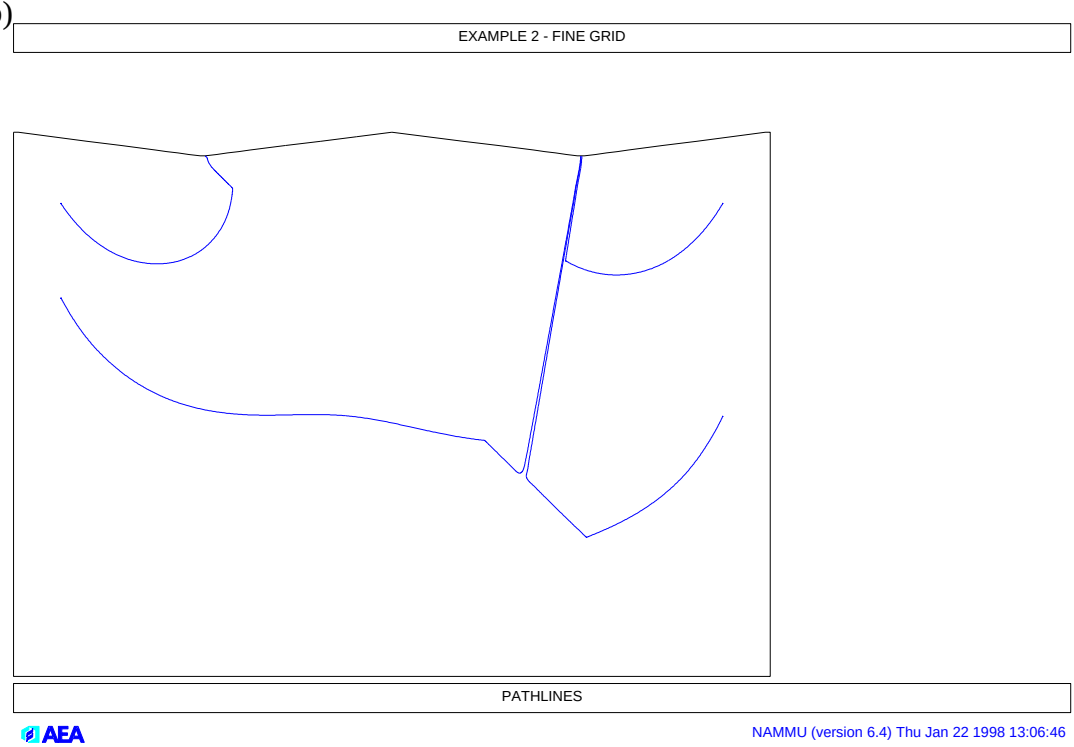


Figure 4.8 Pathlines calculated on each of the grids shown in Figures 4.1b and 4.2b.

Dataset 4.1

```
   /* NAMMU TEST CASE HYDRO2.FINE                                  */
   /*                                                              */
   /* EXAMPLE 2 - STEADY GROUNDWATER FLOW IN A COMPLICATED         */
   /*             DOMAIN - FINE GRID                               */

   /* SPACE ALLOCATION                                             */
   /* INTEGER WORKSPACE  600000                                    */
   /* REAL WORKSPACE     350000                                    */

   /* SOURCE FILES                                                 */
   /* COMPILED FILES                                               */
   /* LIBRARY FILES                                                */

   /* INPUT DATA FILES                                             */
   /* OUTPUT DATA FILES                                            */
   /* 6        nammu/output/hydro2.fine.out                       */
   /* GRAPHICS nammu/output/hydro2.fine.ps                        */

   /* END JOB INFORMATION                                          */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS                      1000
      NODES                         9000
      FRONTWIDTH                     400
      GAUSS POINTS                    13
      INTEGER BC WORKSPACE         40000
      REAL BC WORKSPACE             8000
      PARAMETERS PER FUNCTION TYPE     9
      FUNCTION TYPES PER ELEMENT       3
      VARIABLES                        1
      END

   >> SET VARIABLES
      VARIABLE NAMES 'PRES'
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES

      FLUID DENSITY              998.0

      ROCK TYPE PERMEABILITIES
```

```
      ROCK NAME,    KXX,    KYY,    KXY
      'ROCK'      1.0E-15  1.0E-15  0.0
      'FRACTURE'  1.0E-13  1.0E-13  0.0

      ROCK TYPE PROPERTIES
      ROCK NAME,  POROSITY
      'ROCK'        0.03
      'FRACTURE'    0.03
      END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES

         PATCH SPACING IN FIRST DIRECTION
         SIZE
           1
           4

         PATCH SPACING IN SECOND DIRECTION
         SIZE
           1
           4

         PATCH POSITIONS
         CORNER NUMBER,       COORDINATES
              11        <    0.0      150.0    >
              12        <   10.0      150.0    >
              13        <  300.0      112.5    >
              14        <  395.0      100.0    >
              15        <  405.0      100.0    >
              16        <  500.0      112.5    >
              17        <  800.0      150.0    >
              18        < 1100.0      112.5    >
              19        < 1192.5      100.0    >
              110       < 1207.5      100.0    >
              111       < 1300.0      112.5    >
              112       < 1590.0      150.0    >
              113       < 1600.0      150.0    >
              21        <    0.0     -200.0    >
              22        <   10.0     -200.0    >
              23        <  350.0     -200.0    >
              24        <  630.0     -240.0    >
              25        <  695.0     -200.0    >
              26        <  691.0     -186.0    >
              27        <  736.0      -94.0    >
              28        < 1030.0     -195.0    >
              29        < 1140.5     -186.0    >
              210       < 1154.0     -194.25   >
              211       < 1250.0     -257.0    >
              212       < 1590.0     -200.0    >
```

```
            213       < 1600.0     -200.0    >
            31        <    0.0     -580.0    >
            32        <   10.0     -580.0    >
            33        <  350.0     -580.0    >
            34        <  670.0     -580.0    >
            35        <  970.0     -580.0    >
            36        <  993.0     -498.0    >
            37        <  992.0     -487.0    >
            38        < 1018.0     -396.0    >
            39        < 1090.0     -463.75   >
            310       < 1102.5     -477.5    >
            311       < 1190.0     -580.0    >
            312       < 1590.0     -580.0    >
            313       < 1600.0     -580.0    >
            46        < 1069.8077  -574.8077 >
            47        < 1071.3462  -566.3459 >
            59        < 1082.5     -587.5    >
            510       < 1084.0385  -579.0385 >
            66        < 1052.5     -670.0    >
            67        < 1064.0     -689.25   >
            68        < 1120.0     -745.0    >
            69        < 1163.0     -668.0    >
            610       < 1166.0     -661.0    >
            71        <    0.0    -1000.0    >
            72        <   10.0    -1000.0    >
            73        <  350.0    -1000.0    >
            74        <  670.0    -1000.0    >
            75        <  900.0    -1000.0    >
            76        <  992.5    -1000.0    >
            77        < 1007.5    -1000.0    >
            78        < 1100.0    -1000.0    >
            79        < 1400.0    -1000.0    >
            710       < 1495.0    -1000.0    >
            711       < 1505.0    -1000.0    >
            712       < 1590.0    -1000.0    >
            713       < 1600.0    -1000.0    >

/*------------------------------------------------------------ */
/* SQQ9 IS A FOUR-SIDED PATCH BUILT FROM 9-NODE QUADRILATERAL*/
/* ELEMENTS. TR69 IS A THREE-SIDED PATCH BUILT FROM 9-NODE   */
/* QUADRILATERAL ELEMENTS AND 6 NODE TRIANGULAR ELEMENTS.    */
/*------------------------------------------------------------*/

          PATCH TOPOLOGY
          PATCH TYPE,        CORNERS,          INDICES,  ROCK NAME
            'SQQ9'    <  11  21  22  12 >   <2 1>     'ROCK'
            'SQQ9'    <  12  22  23  13 >   <2 2>     'ROCK'
            'TR69'    <  23  24  13     >   <2 2>     'ROCK'
            'SQQ9'    <  13  24  25  14 >   <2 2>     'ROCK'
            'SQQ9'    <  14  25  26  15 >   <2 1>     'FRACTURE'
            'SQQ9'    <  15  26  27  16 >   <2 2>     'ROCK'
            'TR69'    <  17  27  16     >   <2 2>     'ROCK'
            'SQQ9'    <  17  27  28  18 >   <2 2>     'ROCK'
            'SQQ9'    <  18  28  29  19 >   <2 2>     'ROCK'
```

```
         'SQQ9'    <  19  29 210 110 >   <2 1>     'FRACTURE'
         'SQQ9'    < 110 210 211 111 >   <2 2>     'ROCK'
         'SQQ9'    < 111 211 212 112 >   <2 2>     'ROCK'
         'SQQ9'    < 112 212 213 113 >   <2 1>     'ROCK'
         'SQQ9'    <  21  31  32  22 >   <2 1>     'ROCK'
         'SQQ9'    <  22  32  33  23 >   <2 2>     'ROCK'
         'SQQ9'    <  23  33  34  24 >   <2 2>     'ROCK'
         'TR69'    <  34  35  24     >   <2 2>     'ROCK'
         'SQQ9'    <  24  35  36  25 >   <2 2>     'ROCK'
         'SQQ9'    <  25  36  37  26 >   <2 1>     'FRACTURE'
         'SQQ9'    <  26  37  38  27 >   <2 2>     'ROCK'
         'TR69'    <  28  38  27     >   <2 2>     'ROCK'
         'SQQ9'    <  28  38  39  29 >   <2 2>     'ROCK'
         'SQQ9'    <  29  39 310 210 >   <2 1>     'FRACTURE'
         'SQQ9'    < 210 310 311 211 >   <2 2>     'ROCK'
         'SQQ9'    < 211 311 312 212 >   <2 2>     'ROCK'
         'SQQ9'    < 212 312 313 213 >   <2 1>     'ROCK'
         'SQQ9'    <  35  66  46  36 >   <2 2>     'ROCK'
         'SQQ9'    <  36  46  47  37 >   <2 1>     'FRACTURE'
         'SQQ9'    <  37  47  39  38 >   <2 2>     'ROCK'
         'SQQ9'    <  66  67  59  46 >   <1 2>     'FRACTURE'
         'SQQ9'    <  46  59 510  47 >   <1 1>     'FRACTURE'
         'SQQ9'    <  47 510 310  39 >   <1 2>     'FRACTURE'
         'SQQ9'    <  67  68  69  59 >   <2 2>     'ROCK'
         'SQQ9'    <  59  69 610 510 >   <2 1>     'FRACTURE'
         'SQQ9'    < 510 610 311 310 >   <2 2>     'ROCK'
         'SQQ9'    <  31  71  72  32 >   <2 1>     'ROCK'
         'SQQ9'    <  32  72  73  33 >   <2 2>     'ROCK'
         'SQQ9'    <  33  73  74  34 >   <2 2>     'ROCK'
         'SQQ9'    <  34  74  75  35 >   <2 2>     'ROCK'
         'SQQ9'    <  35  75  76  66 >   <2 2>     'ROCK'
         'SQQ9'    <  66  76  77  67 >   <2 1>     'FRACTURE'
         'SQQ9'    <  67  77  78  68 >   <2 2>     'ROCK'
         'TR69'    <  78  79  68     >   <2 2>     'ROCK'
         'SQQ9'    <  68  79 710  69 >   <2 2>     'ROCK'
         'SQQ9'    <  69 710 711 610 >   <2 1>     'FRACTURE'
         'SQQ9'    < 610 711 712 311 >   <2 2>     'ROCK'
         'TR69'    < 312 712 311     >   <2 2>     'ROCK'
         'SQQ9'    < 312 712 713 313 >   <2 1>     'ROCK'
      END

>> SET BOUNDARY CONDITIONS

/*   ************ PRESSURE BOUNDARY SPECIFICATION **********   */
/*   ********************* TOP BOUNDARY ********************   */
   >> SPECIFIED VALUE

      >> VALUE VARYING LINEARLY WITH POSITION
         VARIABLES    'PRES'
         BASE VALUES     0.0
         Y FACTORS    9733.5
         END

         >> SELECT BOUNDARY SEGMENT
```

```
            START POINT     0.0   150.0
            MID POINT     800.0   150.0
            END POINT    1600.0   150.0
            PRECISION       1.0E-01
            END


>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH    300
      NUMBER OF ITERATIONS    1
      END

      >> GROUNDWATER FLOW
         END


>> OUTPUT DATA

   >> PAGE SETUP
      LANDSCAPE
      END

   >> SET OUTPUT OPTIONS
      HEADING          'EXAMPLE 2 - FINE GRID'
      BOUNDARY COLOUR  'BLACK'
      GRID COLOUR      'BLACK'
      END

   >> SET ROCK STYLES
      ROCK STYLES
      ROCK NAME,  COLOUR
      'ROCK'      'YELLOW'
      'FRACTURE'  'RED'
      END

   >> PLOT BOUNDARY
      END

   >> PLOT GRID
      END

   >> PLOT GRID
      SHADE
      CAPTION  'ROCK TYPES'
      END

   >> CHECK GRID
      MAX JACOBIAN DETERMINANT RATIO    0.5
      MAX SIDE RATIO                  350.0
      END

   >> PLOT CONTOURS
```

```
   VARIABLE            'PRES'
   NUMBER OF CONTOURS  10
   COLOURS             'BLACK'
   KEY TITLE           'RESIDUAL PRESSURE'
   CAPTION             'RESIDUAL PRESSURE CONTOURS'
   END

>> PLOT GRID
   SHADE
   X LIMITS OF ZOOM    1000.0 1200.0
   Y LIMITS OF ZOOM    -500.0 -700.0

>> PLOT CONTOURS
   VARIABLE            'PRES'
   NUMBER OF CONTOURS  30
   COLOURS             'BLUE' 'GREEN'
   X LIMITS OF ZOOM    1000.0 1200.0
   Y LIMITS OF ZOOM    -500.0 -700.0
   USE LOCAL EXTREMA
   KEY TITLE           'RESIDUAL PRESSURE'
   CAPTION             'RESIDUAL PRESSURE CONTOURS'
   SUPERIMPOSE
   END


>> DRAW LINE GRAPH
   VARIABLE 'PRES'
   START POINT           0.0  -200.0
   END POINT          1600.0  -200.0
   NUMBER OF POINTS     200
   X AXIS LABEL RANGE     0.0  1600.0
   NO SYMBOLS
   JOIN POINTS
   PLOT LITHOLOGY
   CAPTION             'RESIDUAL PRESSURE PROFILE AT Y=-200M'
   END

>> PATHLINES
   NUMBER OF PATHS                4
   X COORDINATES OF PATHS       100.0   100.0  1500.0  1500.0
   Y COORDINATES OF PATHS         0.0  -200.0     0.0  -450.0
   TIMES IN YEARS
   MAXIMUM NUMBER OF TIMESTEPS  2000
   ACCURACY PARAMETER             0.5
   NO KEY
   CAPTION                    'PATHLINES'
   END


>> STOP
```

5 EXAMPLE 3: TRANSIENT COUPLED GROUNDWATER FLOW AND HEAT CONDUCTION (HYDROCOIN LEVEL 1 TEST CASE 4)

This third example is also taken from the international HYDROCOIN project [15]. It involves the transient thermal convection of water in a saturated permeable medium containing a heat source with a decaying power output. The background to the example and the modelling assumptions made in formulating an appropriate set of equations are presented in Appendix E.

The approximations used in deriving the mathematical model result in a different set of equations to the standard form solved by NAMMU (see Reference [8]). However, parameters may be chosen such that the equation system used by NAMMU closely approximates that for the test problem. In a previous study [3], it was shown that it is appropriate to set both the fluid specific heat and the flowing porosity to zero during the solution of the matrix equations. This choice gives a close approximation to the required system of equations providing that changes in density are small. More precisely, the condition $\beta T \ll 1$ should be satisfied over the entire domain for all times, where β is the thermal expansion coefficient and T is the rise in temperature. Indeed, this approximation is found to be consistent, since βT is 0.03 at most. For post-processing and producing pathlines it is necessary to restore a value of 10^{-4} for the porosity.

A listing of the input file used for this example is given in Dataset 5.1. In this Section, some of the important NAMMU options relevant to transient problems are explained, with this input dataset used as an illustration. It should be noted that a number of NAMMU options that are of more general interest also arise in this example, such as user-supplied routines, and will receive some explanation here.

5.1 Specifying the Model

In order to specify the model, a number of tasks have to be performed: various parameters need to be set, a finite-element mesh has to be generated, the behaviour of the heat source has to be defined and suitable boundary conditions have to be set. Each of these input stages is covered in the explanations below.

5.1.1 Setting the Geometry and Variables

Almost at the very start of the input file the coordinate system is specified by including the keyword `CYLINDRICAL GEOMETRY` under the `>> SET OPTIONS` command. Following a number of limits setting the size of the problem, the variables to be solved for are set. For coupled groundwater flow and heat transport problems the first two variables must be pressure and temperature, in that order. To ensure that this is the case the following instructions are used:

```
>> SET VARIABLES
   VARIABLE NAMES  'PRES' 'TEMP'
```

5.1.2 Specifying the Physical Properties

The various input parameters that are provided in Table E.1 are specified in the NAMMU dataset using the command ≫ `PHYSICAL PROPERTIES`. Each of these parameters is specified using the appropriate keyword and the value. For example, the viscosity is specified to be independent of temperature by setting the constant δ_1, as defined in equation 20 in the NAMMU Technical Overview [8], to zero using the following instruction:

```
DELTA    0.0
```

5.1.3 Defining a Heat Source

The spatial distribution and time-dependent behaviour of the heat source are also specified through the command ≫ `PHYSICAL PROPERTIES` with the keyword `USER HEAT SOURCE`. This keyword instructs NAMMU that the heat source is defined in FORTRAN subroutines provided by the user. In this case, the user needs to provide two subroutines, HEATFN and HTINT. A description of these user subroutines is available in the NAMMU Reference Manual [7].

In order to define the heat source term using these routines, it is necessary to separate the spatial dependence of the source from its time-dependent part. The spatially dependent part is then specified in the argument QH of HEATFN, while the integral of the time-varying part is assigned to the argument HN in the HTINT routine. Here, the heat source term may be separated such that

$$QH = \frac{3Q_0}{4\pi A^3}\Theta\left(A - R\right)$$

and

$$HN = \left(1 - \exp\left(-\lambda t\right)\right)/\lambda,$$

where Θ is the heaviside (or unit step) function, and $R = \sqrt{r^2 + z^2}$ is the spherical radial coordinate. The other quantities are as defined in Appendix E. Examples of these two user routines are appended at the end of this Section. It may be noted that the multiplying constant in the source term could equally have been included in the factor HN instead of QH, as these two terms are multiplied within the program.

Source terms for other quantities such as radionuclides can also be specified using user routines. These routines allow the user a good deal of flexibility without requiring a knowledge of the internal workings of the program. A more complete description of how to implement user routines is given in Section 11.

5.1.4 Generation of a Grid of Patches Including Triangles

The finite-element mesh is again generated using patches, and is shown in Figure 5.1. A semicircular domain has been chosen, extending to a radius of 3000m – twelve times the

repository radius. The domain is divided into 8 segments, each comprising 22 rectangles and a triangle. Grading is used to concentrate the elements in the vicinity of the repository.

The triangular patches are used in the region surrounding the origin. The patch type `'TRT6'` has been specified; this is constructed from triangular elements.

5.1.5 Boundary Conditions and Initial Values

The boundary conditions imposed are $P^{\mathrm{R}}(r = 0) = 0$, $P^{\mathrm{R}}(r = 3000\mathrm{m}) = 0$ and $\partial T/\partial r(r = 3000\mathrm{m}) = 0$. The first of these conditions is set using the commands ≫ `SPECIFIED VALUE` and ≫ `CONSTANT VALUE`, with the position specified by:

```
>> SELECT POINT
   COORDINATES  0.0  0.0
   TOLERANCE    1.0E-4
```

The second condition is specified using the command ≫ `SELECT BOUNDARY SEGMENT`, which was described previously in Section 4. The last condition is set by default.

To set the initial values, $P^{\mathrm{R}} = T = 0$ everywhere, the following subcommands of ≫ `SET INITIAL GUESS` are used:

```
>> INITIAL VALUES
   VARIABLES  'PRES' 'TEMP'
   VALUES       0.0    0.0
```

5.2 Solver Options for Transient Problems

The user has four options when choosing a solver for time-dependent problems. These are invoked by the commands:

1. ≫ `CRANK NICHOLSON`
2. ≫ `FAST LINEAR TRANSIENT`
3. ≫ `TRANSIENT`
4. ≫ `TIME STEP`

A Crank-Nicholson algorithm is used in the first two of these options, and Gear's Method is used in the last two. As its name implies, ≫ `FAST LINEAR TRANSIENT` can **only** be used for **linear** problems e.g. ≫ `NUCLIDE TRANSPORT`. The options ≫ `TRANSIENT` and ≫ `CRANK NICHOLSON` have both been designed to be robust in terms of stability, and

to use automatic algorithms to reduce the amount of input required from the user. Gear's method is most suited for diffusion-dominated problems and systems that are 'stiff' (i.e. systems that are governed by widely separated time constants); the Crank-Nicholson solver is suitable for transport and advection problems.

The example has been chosen to illustrate the ≫ TRANSIENT option. This option is selected as a subcommand of ≫ SOLVER DATA, and in turn has a number of subcommands that specify the type of problem to be solved. Here, the appropriate option is ≫ GROUNDWATER FLOW AND HEAT TRANSPORT. A number of keywords can also be assigned values, some of the more useful of these are:

- FINAL TIME – sets the time at the end of the final time-step;
- FINAL TIMESTEP – sets an upper limit for the number of time-steps;
- ESSENTIAL TIMES – sets the times at which a time-step must end. The solver will adjust the time-step size to cause time-steps to end at the ESSENTIAL TIMES. This ensures that the global freedoms are available for certain specified times for post-processing.

By default, the global freedom vector (i.e. the values of the variables at all nodes in the grid) is saved at the end of each time-step to unit 50. If NAMMU has already been run and the global freedom information has been saved, then it is possible to restore these global freedoms and restart the time-dependent calculation at the last time-step using appropriate keywords (see the NAMMU Commands Reference Manual [7]). Options for saving and restoring the model and global freedoms vector are explained in detail in the next Section.

5.3 Useful Output Options for Transient Problems

The output required for verification purposes [15] includes plots of temperature and pressure as functions of both time and space, together with a number of pathlines. These are produced using subcommands of ≫ OUTPUT DATA.

5.3.1 Variables as a Function of Time

The values of any variable can be plotted against time for a specified point using the command ≫ PLOT TIME EVOLUTION. For example, to produce a plot of the time evolution of the residual pressure at $(r,\ z) = (0,\ 250\text{m})$ the following instructions are used:

```
>> PLOT TIME EVOLUTION
   VARIABLE       'PRES'
   COORDINATES     0.0 250.0
   FIRST TIMESTEP  1
   LAST TIMESTEP   68
   READ FROM UNIT  50
```

```
   LOG TIME SCALE
   CAPTION         'TIME EVOLUTION OF PRES AT (0,250)'
   END
```

The variable is plotted from the specified FIRST TIMESTEP to the LAST TIMESTEP, with a symbol being plotted for the value of the variable at each time-step in that interval. Note that if the LAST TIMESTEP is specified to be greater than the number of time-steps that were performed, then NAMMU will plot up to the last timestep performed. A logarithmic scale for the time axis may be selected using the keyword LOG TIME SCALE. Time evolution plots of temperature and pressure produced in this way are shown in Figures 5.2 and 5.3, respectively.

The keyword READ FROM UNIT 50 instructs NAMMU to read the variables from a file allocated to unit 50. By default the solver will have stored the global freedoms on unit 50 at each time-step. However, it is also possible to read the global freedoms that were saved in a file during a previous run. This is achieved by allocating a different unit number to the file in the job information [11] and then reading variables from that unit.

5.3.2 Variables as a Function of Distance

Plots of a variable against distance at a given time are produced using a combination of the ≫ SELECT TIME and ≫ DRAW LINE GRAPH commands. First, a time is selected. This may be specified in terms of either the number of a time-step or as an actual time. Again, the global freedoms are restored from a specified unit at the required time. If the selected time falls between two time-steps the variables at that time are obtained by linear interpolation. Thus, to plot variables at a time of 100 years, the following commands would be used:

```
>> SELECT TIME
   TIME           3.1558E9
   READ FROM UNIT 50
```

Once the time has been selected, a line graph can be plotted by specifying a line through the domain using the START POINT and END POINT keywords. The option ≫ DRAW LINE GRAPH is very versatile. For instance, it is possible to superimpose a number of profiles of a variable at different times onto the same graph. To do this, a ≫ SELECT TIME and a ≫ DRAW LINE GRAPH command is made at each required time, but at every selected time following the first, the SUPERIMPOSE keyword is included under ≫ DRAW LINE GRAPH. Also, in order to ensure that the ranges of variable (y) and abscissa (x) are identical for successive line graphs, the keywords VARIABLE LIMITS and X AXIS LABEL RANGE should be given the same values. Examples of how to superimpose line graphs are given in Dataset 5.1. The results for the temperature and pressure rises as a function of distance are given in Figures 5.4 and 5.5.

5.3.3 Pathlines

Travel times for groundwater to reach the 'surface', which is taken to be the plane $z = 1000$m can be calculated using the ≫ PATHLINES command, which has already received some explanation in subsection 4.5.3. For transient problems values should be supplied for the START TIME and FINISH TIME keywords. The start time of the path is important since the Darcy velocity is a function of time as well as space in this case. It is also essential that keyword TRANSIENT VELOCITY FIELD is included to ensure that variations of the velocity field in time as well as space are considered in computing pathlines. Without this keyword pathlines are computed on the basis of an instantaneous velocity field, which by default is that at the final time. Examples of pathline plots are shown in Figure 5.6.

Figures for Section 5

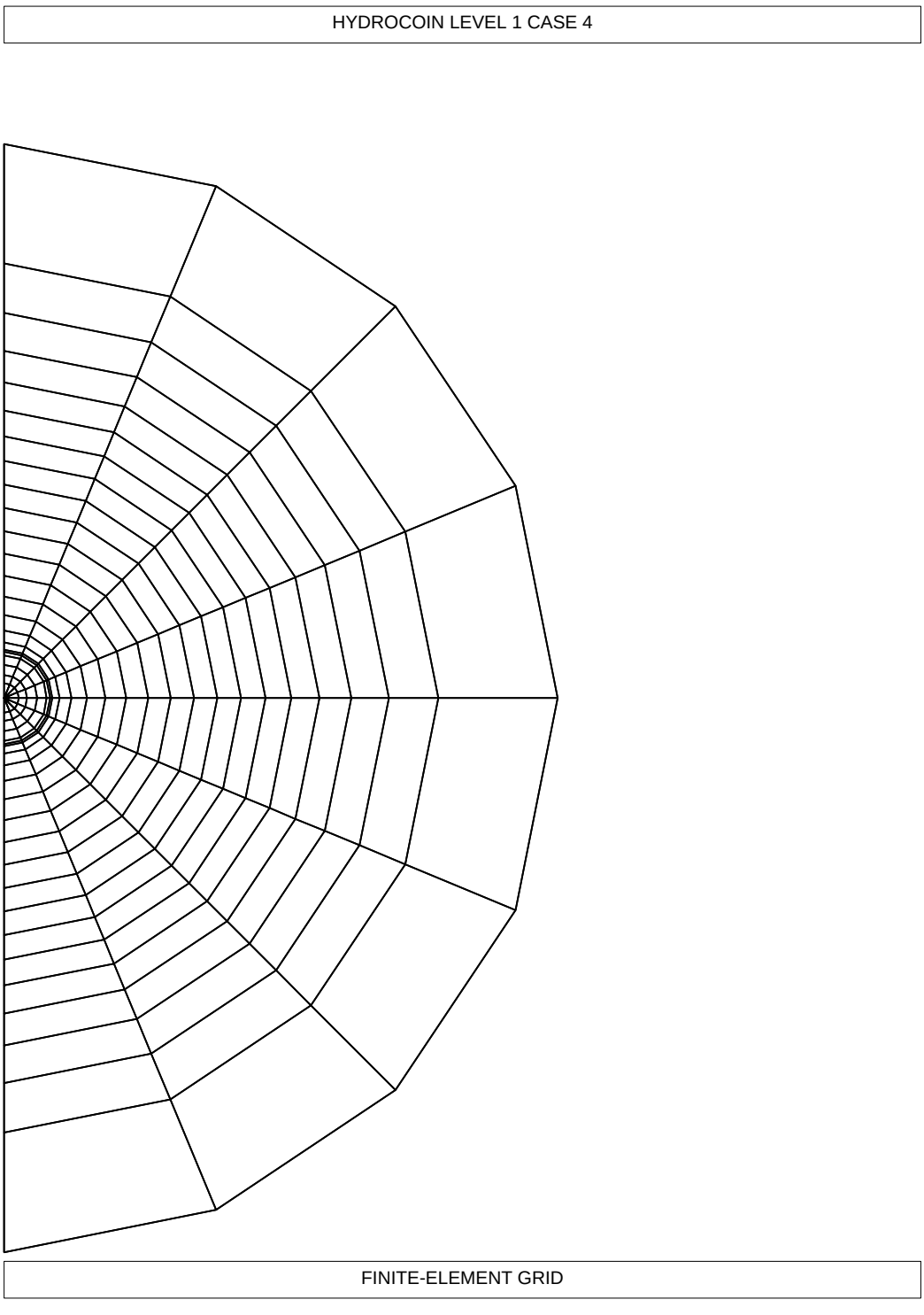


Figure 5.1 The refined finite-element grid.

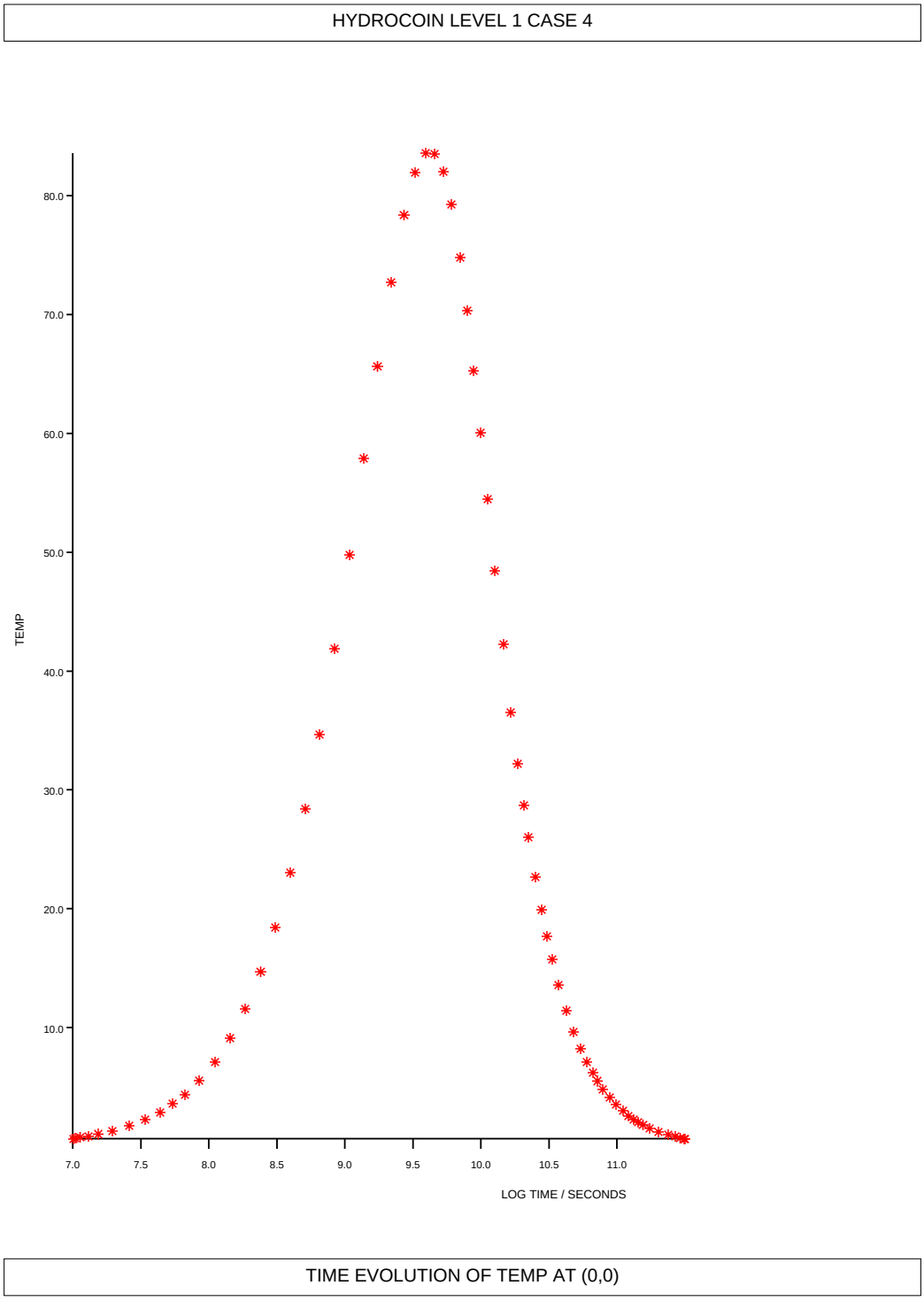


Figure 5.2 Time evolution of the temperature rise at the origin.

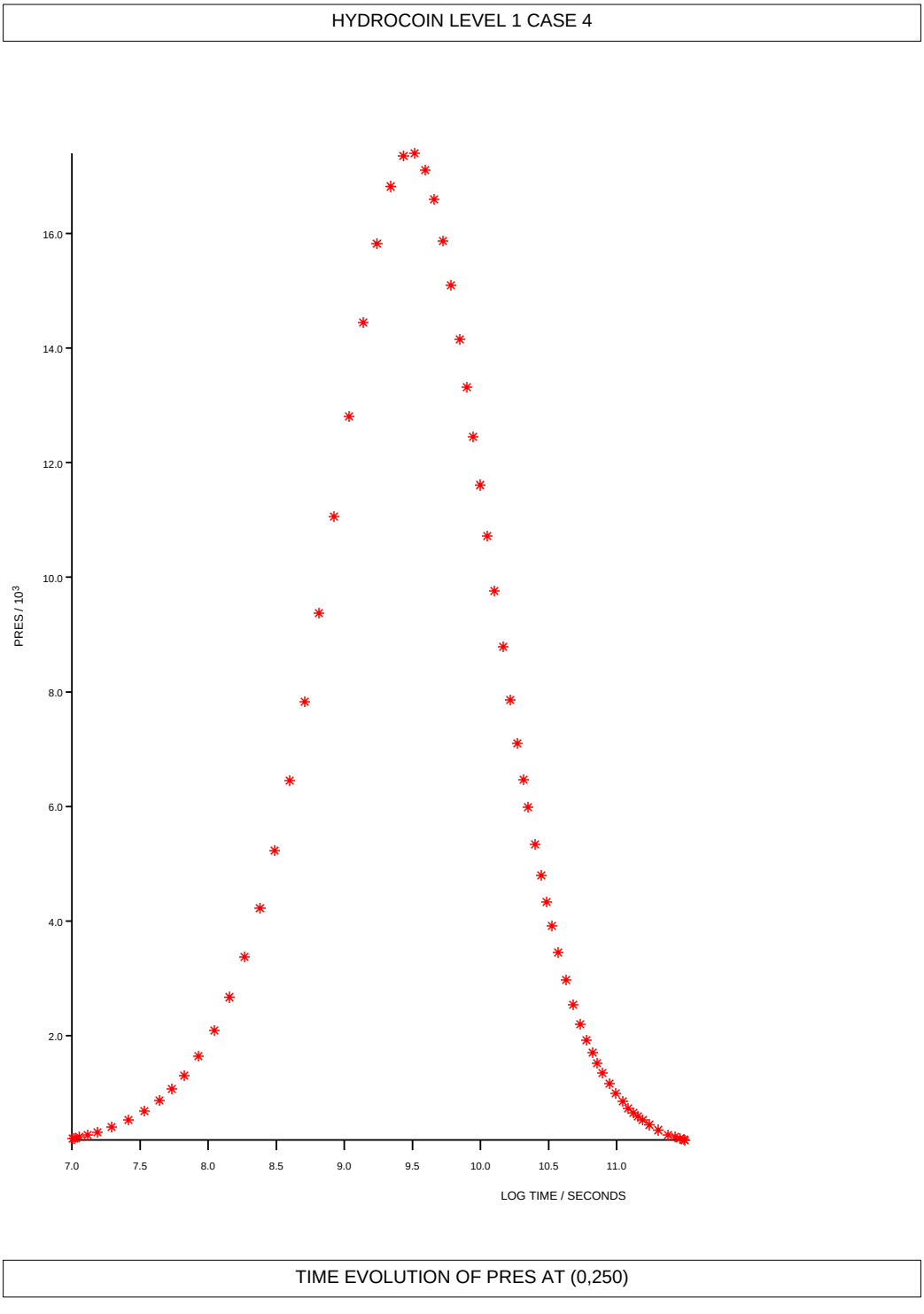


Figure 5.3 **Time evolution of the pressure rise on the vertical centreline, $r = 0$, at a depth $z = 250\text{m}$.**

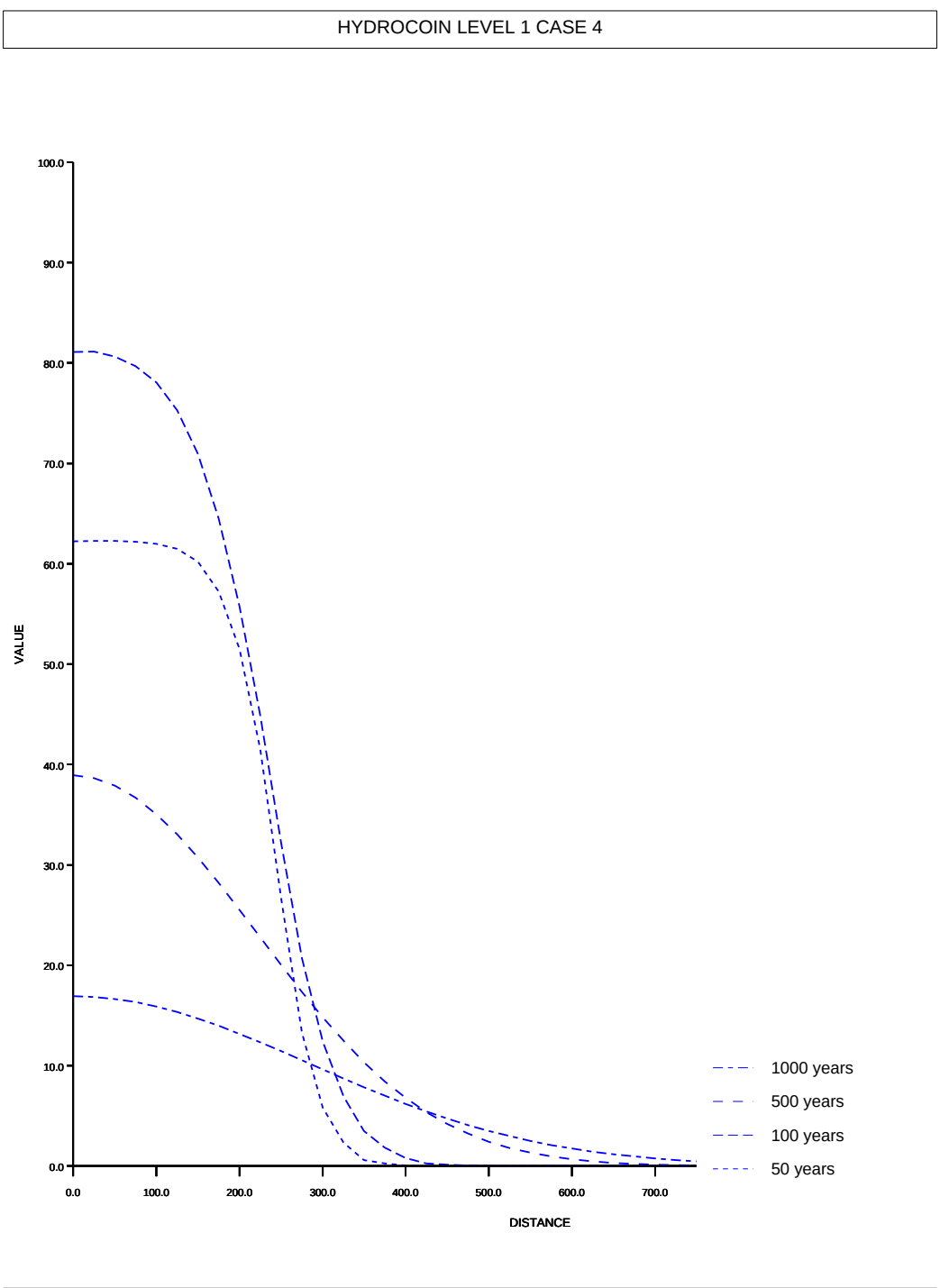


Figure 5.4 **Distribution of the temperature rise along the vertical centerline, $r = 0$, at 50, 100, 500, and 1000 years.**

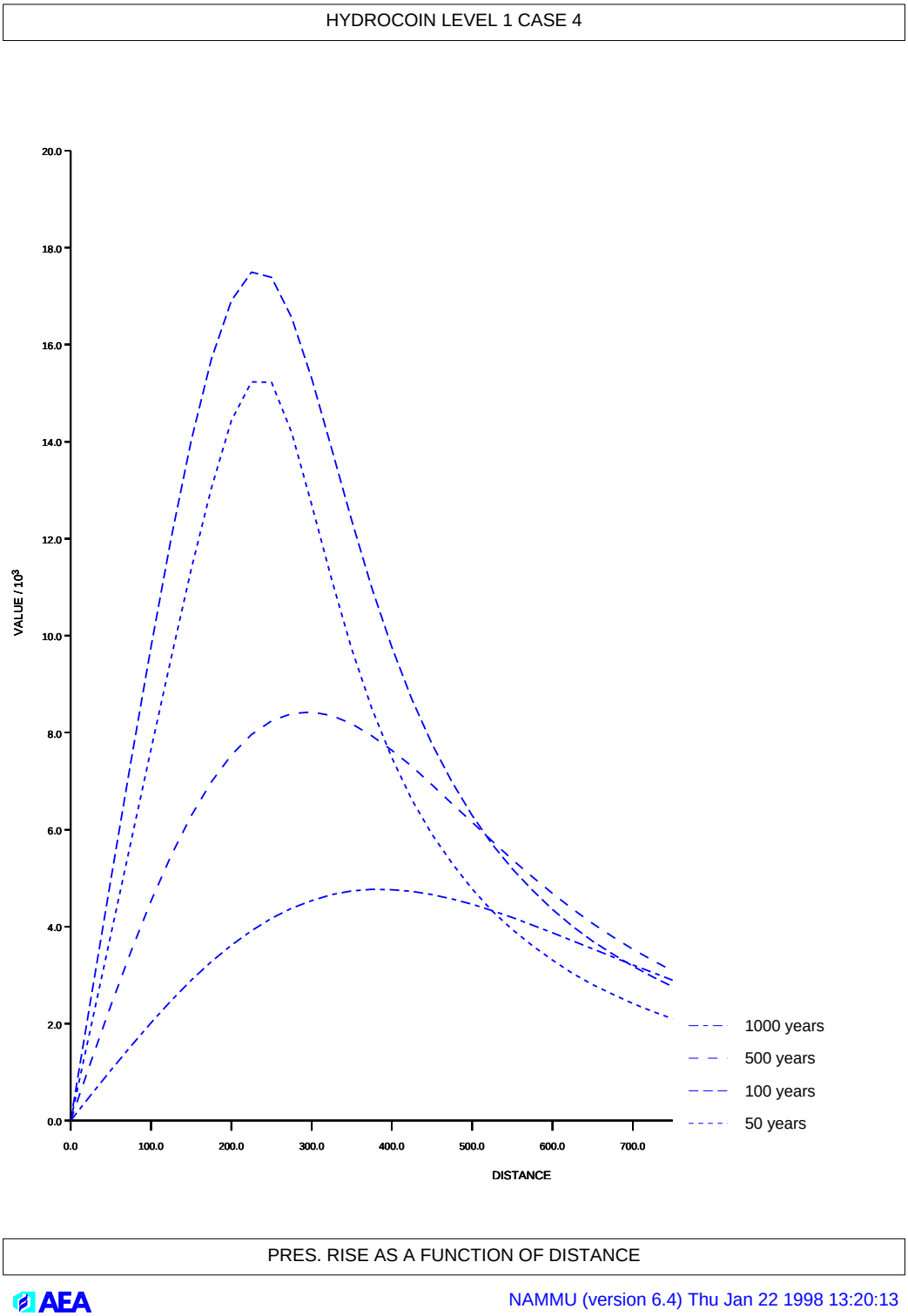


Figure 5.5 **Distribution of the pressure rise along the vertical centerline, $r = 0$, at 50, 100, 500, and 1000 years.**

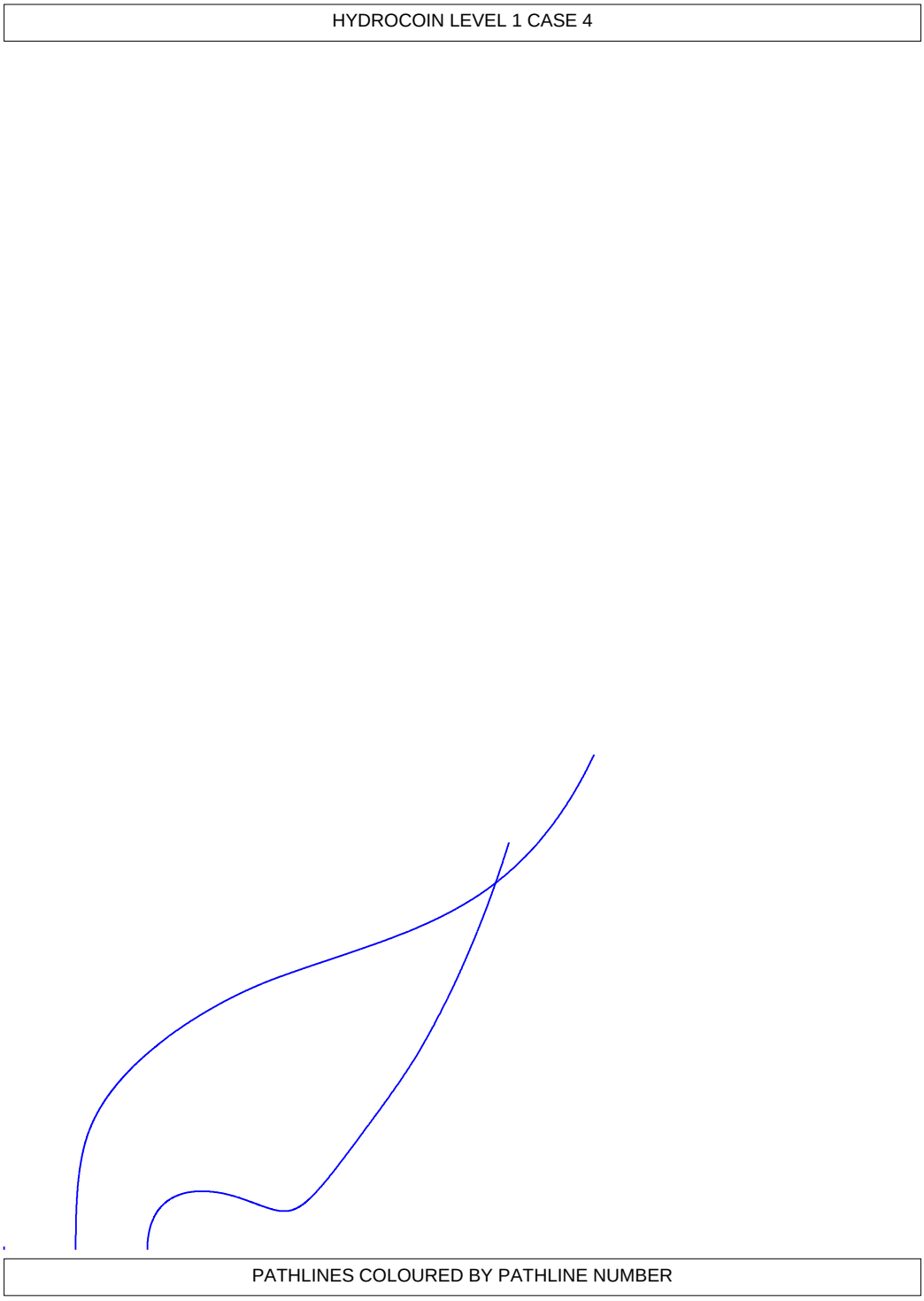


Figure 5.6 **Pathlines starting at** $z = 0$; $r = 0,\ 125,\ 250$m; **from** $t = 100$ **years.**

Dataset 5.1

```
   /* NAMMU TEST CASE HYDRO4                                          */
   /*                                                                 */
   /* ++++++++++++++++++++++ DATASET 5.1 ++++++++++++++++++++++       */
   /*                                                                 */
   /* EXAMPLE 3 : TRANSIENT COUPLED GROUNDWATER FLOW AND              */
   /*             HEAT CONDUCTION                                     */
   /* INPUT DATA FILE FOR HYDROCOIN: LEVEL 1 CASE 4                   */

   /* SPACE ALLOCATION                                                */
   /* INTEGER WORKSPACE  400000                                       */
   /* REAL WORKSPACE     600000                                       */

   /* INLINE FORTRAN
C +-------------------------------------------------------------------+
C | FIG 5.1: SPATIAL DEPENDENT PART OF THE HEAT SOURCE FOR EXAMPLE 3 |
C +-------------------------------------------------------------------+
      SUBROUTINE HEATFN(QH,R,NSD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION R(NSD)
C
      RR = SQRT(R(1)**2 + R(2)**2)
      IF (RR .LE. 250.0D0) THEN
        AA = 3.1415927D0 * 250.0D0**3
        QH = 0.75D7 / AA
      ELSE
        QH = 0.0D0
      END IF
C
      RETURN
      END

C
C +-------------------------------------------------------------------+
C | FIG 5.2: INTEGRATED TIME DEPENDENT HEAT SOURCE FOR EXAMPLE 3     |
C +-------------------------------------------------------------------+
      SUBROUTINE HTINT(TIME,HN)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      RLMBD = 7.3215E-10
      HN = (1.0D0 - EXP(-RLMBD * TIME)) / RLMBD
C
      RETURN
      END
                                                                      */
   /* SOURCE FILES                                                    */
   /* COMPILED FILES                                                  */
   /* LIBRARY FILES                                                   */

   /* OUTPUT DATA FILES                                               */
   /* 6        nammu/output/hydro4.out                                */
   /* GRAPHICS nammu/output/hydro4.ps                                 */
```

```
   /* END JOB INFORMATION                                          */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      CYLINDRICAL GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS                          400
      NODES                            3600
      FRONTWIDTH                        400
      INTEGER BC WORKSPACE            10000
      REAL BC WORKSPACE                2000
      PARAMETERS PER FUNCTION TYPE        9
      FUNCTION TYPES PER ELEMENT          3
      VARIABLES                           2
      END

   >> SET VARIABLES
      VARIABLE NAMES  'PRES' 'TEMP'
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      DELTA                                  0.0
      FLUID HEAT CAPACITY                    0.0
      FLUID THERMAL EXPANSION COEFFICIENT  3.85E-4
      VISCOSITY                            6.529E-4
      FLUID DENSITY                        9.922E2

      ROCK TYPE PERMEABILITIES
      ROCK NUMBER,   KXX,    KYY
           1       1.0E-16 1.0E-16

      ROCK TYPE PROPERTIES
      ROCK NUMBER,  POROSITY, HEAT CONDUCTIVITY, DENSITY, SPECIFIC HEAT
           1          0.0          2.51           2.6E3      8.79E2

      USER HEAT SOURCE
      END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         PATCH SPACING IN FIRST DIRECTION
         SIZE,  GRADE POWERS
```

```
  1     < 1.0 1.0 >

PATCH SPACING IN SECOND DIRECTION
SIZE,  GRADE POWERS
  1    < 1.0 1.0 >
  4    < 1.0 2.0 >
 18    < 2.0 0.5 >

PATCH POSITIONS
CORNER NUMBER,        COORDINATES
      1         <    0.0      80.0  >
      2         <   30.61     73.91 >
      3         <   56.57     56.57 >
      4         <   73.91     30.61 >
      5         <   80.0       0.0  >
      6         <   73.91    -30.61 >
      7         <   56.57    -56.57 >
      8         <   30.61    -73.91 >
      9         <    0.0     -80.0  >
     11         <    0.0     250.0  >
     12         <   95.67    230.97 >
     13         <  176.78    176.78 >
     14         <  230.97     95.67 >
     15         <  250.0       0.0  >
     16         <  230.97    -95.67 >
     17         <  176.78   -176.78 >
     18         <   95.67   -230.97 >
     19         <    0.0    -250.0  >
     21         <    0.0    3000.0  >
     22         < 1148.05   2771.64 >
     23         < 2121.32   2121.32 >
     24         < 2771.64   1148.05 >
     25         < 3000.0       0.0  >
     26         < 2771.64  -1148.05 >
     27         < 2121.32  -2121.32 >
     28         < 1148.05  -2771.64 >
     29         <    0.0   -3000.0  >
     31         <    0.0       0.0  >

PATCH TOPOLOGY
PATCH TYPE,    CORNERS,     INDICES
  'SQQ9'    < 1  2 12 11>    <1 2>
  'SQQ9'    < 2  3 13 12>    <1 2>
  'SQQ9'    < 3  4 14 13>    <1 2>
  'SQQ9'    < 4  5 15 14>    <1 2>
  'SQQ9'    < 5  6 16 15>    <1 2>
  'SQQ9'    < 6  7 17 16>    <1 2>
  'SQQ9'    < 7  8 18 17>    <1 2>
  'SQQ9'    < 8  9 19 18>    <1 2>
  'SQQ9'    <11 12 22 21>    <1 3>
  'SQQ9'    <12 13 23 22>    <1 3>
  'SQQ9'    <13 14 24 23>    <1 3>
  'SQQ9'    <14 15 25 24>    <1 3>
  'SQQ9'    <15 16 26 25>    <1 3>
```

```
        'SQQ9'    <16 17 27 26>    <1 3>
        'SQQ9'    <17 18 28 27>    <1 3>
        'SQQ9'    <18 19 29 28>    <1 3>
        'TRT6'    < 1 31  2   >    <1 1>
        'TRT6'    < 2 31  3   >    <1 1>
        'TRT6'    < 3 31  4   >    <1 1>
        'TRT6'    < 4 31  5   >    <1 1>
        'TRT6'    < 5 31  6   >    <1 1>
        'TRT6'    < 6 31  7   >    <1 1>
        'TRT6'    < 7 31  8   >    <1 1>
        'TRT6'    < 8 31  9   >    <1 1>
      END

>> SET BOUNDARY CONDITIONS

/*   ************ PRESSURE BOUNDARY SPECIFICATION **********   */
/*   ********************** ORIGIN ************************   */
   >> SPECIFIED  VALUE

      >> CONSTANT VALUE
         VARIABLES  'PRES'
         VALUES     0.0
         END

         >> SELECT POINT
            COORDINATES  0.0  0.0
            TOLERANCE    1.0E-4
            END

/*   ********************* OUTER BOUNDARY *****************   */
      >> CONSTANT VALUE
         VARIABLES  'PRES'
         VALUES      0.0
         END

         >> SELECT BOUNDARY SEGMENT
            END POINT       0.0   3000.0
            MID POINT    2121.32  2121.32
            START POINT  3000.0      0.0
            PRECISION       1.0E-1
            END

      >> CONSTANT VALUE
         VARIABLES  'PRES'
         VALUES      0.0
         END

         >> SELECT BOUNDARY SEGMENT
            END POINT       0.0  -3000.0
            MID POINT    2121.32 -2121.32
            START POINT  3000.0      0.0
            PRECISION       1.0E-1
            END
```

```
   >> SET INITIAL GUESS

      >> INITIAL VALUES
         VARIABLES  'PRES' 'TEMP'
         VALUES      0.0    0.0
         END


>> SOLVER DATA

   >> TRANSIENT
      FINAL TIME              3.15576E11
      MAXIMUM FRONTWIDTH     400
      NUMBER OF TIMESTEPS     80
      CONVERGENCE CRITERION    1.0E-3
      NUMBER OF ITERATIONS     3
      END

      >> GROUNDWATER FLOW AND HEAT TRANSPORT


>> OUTPUT DATA

   >> SET PLOT OPTIONS
      HEADING            'HYDROCOIN LEVEL 1 CASE 4'
      BOUNDARY COLOUR    'BLACK'
      GRID COLOUR        'BLACK'
      LINE THICKNESS     0.3
      END

   >> PLOT GRID
      END

   /*   *********** VARIABLES AS A FUNCTION OF TIME  **********   */

   >> PLOT TIME EVOLUTION
      VARIABLE           'TEMP'
      COORDINATES         0.0  0.0
      FIRST TIMESTEP      1
      LAST TIMESTEP      68
      READ FROM UNIT     50
      LOG TIME SCALE
      CAPTION            'TIME EVOLUTION OF TEMP AT (0,0)'
      END

   >> PLOT TIME EVOLUTION
      VARIABLE           'PRES'
      COORDINATES         0.0 250.0
      FIRST TIMESTEP      1
      LAST TIMESTEP      68
      READ FROM UNIT     50
      LOG TIME SCALE
      CAPTION            'TIME EVOLUTION OF PRES AT (0,250)'
      END
```

```
/*   ********* VARIABLES AS A FUNCTION OF DISTANCE *********   */
/* RESET KEY VIEWPORT FOR LINE GRAPH KEYS */

>> SET VIEWPORT
   VERTICAL KEY VIEWPORT
   ORIGIN    0.76  0.2
   SIZE      0.24  0.85

>> SELECT TIME
   TIME             1.57788E9
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'TEMP'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0  100.0
   LINE STYLE           1
   NO SYMBOLS
   JOIN POINTS
   CAPTION             'TEMP. RISE AS A FUNCTION OF DISTANCE'
   TITLE               '50 years'
   END

>> SELECT TIME
   TIME             3.15576E9
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'TEMP'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0  100.0
   LINE STYLE           2
   NO SYMBOLS
   JOIN POINTS
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               '100 years'
   END

>> SELECT TIME
   TIME             1.57788E10
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'TEMP'
```

```
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   VARIABLE LIMITS      0.0  100.0
   X AXIS LABEL RANGE   0.0  750.0
   LINE STYLE           3
   NO SYMBOLS
   JOIN POINTS
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               '500 years'
   END

>> SELECT TIME
   TIME             3.1557E10
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'TEMP'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0  100.0
   LINE STYLE           4
   NO SYMBOLS
   JOIN POINTS
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               '1000 years'
   END

>> SELECT TIME
   TIME             1.57788E9
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'PRES'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0   20.0E3
   LINE STYLE           1
   NO SYMBOLS
   JOIN POINTS
   CAPTION             'PRES. RISE AS A FUNCTION OF DISTANCE'
   TITLE               '50 years'
   END

>> SELECT TIME
   TIME             3.15576E9
   READ FROM UNIT  50
   END
```

```
>> DRAW LINE GRAPH
   VARIABLE            'PRES'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0   20.0E3
   LINE STYLE           2
   NO SYMBOLS
   JOIN POINTS
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               '100 years'
   END

>> SELECT TIME
   TIME             1.57788E10
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'PRES'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0   20.0E3
   LINE STYLE           3
   NO SYMBOLS
   JOIN POINTS
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               '500 years'
   END

>> SELECT TIME
   TIME             3.1557E10
   READ FROM UNIT  50
   END

>> DRAW LINE GRAPH
   VARIABLE            'PRES'
   START POINT          0.0    0.0
   END POINT            0.0  750.0
   NUMBER OF POINTS    31
   X AXIS LABEL RANGE   0.0  750.0
   VARIABLE LIMITS      0.0   20.0E3
   LINE STYLE           4
   NO SYMBOLS
   JOIN POINTS
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               '1000 years'
   END
```

```
>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      ROCK TYPE PROPERTIES
      ROCK NUMBER, POROSITY
           1        1.0E-4
      END


>> OUTPUT DATA

   >> PATHLINES
      NUMBER OF PATHS                  3
      X COORDINATES OF PATHS           0.0  125.0  250.0
      Y COORDINATES OF PATHS           0.0    0.0    0.0
      NO BOUNDARY
      X LIMITS OF ZOOM                 0.0 1200.0
      Y LIMITS OF ZOOM                 0.0 1000.0
      TRANSIENT VELOCITY FIELD
      START TIME                     100.0
      FINISH TIME                  10000.0
      READ FROM UNIT                  50
      TIMES IN YEARS
      MAXIMUM NUMBER OF TIMESTEPS   2000
      ACCURACY PARAMETER               0.1
      NO KEY
      END


>> STOP
```

6 EXAMPLE 4: RADIONUCLIDE TRANSPORT IN A STEADY GROUNDWATER FLOW (CEC PACOMA PROJECT)

An important application of groundwater flow and transport modelling is the performance assessment of underground repositories for radioactive waste. Assessments often presuppose that the transport of radionuclides to the surface takes place along unique pathways determined by the groundwater flow in the vicinity of the repository. An illustrative example of how NAMMU can be used to determine such pathways, and the associated radionuclide transit-times, is considered in this Section. It also demonstrates how a simplified geological model can be derived from information on the surface geology, stratigraphy and hydrogeological properties of a real location.

The example involves the simulation of groundwater flow and radionuclide transport from a hypothetical repository located in the clay layer beneath the Harwell site. The findings of a detailed study of this example have been reported elsewhere [17]. In this study, a two-dimensional vertical cross section consisting of three rock types is chosen to model the local geological features. The cross section runs approximately at right-angles to the direction in which various strata outcrop to the surface and parallel to the anticipated horizontal flow pattern. Figure 6.1 shows the geology of this cross section. The various rock strata may be broadly classified as comprising layers of high hydraulic conductivity (Chalk, Corallian and Greensand) separated by layers of low hydraulic conductivity (Gault and Kimmeridge Clay). The hypothetical repository is positioned 135m below the topographic surface in the middle of a band of Gault and Kimmeridge Clay. This clay is overlaid by permeable Chalk and Upper Greensand, and rests upon a permeable Corallian layer, which in turn rests on the almost impervious Oxford Clay.

A simplified model for the geological configuration is obtained by combining the Chalk and Upper Greensand into a single layer of high permeability, and combining the Lower Greensand with the Gault and Kimmeridge Clay into a layer of low permeability. This results in a three-layer model which is shown in Figure 6.2, and is illustrated further by shading the rock strata differently in Figure 6.3. Before any transport calculations are made using a model of this sort, it is good practice to validate the assumptions made. This can only be done by taking into account the more complex five layer model, including the upper and lower Greensand layers, and comparing the results of a groundwater flow calculation [18].

The upper boundary of the section is taken to be the phreatic surface (water table), which does not coincide with the physical surface. On the base of the Corallian, the Oxford Clay is taken to be impermeable, and so it can be excluded from the model. The left hand boundary corresponds to the SSW extreme of the section, and coincides with the observed groundwater divide where a no-flow condition is specified. Also, the right boundary, corresponding to the NNE limit of the section, is at a point of low groundwater head with zero horizontal flow and is specified to be impermeable.

6.1 Groundwater Flow Modelling

Before any transport modelling, the groundwater flow model should be checked for accuracy, and calculations should be performed to assess the relative importance of the different physical effects. Dataset 6.1 corresponds to a preliminary investigation of the groundwater flow as modelled by a three layer configuration. It includes a few of the more advanced features of NAMMU, which are discussed in the following subsections.

6.1.1 Streamlines

Any inadequacies in the refinement of the grid can often be diagnosed by plotting streamlines derived from the calculated pressure field. This is achieved by first solving for the pressure, and then solving for the streamfunction variable `'STFN'`. These require separate ≫ `SOLVER DATA` phases, with the solution for the groundwater flow always being undertaken first. To do so, the solver should be invoked with the commands:

```
>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH    250
      NUMBER OF ITERATIONS   2
      SAVE GLOBAL FREEDOMS
      END

      >> GROUNDWATER FLOW
         END
```

This is explained further in the NAMMU Reference Manual [7].

Once the pressure field has been obtained, the next step is to compute the boundary values of the streamfunction from the integral of the normal velocity along the boundary. This integration is performed only at nodes for which a Dirichlet condition for the streamfunction has been specified, and so it is necessary to initially specify dummy boundary conditions of the specified value type for the streamfunction along the boundary. The calculation of streamlines requires the finite-element consistent flux formulation, which is specified by the `CONSISTENT FLUX` keyword of ≫ `SET NAMMU OPTIONS`. The boundary values are computed with the following commands:

```
>> SOLVER DATA

   >> COMPUTE BOUNDARY VALUES
      BOUNDARY FUNCTION  'STFN'
      END

      >> STREAMFUNCTION CALCULATION
         END
```

Finally, these commands are followed by instructions to solve for the streamfunction variable:

```
>> STEADY STATE
   MAXIMUM FRONT WIDTH   250
   NUMBER OF ITERATIONS   2
   CONVERGENCE CRITERION 1.0E-15
   END

   >> STREAMFUNCTION CALCULATION
      END
```

Streamlines can then be visualised by plotting contours of the variable `'STFN'`.

Streamlines generated on a poorly refined grid may exhibit spurious oscillations, as appear in the upper aquifer shown in Figure 6.4. Difficulties of this kind arise because the elements are elongated, and ill-suited to representing variations that are actually localised within a region covered by only a small part of the element. By careful adjustment of the finite-element grid, these unphysical oscillations can be reduced, as shown in Figure 6.5.

Plotting streamlines also provides a good indication of the sensitivity of the results to physical effects, such as the shape of the phreatic surface. Abrupt changes in the flow direction and speed are observed in the vicinity of changes in the slope of the water table. Tests should be carried out to discover whether these changes result from modelling the slope to be discontinuous, or from the actual contracting thickness of the upper aquifer.

6.1.2 Flow Vectors

NAMMU includes a very flexible facility for visualising the flow field by means of plotting velocity arrows. To aid interpretation of these plots it is possible to present the vectors in several different ways: (i) as vectors with length proportional to the velocity, (ii) as vectors coloured according to rock types, (iii) as constant-length vectors coloured according to the magnitude of the velocity (which can help to resolve details of the flow in regions where the velocities are much smaller than the overall maximum).

The region on which the vectors are to be plotted, and the points at which velocity arrows are to be drawn, are selected with ≫ `SET PLOT POINTS` in the following way:

```
>> SET PLOT POINTS

   >> SELECT REGULAR ARRAY OF POINTS
      X LIMITS           0.0 13000.0
      Y LIMITS        -110.0   140.0
      NUMBER OF X POINTS 50
      NUMBER OF Y POINTS 50
```

The vectors are then plotted on this slice by the following commands:

```
>> PLOT VELOCITY ARROWS
   CONSTANT LENGTH VECTORS
   COLOUR USING LOG OF VECTOR MAGNITUDE
```

together with other keywords that specify the colours and length scale of the arrows. To present the vectors in the styles suggested above it is necessary to use the keywords `CONSTANT LENGTH VECTORS` and `COLOUR USING LOG OF VECTOR MAGNITUDE`. Figure 6.6 shows constant length velocity arrows which have been shaded in four colour bands according to the magnitude of the logarithm of the Darcy velocity.

6.1.3 Flow Pathlines

Plots of streamlines and velocity arrows provide a general picture of the flow paths in the region. However, in studies of contaminant migration what is needed is the path followed by a contaminant released at a specific location, usually the site of a repository, under the assumption that advection by the flow alone is responsible for transport of the contaminant. Figure 6.7 shows a plot of pathlines originating from various locations in the three layers, and was generated using the ≫ `PATHLINES` command. These show, for example, that the path starting at the repository (positioned toward the left side of the clay layer) leads downwards through the clay, up-dips along the Corallian aquifer, and eventually emerges upwards through the clay to the surface.

Keywords are available to colour the pathlines according to pathline number, rock type, time or velocity. Details may be found in the NAMMU Reference Manual [7].

6.2 Radionuclide Transport Modelling

6.2.1 Transport Modelling on Sub-regions

The calculation of contaminant migration is much more computationally demanding than that of groundwater flow because of the many time steps and the finer grids that are required for accurate solutions. However, in some cases it may be feasible to carry out calculations of contaminant transport on a sub-region of the model used for groundwater flow, and so reduce the computational cost. A further possibility for reducing computational costs is element renumbering to reduce the frontwidth of the equation matrix, as discussed in subsection 6.2.3.

In this instance, two sub-regions might be considered initially. The first is along the flow pathline originating at the repository, that is the Clay/Corallian sub-region BFGLMHDCB on Figure 6.2. This will test the assumption that migration is predominantly in the direction of flow. Should this assumption prove to be valid, then all transport calculations could be performed on this much more confined sub-region. The second sub-region is the Chalk

region AEJNKFBA on Figure 6.2, which is used to investigate an alternative pathway for the advection through the Chalk of any contaminant that diffuses upwards through the Clay layer.

6.2.2 Saving and Restoring of Model and Results

A very useful feature of the NAMMU package is the ability to save the model and global freedom vector from one run and then to restore them in a later run. This facility can be used for example to post-process results without having to recompute the solution. For example, the pressure field obtained from a groundwater flow calculation can be restored for use in a transport calculation.

The model and boundary conditions may be saved on disk in either the MODEL DATA or OUTPUT DATA phase using the commands:

```
>> SAVE MODEL
   SAVE ON UNIT  49
```

The model data is then written to unit number 49 (i.e. FORTRAN stream 49), which should have been assigned to a named file in the job information at the head of the input file.

Likewise, the global freedoms can be saved in the OUTPUT DATA phase by the commands:

```
>> SAVE GLOBAL FREEDOMS
   SAVE ON UNIT  50
```

The global freedoms may also be saved as part of the various solver options. Details may be found in the NAMMU Reference Manual [7]. The global freedoms and model information are saved in unformatted form, and so are machine-dependent.

The model and boundary conditions, saved in a previous run, can be restored in the MODEL DATA phase using the commands:

```
>> RESTORE MODEL
   READ FROM UNIT  34
```

Unit 34 is identified with the appropriate data file in the instructions at the start of the input file. Similarly the global freedoms can be restored with the command >> `RESTORE GLOBAL FREEDOMS`. It is often desirable to restore a solution calculated on one grid, for example in radionuclide modelling to restore the pressure solution from a regional flow model to a smaller grid for radionuclide transport calculations. This can be done using the `INTERPOLATE` keyword (see the NAMMU Reference Manual).

For time-dependent calculations, it is possible to restore the global freedoms at a specified time, and then restart the calculation. The global freedoms can also be restored at selected times and used for post-processing, as discussed in subsection 5.3.2. If these global freedoms describe a variable density or unsaturated flow field one or more of the keywords of ≫ SET PLOT OPTIONS may be required. Similar keywords are available for solver options which use global freedoms that may have been calculated in an earlier run e.g. ≫ NUCLIDE TRANSPORT.

6.2.3 Element Renumbering

The final stage of model generation for models containing many elements is to renumber the elements efficiently to give as small a frontwidth as possible in the matrix to be solved. The cost of a run is proportional to the mean frontwidth squared times the total number of freedoms, and the memory required in-core is the maximum frontwidth squared. Clearly it is worth spending some time and effort to reduce the frontwidth, if these costs can be significantly reduced.

There are two alternative renumbering schemes available in the NAMMU package, both based on Sloan's Algorithm. The relative effects of renumbering with each option may be tested using the ≫ COST subcommand of ≫ OUTPUT DATA.

An example of the commands appropriate to the renumbering stage is given below:

```
>> RENUMBER ELEMENTS

   >> SLOAN ALGORITHM
      END
```

6.2.4 Solution Procedure

The procedure for calculating contaminant migration on a sub-region of the finite-element grid using NAMMU is summarised as follows:

1. **Save model and global freedoms from a groundwater flow calculation.** The model should be saved using the command ≫ SAVE MODEL. The pressure field should be computed on the full domain, and the global freedom vector saved using the option ≫ SAVE GLOBAL FREEDOMS. This latter command is explained in subsection 6.2.2.

2. **Create a new input file and declare a nuclide variable.** In a new input file, the variables should be set to include a variable to represent the contaminant concentration. Normally the variable name 'NUC1' is used for this purpose, and is by default the sixth in the variable list.

3. **Specify the radionuclide physical properties.** Data relevant to radionuclide transport is supplied through the keyword `DECAY CONSTANT`, and the table keyword `ROCK TYPE NUCLIDE PROPERTIES`. In the latter, the dispersion coefficients, the tortuosities and the sorption coefficients are set.

4. **Generate a refined grid for a sub-region.** An appropriate grid for the sub-region is specified in the new input file. Substantial refinement of the local mesh in the vicinity of the repository is often necessary to resolve the migration of the contaminant accurately. An insufficiently refined grid may lead to ripples in the contours of concentration.

5. **Restore and interpolate the global freedoms on the new grid.** The global freedoms are restored to the new input file using ≫ `RESTORE GLOBAL FREEDOMS` (a subcommand of ≫ `SET INITIAL GUESS`), and the pressure field is interpolated onto the current grid by including the keyword `INTERPOLATE` and other related keywords to supply information about the model for which the pressure field was obtained. The velocity field can then be computed on the new grid.

6. **Define a source of contaminant.** The source of contaminant may be specified in a number of ways. For a constant source of contaminant a Dirichlet boundary condition may be applied on a restricted region of the domain. For instance, a fixed contaminant concentration of unity over a restricted region can be specified as follows:

```
>> SET BOUNDARY CONDITIONS
   >> SPECIFIED VALUE
      >> CONSTANT VALUE
         VARIABLES 'NUC1'
         VALUES      1.0

         >> CALL SUBROUTINE USLECT
```

   Here the user routine USLECT is used to define the extent of the contaminant source (an example of this routine is listed in Dataset 6.2 at the end of this Section). An alternative is to specify a contaminant source in much the same way as was described in subsection 5.1.3 for a source of heat. The keyword `USER NUCLIDE SOURCE` is included under the ≫ `PHYSICAL PROPERTIES` command, and two user routines, SRCXY and SRCT, are supplied (see subsection 11.1.3 for examples). Again, these specify the spatial variation and the time integral of the source, respectively.

7. **Set contaminant boundary conditions.** The possible boundary conditions for the radionuclide transport equations are:

   - zero concentration far from a source;

   - zero flux, appropriate to impermeable boundaries;

- zero dispersive flux, appropriate when solute is expected to pass through the boundary by advection alone. The way in which an imposed advective flux condition (zero dispersive flux) is set using NAMMU is described in subsection 6.2.8.

8. **Solve transport equations.** The time-dependent solution of the transport equation is then obtained by a fully implicit method. This option is selected by the following commands:

```
>> SOLVER DATA
   >> FAST LINEAR TRANSIENT
      >> NUCLIDE TRANSPORT
```

   together with keywords that specify the frequency at which the global freedoms are saved and printed. For nuclide transport calculations, the solver option ≫ `FAST LINEAR TRANSIENT` is usually considerably faster than ≫ `CRANK NICHOLSON`, but it uses considerably more memory. As the name implies, ≫ `FAST LINEAR TRANSIENT` can only be used on linear problems such as nuclide transport. Time-dependent boundary conditions are not supported under ≫ `FAST LINEAR TRANSIENT`.

6.2.5 Choice of Time Step

To simulate accurately the transport of a contaminant the maximum mesh spacing should be chosen to ensure a mesh Peclet number $\mathrm{Pe_m}$ of order 1, where

$$\mathrm{Pe_m} = \frac{v\,\Delta x}{D} \qquad \Longrightarrow \qquad \Delta x \approx \frac{D}{v},$$

where v is the average pore water velocity, Δx is the mesh spacing and D is the diffusion/dispersion coefficient.

For the solution of the time-dependent equations the time-step should be less than the mesh transit time, such that

$$\Delta t = \frac{\Delta x}{v} \approx \frac{D}{v^2}.$$

In the Corallian, the longitudinal dispersion dominates diffusion and so it can be assumed that $D \approx \alpha_{\mathrm{L}} v$, where α_{L} is the longitudinal dispersion length. Thus, for a typical average pore velocity of around $10^{-9}\mathrm{ms}^{-1}$ and using a longitudinal dispersion length of 88m, the time-step should be of the order $\Delta t = 10^{11}$s. In order to get accurate results Δt was set to $2.5\,10^{10}$s in Dataset 6.2.

In systems for which the migration of a nuclide is retarded by sorption, this estimate of the appropriate time-step must be modified. The effect of sorption is to scale time in proportion to the retention factor R, so that the mesh transit time becomes $R\Delta t$.

6.2.6 Results for a Notional Contaminant

As a first step in simulating radionuclide migration, it is recommended that a constant source of a notional contaminant of unit concentration be considered, with the effects of radioactive decay and sorption neglected for the time being. The purpose of such calculations is to establish the relative magnitudes of physical effects, such as advection against diffusion. An example of this type of investigation is provided in Dataset 6.2.

A further benefit of studying such a constant source of a notional contaminant, is that the results obtained simulate the response of the system to a step change in contamination, and by differentiating those results with respect to time, the response of the system to a delta function or impulse source of contaminant is obtained. As described in Appendix F, the significance of this derived response function is that, since the migration is governed by linear equations, the effect of an arbitrary time-dependent source may then be deduced by computing the convolution of that source with the response function. Figure 6.8 shows the contaminant distribution for the Clay/Corallian sub-region. These results were computed with natural (zero total flux) conditions on each boundary except the segments LM and BF, where a zero concentration condition was applied. From Figure 6.8 it is clear that transport upwards toward the chalk aquifer is as important as that downward towards the Corallian, so that an assumption of advection along the flow pathline being the primary transport mechanism is in question.

The extra path for contaminant migration by diffusion through the Clay motivates an investigation of transport in the Chalk sub-region. The flux into the Chalk is provided by imposing a unit concentration of contaminant on a small section of the lower boundary. Both zero concentration and zero flux conditions at the surface were examined. Figure 6.9 illustrates that for either boundary condition, contaminants are transmitted rapidly to the surface, reaching the surface within about 10^9s.

These findings suggest that release of nuclide occurs into both upper and lower aquifers at much the same time. Thus, a complete calculation of transport over a region that comprises the three layers is unavoidable. However, it is not necessary to consider the entire grid, instead the sub-region AWYD on Figure 6.2 can be chosen for this calculation.

Figure 6.10 shows the migration of the cloud of contaminant through the layers, in which the contour of contaminant having concentration of 10^{-4} has been superimposed at successive times after release. The way in which such a plot is produced is similar to that described in subsection 5.3.2, except that at each time increment a contour is plotted rather than a line profile. This Figure reveals that there are three pathways for contaminant to reach the surface. Not only does the contaminant emerge at the surface through the chalk above the repository and through the Clay outcrop suggested by flow pathlines, but also through the Chalk layer between the Harwell site and the Clay outcrop, namely by diffusion from the Corallian aquifer through the central clay layer.

Again, the effect of surface boundary conditions can be investigated by considering con-

ditions of both zero concentration and zero dispersive flux of contaminant. The second condition is considered to be the more realistic, and its imposition is discussed in subsection 6.2.8.

6.2.7 Realistic Nuclides and Nuclide Chains

The results of the transport of a notional contaminant can be assessed by integrating the flux of contaminant over the surface. This also provides a useful check of the accuracy of the results, since the total flux through the surface should equate to the flux of contaminant from the repository once a steady state has been reached.

As described in Appendix F, the results for a notional contaminant can be used as the basis for computing the nuclide concentration arising from a general source term. To do this, one needs to differentiate with respect to time the concentrations of contaminant to derive a response function that represents the migration of an instantaneous release of contaminant. For a nuclide that is (i) released from a repository over a short time compared with the time scale for migration; (ii) poorly sorbed in the strata; (iii) stable to decay over the time scale for migration, then the response function should closely resemble the migration of that nuclide.

In cases when sorption is significant and the time scale for radioactive decay is less than or comparable to that for migration, then these effects must be taken into consideration. For each nuclide or nuclide chain it is necessary to create a new NAMMU input file, which should consist of the following phases:

1. **Specify a single nuclide or a nuclide chain.** The command ≫ `SET NAMMU OPTIONS` is used to specify the number of nuclides in a chain of parent and daughter nuclides, and to identify the position of the first nuclide variable in the variable list. For instance, if a chain of two nuclides were to be considered then the following commands would be appropriate:

```
>> SET NAMMU OPTIONS
   NUMBER OF NUCLIDES    2
   VARIABLE NUMBER OF FIRST NUCLIDE  6

>> SET VARIABLES
   VARIABLE NAMES 'PRES' 'TEMP' 'UVEL' 'VVEL' 'STFN' +
                  'NUC1' 'NUC2'
```

   NAMMU treats the first nuclide variable as the head of the chain, so that this example represents the chain `NUC1` to `NUC2`. Since the number of variables now exceeds the default of six the maximum number must be reset in ≫ `SET LIMITS`. The default option is to solve for a single nuclide in variable position six.

2. **Specify the radionuclide physical properties.** The amount of sorption is determined by the sorption coefficient K_d, and is related to the nuclide retention, R, defined in

the NAMMU Technical Overview [8] by the expression

$$R = 1 + (1 - \phi)K_d/\phi.$$

The quantity K_d is specified in column SORPTION COEFFICIENTS of the keyword table ROCK TYPE NUCLIDE PROPERTIES.

3. **Generate a refined grid for a sub-region.**

4. **Restore and interpolate global freedoms onto the new grid.**

5. **Define a source of radionuclide.** The source is usually defined over an area of the model. It is possible to set the time-dependent source at a point, but this point must correspond to a single node of the grid.

6. **Set radionuclide boundary conditions.**

7. **Solve transport equations.** The time-dependent equations can be solved using the Crank-Nicholson method by invoking the fast linear solver as described in subsection 6.2.4 or the conventional Crank-Nicholson solver as described in the NAMMU Reference Manual, along with the choice of a suitable time-step as advised in subsection 6.2.5. Gear's method may also be used. It is not necessary to issue any special instructions for a nuclide chain in the solver data, since the variable specified by the keyword NUCLIDE will be over-ridden by the parent nuclide of the chain identified in >> SET NAMMU OPTIONS.

6.2.8 Generalised Flux Boundary Conditions

NAMMU contains an option for specifying boundary conditions of the flux type quite generally using the subcommand ≫ GENERALISED FLUX LAW. The boundary fluxes may be specified by means of a number of functions supplied in a user routine BFIELD, or by simply assigning values to the terms that contribute to the boundary integral in the weak form of the governing equations. The most common of these boundary conditions is the zero dispersive flux boundary condition. Normally this boundary condition is set by specifying the keyword ZERO DISPERSIVE FLUX as shown below and in Section 9.2.3.

```
>> GENERALISED FLUX LAW
   VARIABLES    'NUC1'
   ZERO DISPERSIVE FLUX
   >> SELECT BOUNDARY SEGMENT
      START POINT   2508.7  107.9
      MID POINT     9578.8   72.9
      END POINT    13000.0   56.8
```

If a condition other than zero dispersive flux is required the keyword USER DEFINED FLUX should be used and two user routines (GFR2NU and GJR2NU in the current case)

must be supplied. The keywords REAL PARAMETERS, INTEGER PARAMETERS and IDENTIFICATION NUMBER may be used to pass parameters to the routines GFR2NU and GJR2NU. This is illustrated in the example routines given in subsection 11.2.1. The routines GFR2NU and GJR2NU included in Dataset 6.2 and discussed in subsection 11.2.1 set the boundary condition of no flow of nuclide is the groundwater flow is into the model and zero dispersive flux for the nuclide if the groundwater flow is out of the model.

6.2.9 Calculating Integrals of Surface Flux

The flux across the surface is calculated using the command ≫ CALCULATE LINE INTEGRAL. The keywords DARCY VELOCITY and NORMAL COMPONENT indicate that the quantity to be integrated is the component of the darcy velocity normal to the line along which the integration is performed.

```
>> CALCULATE LINE INTEGRAL
   DARCY VELOCITY
   NORMAL COMPONENT
   NUMBER OF POINTS PER SEGMENT 100

   SEGMENTS
   SEGMENT END POINTS
     < 2508.7  107.91 >
     < 8818.6  81.61 >
```

The segment of the chalk surface AJ, as labelled in Figure 6.2, is specified above.

Figures for Section 6

Figure 6.1 A geological cross-section SSW–NNE through the Harwell site.

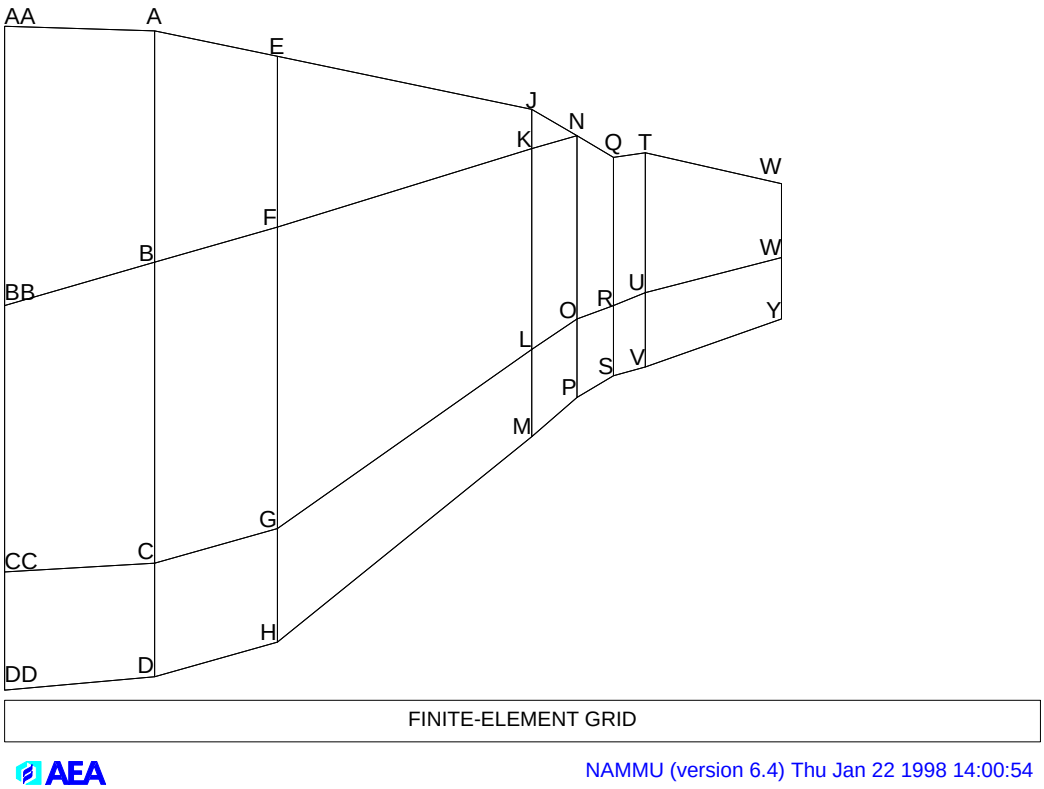


Figure 6.2 The coarse grid of patches chosen to model the vertical section in Figure 6.1.

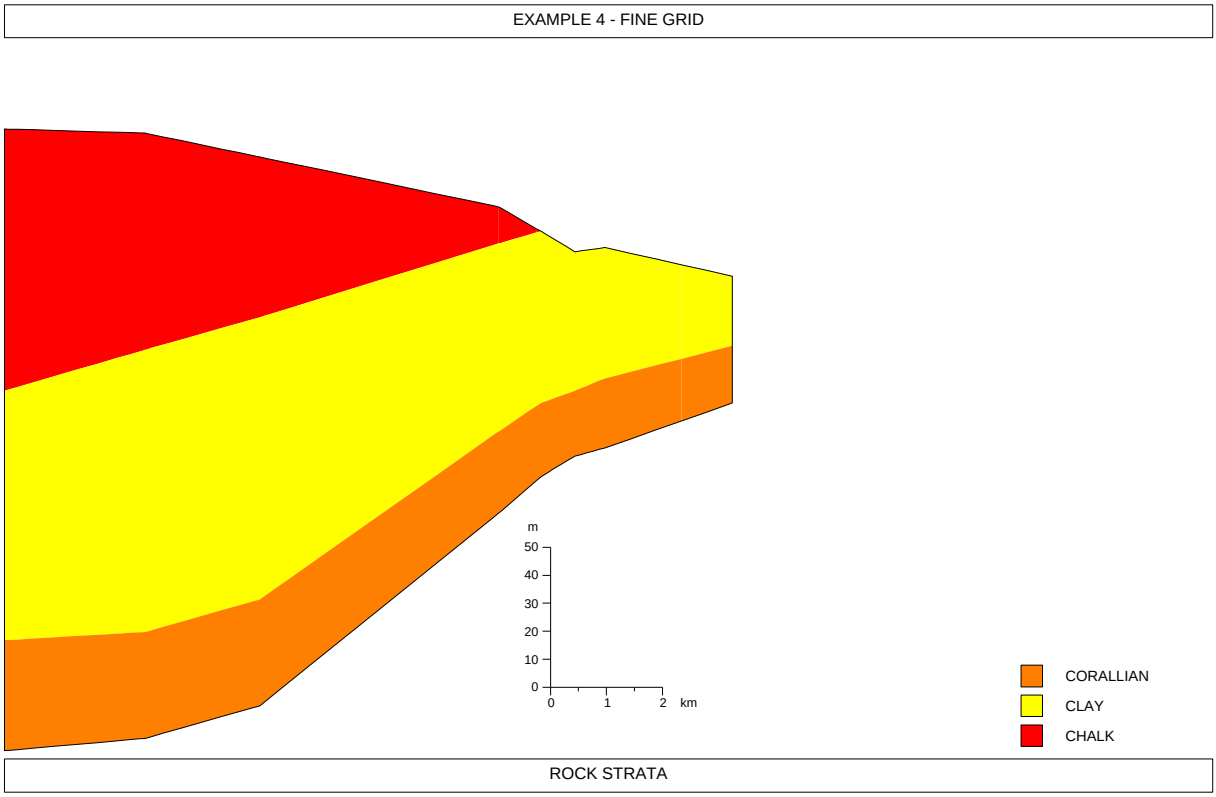


Figure 6.3 **A refined grid shaded according to the rock type. The layers are from top to bottom: Chalk, Clay and Corallian.**

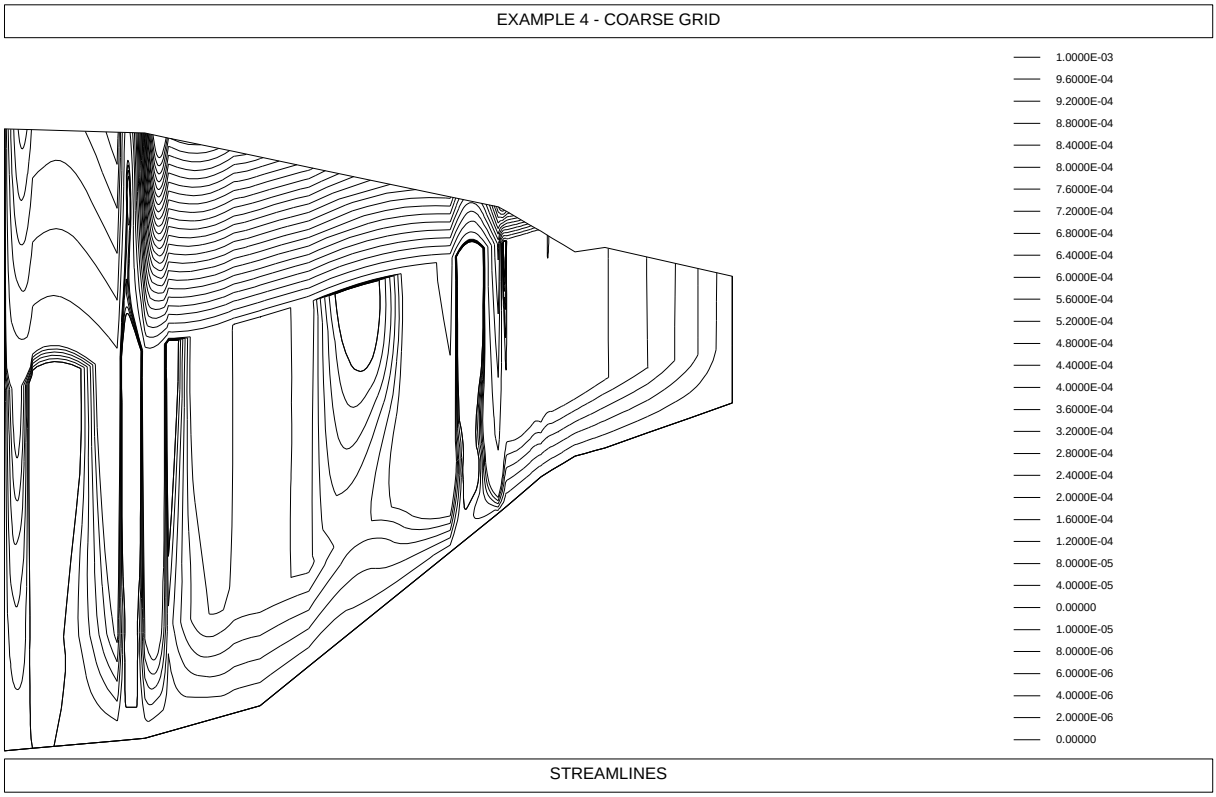


Figure 6.4 **Streamlines of groundwater flow for an inadequately refined finite-element grid.**

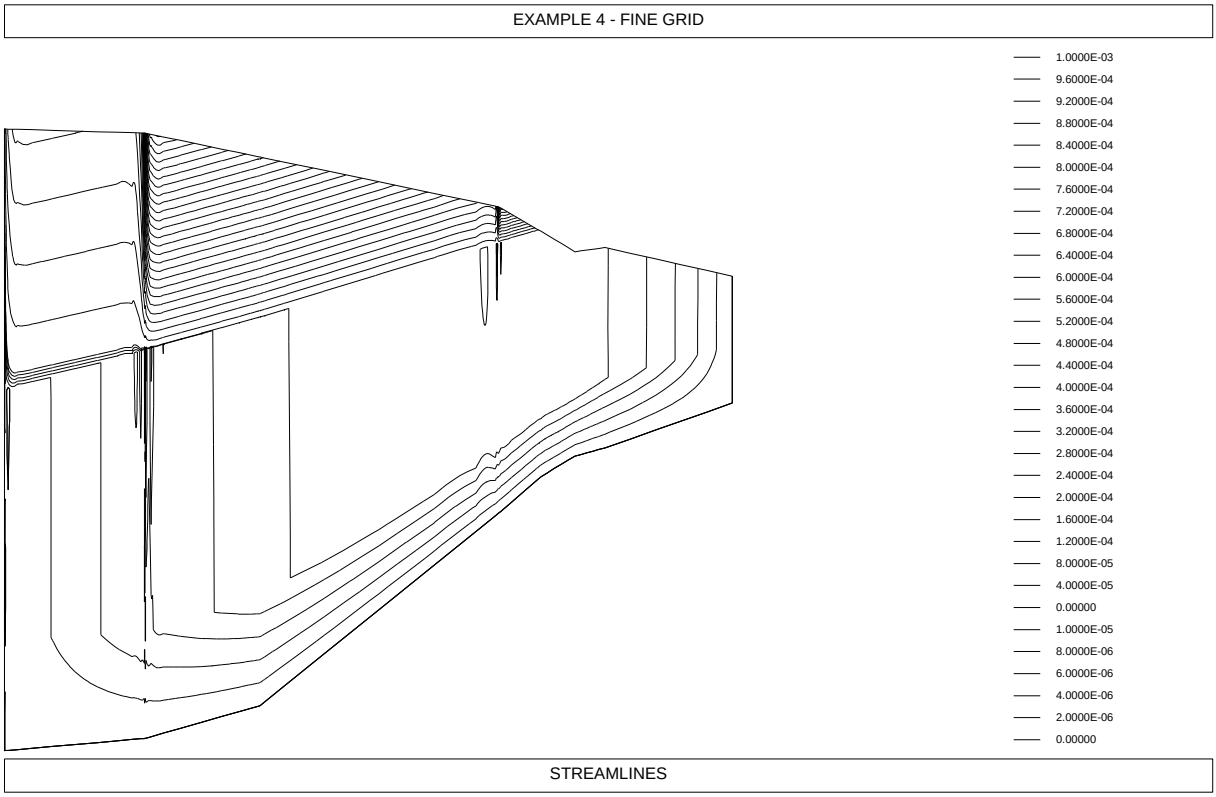


Figure 6.5 Groundwater flow calculation for a more refined grid.

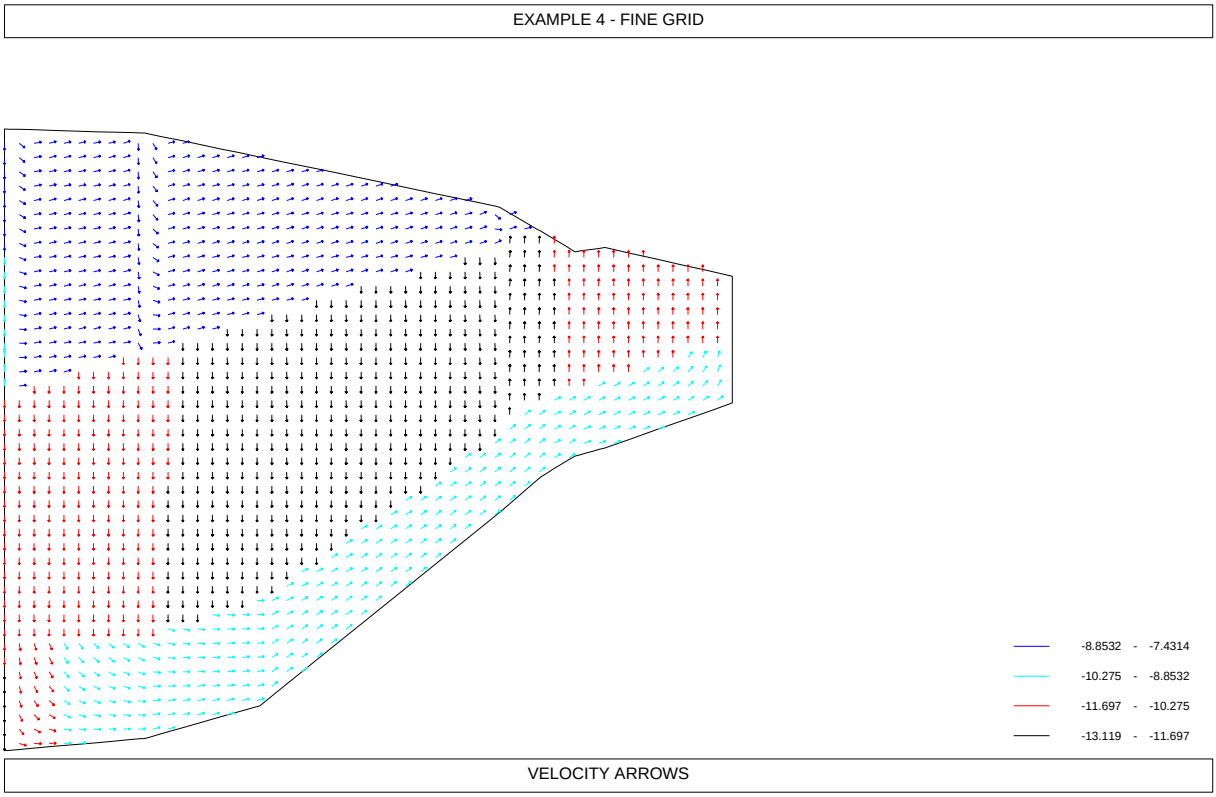


Figure 6.6 **Constant length velocity arrows shaded in four bands according to the logarithm of the Darcy velocity.**

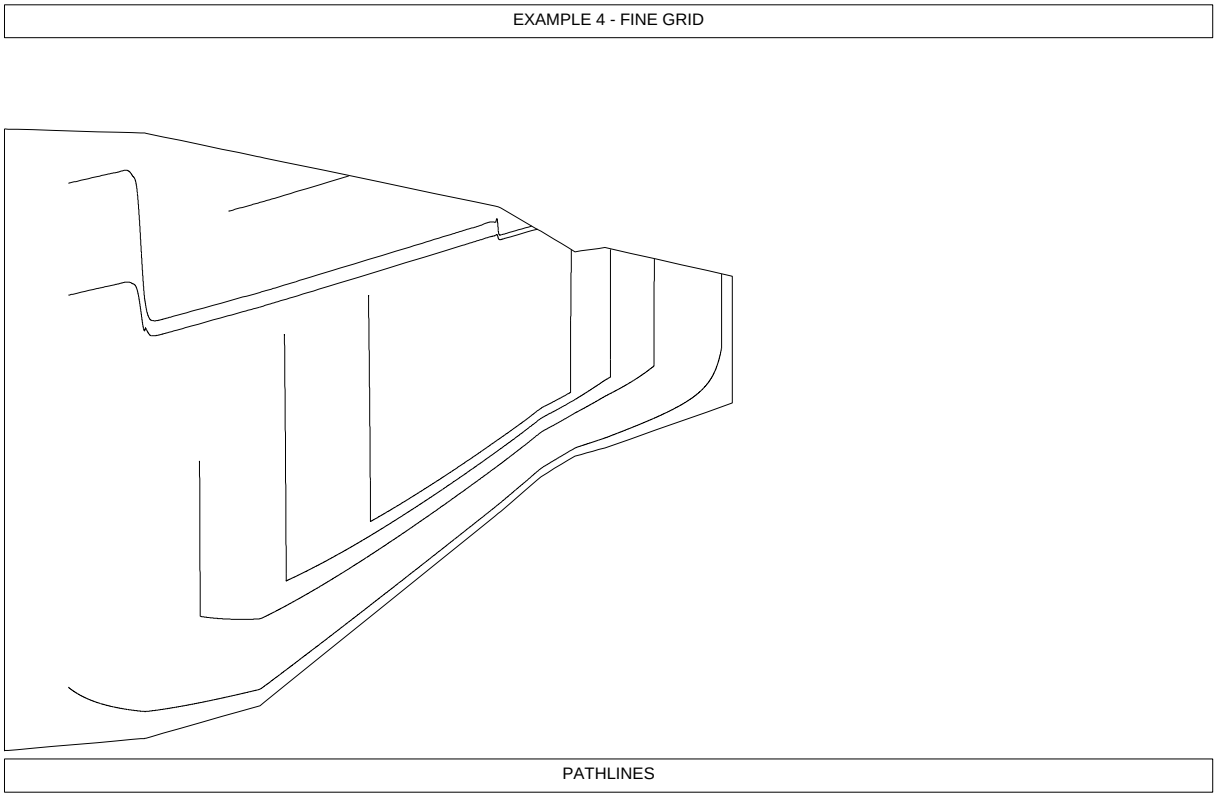


Figure 6.7 **Pathlines originating at various locations in the three layers. For this steady problem, the pathlines are identical to streamlines and provide a check on accuracy.**

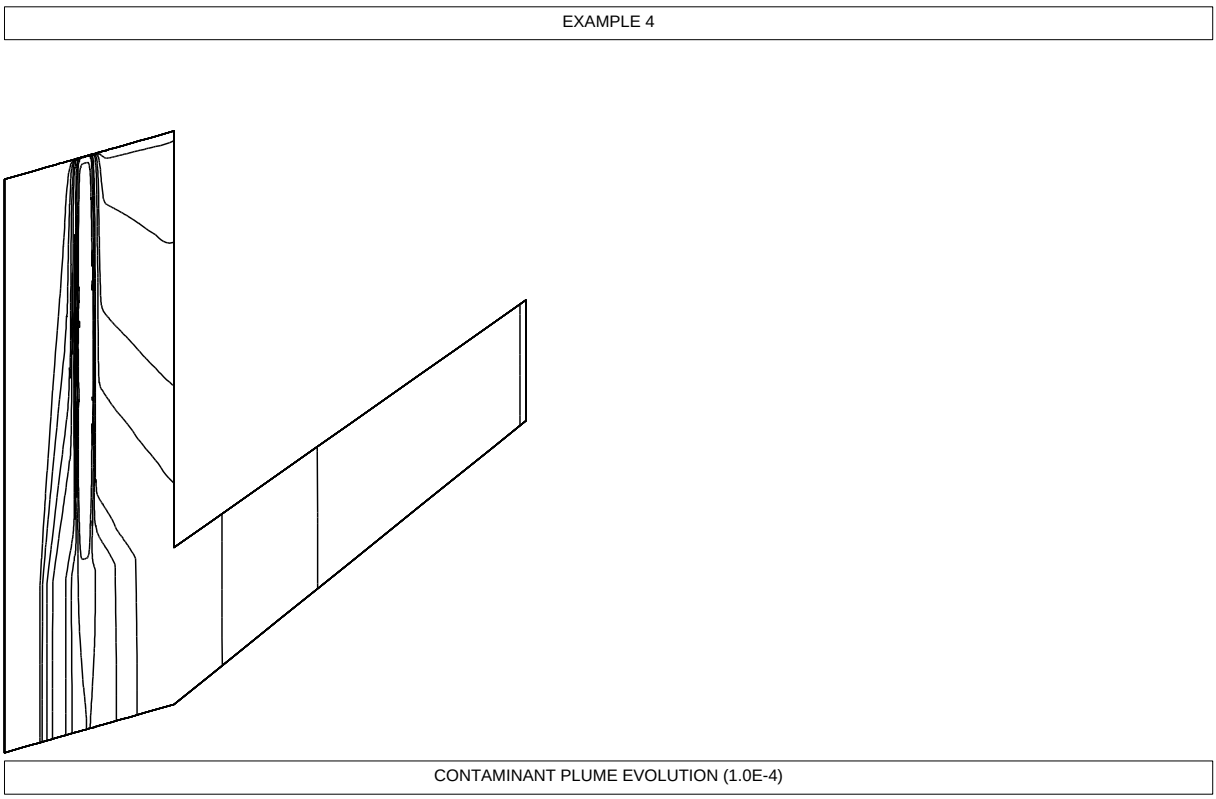
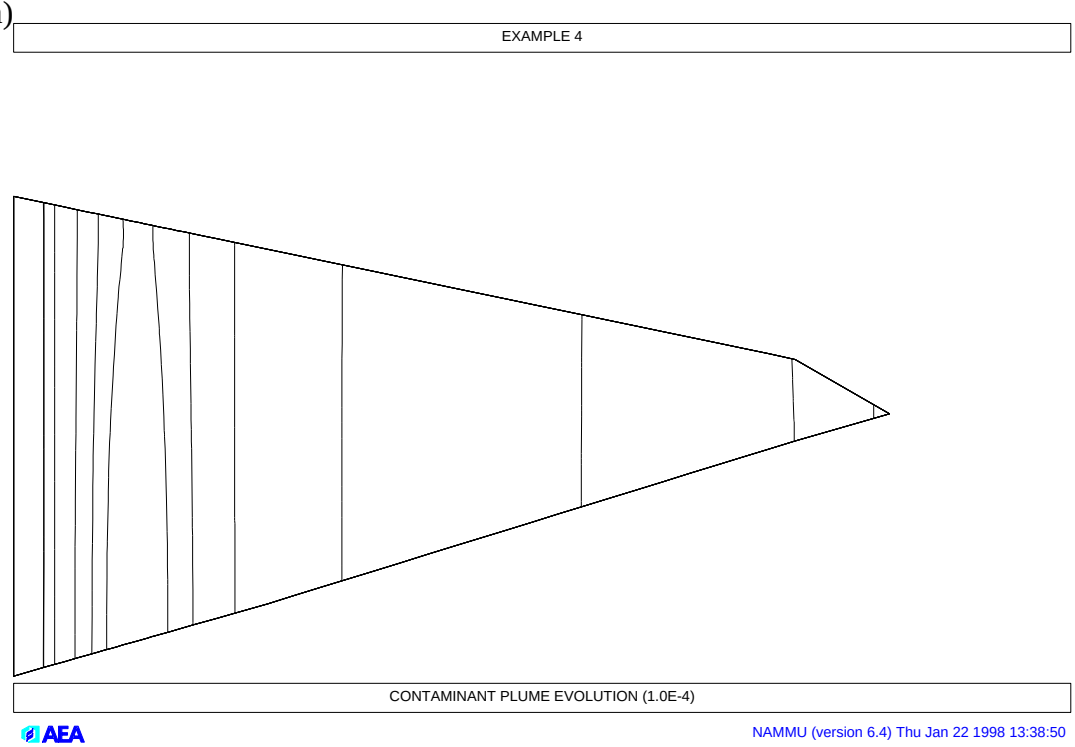


Figure 6.8 **Evolution of the contaminant cloud for the Clay-Corallian sub-region. A zero contaminant concentration boundary condition is applied on the segments BF and LM (see Figure 6.2). The contour representing a contaminant concentration of 10^{-4} is plotted at times $t = 2.5 \times 10^{11}$, 5×10^{11}, 7.5×10^{11}, 10^{12}, 2×10^{12}, 3×10^{12}, 5×10^{12}, and 10^{13}s.**

(a)



(b)

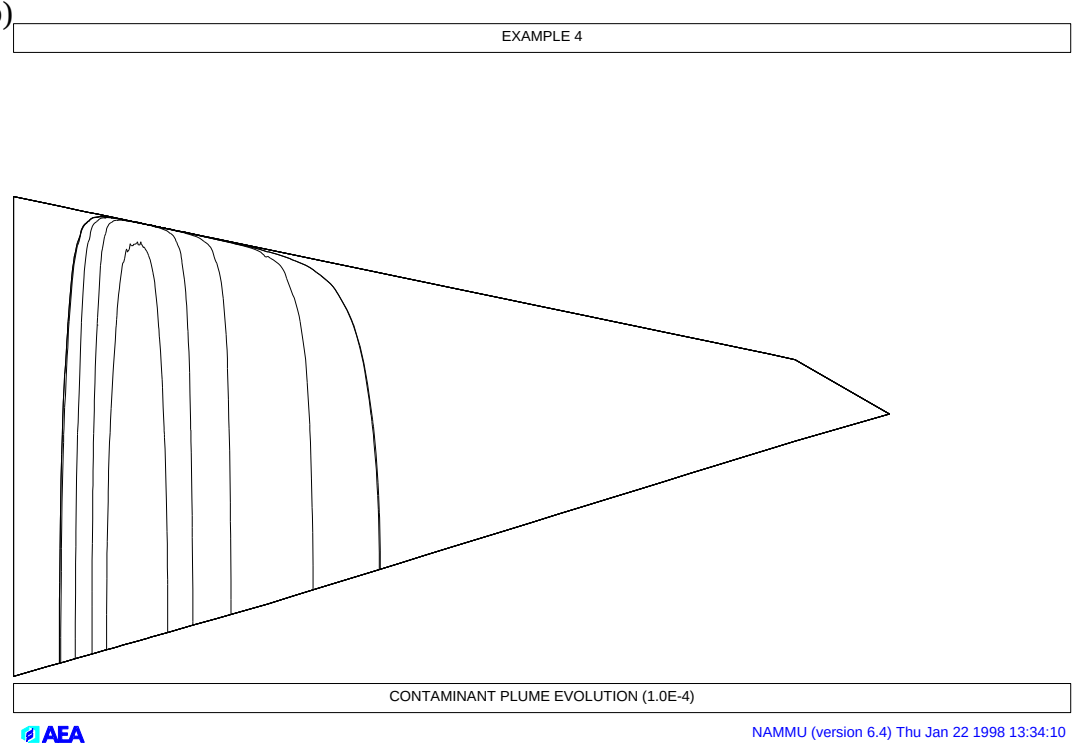


Figure 6.9 **Evolution of the contaminant cloud for the Chalk sub-region. Results are shown for both a) zero flux and b) zero concentration of contaminant on the upper surface. The contour representing a contaminant concentration of 10^{-4} is plotted at times $t = 3.0 \times 10^8$, 1.5×10^9, 4.5×10^9, 1.5×10^{10}, 4.5×10^{10} and 7.5×10^{10}s.**

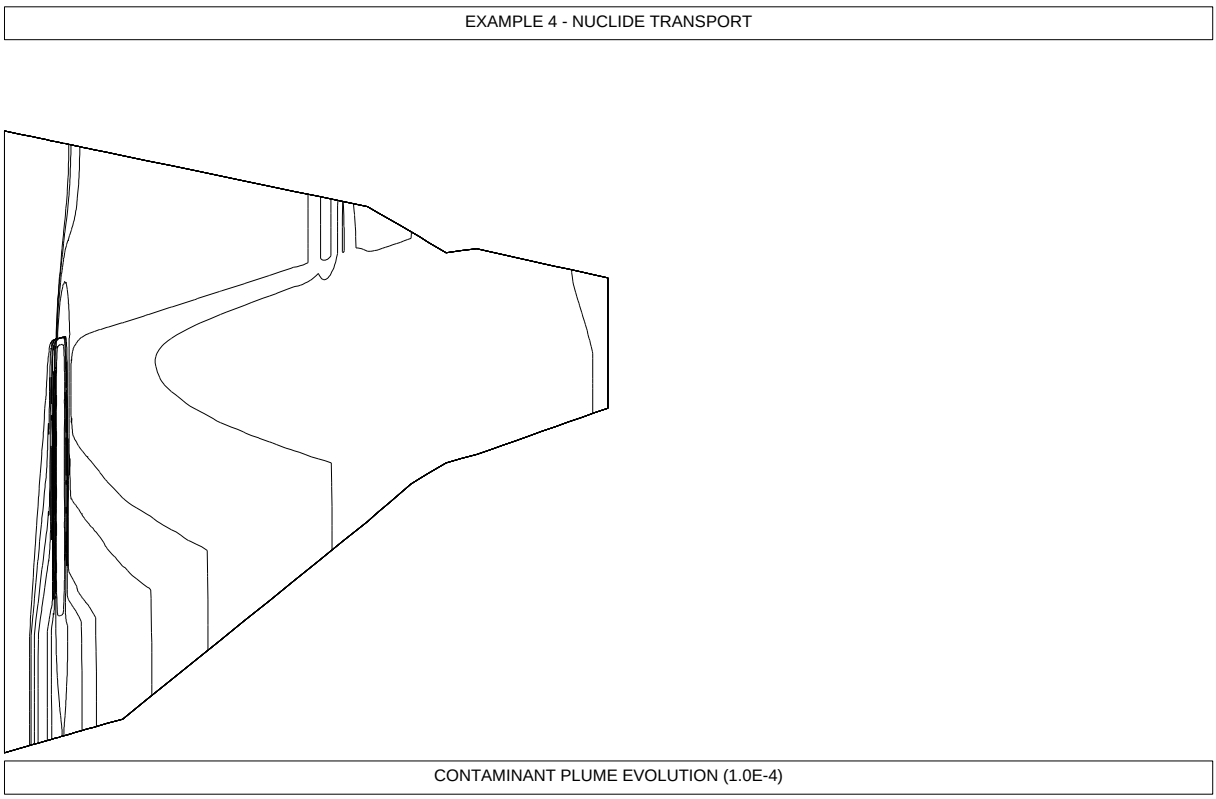


Figure 6.10 **Evolution of the contaminant cloud from the repository for a zero dispersive flux condition at the surface. The contour representing a contaminant concentration of 10^{-4} is plotted at times $t = 2.5 \times 10^{11}$, 5×10^{11}, 7.5×10^{11}, 10^{12}, 2×10^{12}, 3×10^{12}, 5×10^{12} and 10^{13}.**

Dataset 6.1

```
   /* NAMMU TEST CASE PACOMA.FINE                                  */
   /*                                                              */
   /* EXAMPLE 4 - PACOMA GROUNDWATER FLOW - FINE GRID              */

   /* SPACE ALLOCATION                                             */
   /* INTEGER WORKSPACE  500000                                    */
   /* REAL WORKSPACE     500000                                    */

   /* SOURCE FILES                                                 */
   /* COMPILED FILES                                               */
   /* LIBRARY FILES                                                */

   /* INPUT DATA FILES                                             */
   /* OUTPUT DATA FILES                                            */
   /* 6        nammu/output/pacoma.fine.out                       */
   /* 49       nammu/output/pacoma.fine.grid                      */
   /* 50       nammu/output/pacoma.fine.gf                        */
   /* GRAPHICS nammu/output/pacoma.fine.ps                        */

   /* END JOB INFORMATION                                          */


>> NAMMU

   >> SET NAMMU OPTIONS
      CONSISTENT FLUX
      END

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS                        400
      NODES                          3600
      FRONTWIDTH                      400
      GAUSS POINTS                     13
      INTEGER BC WORKSPACE           5000
      REAL BC WORKSPACE              1000
      PARAMETERS PER FUNCTION TYPE      9
      FUNCTION TYPES PER ELEMENT        3
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      FLUID DENSITY                    992.0
      MOLECULAR DIFFUSION COEFFICIENTS   6.0E-10

      ROCK TYPE PERMEABILITIES
```

```
      ROCK NAME,      KXX,     KYY
       'CHALK'      3.3E-13  3.3E-13
       'CLAY'       1.3E-17  8.2E-19
       'CORALLIAN'  5.2E-13  5.2E-13

      ROCK TYPE PROPERTIES
      ROCK NAME,    POROSITY
       'CHALK'        0.37
       'CLAY'         0.31
       'CORALLIAN'    0.34

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TORTUOSITIES,  LONGITUDINAL DISPERSION LENGTHS
       'CHALK'         100.0                    82.0
       'CLAY'            2.73                    0.0
       'CORALLIAN'     100.0                    88.0

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TRANSVERSE DISPERSION LENGTHS
       'CHALK'                  8.2
       'CLAY'                   0.0
       'CORALLIAN'              8.8
      END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         PATCH SPACING IN FIRST DIRECTION
         SIZE,  GRADE POWERS
           1    < 1.0 1.0 >
           5    < 2.5 1.5 >

         PATCH SPACING IN SECOND DIRECTION
         SIZE,  GRADE POWERS
          12    < 2.5 2.2 >
          10    < 2.4 1.7 >
           8    < 2.0 2.5 >
           5    < 2.5 1.5 >
           5    < 1.0 1.0 >
           1    < 1.0 1.0 >

         PATCH POSITIONS
         CORNER NUMBER,   COORDINATES
               11       <  0.0  15.2   >
               12       <  3.3  15.1   >
               13       <  6.0  14.515 >
               14       < 11.6  13.3   >
               21       <  0.0   8.8   >
               22       <  3.3   9.8   >
               23       <  6.0  10.6   >
               24       < 11.6  12.4   >
```

```
            25       < 12.6  12.7   >
            26       < 13.4  12.2   >
            27       < 14.1  12.3   >
            28       < 17.1  11.6   >
            31       <  0.0   2.7   >
            32       <  3.3   2.9   >
            33       <  6.0   3.7   >
            34       < 11.6   7.8   >
            35       < 12.6   8.5   >
            36       < 13.4   8.8   >
            37       < 14.1   9.1   >
            38       < 17.1   9.9   >
            41       <  0.0   0.0   >
            42       <  3.3   0.3   >
            43       <  6.0   1.1   >
            44       < 11.6   5.8   >
            45       < 12.6   6.7   >
            46       < 13.4   7.2   >
            47       < 14.1   7.4   >
            48       < 17.1   8.5   >

      PATCH TOPOLOGY
      PATCH TYPE,      CORNERS,        INDICES, ROCK NAME
        'SQQ9'    < 11  21  22  12 >   <1 1>    'CHALK'
        'SQQ9'    < 12  22  23  13 >   <1 2>    'CHALK'
        'SQQ9'    < 13  23  24  14 >   <1 3>    'CHALK'
        'TR69'    < 24  25  14     >   <2 6>    'CHALK'
        'SQQ9'    < 21  31  32  22 >   <1 1>    'CLAY'
        'SQQ9'    < 22  32  33  23 >   <1 2>    'CLAY'
        'SQQ9'    < 23  33  34  24 >   <1 3>    'CLAY'
        'SQQ9'    < 24  34  35  25 >   <1 4>    'CLAY'
        'SQQ9'    < 25  35  36  26 >   <1 5>    'CLAY'
        'SQQ9'    < 26  36  37  27 >   <1 5>    'CLAY'
        'SQQ9'    < 27  37  38  28 >   <1 5>    'CLAY'
        'SQQ9'    < 31  41  42  32 >   <1 1>    'CORALLIAN'
        'SQQ9'    < 32  42  43  33 >   <1 2>    'CORALLIAN'
        'SQQ9'    < 33  43  44  34 >   <1 3>    'CORALLIAN'
        'SQQ9'    < 34  44  45  35 >   <1 4>    'CORALLIAN'
        'SQQ9'    < 35  45  46  36 >   <1 5>    'CORALLIAN'
        'SQQ9'    < 36  46  47  37 >   <1 5>    'CORALLIAN'
        'SQQ9'    < 37  47  48  38 >   <1 5>    'CORALLIAN'
      END

>> SET BOUNDARY CONDITIONS

/*   ************ PRESSURE BOUNDARY SPECIFICATION **********   */
/*   ********************* TOP BOUNDARY ********************   */
   >> SPECIFIED VALUE

      >> VALUE VARYING LINEARLY WITH POSITION
         VARIABLES    'PRES'
         BASE VALUES  -1096082.3
         Y FACTORS      142132.4
         END
```

```
         >> SELECT BOUNDARY SEGMENT
            START POINT   0.0  15.2
            MID POINT    13.4  12.2
            END POINT    17.1  11.6
            PRECISION     1.0E-4
            END

/*   ********* STREAMFUNCTION BOUNDARY SPECIFICATION *******   */
/*   ******************** TOP BOUNDARY ********************   */
   >> SPECIFIED VALUE

      >> CONSTANT VALUE
         VARIABLES  'STFN'
         VALUES     99.9
         END

         >> SELECT BOUNDARY SEGMENT
            START POINT   0.0  15.2
            MID POINT    13.4  12.2
            END POINT    17.1  11.6
            PRECISION     1.0E-4
            END

/*   ***************** BOTTOM BOUNDARY ********************   */
   >> SPECIFIED VALUE

      >> CONSTANT VALUE
         VARIABLES  'STFN'
         VALUES     99.9
         END

         >> SELECT BOUNDARY SEGMENT
            START POINT   0.0   0.0
            MID POINT    13.4   7.2
            END POINT    17.1   8.5
            PRECISION     1.0E-4
            END

/*   ***************** LEFT BOUNDARY ********************   */
   >> SPECIFIED VALUE

      >> CONSTANT VALUE
         VARIABLES  'STFN'
         VALUES     99.9
         END

         >> SELECT LINE
            START POINT   0.0   0.0
            END POINT     0.0  15.2
            PRECISION     1.0E-4
            END

/*   ***************** RIGHT BOUNDARY ********************   */
```

```
      >> SPECIFIED VALUE

         >> CONSTANT VALUE
            VARIABLES  'STFN'
            VALUES     99.9
            END

            >> SELECT LINE
               START POINT  17.1   8.5
               END POINT    17.1  11.6
               PRECISION     1.0E-4
               END

   >> MAP GRID

      >> CHANGE ORIGIN
         MOVE TO  0.0  7.7117
         END

      >> SCALE COORDINATES
         DIVIDE X BY  1.3154E-3
         DIVIDE Y BY  6.8468E-2
         END

      >> SAVE MODEL
         SAVE ON UNIT 49

>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH    250
      NUMBER OF ITERATIONS    2
      END

      >> GROUNDWATER FLOW
         END


>> SOLVER DATA

   >> COMPUTE BOUNDARY VALUES
      BOUNDARY FUNCTION  'STFN'
      END

      >> STREAMFUNCTION CALCULATION
         END

   >> STEADY STATE
      MAXIMUM FRONTWIDTH     250
      NUMBER OF ITERATIONS     2
      CONVERGENCE CRITERION    1.0E-15
      END

      >> STREAMFUNCTION CALCULATION
```

```
      END


>> OUTPUT DATA

   >> SAVE GLOBAL FREEDOMS
      SAVE ON UNIT 50
      END

   >> PAGE SETUP
      LANDSCAPE
      END

   >> SET OUTPUT OPTIONS
      HEADING                   'EXAMPLE 4 - FINE GRID'
      BOUNDARY COLOUR           'BLACK'
      GRID COLOUR               'BLACK'
      COORDINATE SCALE FACTORS     1.0   50.0
      END

   >> SET ROCK STYLES
      ROCK STYLES
      ROCK NAME,   COLOUR
      'CHALK'      'RED'
      'CLAY'       'YELLOW'
      'CORALLIAN'  'ORANGE'
      END

   >> PLOT GRID
      SHADE
      CAPTION  'ROCK STRATA'
      END

      >> PLOT SCALE
         POSITION      9750.0  -90.0
         DIVISIONS        2      5
         SUBDIVISIONS     2      1
         END

   >> PLOT CONTOURS
      VARIABLE            'STFN'
      CONTOUR VALUES       0.0 TO 1.0E-5 BY 2.0E-6 +
                           0.0 TO 1.0E-3 BY 4.0E-5
      COLOURS             'BLACK'
      CAPTION             'STREAMLINES'
      END

   >> SET PLOT POINTS

      >> SELECT REGULAR ARRAY OF POINTS
         X LIMITS               0.0  13000.0
         Y LIMITS            -110.0    140.0
         NUMBER OF X POINTS    50
         NUMBER OF Y POINTS    50
```

```
      END

   >> PLOT VELOCITY ARROWS
      CONSTANT LENGTH VECTORS
      NUMBER OF INTERVALS   4
      ARROW SCALE          25.0
      ARROWHEAD ANGLE      40.0
      COLOUR USING LOG OF VECTOR MAGNITUDE
      COLOURS              'BLACK' 'RED' 'CYAN' 'BLUE'
      CAPTION              'VELOCITY ARROWS'
      END

   >> PATHLINES
      NUMBER OF PATHS             7
      X COORDINATES OF PATHS   3483.7 1140.0 1140.0 4000.0 1140.0 5000.0 6500.0
      Y COORDINATES OF PATHS     -9.3   90.0   50.0   80.0  -90.0   36.0   50.0
      TIMES IN YEARS
      MAXIMUM NUMBER OF STEPS  1000
      ACCURACY PARAMETER          0.1
      NO KEY
      COLOURS                  'BLACK'
      CAPTION                  'PATHLINES'
      END


>> STOP
```

Dataset 6.2

```
   /* NAMMU TEST CASE PACOMA.NUC3                                    */
   /*                                                                */
   /* EXAMPLE 4 - NUCLIDE TRANSPORT                                  */
   /*             ZERO DIFFUSIVE FLUX CONDITION AT SURFACE           */
   /*             USER DEFINED GFLUX ROUTINES                        */

   /* SPACE ALLOCATION                                               */
   /* INTEGER WORKSPACE 3000000                                      */
   /* REAL WORKSPACE    3000000                                      */

   /* INLINE FORTRAN
      SUBROUTINE GFR2NU(V,DVDR,R,
     >               E,ER,
     >               NVAR,NDIM,LSP,MXLVEL,MXRHS,
     >               IPAR,NIP,RPAR,NVP,XN,BFLD)
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION V(NVAR,MXLVEL),DVDR(NVAR,NDIM,MXLVEL),
     >          R(NDIM),E(NVAR,MXRHS),ER(NVAR,NDIM,MXRHS)
      DIMENSION QR(3),DQRDV(3,2),DQRDDP(3,3)
      DIMENSION DRHODV(2),DPORDV(2)
      DIMENSION XN(NDIM)
      DIMENSION IPAR(NIP),RPAR(NVP),BFLD(8,5)
      DIMENSION XYINT(2),ANRM(2)
C
      DATA IP/1/,IN/3/,IN1/4/
      DATA IX/1/,IY/2/
      DATA ZERO/0.0D0/
C
      ANX = RPAR(1)
      ANY = RPAR(2)
      BNX = RPAR(3)
      BNY = RPAR(4)
      ANX = ANX / 1.3154E-3
      ANY = ANY / 6.8468E-2
      BNX = BNX / 1.3154E-3
      BNY = BNY / 6.8468E-2
C
      ANUC=V(IN,1)
C
      CALL GWVEL1(RHOF,POROS,QR,DRHODV,DPORDV,
     >                  DQRDV,DQRDDP,S,DSDP,
     >                  V,DVDR,R,NVAR,NDIM,LSP)
C
      XYINT(1) = BNX - ANX
      XYINT(2) = BNY - ANY
      ASIZ = SQRT(XYINT(1)*XYINT(1) + XYINT(2)*XYINT(2))
      ANRM(1) = -XYINT(2) / ASIZ
      ANRM(2) =  XYINT(1) / ASIZ
      QDOTN = QR(IX)*ANRM(1) + QR(IY)*ANRM(2)
C
      IF (QDOTN .GT. ZERO) THEN
```

```
        E(IN,1) = ANUC*QDOTN
        ER(IN,IX,1) = ZERO
        ER(IN,IY,1) = ZERO
      ELSE
        E(IN,1) = ZERO
        ER(IN,IX,1) =ZERO
        ER(IN,IY,1) =ZERO
      END IF
C
      RETURN
      END
      SUBROUTINE GJR2NU(V,DVDR,R,
     >               DEDV,DERDV,DEDVR,DERDVR,
     >               NVAR,NDIM,LSP,MXLVEL,MMAT,
     >               IPAR,NIP,RPAR,NVP,XN,BFLD)
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION V(NVAR,MXLVEL),DVDR(NVAR,NDIM,MXLVEL),
     >          R(NDIM),DEDV(NVAR,NVAR,MMAT),
     >          DERDV(NVAR,NDIM,NVAR,MMAT),
     >          DEDVR(NVAR,NVAR,NDIM,MMAT),
     >          DERDVR(NVAR,NDIM,NVAR,NDIM,MMAT)
      DIMENSION QR(3),DQRDV(3,2),DQRDDP(3,3)
      DIMENSION DRHODV(2),DPORDV(2)
      DIMENSION XN(NDIM)
      DIMENSION IPAR(NIP),RPAR(NVP),BFLD(8,5)
      DIMENSION XYINT(2),ANRM(2)
C
      DATA IP/1/,IN/3/,IN1/4/
      DATA IX/1/,IY/2/
      DATA ZERO/0.0D0/
C
      ANX = RPAR(1)
      ANY = RPAR(2)
      BNX = RPAR(3)
      BNY = RPAR(4)
      ANX = ANX / 1.3154E-3
      ANY = ANY / 6.8468E-2
      BNX = BNX / 1.3154E-3
      BNY = BNY / 6.8468E-2
C
      ANUC=V(IN,1)
C
      CALL GWVEL1(RHOF,POROS,QR,DRHODV,DPORDV,
     >                DQRDV,DQRDDP,S,DSDP,
     >                V,DVDR,R,NVAR,NDIM,LSP)
C
      XYINT(1) = BNX - ANX
      XYINT(2) = BNY - ANY
      ASIZ = SQRT(XYINT(1)*XYINT(1) + XYINT(2)*XYINT(2))
      ANRM(1) = -XYINT(2) / ASIZ
      ANRM(2) =  XYINT(1) / ASIZ
      QDOTN = QR(IX)*ANRM(1) + QR(IY)*ANRM(2)
C
```

```
      IF (QDOTN .GT. ZERO) THEN
        DEDV(IN,IN,1) = QDOTN
        DEDVR(IN,IN,IX,1) = ZERO
        DEDVR(IN,IN,IY,1) = ZERO
        DERDV(IN,IX,IN,1) = ZERO
        DERDV(IN,IY,IN,1) = ZERO
        DERDVR(IN,IX,IN,IX,1) = ZERO
        DERDVR(IN,IX,IN,IY,1) = ZERO
        DERDVR(IN,IY,IN,IX,1) = ZERO
        DERDVR(IN,IY,IN,IY,1) = ZERO
      ELSE
        DEDV(IN,IN,1) = ZERO
        DEDVR(IN,IN,IX,1) = ZERO
        DEDVR(IN,IN,IY,1) = ZERO
        DERDV(IN,IX,IN,1) = ZERO
        DERDV(IN,IY,IN,1) = ZERO
        DERDVR(IN,IX,IN,IX,1) = ZERO
        DERDVR(IN,IX,IN,IY,1) = ZERO
        DERDVR(IN,IY,IN,IX,1) = ZERO
        DERDVR(IN,IY,IN,IY,1) = ZERO
      END IF
C
      RETURN
      END

C  +---------------------------------------------------------------------+
C  | THIS ROUTINE DEFINES THE EXTENT OF REPOSITORY                       |
C  +---------------------------------------------------------------------+
      SUBROUTINE USLECT(XX,NSD,IIN)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION XX(NSD)
C
      IIN = 0
      EPS = 0.01D0
      IF (XX(1) .GT. 3432.4D0 - EPS  .AND.
     >    XX(1) .LT. 3535.0D0 + EPS  .AND.
     >    XX(2) .GT. -14.63D0 - EPS  .AND.
     >    XX(2) .LT. -3.968D0 + EPS)  IIN = 1
C
      RETURN
      END

                                                                      */
   /* SOURCE FILES                                                    */
   /* COMPILED FILES                                                  */
   /* LIBRARY FILES                                                   */

   /* INPUT DATA FILES                                                */
   /* 33 nammu/output/pacoma.fine.grid                               */
   /* 48 nammu/output/pacoma.fine.gf                                 */
   /* OUTPUT DATA FILES                                               */
   /* 6        nammu/output/pacoma.nuc3.out                           */
   /* GRAPHICS nammu/output/pacoma.nuc3.ps                            */
```

```
   /* END JOB INFORMATION                                          */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      LEVELS                            3
      ELEMENT MATRICES                  2
      ELEMENTS                        700
      NODES                          3500
      FREEDOMS                      18000
      FRONTWIDTH                      100
      INTEGER BC WORKSPACE           5000
      REAL BC WORKSPACE              1000
      PARAMETERS PER FUNCTION TYPE      9
      FUNCTION TYPES PER ELEMENT        3
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      FLUID DENSITY                       992.0
      MOLECULAR DIFFUSION COEFFICIENTS     6.0E-10

      ROCK TYPE PERMEABILITIES
      ROCK NAME,      KXX,     KYY
       'CHALK'      3.3E-13  3.3E-13
       'CLAY'       1.3E-17  8.2E-19
       'CORALLIAN'  5.2E-13  5.2E-13

      ROCK TYPE PROPERTIES
      ROCK NAME,    POROSITY
       'CHALK'        0.37
       'CLAY'         0.31
       'CORALLIAN'    0.34

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TORTUOSITIES,  LONGITUDINAL DISPERSION LENGTHS
       'CHALK'         100.0                    82.0
       'CLAY'            2.73                    0.0
       'CORALLIAN'     100.0                    88.0

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TRANSVERSE DISPERSION LENGTHS
       'CHALK'                  8.2
       'CLAY'                   0.0
       'CORALLIAN'              8.8
      END
```

```
>> MODEL DATA

  >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         PATCH SPACING IN FIRST DIRECTION
         SIZE,  GRADE POWERS
           2    < 1.0 1.0 >
           8    < 1.0 1.0 >
           4    < 1.0 1.0 >

         PATCH SPACING IN SECOND DIRECTION
         SIZE,  GRADE POWERS
          30    < 0.6 0.6 >
          10    < 1.0 1.0 >
           4    < 1.0 1.0 >
           2    < 1.0 1.0 >

         PATCH POSITIONS
         CORNER NUMBER,   COORDINATES
               11       <  3.3  15.1   >
               12       <  6.0  14.515 >
               13       < 11.6  13.3   >
               14       < 12.1  13.0   >
               21       <  3.3   9.8   >
               22       <  6.0  10.6   >
               23       < 11.6  12.4   >
               24       < 12.1  12.55  >
               25       < 12.6  12.7   >
               26       < 13.4  12.2   >
               27       < 14.1  12.3   >
               28       < 17.1  11.6   >
               31       <  3.3   2.9   >
               32       <  6.0   3.7   >
               33       < 11.6   7.8   >
               34       < 12.1   8.15  >
               35       < 12.6   8.5   >
               36       < 13.4   8.8   >
               37       < 14.1   9.1   >
               38       < 17.1   9.9   >
               41       <  3.3   0.3   >
               42       <  6.0   1.1   >
               43       < 11.6   5.8   >
               44       < 12.1   6.25  >
               45       < 12.6   6.7   >
               46       < 13.4   7.2   >
               47       < 14.1   7.4   >
               48       < 17.1   8.5   >

         PATCH TOPOLOGY
         PATCH TYPE,      CORNERS,       INDICES, ROCK NAME
           'SQQ9'    < 11  21  22  12 >   <1 1>    'CHALK'
```

```
         'SQQ9'    < 12  22  23  13 >   <1 2>    'CHALK'
         'SQQ9'    < 13  23  24  14 >   <1 4>    'CHALK'
         'TRT6'    < 24  25  14     >   <1 4>    'CHALK'
         'SQQ9'    < 21  31  32  22 >   <2 1>    'CLAY'
         'SQQ9'    < 22  32  33  23 >   <2 2>    'CLAY'
         'SQQ9'    < 23  33  34  24 >   <2 4>    'CLAY'
         'SQQ9'    < 24  34  35  25 >   <2 4>    'CLAY'
         'SQQ9'    < 25  35  36  26 >   <2 3>    'CLAY'
         'SQQ9'    < 26  36  37  27 >   <2 4>    'CLAY'
         'SQQ9'    < 27  37  38  28 >   <2 2>    'CLAY'
         'SQQ9'    < 31  41  42  32 >   <1 1>    'CORALLIAN'
         'SQQ9'    < 32  42  43  33 >   <1 2>    'CORALLIAN'
         'SQQ9'    < 33  43  44  34 >   <1 4>    'CORALLIAN'
         'SQQ9'    < 34  44  45  35 >   <1 4>    'CORALLIAN'
         'SQQ9'    < 35  45  46  36 >   <1 3>    'CORALLIAN'
         'SQQ9'    < 36  46  47  37 >   <1 4>    'CORALLIAN'
         'SQQ9'    < 37  47  48  38 >   <1 2>    'CORALLIAN'
      END

   >> RENUMBER ELEMENTS

      >> SLOAN ALGORITHM
         END

>> SET BOUNDARY CONDITIONS

/* ****** ZERO DIFFUSIVE FLUX CONDITION ON TOP SURFACE ********* */
   >> GENERALISED FLUX LAW
      VARIABLES                'NUC1'
      USER DEFINED FLUX
      REAL PARAMETERS           3.3   15.1    6.0   14.515
      END

      >> SELECT LINE
         START POINT   3.3  15.1
         END POINT     6.0  14.515
         PRECISION     1.0E-4
         END

   >> GENERALISED FLUX LAW
      VARIABLES                'NUC1'
      USER DEFINED FLUX
      REAL PARAMETERS           6.0   14.515 11.6   13.3
      END

      >> SELECT LINE
         START POINT   6.0  14.515
         END POINT    11.6  13.3
         PRECISION     1.0E-4
         END

   >> GENERALISED FLUX LAW
      VARIABLES                'NUC1'
      USER DEFINED FLUX
```

```
      REAL PARAMETERS            11.6   13.3   12.6   12.7
      END

      >> SELECT LINE
         START POINT  11.6  13.3
         END POINT    12.6  12.7
         PRECISION     1.0E-4
         END

   >> GENERALISED FLUX LAW
      VARIABLES                  'NUC1'
      USER DEFINED FLUX
      REAL PARAMETERS            12.6   12.7   13.4   12.2
      END

      >> SELECT LINE
         START POINT  12.6  12.7
         END POINT    13.4  12.2
         PRECISION     1.0E-4
         END

   >> GENERALISED FLUX LAW
      VARIABLES                  'NUC1'
      USER DEFINED FLUX
      REAL PARAMETERS            13.4   12.2   14.1   12.3
      END

      >> SELECT LINE
         START POINT  13.4  12.2
         END POINT    14.1  12.3
         PRECISION     1.0E-4
         END

   >> GENERALISED FLUX LAW
      VARIABLES                  'NUC1'
      USER DEFINED FLUX
      REAL PARAMETERS            14.1   12.3   17.1   11.6
      END

      >> SELECT LINE
         START POINT  14.1  12.3
         END POINT    17.1  11.6
         PRECISION     1.0E-4
         END

>> MAP GRID

   >> CHANGE ORIGIN
      MOVE TO  0.0  7.7117
      END

   >> SCALE COORDINATES
      DIVIDE X BY  1.3154E-3
      DIVIDE Y BY  6.8468E-2
```

```
      END

/*   ********* SPECIFY THE CONTAMINANT SOURCE **********   */
>> MODIFY BOUNDARY CONDITIONS

   >> SPECIFIED VALUE

      >> CONSTANT VALUE
         VARIABLES  'NUC1'
         VALUES     1.0

      >> CALL SUBROUTINE USLECT
         END

/*  ** INTERPOLATE THE PRESSURE FIELD ONTO THE NEW GRID **  */
 >> SET INITIAL GUESS

    >> RESTORE GLOBAL FREEDOMS
       READ FROM UNIT 48
       INTERPOLATE
       READ MODEL FROM UNIT 33
       END


>> SOLVER DATA

   >> FAST LINEAR TRANSIENT
      NUMBER OF TIMESTEPS          1
      TIMESTEP SIZE                1.0E5
      SAVE ON UNIT                51
      END

      >> NUCLIDE TRANSPORT
         END


>> SOLVER DATA

   >> FAST LINEAR TRANSIENT
      NUMBER OF TIMESTEPS          400
      TIMESTEP SIZE                2.5E10
      INITIAL TIME                 1.0E5
      NUMBER OF TIMESTEPS PER PRINT 1000
      NUMBER OF TIMESTEPS PER SAVE  10
      END

      >> NUCLIDE TRANSPORT
         END


>> OUTPUT DATA

   >> PAGE SETUP
      LANDSCAPE
```

```
   END

>> SET OUTPUT OPTIONS
   HEADING                   'EXAMPLE 4 - NUCLIDE TRANSPORT'
   BOUNDARY COLOUR           'BLACK'
   GRID COLOUR               'BLACK'
   COORDINATE SCALE FACTORS  1.0  50.0
   END

>> PLOT GRID
   CAPTION  'NUCLIDE CALCULATION SUBGRID'
   END

/*   ** PLOT CONTOURS OF CONTAMINANT FOR SELECTED TIMESTEPS **   */
>> SELECT TIME
   TIMESTEP        10
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   NO KEY
   CAPTION         'CONTAMINANT PLUME EVOLUTION (1.0E-4)'
   END

>> SELECT TIME
   TIMESTEP        20
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

>> SELECT TIME
   TIMESTEP        30
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

>> SELECT TIME
   TIMESTEP        40
   READ FROM UNIT  50
```

```
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

>> SELECT TIME
   TIMESTEP        80
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

>> SELECT TIME
   TIMESTEP       120
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

>> SELECT TIME
   TIMESTEP       200
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

>> SELECT TIME
   TIMESTEP       400
   READ FROM UNIT  50
   END

>> PLOT CONTOURS
   VARIABLE        'NUC1'
   CONTOUR VALUES  1.0E-4
   COLOURS         'BLACK'
```

```
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER, NO KEY
   END

/*   ****** CALCULATE FLUX THROUGH  ******   */
/*   ********* THE CHALK ABOVE THE REPOSITORY ***********   */
>> CALCULATE LINE INTEGRAL
   DARCY VELOCITY
   NORMAL COMPONENT
   NUMBER OF SEGMENTS               1
   NUMBER OF POINTS PER SEGMENT   100

   SEGMENTS
   SEGMENT END POINTS
   < 2508.7  107.91 >
   < 8818.6   81.61 >
   END

>> CALCULATE LINE INTEGRAL
   DARCY VELOCITY
   NORMAL COMPONENT
   NUMBER OF SEGMENTS               1
   NUMBER OF POINTS PER SEGMENT   100

   SEGMENTS
   SEGMENT END POINTS
   < 8818.6   81.61  >
   < 9578.8   72.856 >
   END


>> STOP
```

7 EXAMPLE 5: THREE-DIMENSIONAL STEADY GROUNDWATER FLOW (3D FLOW MODEL FOR PACOMA)

In some instances, it may be necessary to consider three-dimensional effects in groundwater flow. Reasons for having to include an extra spatial dimension may be related to complex geological formations or irregular features of the surface topography, such as valleys. A way of assessing the relative importance of three-dimensional effects within the flow is to generate a series of two-dimensional vertical sections parallel to the anticipated flow, together with a number of mutually orthogonal vertical sections. Regions of the flow field in which the flows in the orthogonal sections are of comparable magnitude correspond to a three-dimensional flow.

Conversely, a three-dimensional study may be used to verify that the regional groundwater flow is predominantly two-dimensional in other situations, and hence to determine the appropriate alignment for two-dimensional sections.

The example given here is an extension of the PACOMA study, discussed in Section 6, into a preliminary three-dimensional investigation of the groundwater flow beneath the Harwell site. The dataset constructed for this Example, Dataset 7.1, is intended only as an illustration for the NAMMU facilities available in three-dimensional geometries, and not as a detailed model of the region. An example of a more complicated three-dimensional model has been reported in Reference [18].

7.1 Specifying a Model in Three Dimensions

The intention to use a three-dimensional geometry is declared by the following subcommands of ≫ NAMMU:

```
>> SET OPTIONS
   THREE DIMENSIONS
```

and

```
>> SET LIMITS
   SPACE DIMENSIONS  3
```

It is likely that the size of the three-dimensional problem will be greater than that allowed for in the defaults, in which case it is necessary to assign suitable values to other keywords of ≫ SET LIMITS.

7.1.1 Grid Generation

The addition of a third spatial dimension introduces extra conceptual difficulty in generating the grid for what is perhaps a complex geological model. However, by constructing the grid from layers or vertical slices this task becomes more tractable.

For instance, the grid may be set up by joining together several parallel vertical sections, where each has been sub-divided into quadrilateral patches to fit the boundaries and interfaces between different rock strata. Quadrilateral patches on adjacent sections can be joined using either brick or prism three-dimensional patches.

In Section 4, the importance of adhering to a logical coordinate numbering system was stressed. Those remarks also apply here. Coordinates should be identified by a cross-section number, layer (or horizontal row) number and a block (or vertical column) number. This makes it easier to determine whether a quadrilateral in one section is to be joined to another quadrilateral in an adjacent section, in which case a brick element type is used, or to a simple line by a prism element type. Of course, prismatic patches can also be used to connect triangular patches on adjacent sections.

It is strongly advised that the two-dimensional grids that form each cross section should be checked prior to any joining, by plotting the boundary, the grid and shading according to the rock types.

Three-dimensional patch vertices can be specified largely by manipulating the corresponding specifications of the two-dimensional patches. For example, the following data for two quadrilateral patches on adjacent sections,

```
PATCH TYPE,     CORNERS,        INDICES,  ROCK NAME
  'SQQ9'   < 111 112 122 121 >  < 1 1 >    'ROCK'
  'SQQ9'   < 211 212 222 221 >  < 1 1 >    'ROCK'
```

may be combined to specify a single brick:

```
PATCH TYPE,            CORNERS,              INDICES, ROCK NAME
 'BKBQ'  < 111 112 122 121 211 212 222 221 >  < 1 1 1 > 'ROCK'
```

Note that in this latter patch specification an extra integer is supplied in the `INDICES` column, corresponding to the third local coordinate direction. The relationship between the order in which the corners are input and the orientation of both brick and prism type patches is illustrated in the NAMMU Reference Manual [7]. Particular care must be taken to ensure that the model data are consistent with these conventions, not only for the purposes of refinement, but also to have the correct orientation of prismatic patches. Also, at this stage the property type of the patch must be specified to correspond to that of one or the other of the two-dimensional patches from which the patch was constructed.

Any errors that occur in forming the slabs between cross-sections usually result in an obviously wrong topology that can be identified by the option ≫ `CHECK GRID` or by output from the grid plotting options discussed in subsection 7.2. Errors in the input of the property types are most readily observed by separately plotting the elements with each property type, as described in subsection 7.2.1. Common features that can be detected with such plots

are unphysical jagged edges to a rock stratum and poorly connected sections of a layer. Such features may not have been apparent from inspecting only the vertical cross-sections. To correct these errors, the user must decide whether to change the property types of the offending patches, or sub-divide these patches and change the property types of the new patches (for example, divide a cuboid patch into two prisms).

7.1.2 Surface Boundary Conditions

In order to model realistic sites, one needs to be able to impose boundary conditions over specified surfaces of the model. In some idealised cases, the boundary conditions can be set very simply on planar surfaces. In these cases, the surface is specified using the option ≫ SELECT AREA. Here is a simple example:

```
>> SELECT AREA
   >> VERTICES
      X VALUES  0.0  1.0  1.0  0.0
      Y VALUES  0.0  0.0  1.0  1.0
      Z VALUES  0.0  0.0  0.0  0.0
```

This defines a square region with vertices at the points $(0, 0, 0)$, $(1, 0, 0)$, $(1, 1, 0)$, $(0, 1, 0)$. In more realistic models, however, the surface topography of the grid is more complex. In order to facilitate the generation of these more complex models, NAMMU is equipped with a quite general option for selecting surfaces of the model as a list of nodes. Such a list is the appropriate format for specifying fixed pressure boundary conditions. When the option is invoked using the ≫ SELECT SURFACE command, all the nodes lying on the surface of the grid are assembled. Subsections of this list of nodes may then be identified with parts of the surface which lie in a particular region or have a particular orientation (for example, the top surface). This is done using a number of ≫ RESTRICT SURFACE SELECTION subcommands which allow the user to restrict the selection to a particular Cartesian sub-region, and accept only nodes whose normal vector is oriented within a specified angular tolerance of a reference vector. For example, the following commands select the nodes in a region of the top surface of a model:

```
>> SELECT SURFACE
   >> RESTRICT SURFACE SELECTION
      X LIMITS  -6.0   28.0
      Y LIMITS   0.0   27.0
      Z LIMITS  39.9  120.0
      SURFACE NORMAL  0.0  0.0  1.0
      TOLERANCE ANGLE  88.0
      PRECISION  0.001
```

Note:

- The ≫ SELECT SURFACE command automatically sums the directed normal at each node over all the elements on which the node is found. For nodes on the surface of the mesh the sum will be non-zero, and hence the command also provides a useful check to ensure there are no internal surfaces within the model. For nodes on the edge of the grid surface the normal is taken as a combination of the normal directions on each of the adjacent element faces. If the vertical components of the normal directions on the adjacent faces are nearly opposite, then the normal direction at the node may be below the horizon and so will not satisfy the surface selection criterion. This is most likely to occur when there are prismatic patches on the edge of the grid.

- When prismatic patches are present on the edge of the surface the normal along this edge may not satisfy the surface selection criterion, and so it may be necessary to select this edge separately using ≫ SELECT LINE. This sharp edge of the region is shown clearly in the boundary plot reproduced in Figure 7.1.

The command ≫ SELECT PATCH FACES is a useful alternative to ≫ SELECT SURFACE. The patch faces to be selected are specified in terms of the corner numbers used to define them in the PATCH TOPOLOGY table.

7.2 Useful Output Options in 3D

For a large three-dimensional model it is not practical to plot the whole grid. Instead the ≫ OUTPUT DATA options for plotting a number of grid slices or perspective views of both the external surfaces and the interfaces between different rock types should be used. These options, together with those for visualising the solution, are detailed below. However, three-dimensional models are often best viewed using a visualisation package such as Avizier.

7.2.1 Plotting Grid Slices

Besides plotting any layers or vertical sections used in constructing the three-dimensional grid, it is also useful to examine arbitrary cross-sections of the grid. This is done by plotting slices through the grid, which represent the intersection of the element boundaries with a given plane. To specify the required slice, the user must first define the position and direction from which it is viewed using the command ≫ SET PROJECTION, and then define the plane of the slice. An example of a vertical slice through a grid is illustrated:

```
>> SET PROJECTION
   EYE POSITION   1.0E4  -1.0E6  0.0
   PAPER VECTOR  -1.0E4   1.0E6  0.0
   PAPER VERTICAL   0.0    0.0   1.0
>> PLOT GRID SLICE
   PLANE PARAMETERS  0.0  1.0  0.0  -1.0E4
   SHADE
```

Here, the keyword PLANE PARAMETERS specifies the plane $y = 10$km. By including the keyword SHADE, the elements will by default be shaded according to their rock types. The large magnitude of the y coordinate of the EYE POSITION ensures the projection is near parallel, that is effectively a projection from minus infinity along the y direction. Examples of vertical grid slices are shown in Figures 7.2 and 7.3.

In order to check the grid visually many slices should be plotted. Normally, slices should be taken along three mutually orthogonal sets of planes, with two sets of vertical planes and perhaps a more limited set of horizontal planes. It may be necessary to use the zoom facilities of ≫ SET PLOT OPTIONS to examine regions where the elements are very small.

7.2.2 Plotting the Grid Surface

As a further check the grid surface should be plotted from various viewpoints. Again, the user must first set the viewpoint and then invoke the option ≫ PLOT GRID SURFACE. The following example corresponds to a viewpoint vertically above the grid:

```
>> SET PROJECTION
   EYE POSITION    0.0   0.0   1.0E7
   PAPER VECTOR    0.0   0.0  -1.0E7
   PAPER VERTICAL  0.0   1.0   0.0

>> PLOT GRID SURFACE
```

7.2.3 Plotting Elements of Each Property Type

We have already described in subsection 4.5.1 how cross-sections can be shaded according to rock types. Another way of checking that the model matches the geology is to plot separately the elements with each property type. A convenient way of producing such a plot is to plot the surface of each rock type from an appropriate viewpoint, say from above the model. After setting a projection, as described in subsection 7.2.2, the elements of each property are selected as follows:

```
>> SET PLOT CRITERION

   >> SELECT ON PROPERTY TYPES
      VALUE 3
      END

>> PLOT GRID SURFACE
   USE PLOT CRITERION
   CAPTION  'STRATA SURFACE - CORALLIAN'
   END
```

In this example, only those elements of the grid that have a property type set to '3' will be plotted. The VALUE '3' refers to the third row in the ROCK TYPE PERMEABILITIES

keyword table. The output from these commands is shown in Figure 7.4.

7.2.4 Flow Visualisation

Having obtained a satisfactory model, the next stage is to build an understanding of the flow-field calculated from it. This is not always easy in three dimensions and a variety of output options should be used. One option is to plot pathlines on a grid slice (Figure 7.5). Another is to plot contours on sections using the command ≫ `PLOT CONTOURS ON SLICE`. The slice is defined using the keywords `ORIGIN`, `FIRST DEFINING POINT` and `SECOND DEFINING POINT`.

```
>> PLOT CONTOURS ON SLICE
   HEAD
   ORIGIN                  9800.0   2500.0  -140.0
   FIRST DEFINING POINT    15000.0  14300.0  -140.0
   SECOND DEFINING POINT   9800.0   2500.0   110.0
```

The contours plotted using these keywords, as viewed from an oblique angle, are shown in Figure 7.6.

Another useful option is to plot velocity arrows on slices. Possible ways of presenting velocity arrows discussed in subsection 6.1.2, The slice on which the vectors are to be plotted, and the points at which velocity arrows are to be drawn, are selected with ≫ `SET PLOT POINTS`. The vectors are then plotted on this slice by the following commands:

```
>> PLOT VECTORS
   CONSTANT LENGTH VECTORS
   COLOUR USING LOG OF VECTOR MAGNITUDE
```

Figure 7.7 shows velocity vectors plotted on the grid slice selected above.

In general, plots of the flow on vertical slices are good for presenting flow in aquifers, since the flow is often nearly along the long axis of the layer; horizontal slices through the grid are good for flow in aquitards, as the flow is often predominantly nearly vertical.

Projections of pathlines may be plotted from various viewpoints. This is done using the same commands that were described in subsection 4.5.3, together with selecting the required projection using the ≫ `SET PROJECTION` command.

Figures for Section 7

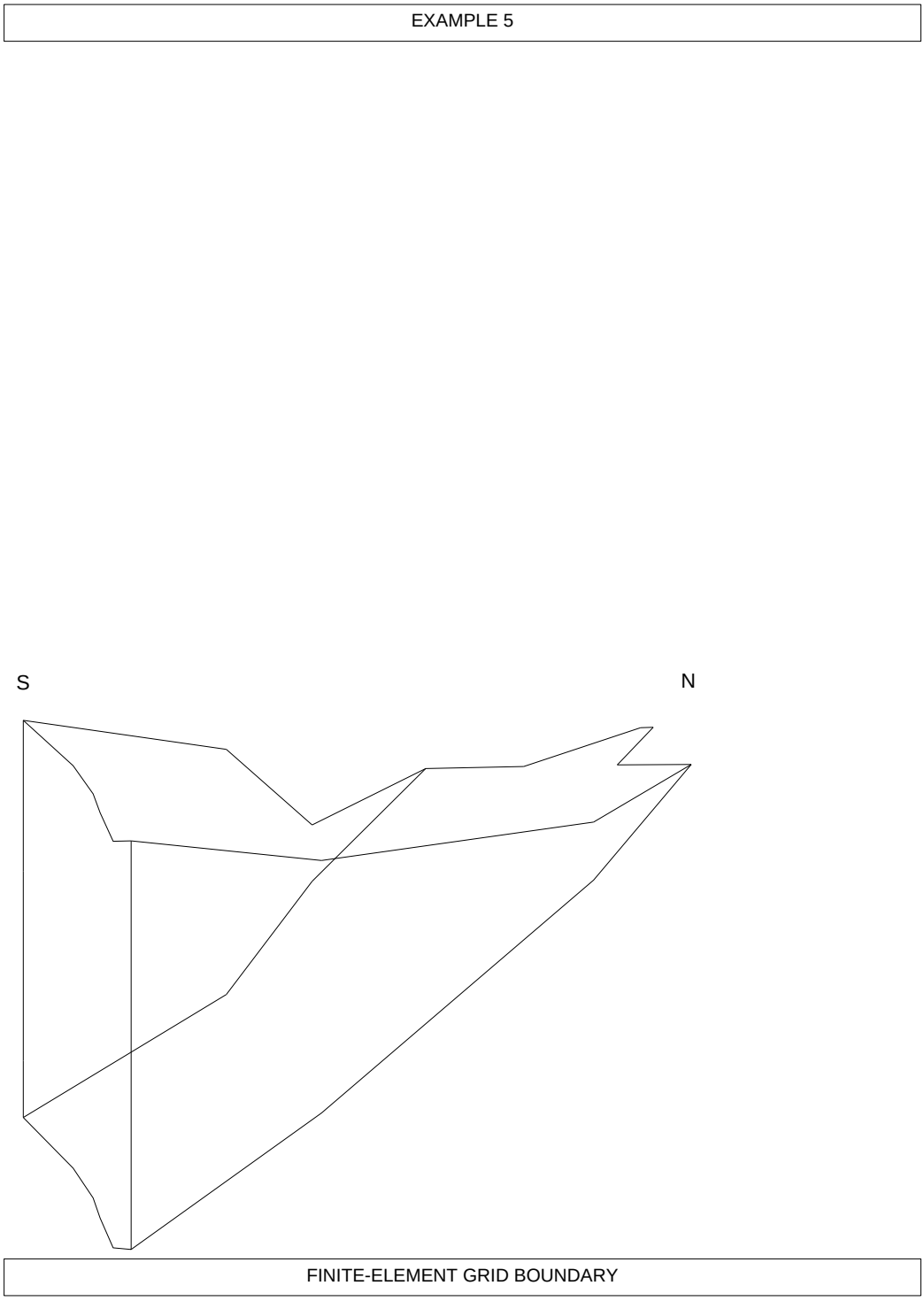


Figure 7.1 The boundary of the three-dimensional domain shown from an oblique projection.

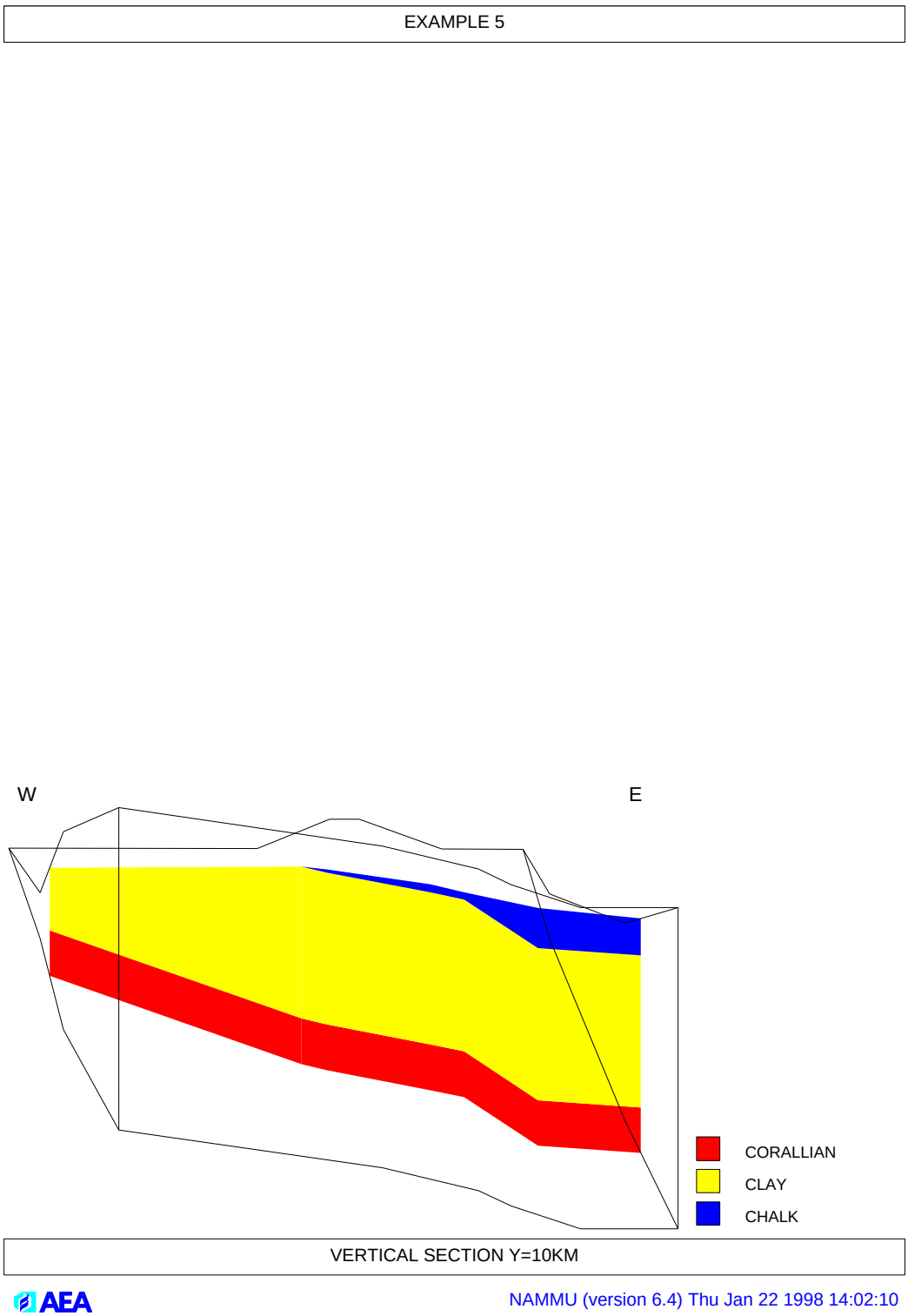


Figure 7.2 **A vertical section through the grid at $y = 10\text{km}$. The lower layer is the Corallian aquifer, while successively higher layers are Clay and Chalk.**

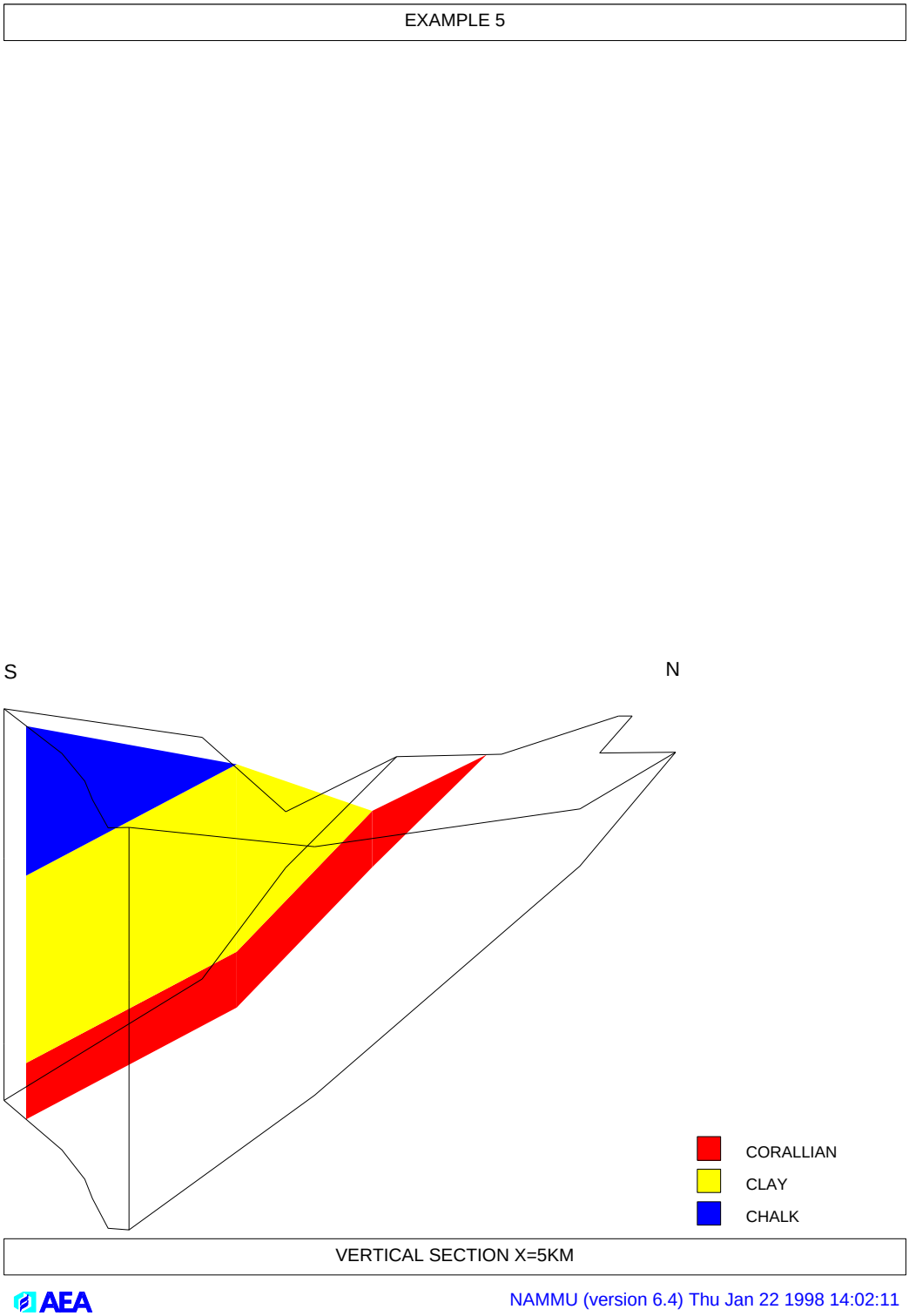


Figure 7.3 A vertical grid slice at $x = 5\text{km}$.

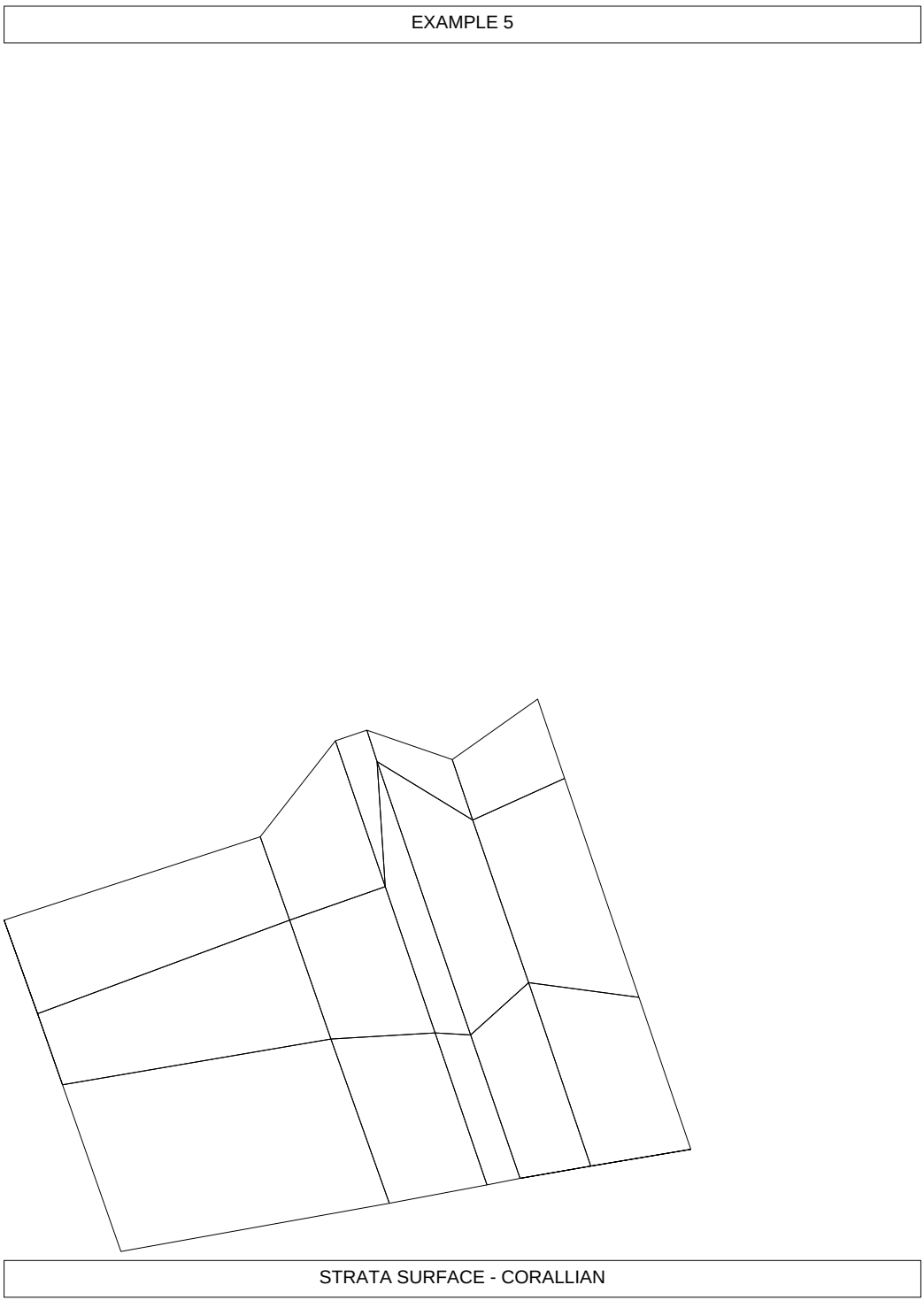


Figure 7.4 The surface of the Corallian aquifer, as seen from above.

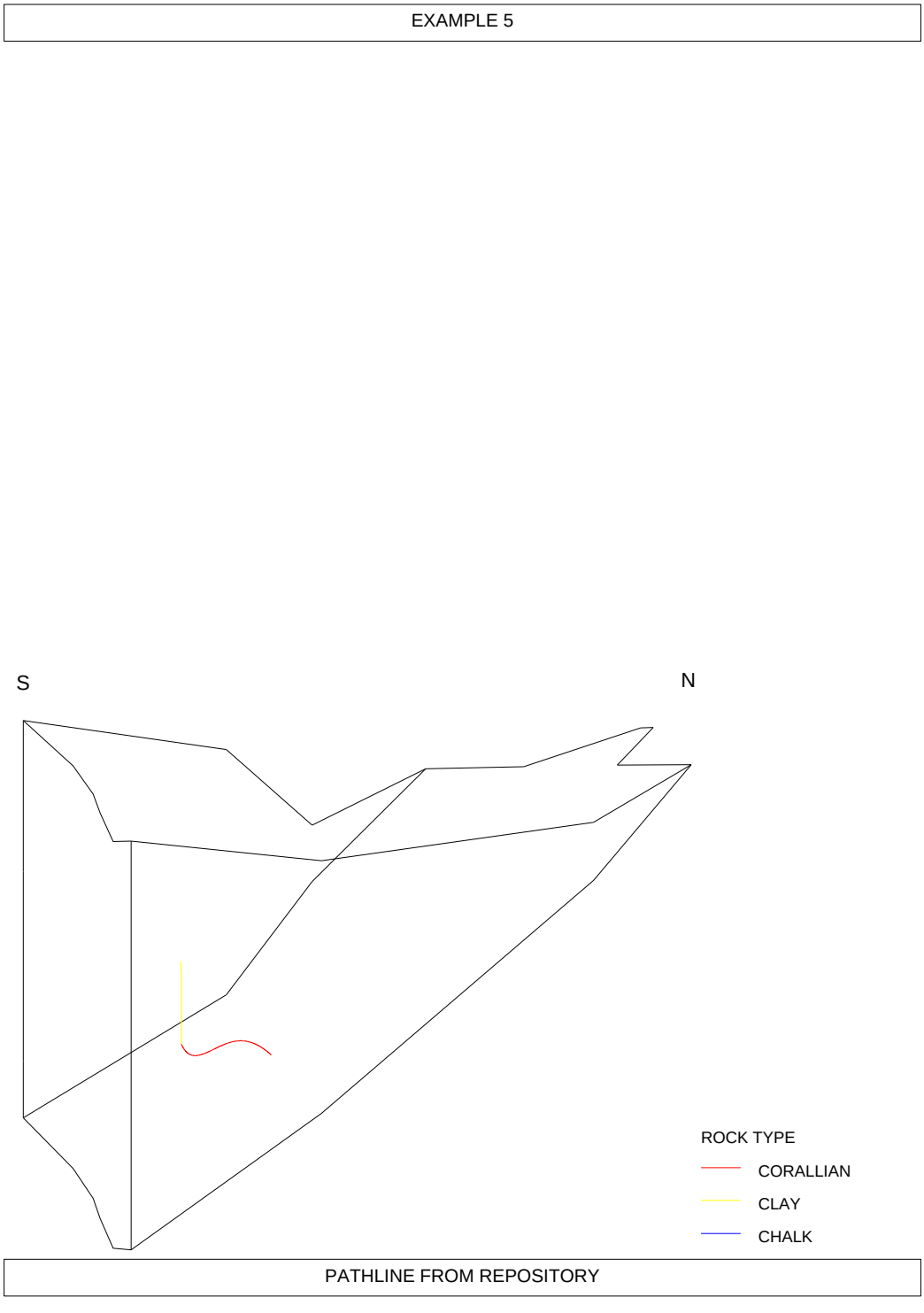


Figure 7.5 A pathline from the repository.

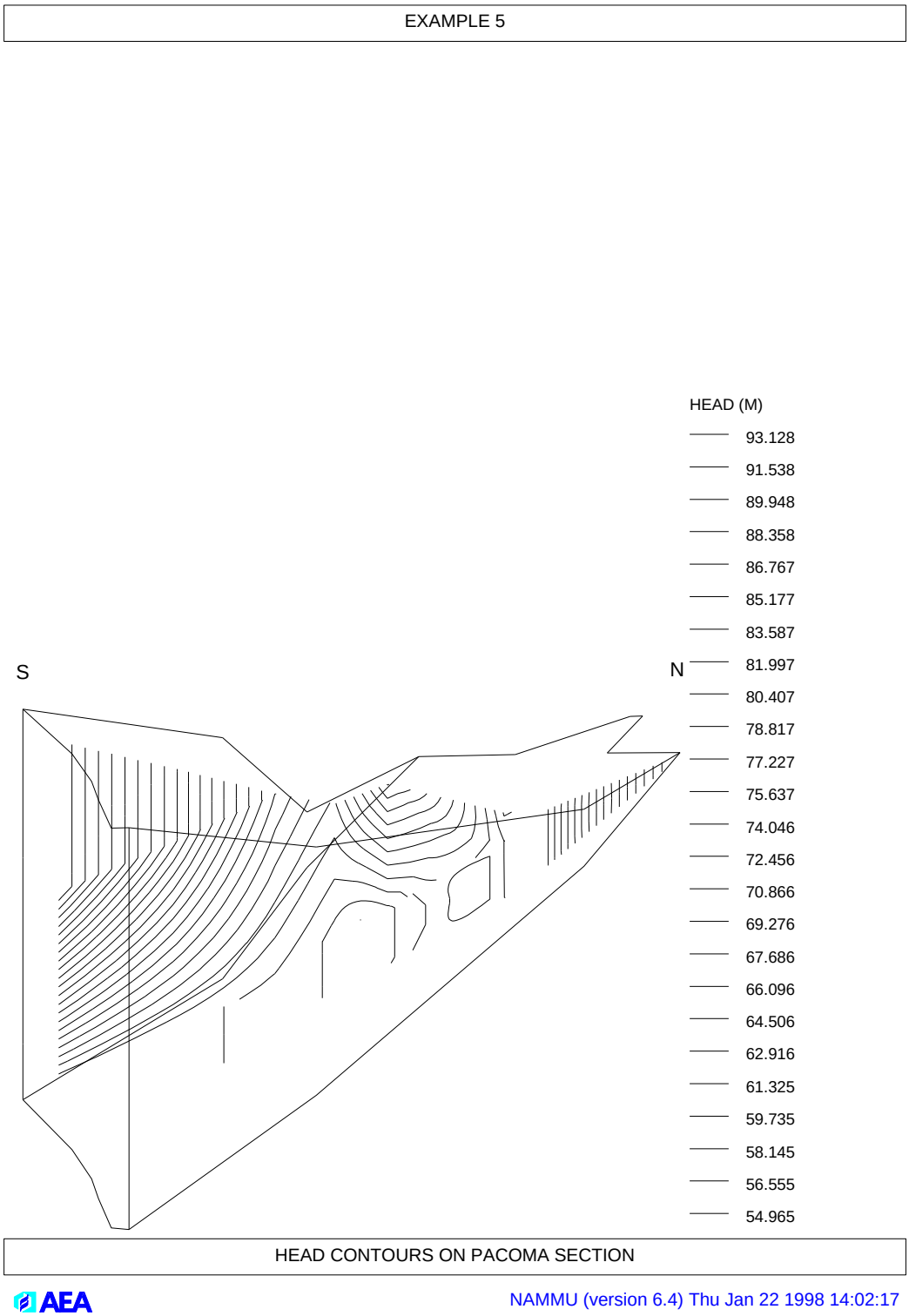


Figure 7.6 **A plot of head contours on the slice used in the two-dimensional study of Section 6.**

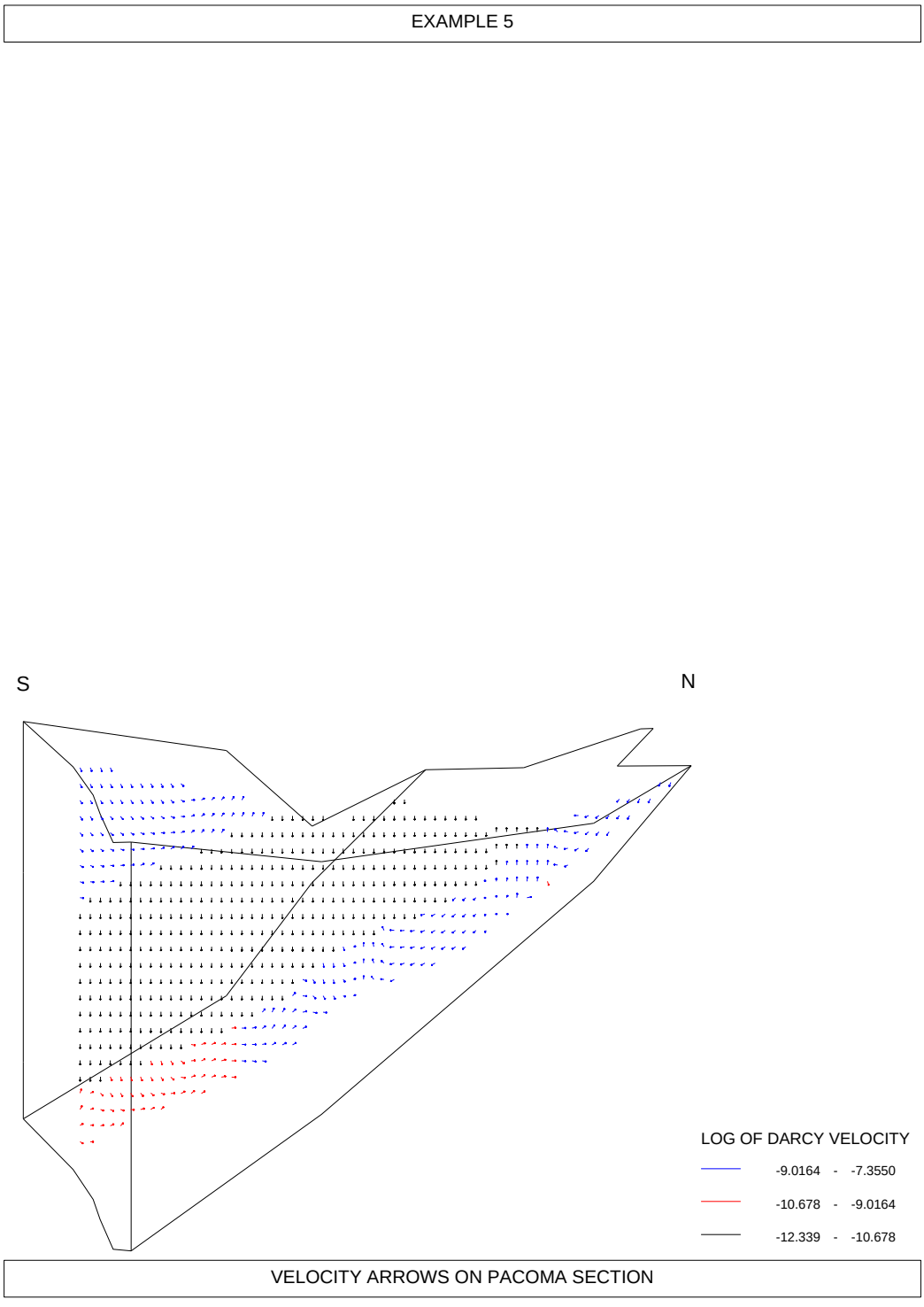


Figure 7.7 **Velocity vectors plotted on the slice used in the two-dimensional study of Section 6.**

Dataset 7.1

```
   /* NAMMU TEST CASE PACOMA3D                                          */
   /*                                                                   */
   /* EXAMPLE 5 : THREE DIMENSIONAL STEADY GROUNDWATER FLOW             */

   /* SPACE ALLOCATION                                                  */
   /* INTEGER WORKSPACE  350000                                         */
   /* REAL WORKSPACE     250000                                         */

   /* INLINE FORTRAN                                                    */
   /* SOURCE FILES                                                      */
   /* COMPILED FILES                                                    */
   /* LIBRARY FILES                                                     */

   /* INPUT DATA FILES                                                  */
   /* OUTPUT DATA FILES                                                 */
   /* 6        nammu/output/pacoma3d.out                                */
   /* GRAPHICS nammu/output/pacoma3d.ps                                 */

   /* END JOB INFORMATION                                               */


>> NAMMU

   >> SET OPTIONS
      THREE DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS                      40
      NODES                       1080
      SPACE DIMENSIONS               3
      FRONTWIDTH                   400
      LEVELS                         3
      INTEGER BC WORKSPACE        5000
      REAL BC WORKSPACE           1000
      FUNCTION TYPES PER ELEMENT     3
      VARIABLES                      1
      END

   >> SET VARIABLES
      VARIABLE NAMES  'PRES'
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      FLUID DENSITY                     992.0
      MOLECULAR DIFFUSION COEFFICIENTS    6.0E-10

      ROCK TYPE PERMEABILITIES
```

```
      ROCK NAME,       KXX,      KYY,      KZZ
       'CHALK'       3.3E-13   3.3E-13   3.3E-13
       'CLAY'        1.3E-17   1.3E-17   8.2E-19
       'CORALLIAN'   5.2E-13   5.2E-13   5.2E-13

      ROCK TYPE PROPERTIES
      ROCK NAME,    POROSITY
       'CHALK'        0.37
       'CLAY'         0.31
       'CORALLIAN'    0.34

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TORTUOSITIES,  LONGITUDINAL DISPERSION LENGTHS
       'CHALK'         100.0                    82.0
       'CLAY'            2.73                    0.0
       'CORALLIAN'     100.0                    88.0

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TRANSVERSE DISPERSION LENGTHS
       'CHALK'                  8.2
       'CLAY'                   0.0
       'CORALLIAN'              8.8
      END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         PATCH POSITIONS
         CORNER NUMBER,        COORDINATES
               11        <   0.0     0.0   -95.0 >
               12        <  12.9     2.3  -120.0 >
               13        <  17.6     3.2  -135.0 >
               14        <  19.2     3.5  -145.0 >
               15        <  22.6     4.1  -160.0 >
               16        <  27.4     4.9  -160.0 >
               21        <   0.0     0.0   -65.0 >
               22        <  12.9     2.3   -90.0 >
               23        <  17.6     3.2  -105.0 >
               24        <  19.2     3.5  -115.0 >
               25        <  22.6     4.1  -130.0 >
               26        <  27.4     4.9  -130.0 >
               31        <   0.0     0.0    35.0 >
               32        <  12.9     2.3    10.0 >
               33        <  17.6     3.2    -5.0 >
               34        <  19.2     3.5   -15.0 >
               35        <  22.6     4.1   -30.0 >
               36        <  27.4     4.9   -30.0 >
               41        <   0.0     0.0   115.0 >
               42        <  12.9     2.3    90.0 >
               43        <  17.6     3.2    75.0 >
               44        <  19.2     3.5    65.0 >
```

```
     45       <  22.6     4.1    50.0 >
     46       <  27.4     4.9    50.0 >
    111       <  -2.8     8.0   -30.0 >
    112       <  10.1    10.2   -55.0 >
    113       <  15.1    10.5   -65.0 >
    114       <  16.8    10.4   -70.0 >
    115       <  19.6    12.9   -80.0 >
    116       <  24.9    12.2   -90.0 >
    121       <  -2.8     8.0     0.0 >
    122       <  10.1    10.2   -25.0 >
    123       <  15.1    10.5   -35.0 >
    124       <  16.8    10.4   -40.0 >
    125       <  19.6    12.9   -50.0 >
    126       <  24.9    12.2   -60.0 >
    131       <  -2.8     8.0   100.0 >
    132       <  10.1    10.2    75.0 >
    133       <  15.1    10.5    65.0 >
    134       <  16.8    10.4    60.0 >
    135       <  19.6    12.9    50.0 >
    136       <  24.9    12.2    40.0 >
    211       <  -4.0    11.4    30.0 >
    212       <   8.1    15.9    30.0 >
    213       <  12.7    17.5    30.0 >
    214       <  12.3    23.5    70.0 >
    215       <  16.9    20.7    30.0 >
    216       <  21.3    22.7    30.0 >
    221       <  -4.0    11.4    60.0 >
    222       <   8.1    15.9    60.0 >
    223       <  12.7    17.5    60.0 >
    224       <  12.3    23.5   100.0 >
    225       <  16.9    20.7    60.0 >
    226       <  21.3    22.7    60.0 >
    311       <  -5.6    15.9    90.0 >
    312       <   6.7    19.9    90.0 >
    313       <  10.3    24.5   110.0 >
    314       <  11.8    25.0   110.0 >
    315       <  15.9    23.6    90.0 >
    316       <  20.0    26.5    90.0 >

PATCH TOPOLOGY
PATCH TYPE,                CORNERS,                ROCK NAME
  'BKBQ'    <  11  12  22  21 111 112 122 121 >  'CORALLIAN'
  'BKBQ'    <  12  13  23  22 112 113 123 122 >  'CORALLIAN'
  'BKBQ'    <  13  14  24  23 113 114 124 123 >  'CORALLIAN'
  'BKBQ'    <  14  15  25  24 114 115 125 124 >  'CORALLIAN'
  'BKBQ'    <  15  16  26  25 115 116 126 125 >  'CORALLIAN'
  'BKBQ'    <  21  22  32  31 121 122 132 131 >  'CLAY'
  'BKBQ'    <  22  23  33  32 122 123 133 132 >  'CLAY'
  'BKBQ'    <  23  24  34  33 123 124 134 133 >  'CLAY'
  'BKBQ'    <  24  25  35  34 124 125 135 134 >  'CLAY'
  'BKBQ'    <  25  26  36  35 125 126 136 135 >  'CLAY'
  'PRPQ'    <  31 131  41  32 132  42         >  'CHALK'
  'PRPQ'    <  32 132  42  33 133  43         >  'CHALK'
  'PRPQ'    <  33 133  43  34 134  44         >  'CHALK'
```

```
         'PRPQ'    <  34 134  44  35 135  45         >  'CHALK'
         'PRPQ'    <  35 135  45  36 136  46         >  'CHALK'
         'BKBQ'    < 111 112 122 121 211 212 222 221 >  'CORALLIAN'
         'BKBQ'    < 112 113 123 122 212 213 223 222 >  'CORALLIAN'
         'BKBQ'    < 113 114 124 123 213 214 224 223 >  'CORALLIAN'
         'BKBQ'    < 114 115 125 124 214 215 225 224 >  'CORALLIAN'
         'BKBQ'    < 115 116 126 125 215 216 226 225 >  'CORALLIAN'
         'PRPQ'    < 121 221 131 122 222 132         >  'CLAY'
         'PRPQ'    < 122 222 132 123 223 133         >  'CLAY'
         'PRPQ'    < 123 223 133 124 224 134         >  'CLAY'
         'PRPQ'    < 124 224 134 125 225 135         >  'CLAY'
         'PRPQ'    < 125 225 135 126 226 136         >  'CLAY'
         'PRPQ'    < 211 311 221 212 312 222         >  'CORALLIAN'
         'PRPQ'    < 212 312 222 213 313 223         >  'CORALLIAN'
         'PRPQ'    < 213 313 223 214 314 224         >  'CORALLIAN'
         'PRPQ'    < 214 314 224 215 315 225         >  'CORALLIAN'
         'PRPQ'    < 215 315 225 216 316 226         >  'CORALLIAN'
       END

 >> SET BOUNDARY CONDITIONS

/*  *****  TOP SURFACE PRESSURE BOUNDARY SPECIFICATION *****  */
    >> SPECIFIED VALUE

       >> VALUE VARYING LINEARLY WITH POSITION
          BASE VALUES     0.0
          Z FACTORS    9371.52
          VARIABLES    'PRES'
          END

          >> SELECT SURFACE

             >> RESTRICT SURFACE SELECTION
                X LIMITS         -6.0   28.0
                Y LIMITS          0.0   27.0
                Z LIMITS         39.0  120.0
                SURFACE NORMAL    0.0    0.0    1.0
                TOLERANCE ANGLE  88.0
                PRECISION         0.001
                END

/*  ********** SURFACE BOUNDARY CONDITION FOR EDGE ********  */
/*  ****************** OF PRISMATIC PATCHES ***************  */
    >> SPECIFIED VALUE

       >> VALUE VARYING LINEARLY WITH POSITION
          BASE VALUES     0.0
          Z FACTORS    9371.52
          VARIABLES    'PRES'
          END

          >> SELECT LINE
             START POINT   -5.6   15.9   90.0
             END POINT      6.7   19.9   90.0
```

```
         PRECISION      0.001
         END

>> SPECIFIED VALUE

   >> VALUE VARYING LINEARLY WITH POSITION
      BASE VALUES  0.0
      Z FACTORS    9371.52
      VARIABLES  'PRES'
      END

      >> SELECT LINE
         START POINT    6.7   19.9   90.0
         END POINT     10.3   24.5  110.0
         PRECISION      0.001
         END

>> SPECIFIED VALUE
   >> VALUE VARYING LINEARLY WITH POSITION
      BASE VALUES     0.0
      Z FACTORS    9371.52
      VARIABLES    'PRES'
      END

      >> SELECT LINE
         START POINT   10.3   24.5  110.0
         END POINT     11.8   25.0  110.0
         PRECISION      0.001
         END

>> SPECIFIED VALUE

   >> VALUE VARYING LINEARLY WITH POSITION
      BASE VALUES  0.0
      Z FACTORS    9371.52
      VARIABLES  'PRES'
      END

      >> SELECT LINE
         START POINT   11.8   25.0  110.0
         END POINT     15.9   23.6   90.0
         PRECISION      0.001
         END

>> SPECIFIED VALUE

   >> VALUE VARYING LINEARLY WITH POSITION
      BASE VALUES     0.0
      Z FACTORS    9371.52
      VARIABLES    'PRES'
      END

      >> SELECT LINE
         START POINT   15.9   23.6   90.0
```

```
            END POINT     20.0   26.5   90.0
            PRECISION      0.001
            END

   /*  **** SCALE THE X AND Y COORDINATES TO REAL DIMENSIONS *****  */
   >> MAP GRID

      >> SCALE COORDINATES
         DIVIDE X BY  1.0000E-3
         DIVIDE Y BY  1.0000E-3
         END


>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH   200
      END

      >> GROUNDWATER FLOW
         END


>> OUTPUT DATA

   >> SET OUTPUT OPTIONS
      HEADING                    'EXAMPLE 5'
      BOUNDARY COLOUR            'BLACK'
      GRID COLOUR                'BLACK'
      COORDINATE SCALE FACTORS  1.0 1.0 75.0
      END

   >> SET ROCK STYLES
      ROCK STYLES
      ROCK NAME,   COLOUR
      'CHALK'      'BLUE'
      'CLAY'       'YELLOW'
      'CORALLIAN'  'RED'
      END

   /*   *************** SET AN OBLIQIUE VIEWPOINT *************   */
   >> SET PROJECTION
      EYE POSITION     1.0E6   2.7E4   600.0
      PAPER VECTOR    -1.0E6  -2.7E4  -600.0
      PAPER VERTICAL   0.0     0.0       1.0
      END

   >> PLOT BOUNDARY
      END

   >> PLOT TEXT
      TEXT   'S'
      POSITION  9800.0   0.0  130.0
```

```
>> PLOT TEXT
   TEXT   'N'
   POSITION  20200.0  26100.0  130.0

/*   *************** PLOT VERTICAL SLICES ****************   */
>> SET PROJECTION
   EYE POSITION     1.0E4 -1.0E6  0.0
   PAPER VECTOR    -1.0E4  1.0E6  0.0
   PAPER VERTICAL   0.0    0.0    1.0
   END

>> PLOT GRID SLICE
   SHADE
   PLANE PARAMETERS   0.0  1.0  0.0 -1.0E4
   CAPTION           'VERTICAL SECTION Y=10KM'
   END

>> PLOT BOUNDARY
   SUPERIMPOSE
   NO CAPTION
   END

>> PLOT TEXT
   TEXT   'W'
   POSITION  -5000.0  5000.0 120.0

>> PLOT TEXT
   TEXT   'E'
   POSITION  25000.0 5000.0 120.0

>> SET PROJECTION
   EYE POSITION     1.0E6  0.0    0.0
   PAPER VECTOR    -1.0E6  0.0    0.0
   PAPER VERTICAL   0.0    0.0    1.0
   END

>> PLOT GRID SLICE
   SHADE
   PLANE PARAMETERS   1.0  0.0  0.0 -5.0E3
   CAPTION           'VERTICAL SECTION X=5KM'
   END

>> PLOT BOUNDARY
   SUPERIMPOSE
   NO CAPTION
   END

>> PLOT TEXT
   TEXT   'S'
   POSITION  9800.0   0.0  130.0

>> PLOT TEXT
   TEXT   'N'
   POSITION  20200.0  26100.0  130.0
```

```
>> SET PROJECTION
   EYE POSITION     0.0    0.0    1.0E7
   PAPER VECTOR     0.0    0.0   -1.0E7
   PAPER VERTICAL   0.0    1.0    0.0
   END

>> SET PLOT CRITERION

   >> SELECT ON PROPERTY TYPES
      VALUE  3
      END

>> PLOT GRID SURFACE
   USE PLOT CRITERION
   CAPTION  'STRATA SURFACE - CORALLIAN'
   END

>> SET PROJECTION
   EYE POSITION    0.0E4  0.0E4  1.0E7
   PAPER VECTOR    0.0    0.0   -1.0E7
   PAPER VERTICAL  0.0    1.0    0.0
   END

>> SET PLOT CRITERION

   >> SELECT ON PROPERTY TYPES
      VALUE 1
      END

>> PLOT GRID SURFACE
   USE PLOT CRITERION
   CAPTION  'STRATA SURFACE - CHALK'
   END

>> SET PROJECTION
   EYE POSITION     1.0E6  2.7E4  600.0
   PAPER VECTOR    -1.0E6 -2.7E4 -600.0
   PAPER VERTICAL   0.0    0.0      1.0
   END

>> PATHLINES
   NUMBER OF PATHS                1
   X COORDINATES OF PATHS      11400.0
   Y COORDINATES OF PATHS       6500.0
   Z COORDINATES OF PATHS        -12.0
   TIMES IN YEARS
   MAXIMUM NUMBER OF TIMESTEPS   750
   ACCURACY PARAMETER              0.1
   COORDINATE SCALES               1.0  1.0  100.0
   COLOUR USING ROCK TYPE
   CAPTION                    'PATHLINE FROM REPOSITORY'
   KEY TITLE                  'ROCK TYPE'
   END
```

```
>> PLOT TEXT
   TEXT   'S'
   POSITION  9800.0   0.0  130.0

>> PLOT TEXT
   TEXT   'N'
   POSITION  20200.0  26100.0  130.0

>> SET PROJECTION
   EYE POSITION     0.0    0.0    1.0E8
   PAPER VECTOR     0.0    0.0   -1.0E8
   PAPER VERTICAL   0.0    1.0    0.0
   END

>> SET PLOT CRITERION

   >> SELECT ON PROPERTY TYPES
      VALUE 3
      END

>> PLOT CONTOURS ON SURFACE
   HEAD
   NUMBER OF CONTOURS  15
   COLOURS             'BLACK'
   USE PLOT CRITERION
   CAPTION             'HEAD CONTOURS IN CORALLIAN'
   KEY TITLE           'HEAD (M)'
   END

>> SET PROJECTION
   EYE POSITION     0.0    0.0    1.0E8
   PAPER VECTOR     0.0    0.0   -1.0E8
   PAPER VERTICAL   0.0    1.0    0.0
   END

>> SET PLOT CRITERION

   >> SELECT ON PROPERTY TYPES
      VALUE 2
      END

>> PLOT CONTOURS ON SURFACE
   HEAD
   NUMBER OF CONTOURS  15
   COLOURS             'BLACK'
   USE PLOT CRITERION
   CAPTION             'HEAD CONTOURS IN CLAY'
   KEY TITLE           'HEAD (M)'
   END

>> SET PROJECTION
   EYE POSITION    0.0    0.0    1.0E8
   PAPER VECTOR    0.0    0.0   -1.0E8
```

```
   PAPER VERTICAL  0.0    1.0    0.0
   END

>> SET PLOT CRITERION

   >> SELECT ON PROPERTY TYPES
      VALUE 1
      END

>> PLOT CONTOURS ON SURFACE
   HEAD
   NUMBER OF CONTOURS  15
   COLOURS             'BLACK'
   USE PLOT CRITERION
   CAPTION             'HEAD CONTOURS IN CHALK'
   KEY TITLE           'HEAD (M)'
   END

>> SET PROJECTION
   EYE POSITION     1.0E6  2.7E4  600.0
   PAPER VECTOR    -1.0E6 -2.7E4 -600.0
   PAPER VERTICAL   0.0    0.0      1.0
   END

>> PLOT CONTOURS ON SLICE
   HEAD
   ORIGIN                 9800.0   2500.0  -140.0
   FIRST DEFINING POINT   15000.0  14300.0  -140.0
   SECOND DEFINING POINT  9800.0   2500.0   110.0
   NUMBER OF CONTOURS  25
   COLOURS             'BLACK'
   CAPTION             'HEAD CONTOURS ON PACOMA SECTION'
   KEY TITLE           'HEAD (M)'
   END

>> PLOT TEXT
   TEXT   'S'
   POSITION  9800.0   0.0  130.0

>> PLOT TEXT
   TEXT   'N'
   POSITION  20200.0  26100.0  130.0

>> SET PLOT POINTS

   >> SELECT PLANE OF POINTS
      NUMBER OF POINTS IN FIRST DIRECTION      60
      NUMBER OF POINTS IN SECOND DIRECTION     50
      FIRST DEFINING POINT                  20200.0  26100.0  -140.0
      SECOND DEFINING POINT                  9800.0   2500.0   277.0
      ORIGIN                                 9800.0   2500.0  -140.0
      END

>> PLOT VECTORS
```

```
      CONSTANT LENGTH VECTORS
      NUMBER OF INTERVALS    3
      ARROW SCALE            1.0E4
      ARROWHEAD ANGLE       40.0
      COLOUR USING LOG OF VECTOR MAGNITUDE
      COLOURS              'BLACK' 'RED' 'BLUE'
      CAPTION              'VELOCITY ARROWS ON PACOMA SECTION'
      KEY TITLE            'LOG OF DARCY VELOCITY'
      END

   >> PLOT TEXT
      TEXT   'S'
      POSITION  9800.0   0.0  130.0

   >> PLOT TEXT
      TEXT   'N'
      POSITION  20200.0  26100.0  130.0


>> STOP
```

8 EXAMPLE 6: THE MIXED-ELEMENT FORMULATION (TOTH TEST CASE)

The mixed-element formulation is designed to ensure mass-conservation on an element-by-element basis. Standard formulations ensure mass-conservation globally. Solutions and pathlines calculated using standard formulations may be more accurate than those computed with a mixed formulation but they are generally less robust. The use of mixed elements is particularly beneficial in pathline calculations. When using a standard formulation there are discontinuities in velocity at the interfaces between different elements. If the velocities on adjacent faces are oppositely directed the pathlines may become 'stuck' at an element boundary.

In NAMMU the flow equation may be solved using the mixed formulation when using the ≫ `GROUNDWATER FLOW`, ≫ `SALT TRANSPORT` or ≫ `SALT AND HEAT TRANSPORT` options. A mixed-element ≫ `GROUNDWATER FLOW` or ≫ `SALT TRANSPORT` calculation may be used to provide the velocity field for a ≫ `NUCLIDE TRANSPORT` calculation. The mixed-element formulation solves the conservative form of the flow equation which is given in the NAMMU Technical Overview [8]. The keywords required to select the conservative form of the flow equation are described in Section 8.2.

The mixed-element formulation is currently restricted to Cartesian geometry. In two-dimensions, quadrilateral (QMX2) and triangular (TMX2) elements are available. In three-dimensions, cuboid (CBMX), prism (PRMX) and tetrahedral (TTMX) elements are available. These may be used with any of the standard patches with the following exception. BT6, BT24 and PT10 patches must be composed of TTMX elements. These are the only patches in which TTMX elements may be used. In three-dimensions, mixed elements must have planar faces. The use of tetrahedral mixed elements removes the requirement for the patch faces to be planar when BT6, BT24 and PT10 patches are used.

The example given below is the well known Toth Test Case [19]. This test case is an example of regional constant-density groundwater flow for which an analytic solution exists. The full definition and the analytic solution are given in Appendix G.

8.1 Generating a Model using the Mixed-Element Formulation

8.1.1 Setting up the Variables

The conservative form of the flow equation is solved using the pressure and the mass flux normal to the face or side of the element as variables. The mass flux is a vector variable which has components parallel to the coordinate axes. In the mixed-element formulation, the pressure is piecewise discontinuous. In two-dimensions, the horizontal component of the flux (FX) is interpolated by a basis function that varies linearly in the x-direction and is constant in the y-direction. The vertical component of the flux (FY) is interpolated by a basis function that varies linearly in the y-direction and is constant in the x-direction. Pressure freedoms are present at the node in the centre of the element and flux freedoms are present at the mid-side or mid-face nodes. It should be remembered that FX and FZ are

components of the mass flux and *not* components of the velocity.

In Dataset 8.1 the variables are set up in the following way:

```
 >> SET LIMITS
    VARIABLES                    4
       .
       .
       .

>> SET VARIABLES
   VARIABLE NAMES   'PRES'  'TEMP'  'FX'  'FY'

   VECTORS
   X COMPONENT, Y COMPONENT
      'FX'         'FY'

   END

>> SET INTERPOLATION TYPES
   BASIS FUNCTION TYPES  2  1  3  4
   ELEMENT NAME          'QMX2'
```

The components of the flux variable are declared using the VARIABLE NAMES keyword. The VECTORS table defines the components of the vector variable. Four variables are defined in Dataset 8.1 even though the groundwater flow calculation only requires the pressure and the flux. For ≫ GROUNDWATER FLOW amd ≫ SALT TRANSPORT calculations, the solver expects the components of the flux to be variables 3 and 4 in two-dimensions and variables 3, 4 and 5 in three dimensions. The easiest and safest way of ensuring that the flux variables are in the correct place is to declare them as variables 3, 4 (and 5) in the ≫ SET VARIABLES command. For ≫ SALT AND HEAT TRANSPORT, the solver expects the components of the flux to be variables 4 and 5 in two-dimensions and variables 4, 5 and 6 in three dimensions.

Four basis function types are required. The default value of FUNCTION TYPES PER ELEMENT under ≫ SET LIMITS in NAMMU is 4. For three-dimensional mixed-element calculations, the value of FUNCTION TYPES PER ELEMENT must be increased to 5 because five basis function types are required. The variable 'TEMP' has been declared to have interpolation type 1. Interpolation type 1 is a conventional linear basis function where the freedom is present at the corner nodes of the element. Interpolation type 1 should be used for the concentration variable in salt transport calculations and for the nuclide variable(s) in nuclide transport calculations. A variable with interpolation type 1 is using a standard formulation. Details of the basis functions available for each element type may be found in Appendix B.

8.1.2 Grid Generation

The only item in the ≫ CREATE GRID section of the example discussed in this Section that is specific to mixed elements is the keyword

```
QUADRILATERAL ELEMENT TYPE   'QMX2'
```

of the subcommand ≫ GENERATE A GRID OF PATCHES which is required to make NAMMU use the mixed-element type QMX2 instead of the default QAD9 elements. In cases where the finite-elements are distorted, it is recommended that triangular mixed elements are used in preference to quadrilateral mixed elements.

At the end of the ≫ MODEL DATA phase, NAMMU prints out a summary of the model. This summary contains a table listing the nodal coordinates and the freedoms present at each node. A section of this table is given below:

```
 NODE  FREEDOM       COORDINATES              FREEDOMS
        COUNT
------ -------      -----------              --------
     1       1   0.0000E+00 -2.0000E+02    TEMP
     2       2   3.1250E+01 -2.0000E+02    FX      FY
     3       3   6.2500E+01 -2.0000E+02    TEMP
     4       4   9.3750E+01 -2.0000E+02    FX      FY
     5       5   1.2500E+02 -2.0000E+02    TEMP
     6       6   1.5625E+02 -2.0000E+02    FX      FY
     .       .        .           .        .       .
     .       .        .           .        .       .
     .       .        .           .        .       .
```

At nodes where the flux variable is present the table of nodes lists both 'FX' and 'FY', yet the freedom count is only incremented by 1. The table is simply showing that a single flux variable which has components 'FX' and 'FY', parallel to the coordinate axes, is present.

8.1.3 Boundary Conditions

The default boundary condition for the mixed-element formulation of the flow equation is zero pressure. Therefore, no-flow boundary conditions (the default for standard elements) must be set explicitly by setting the flux normal to the boundary to be zero. For example:

```
>> SPECIFIED VALUE

   >> CONSTANT VALUE
      VARIABLES  'FY'
      VALUES     0.0
      END
```

```
>> SELECT LINE
   START POINT     0.0  -200.0
   END POINT    1000.0  -200.0
   PRECISION       1.0E-4
   END
```

sets a no-flow boundary condition along the bottom surface of the model. `'FX'` could have been specified instead of `'FY'` after the `VARIABLES` keyword. NAMMU calculates the flux normal to the boundary automatically and sets the boundary condition on the flux normal to the boundary, not on an individual component of the flux variable.

At the end of the MODEL DATA section, NAMMU prints a summary of the boundary conditions that have been set. The subcommand ≫ `SELECT LINE` selects all nodes that lie on a specified line. NAMMU will therefore attempt to set the Dirichlet boundary condition at all nodes along this line despite the fact that the flux variable is only present at the mid-side nodes. As a result the summary of boundary conditions will contain a number of warning messages. A section of the boundary conditions summary is reproduced below.

```
DIRICHLET BC FOR VARIABLE FY   AT NODE      1 WITH VALUE  0.0000E+00
ABOVE BOUNDARY CONDITION IGNORED: VARIABLE NOT PRESENT
DIRICHLET BC FOR VARIABLE FY   AT NODE      2 WITH VALUE  0.0000E+00
DIRICHLET BC FOR VARIABLE FY   AT NODE      3 WITH VALUE  0.0000E+00
ABOVE BOUNDARY CONDITION IGNORED: VARIABLE NOT PRESENT
```

At the end of the list a warning of the following form is printed.

```
****** WARNING FROM BCNPRT ******
BOUNDARY CONDITIONS IGNORED AT   51 NODES BECAUSE VARIABLES WERE NOT PRESENT
```

In this case nodes 1 and 3 are corner nodes at which the boundary condition cannot be set because the flux variable is not present. The boundary condition is set successfully at node 2 which is a mid-side node. The list of nodes at which the boundary condition is not set should be compared with the list of nodal coordinates to check that they are nodes at which the variable should not be present given the chosen interpolation scheme. Warning messages of the above form may be produced whenever the interpolation scheme chosen means that a variable is not present at all nodes.

When using mixed elements to solve the flow equation it is not possible to set Dirichlet boundary conditions on the pressure in the conventional way. The pressure variable is only present at the node in the centre of the element and so cannot be set in a boundary condition. Instead, a generalised flux law type boundary condition is set on the flux variable. Further details are given in Section 11.2.2.

Dirichlet boundary conditions on the pressure variable are very common when using standard elements. A subcommand exists in NAMMU for use with mixed elements which is equivalent to setting a Dirichlet boundary condition on pressure in standard elements. This subcommand actually uses the specified value of the pressure to set up a generalised flux law boundary condition on the flux variable. It has the following form:

```
>> SPECIFIED VALUE FOR MIXED ELEMENTS
   >> CALL SUBROUTINE BNDVAL
      VARIABLES   'PRES'
```

Most of the subcommands of ≫ SPECIFIED VALUE may be used with ≫ SPECIFIED VALUE FOR MIXED ELEMENTS. Further details are given in the NAMMU Reference Manual /citenamref. In the above example the pressure is specified in the user routine BNDVAL. The subcommand ≫ SPECIFIED VALUE FOR MIXED ELEMENTS should only be used for variables with interpolation type 2 on element types QMX2, TMX2, CBMX, PRMX and TTMX. Dirichlet boundary conditions may be applied in the normal way to variables with other interpolation schemes.

8.2 Mixed-Element Solver Options

The mixed-element formulation for groundwater flow is selected by specifying the keyword MIXED FORMULATION.

```
>> SOLVER DATA

    >> STEADY STATE
       NUMBER OF ITERATIONS  2
       FORCE DIAGONAL PIVOTING
       PIVOT SEARCH         10
       END

       >> GROUNDWATER FLOW
          MIXED FORMULATION
          END
```

When solving the flow equation using the mixed formulation, the solver may have difficulty selecting suitable pivot points in the matrix. The keyword FORCE DIAGONAL PIVOTING usually solves this problem. However, even when this keyword is used, the solver may be very slow because it is using a very large frontwidth. The frontwidth should be restricted to a value that is reasonable for the problem using the keyword MAXIMUM FRONTWIDTH. When the frontwidth is restricted in this way the solver may return warning messages of the form:

```
***** Warning from MA42B/BD *****  INFO(1) = 2
      Numerical criterion not satisfied by      246 pivots
```

If the solution converged satisfactorily these warnings can usually be ignored.

The default formulations for ≫ SALT TRANSPORT and ≫ SALT AND HEAT TRANSPORT are also the standard formulation. The flow equation may be solved using the mixed formulation by specifying the keyword MIXED FORMULATION FOR FLOW.

```
>> SOLVER DATA
   >> STEADY STATE
      MAXIMUM FRONTWIDTH    150
      NUMBER OF ITERATIONS   15
      FORCE DIAGONAL PIVOTING

      >> SALT TRANSPORT
         MIXED FORMULATION FOR FLOW
```

Further details of ≫ SALT TRANSPORT calculations are given in Section 9.

A flow solution calculated using mixed elements may be used in a ≫ NUCLIDE TRANSPORT calculation. If the ≫ NUCLIDE TRANSPORT calculation is performed during the same run as the flow calculation the solver will automatically use the equations appropriate for a mixed-element flow field. When the flow solution is restored from an earlier run, one or more of the keywords given in the ≫ NUCLIDE TRANSPORT section of the NAMMU Reference Manual [7] will be required. It should be noted that ≫ NUCLIDE TRANSPORT calculations using flow fields calculated using ≫ SALT AND HEAT TRANSPORT are currently not supported.

8.3 Output Options

The normal commands and keywords of the ≫ OUTPUT DATA phase may be used with mixed elements. The exception is contour plots of the pressure variable. The piecewise constant nature of the pressure variable (interpolation type 2) means that a conventional unshaded contour plot would not be sensible. The best method for plotting such variables is to use ≫ PLOT CONTOURS or ≫ PLOT CONTOURS ON SLICE with the SHADE keyword. It should be remembered that any variable with interpolation type 1 uses conventional linear interpolation and so may be plotted using conventional unshaded contours.

If the global freedoms are restored for post-processing, keywords of ≫ SET PLOT OPTIONS will be required. If the global freedoms were produced using the MIXED FORMULATION keyword of ≫ GROUNDWATER FLOW, the keyword MIXED FORMULATION FOR FLOW will be required. If the MIXED FORMULATION FOR FLOW option of ≫ SALT TRANSPORT was used, the keyword VARIABLE SALINITY CALCULATION will also be required. If the keyword MIXED FORMULATION FOR FLOW of ≫ SALT AND HEAT TRANSPORT was used, the keyword VARIABLE TEMPERATURE CALCULATION will be required in addition to the keywords already mentioned.

Figures 8.1–8.4 show the output from Dataset 8.1. Figures 8.2–8.4 show the difference

between the analytic solution (Appendix G) and the solution calculated by NAMMU. The discontinuous nature of the pressure and of the vertical component of velocity along the line of the plot may be seen clearly in Figures 8.2 and 8.4. The curve in Figure 8.3 is very different to the other two line graphs because the horizontal component of the velocity varies linearly along the line of the plot.

This series of line graphs also illustrates the use of the `IDENTIFICATION NUMBER` keyword. This keyword is usually used when a single user routine needs to perform a number of different functions.

Figures for Section 8

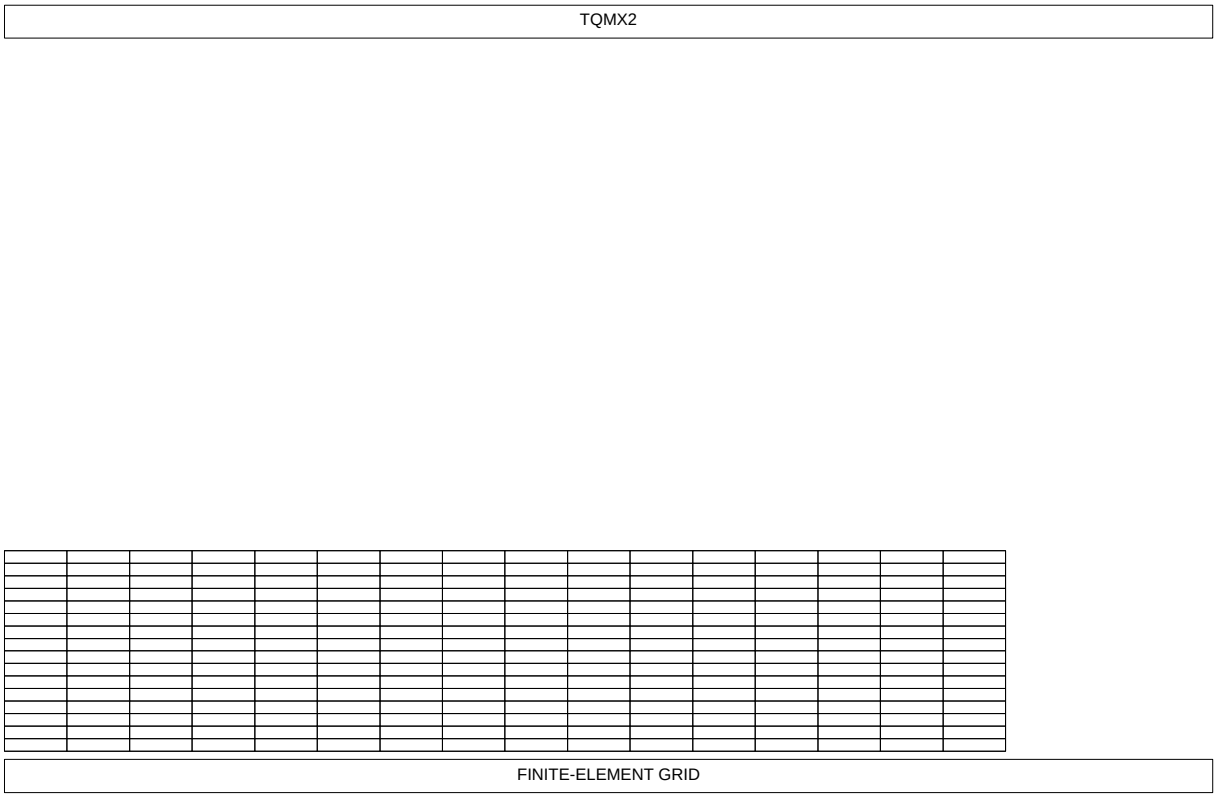


Figure 8.1 Grid used for the Toth Test Case.

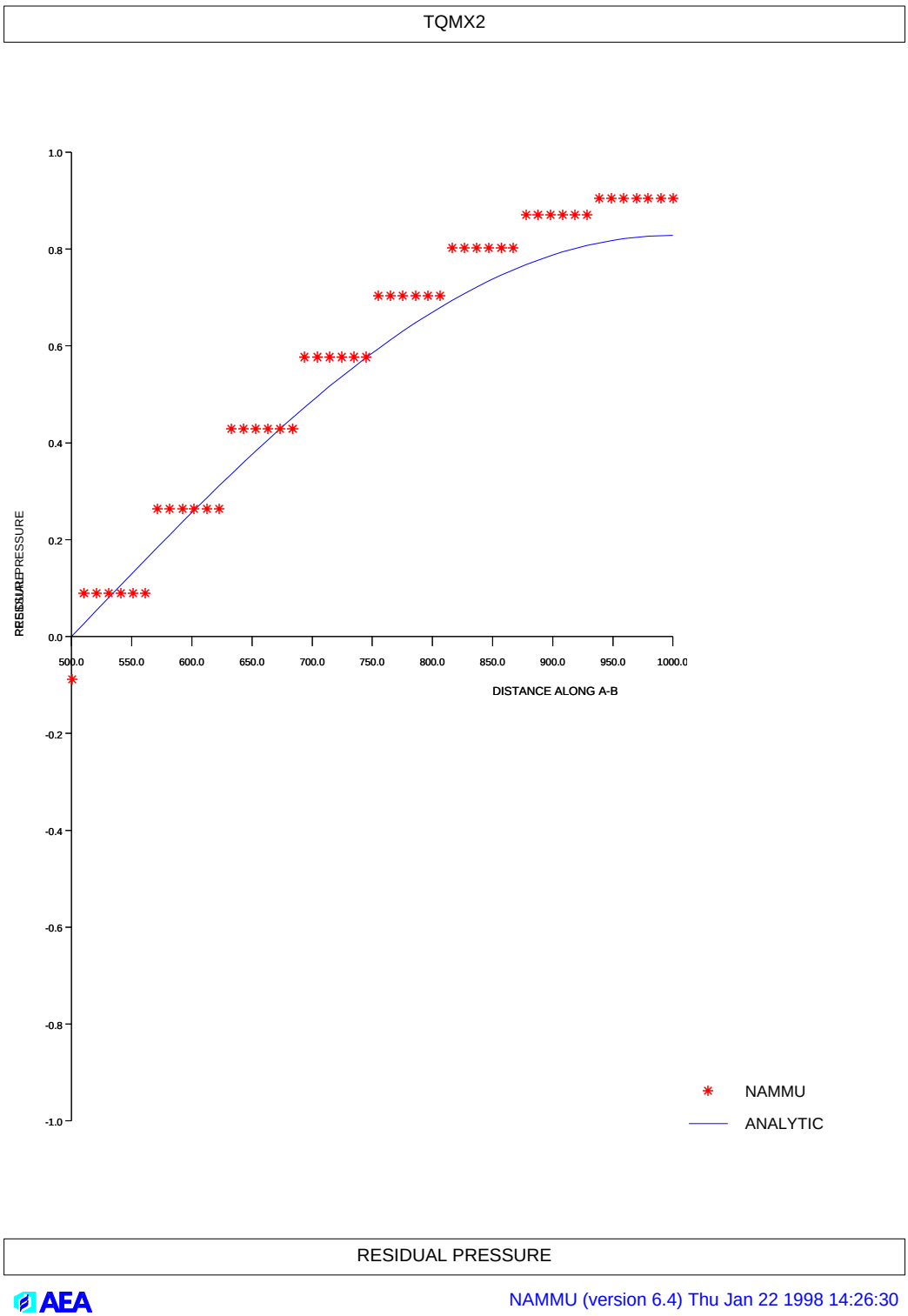


Figure 8.2 **The calculated pressure (symbols) compared with the analytic solution (line).**

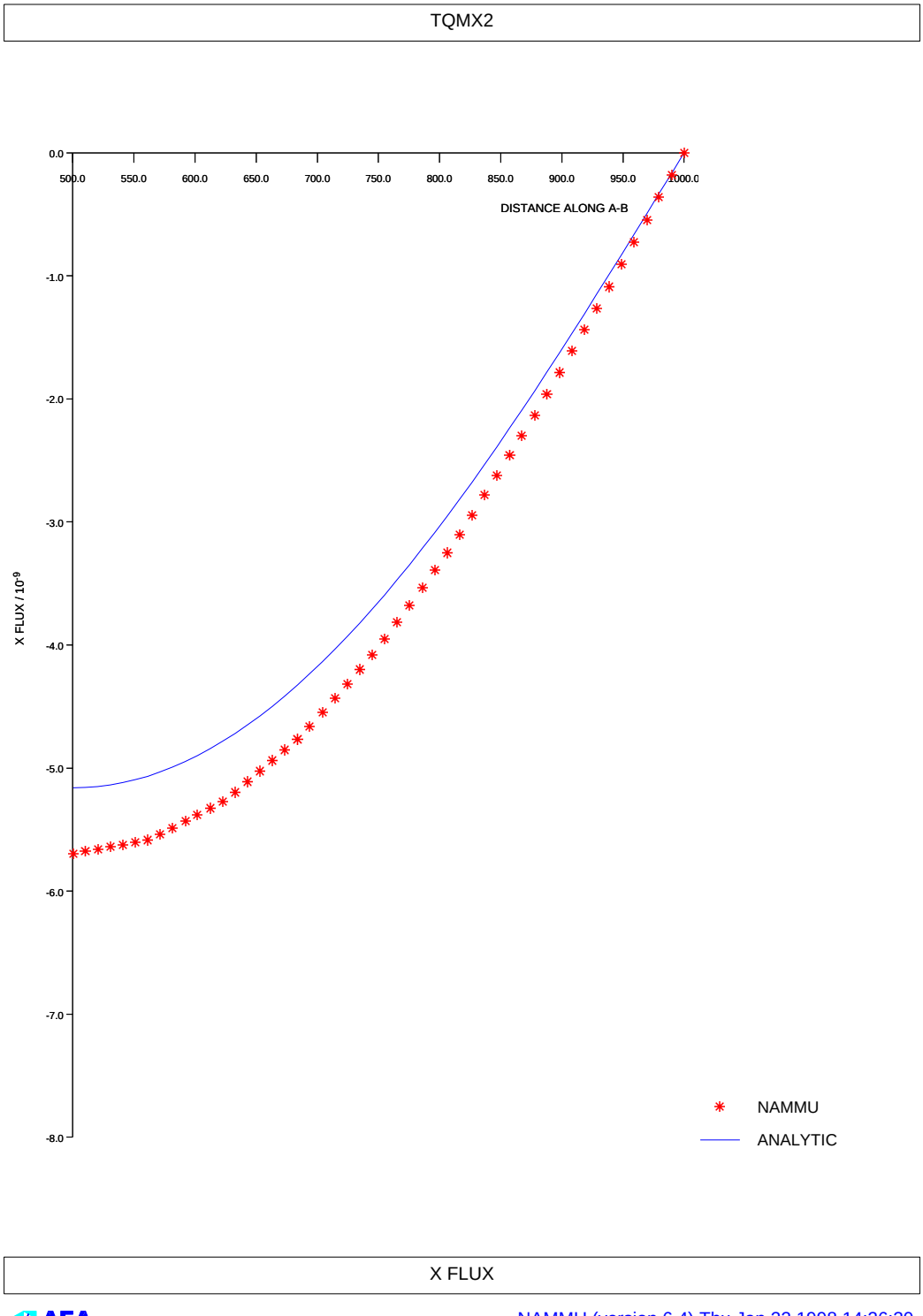


Figure 8.3 The calculated horizontal velocity (symbols) compared with the analytic solution (line).

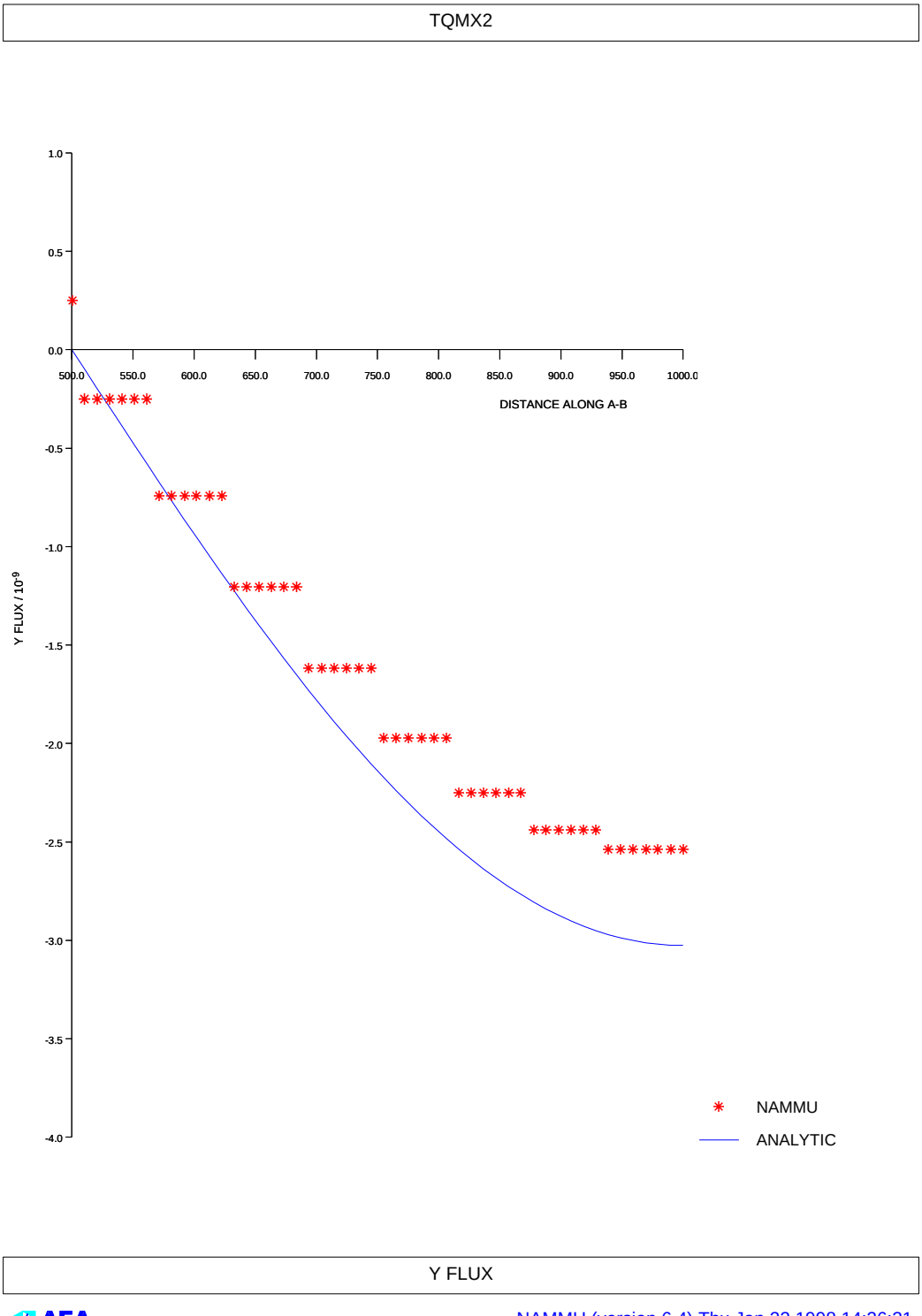


Figure 8.4 The calculated vertical velocity (symbols) compared with the analytic solution (line).

Dataset 8.1

```
/* NAMMU TEST CASE TQMX2                                          */
/*                                                                */
/* TO TEST 2D STEADY-STATE GROUNDWATER FLOW USING QMX2            */
/* MIXED ELEMENTS. THE CASE TESTS THE OPTION TO SPECIFY A         */
/* SPECIFIED VALUE BC FOR PRESSURE. THE CASE ALSO TESTS THE       */
/* USE OF AN ANISOTROPIC PERMEABILITY. THE TEST CASE IS           */
/* BASED ON THE 'TOTH' SOLUTION.                                  */

/* SPACE ALLOCATION                                               */
/* INTEGER WORKSPACE  350000                                      */
/* REAL WORKSPACE     150000                                      */

/* INLINE FORTRAN
   SUBROUTINE BNDVAL(X,NSD,V,IV,NVARS)
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
   DIMENSION X(NSD),V(NVARS)
   PI = ATAN( 1.0D0 ) * 4.0D0
   A = 1000.0D0
   V(1) = -COS( PI * X(1) / A )
   RETURN
   END

   SUBROUTINE SCLUSR(VAL,X,NSD,V,NVAR,DVDR)
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
   DIMENSION X(NSD),V(NVAR),DVDR(NSD,NVAR)
   COMMON /CUIDNO/ IDNO
   PI = ATAN( 1.0D0 ) * 4.0D0
   A  = 1000.0D0
   B  = 200.0D0
   CH = COSH( PI * X(2) * SQRT( A / B ) / A )
   TH = TANH( PI * B * SQRT( A / B ) / A )
   SH = SINH( PI * X(2) * SQRT( A / B ) / A )
   C  = COS( PI * X(1) / A )
   S  = SIN( PI * X(1) / A )
   IF ( IDNO .EQ. 1 ) THEN
     VAL = -( CH + TH * SH ) * C
   ELSE IF ( IDNO .EQ. 2 ) THEN
     VAL = -2.0D-12 * 992.0D0 * PI * ( CH + TH * SH ) * S
   ELSE IF ( IDNO .EQ. 3 ) THEN
     VAL = 1.0D-12 * 992.0D0 * PI * SQRT( 2.0D0 )
  >        * ( SH + TH * CH ) * C
   END IF
   RETURN
   END
                                                                  */
/* SOURCE FILES                                                   */
/* COMPILED FILES                                                 */
/* LIBRARY  FILES                                                 */

/* INPUT DATA FILES                                               */
/* OUTPUT DATA FILES                                              */
/* 6        nammu/output/tqmx2.out                                */
```

```
   /* GRAPHICS nammu/output/tqmx2.ps                              */

   /* END JOB INFORMATION                                         */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS               300
      NODES                 1200
      FREEDOMS              2400
      VARIABLES                4
      INTEGER BC WORKSPACE  2500
      REAL BC WORKSPACE      500
      END

   >> SET VARIABLES
      VARIABLE NAMES  'PRES' 'TEMP' 'FX' 'FY'
      VECTORS
      X COMPONENT, Y COMPONENT
          'FX'         'FY'
      END

   >> SET INTERPOLATION TYPES
      BASIS FUNCTION TYPES  2 1 3 4
      ELEMENT NAME          'QMX2'
      END


>> INITIAL DATA

    >> PHYSICAL PROPERTIES
       FLUID DENSITY 992.0

       ROCK TYPE PERMEABILITIES
       ROCK NUMBER,   KXX,    KYY
            1       2.0E-12 1.0E-12

       ROCK TYPE PROPERTIES
       ROCK NUMBER,  POROSITY
            1         1.0E-4
       END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
```

```
      QUADRILATERAL ELEMENT TYPE  'QMX2'

      PATCH SPACING IN FIRST DIRECTION
      SIZE
       16

      PATCH SPACING IN SECOND DIRECTION
      SIZE
       16

      PATCH POSITIONS
      CORNER NUMBER,    COORDINATES
            11       <    0.0    0.0 >
            12       < 1000.0    0.0 >
            21       <    0.0 -200.0 >
            22       < 1000.0 -200.0 >

      PATCH TOPOLOGY
      PATCH TYPE,     CORNERS
        'SQQ9'    < 21 22 12 11 >
      END

>> SET BOUNDARY CONDITIONS

   >> SPECIFIED VALUE FOR MIXED ELEMENTS

      >> CALL SUBROUTINE BNDVAL
         VARIABLES  'PRES'
         END

         >> SELECT LINE
            START POINT     0.0     0.0
            END POINT    1000.0     0.0
            END

   >> SPECIFIED VALUE

      >> CONSTANT VALUE
         VARIABLES  'FX'
         VALUES     0.0
         END

         >> SELECT LINE
            START POINT     0.0     0.0
            END POINT       0.0  -200.0
            PRECISION       1.0E-4
            END

   >> SPECIFIED VALUE

      >> CONSTANT VALUE
         VARIABLES  'FY'
         VALUES     0.0
         END
```

```
            >> SELECT LINE
               START POINT     0.0  -200.0
               END POINT    1000.0  -200.0
               PRECISION       1.0E-4
               END

      >> SPECIFIED VALUE

         >> CONSTANT VALUE
            VARIABLES  'FX'
            VALUES     0.0
            END

            >> SELECT LINE
               START POINT  1000.0     0.0
               END POINT    1000.0  -200.0
               PRECISION       1.0E-4
               END


>> SOLVER DATA

    >> STEADY STATE
       NUMBER OF ITERATIONS  2
       FORCE DIAGONAL PIVOTING
       PIVOT SEARCH         10
       END

       >> GROUNDWATER FLOW
          MIXED FORMULATION
          END


>> OUTPUT DATA

   >> PAGE SETUP
      LANDSCAPE
      END

   >> PRINT GLOBAL FREEDOMS
      END

   >> SET PLOT OPTIONS
      HEADING 'TQMX2'
      BOUNDARY COLOUR 'BLACK'
      GRID COLOUR     'BLACK'
      END

   >> PLOT GRID
      END

   >> PAGE SETUP
      PORTRAIT
```

```
   END

>> SET VIEWPORT
   VERTICAL KEY VIEWPORT
   ORIGIN    0.76  0.2
   SIZE      0.24  0.85

>> DRAW LINE GRAPH
   CALL SUBROUTINE SCLUSR
   IDENTIFICATION NUMBER  1
   START POINT          500.0     -31.25
   END POINT           1000.0     -31.25
   NUMBER OF POINTS      50
   VARIABLE LIMITS       -1.0       1.0
   X AXIS LABEL RANGE   500.0    1000.0
   X AXIS TITLE        'DISTANCE ALONG A-B'
   Y AXIS TITLE        'RESIDUAL PRESSURE'
   NO SYMBOLS
   CAPTION             'RESIDUAL PRESSURE'
   TITLE               'ANALYTIC'
   END

>> DRAW LINE GRAPH
   VARIABLE            'PRES'
   START POINT          500.0     -31.25
   END POINT           1000.0     -31.25
   NUMBER OF POINTS      50
   X AXIS LABEL RANGE   500.0    1000.0
   VARIABLE LIMITS       -1.0       1.0
   X AXIS TITLE        'DISTANCE ALONG A-B'
   Y AXIS TITLE        'PRESSURE'
   SYMBOLS ONLY
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               'NAMMU'
   END

>> DRAW LINE GRAPH
   CALL SUBROUTINE SCLUSR
   IDENTIFICATION NUMBER  2
   START POINT          500.0     -31.25
   END POINT           1000.0     -31.25
   NUMBER OF POINTS      50
   VARIABLE LIMITS       -8.0E-9   0.0
   X AXIS LABEL RANGE   500.0    1000.0
   X AXIS TITLE        'DISTANCE ALONG A-B'
   Y AXIS TITLE        'X FLUX'
   NO SYMBOLS
   CAPTION             'X FLUX'
   TITLE               'ANALYTIC'
   END

>> DRAW LINE GRAPH
   VARIABLE            'FX'
   START POINT          500.0     -31.25
```

```
   END POINT           1000.0     -31.25
   NUMBER OF POINTS      50
   X AXIS LABEL RANGE   500.0    1000.0
   VARIABLE LIMITS       -8.0E-9   0.0
   X AXIS TITLE        'DISTANCE ALONG A-B'
   Y AXIS TITLE        'X FLUX'
   SYMBOLS ONLY
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               'NAMMU'
   END

>> DRAW LINE GRAPH
   CALL SUBROUTINE SCLUSR
   IDENTIFICATION NUMBER  3
   START POINT          500.0     -31.25
   END POINT           1000.0     -31.25
   NUMBER OF POINTS      50
   VARIABLE LIMITS       -4.0E-9   1.0E-9
   X AXIS LABEL RANGE   500.0    1000.0
   X AXIS TITLE        'DISTANCE ALONG A-B'
   Y AXIS TITLE        'Y FLUX'
   NO SYMBOLS
   CAPTION             'Y FLUX'
   TITLE               'ANALYTIC'
   END

>> DRAW LINE GRAPH
   VARIABLE            'FY'
   START POINT          500.0     -31.25
   END POINT           1000.0     -31.25
   NUMBER OF POINTS      50
   X AXIS LABEL RANGE   500.0    1000.0
   VARIABLE LIMITS       -4.0E-9   1.0E-9
   X AXIS TITLE        'DISTANCE ALONG A-B'
   Y AXIS TITLE        'Y FLUX'
   SYMBOLS ONLY
   SUPERIMPOSE,  NO HEADING,  NO CAPTION,  NO FOOTER
   TITLE               'NAMMU'
   END


>> STOP
```

9 EXAMPLE 7: SALT TRANSPORT (HENRY TEST CASE)

If the region of interest is near to the coast or to salt deposits, the effect of salt on the groundwater flow must be considered. Saline water is denser than fresh water and these density differences lead to flow. This flow, in turn, transports salinity and hence the groundwater flow and transport of salinity are coupled. This results in a set of non-linear coupled equations, which are much more difficult to solve than the ordinary groundwater flow equation. Modelling coupled groundwater flow and transport of salinity is widely recognised to be a difficult problem, particularly if the salinities, and hence density contrasts, are large.

This Section describes the various formulations within NAMMU that are available for solving the coupled groundwater flow and transport of salinity equations. It also makes some general points about using NAMMU to perform such calculations. The example in this Section is a variant of the Henry Test Case [20] and shows how NAMMU can be used to solve a simple coupled groundwater flow and transport of salinity problem.

The Henry Test Case is a simple example of flow in a confined aquifer which directly contacts the sea. The domain and boundary conditions are illustrated in Figure 9.1. The problem uses a single rock type which has a permeability of $1.1892 \times 10^{-12}\,\mathrm{m}^2$ and a porosity of 0.35. All of the dispersion in the case considered here is hydrodynamic, the longitudinal and transverse dispersion lengths being 20m and 2m respectively, with the porewater diffusion coefficient set to zero.

9.1 Numerical Formulations

Two numerical formulations are available for solving the equations that describe coupled groundwater flow and transport of salinity. They are

1. TWO-VARIABLE FORMULATION (Default): This formulation uses the pressure and the concentration variables to solve the coupled equations. It is usually the fastest formulation but may be the least robust.

2. MIXED FORMULATION FOR THE FLOW EQUATION: The mixed element formulation (variables `'PRES'`, `'CONC'`, `'FX'`, `'FY'`; see Section 8) is used for the flow equation and the standard formulation is used for the concentration equation. The variables `'FX'`, `'FY'` (or `'FX'`, `'FY'` and `'FZ'` in 3D) represent the components of the mass flux parallel to the coordinate axes. Pathlines calculated using this formulation are more robust than those calculated using the two-variable formulation, although they may be less accurate.

The equations that describe coupled groundwater flow and transport of salinity are given in the NAMMU Technical Overview [8].

9.2 Specifying the Model

9.2.1 Mixed Interpolation

In regions where the flow is small, Darcy's Law becomes a balance between the vertical component of the pressure gradient and the density variation, both of which may be much larger than the flow. If the same order of interpolation is used for the pressure and the concentration, it is impossible to achieve a pointwise balance between the vertical component of the pressure gradient and the density variation because the two terms behave differently. An average balance integrated over an element is achieved and there may be large ripples in the velocity on the scale of the elements. This problem can be solved by using a lower order interpolation for the concentration variable than for the pressure variable.

It is recommended that linear interpolation is used for the concentration in both formulations. When using standard elements to solve the flow equation, quadratic interpolation should be used for the pressure. When using mixed elements to solve the flow equation, the interpolation schemes described in Section 8.1.1 should be used.

9.2.2 Setting up the variables and grid

In Dataset 9.1 the two-variable (default) formulation is used. The number of variables is set to 2 using the VARIABLES keyword of ≫ SET LIMITS and the two variables are declared using

```
>> SET VARIABLES
   VARIABLE NAMES  'PRES'  'CONC'
```

Interpolation type 1 on element type 'Q9/1' is quadratic and interpolation type 3 is linear. The interpolation types for the variables are declared in the ≫ SET INTERPOLATION TYPES subcommand as follows:

```
>> SET INTERPOLATION TYPES
   BASIS FUNCTION TYPES   1   3
   ELEMENT NAME           'Q9/1'
```

The element type 'Q9/1' must also be specified under the subcommand ≫ GENERATE A GRID OF PATCHES by using the keyword

```
QUADRILATERAL ELEMENT TYPE   'Q9/1'
```

The element type 'Q984' also has both quadratic and linear interpolation schemes and could have been used in place of element type 'Q9/1'. A table of elements and interpolation schemes is given in Appendix B.

In all transport calculations it is important that the mesh Peclet number, Pe_m is of order 1 or smaller (Section 6.2.5). If Pe_m is too large, the solution may be inaccurate or fail to converge properly. In Dataset 9.1 the longitudinal dispersion length is equal to the element size, ensuring that Pe_m is approximately equal to 1 at all times because the dispersion increases as the velocity increases ([8]).

9.2.3 Boundary Conditions

The Henry Test Case contains a $\partial c/\partial n = 0$ (ie zero dispersive flux) boundary condition at the outflow at the top of the right-hand edge of the model (Figure 9.1). The flux term for the concentration equation ([8]) is the total flux (dispersive flux plus advective flux) and so the boundary condition cannot be set by a ≫ SPECIFIED FLUX command. Instead it is set using a generalised flux law boundary condition in the following way:

```
>> GENERALISED FLUX LAW
   VARIABLES  'CONC'
   ZERO DISPERSIVE FLUX
```

The summary of the boundary conditions printed at the end of the MODEL DATA section will contain a number of warnings of the type described in Section 8.1.3. In this case the warnings will refer to the variable 'CONC'. The user should check that all of the nodes at which the Dirichlet boundary condition on 'CONC' is not set are mid-side nodes.

9.3 Solver Options

The two formulations described in Section 9.1 are selected using keywords of the ≫ SALT TRANSPORT subcommand. The keywords are

1. PRES CONC FORMULATION to select the two-variable formulation
2. MIXED FORMULATION FOR FLOW to solve the flow equation using the mixed formulation and the concentration using the standard formulation

If no keyword is supplied NAMMU will use the two-variable formulation and print a warning message.

In releases of NAMMU prior to Release 6.2, the formulation for ≫ SALT TRANSPORT was a zero diffusive flux formulation in which, in addition to solving for the pressure and salt concentration, solved for the velocities along the coordinate axes. Datasets created using Release 6.1 or earlier containing the ≫ SALT TRANSPORT subcommand should not be used in Release 6.2 or later of NAMMU without modification because the boundary conditions contained in an old dataset will be inconsistent with the new form of the salt transport equations.

9.3.1 Initial Conditions

It is important to supply the solver with a suitable initial condition because the salt transport equations are non-linear. One symptom of an inappropriate initial condition is a singular front matrix. Another symptom is failure of the Newton-Raphson iterations to converge. In Dataset 9.1 a suitable initial condition is provided by solving the pressure equation on its own.

The subcommand ≫ CHANGE EQUATION DICTIONARIES is used to select a subset of the equations for solution. The example below solves the pressure equation on its own for the two-variable formulation.

```
>> SOLVER DATA
   >> STEADY STATE
      MAXIMUM FRONTWIDTH   50
      NUMBER OF ITERATIONS  2
      END

     >> SALT TRANSPORT
        PRES CONC FORMULATION
        END

        >> CHANGE EQUATION DICTIONARIES
           VARIABLE SELECT   'PRES'  'CONC'
           EQUATION SELECT   'PRES'
           END
```

The subcommand ≫ CHANGE EQUATION DICTIONARIES has two commonly used keywords. VARIABLE SELECT is used to tell the solver which variables are to be made available to the solver; usually the list of variables used when the full set of equations is solved. EQUATION SELECT tells the solver which variables are to be updated during this solve. The example above solves the salt transport equation for a specified salt distribution, holding the salt variable fixed. This provides a suitable pressure distribution to be used as an initial guess for a fully coupled calculation.

9.3.2 Transient Calculations

NAMMU contains four solver options for transient problems (Section 5.2). The most suitable time-stepping option for use in ≫ SALT TRANSPORT calculations is ≫ CRANK NICHOLSON. Coupled groundwater flow and transport of salinity calculations are highly non-linear so the ≫ FAST LINEAR TRANIENT solver option should never be used for these calculations. The other two time-stepping options use Gear's method to determine the size of the time step. Gear's method is not really suitable for coupled groundwater flow and transport of salinity calculations because here the main control on the size of the time steps is the convergence of the non-linear iterations rather than the error in the solution.

It is often possible to increase the time step as a calculation proceeds because the time

scale over which the solution is changing increases. Changes in the time step size may be implemented using a number of consecutive ≫ CRANK NICHOLSON commands. The convergence of the non-linear iterations must be checked for every time step. In ≫ SALT TRANSPORT calculations, the maximum time step size for which the non-linear iterations will converge sometimes decreases temporarily as the calculation proceeds. If the non-linear iterations fail to converge for any time step all subsequent time steps will be invalid.

It is therefore recommended that the ≫ AUTOMATIC TIMESTEPPING subcommand of ≫ CRANK NICHOLSON is used. This option choses the timestep size automatically depending on the convergence of the non-linear iterations.

9.3.3 Large Density Contrasts

In cases where the density contrasts, and hence non-linearities, are large it may not be possible to provide an initial guess that is close enough to the final solution for the non-linear iterations to converge. In these cases it is necessary to use a parameter-stepping strategy. Such a strategy may also be necessary to provide a suitable initial condition for a transient calculation.

A strategy that is often successful for a calculation with a small diffusion coefficient and the longitudinal dispersion length, α_{L} larger than the transverse dispersion length, α_{T} is:

1. Obtain a solution using a large value of the diffusion coefficient and large values of the dispersion lengths. $\alpha_{\mathrm{L}} = \alpha_{\mathrm{T}} \sim$ size of largest element are often good values to use.
2. Step the diffusion coefficient down to the desired value by using several ≫ SOLVER DATA stages. For each ≫ SOLVER DATA stage the output of the previous solve is used as the initial condition and the diffusion coefficient is reset using the ≫ PHYSICAL PROPERTIES command (see Section 3.14).
3. Reduce α_{L} and α_{T} together in stages until both are equal to the desired value of α_{L}.
4. Reduce α_{T} in stages to the desired value.

9.4 Output

Figures 9.2 and 9.3 show the contour plots of the pressure and the fluid density from Dataset 9.1. ≫ SALT TRANSPORT calculations do not require any special output options when the plotting is done in the same run as the solve. When post-processing global freedoms from ≫ SALT TRANSPORT calculations the keyword VARIABLE SALINITY CALCULATION should be specified under ≫ SET PLOT OPTIONS. Similar keywords exist for specifying that the global freedoms were obtained from an unsaturated or a heat transport calculation. If global freedoms obtained from a ≫ SALT TRANSPORT calculation are restored for use in a nuclide transport calculation the keyword SALT TRANSPORT of the subcommand ≫ NUCLIDE TRANSPORT will be required.

Figures for Section 9

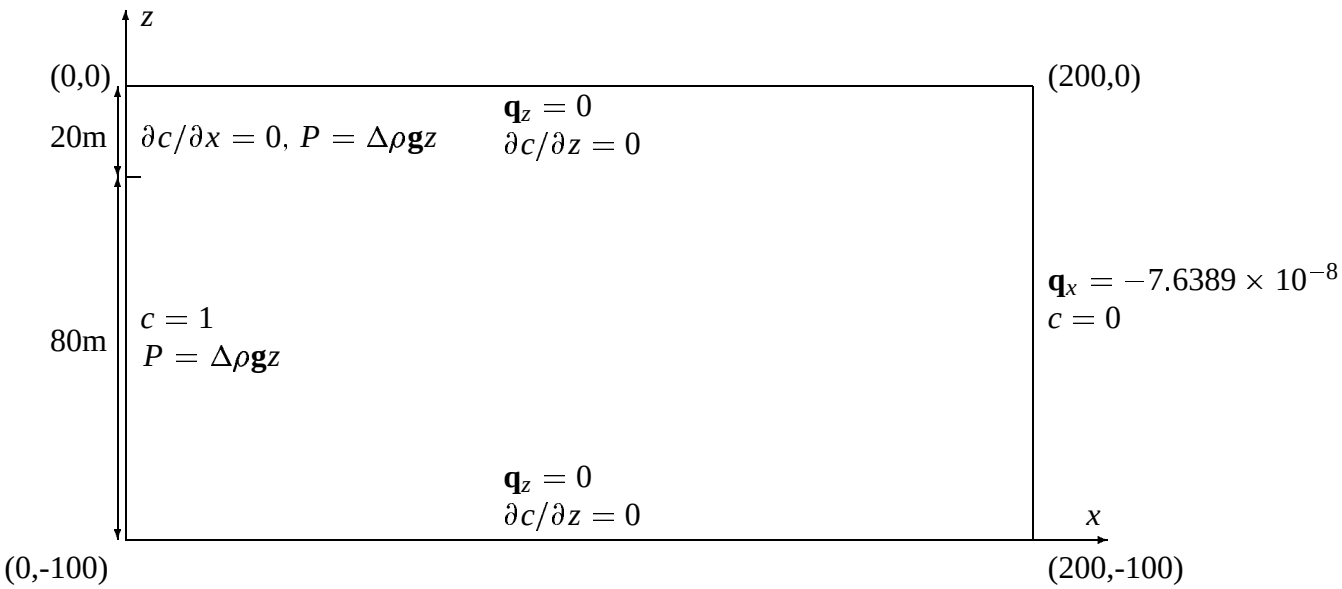


Figure 9.1 Domain and boundary conditions for the Henry Test Case. SI units.

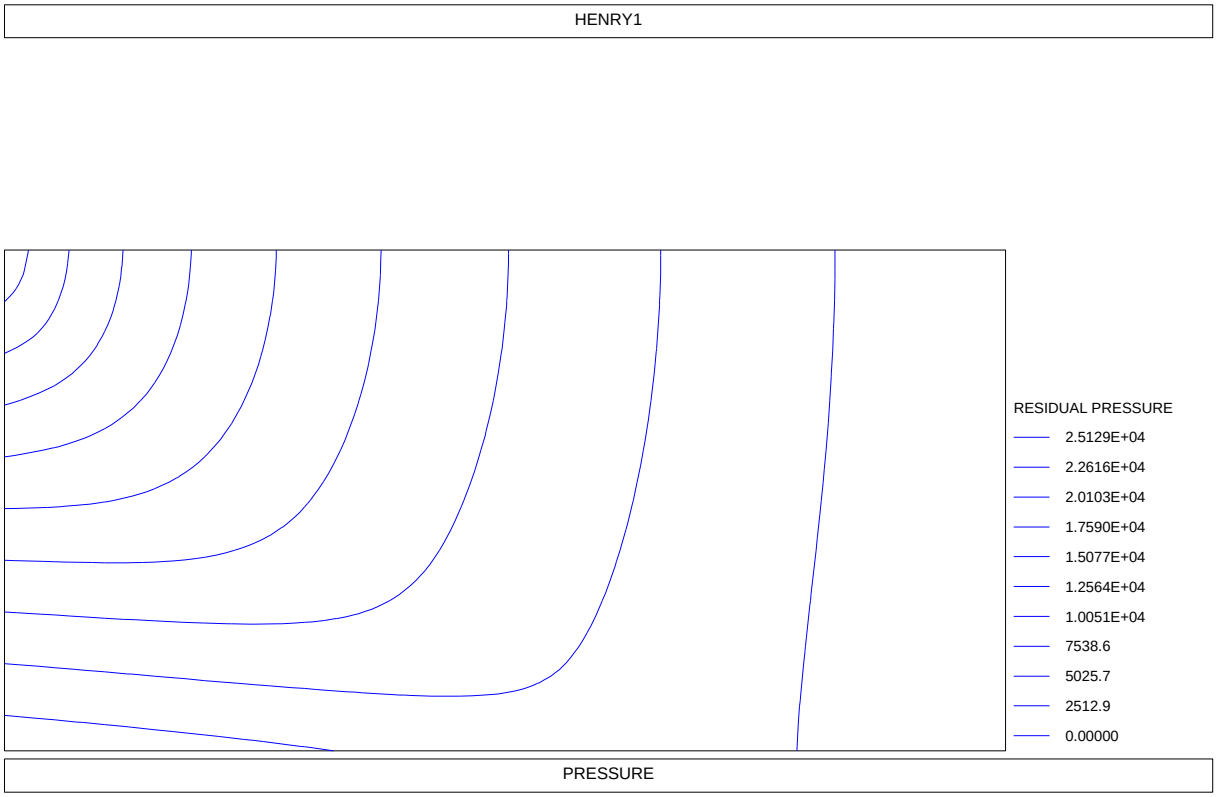


Figure 9.2 Residual pressure contours for the Henry Test Case.

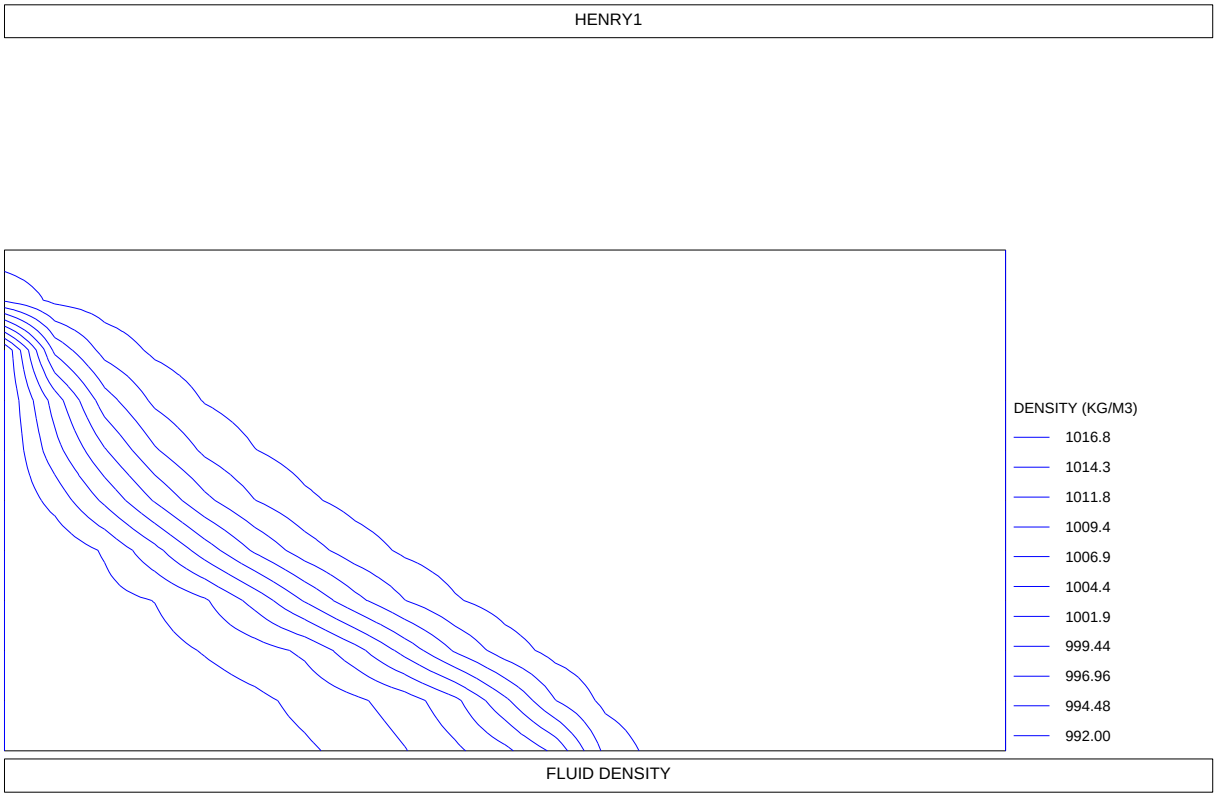


Figure 9.3 Contours of fluid density for the Henry Test Case.

Dataset 9.1

```
   /* NAMMU TEST CASE HENRY1                                          */
   /*                                                                 */
   /* DISPERSION = 20M,2M DIFFUSION = 0                               */
   /* DEFAULT FORMULATION                                             */

   /* SPACE ALLOCATION                                                */
   /* INTEGER WORKSPACE  500000                                       */
   /* REAL WORKSPACE     250000                                       */

   /* INLINE FORTRAN
      SUBROUTINE BNDVAL(X,NSD,V,IV,NVARS)

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)

      DIMENSION X(NSD),V(NVARS)

      COMMON /GRAVIT/ G
      COMMON /REFDEN/ RHOF0
      COMMON /FPSALT/ RHOBRN,ALPHAS,BETAS

      RHO = RHOBRN - RHOF0
      IF (IV .EQ. 1) THEN
        V(IV) = -RHO*G*X(2)
      END IF

      RETURN
      END
                                                                      */
   /* SOURCE FILES                                                    */
   /* COMPILED FILES                                                  */
   /* LIBRARY FILES                                                   */

   /* INPUT DATA FILES                                                */
   /* OUTPUT DATA FILES                                               */
   /* 6        nammu/output/henry1.out                                */
   /* GRAPHICS nammu/output/henry1.ps                                 */

   /* END JOB INFORMATION                                             */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS                      200
      NODES                        1000
      FRONTWIDTH                    100
      INTEGER BC WORKSPACE         2000
```

```
      REAL BC WORKSPACE              400
      PARAMETERS PER FUNCTION TYPE     9
      FUNCTION TYPES PER ELEMENT       3
      VARIABLES                        2
      END

   >> SET VARIABLES
      VARIABLE NAMES  'PRES' 'CONC'
      END

   >> SET INTERPOLATION TYPES
      BASIS FUNCTION TYPES  1 3
      ELEMENT NAME          'Q9/1'
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      DENSITY OF SALT SOLUTION          1016.8
      FLUID DENSITY                      992.0
      SALT DIFFUSION COEFFICIENT           0.0

      ROCK TYPE PERMEABILITIES
      ROCK NAME,    KXX,        KYY,      KXY
      'MATRIX'   1.1893E-12  1.1893E-12   0.0

      ROCK TYPE PROPERTIES
      ROCK NAME,  POROSITY
      'MATRIX'      0.35

      ROCK TYPE PROPERTIES
      ROCK NAME,  LONGITUDINAL DISPERSION LENGTHS OF SALT
      'MATRIX'                20.0

      ROCK TYPE PROPERTIES
      ROCK NAME,  TRANSVERSE DISPERSION LENGTHS OF SALT
      'MATRIX'                2.0
      END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         QUADRILATERAL ELEMENT TYPE   'Q9/1'

         PATCH SPACING IN FIRST DIRECTION
         SIZE
          20

         PATCH SPACING IN SECOND DIRECTION
         SIZE
```

```
          8
          2

        PATCH POSITIONS
        CORNER NUMBER,      COORDINATES
             101         <   0.0  -100.0 >
             102         < 200.0  -100.0 >
             201         <   0.0   -20.0 >
             202         < 200.0   -20.0 >
             301         <   0.0     0.0 >
             302         < 200.0     0.0 >

        PATCH TOPOLOGY
        PATCH TYPE,       CORNERS,        INDICES,   ROCK NAME
          'SQQ9'    < 101 102 202 201 >   < 1  1 >   'MATRIX'
          'SQQ9'    < 201 202 302 301 >   < 1  2 >   'MATRIX'
        END

   >> MODIFY GRID

      >> RENUMBER ELEMENTS

         >> SLOAN ALGORITHM
            END

   >> SET BOUNDARY CONDITIONS

/* RIGHT BOUNDARY - FRESH WATER INPUT */
      >> SPECIFIED VALUE

         >> CONSTANT VALUE
            VARIABLES  'CONC'
            VALUES     0.0
            END

            >> SELECT LINE
               START POINT  200.0 -100.0
               END POINT    200.0    0.0
               PRECISION      1.0E-4
               END

/* PRESSURE = RHO_F*SPECIFIED HORIZONTAL VELOCITY  */
      >> SPECIFIED FLUX

         >> CONSTANT VALUE
            VARIABLES  'PRES'
            VALUES     -7.57779E-5
            END

            >> SELECT LINE
               START POINT  200.0 -100.0
               END POINT    200.0    0.0
               PRECISION      1.0E-4
               END
```

```
/* LEFT BOUNDARY - SALT WATER INTRUSION    */
      >> SPECIFIED VALUE

         >> CONSTANT VALUE
            VARIABLES  'CONC'
            VALUES     1.0
            END

            >> SELECT LINE
               START POINT    0.0 -100.0
               END POINT      0.0  -20.0
               PRECISION      1.0E-4
               END

      >> SPECIFIED VALUE

         >> CALL SUBROUTINE BNDVAL
            VARIABLES  'PRES'
            END

            >> SELECT LINE
               START POINT    0.0    0.0
               END POINT      0.0 -100.0
               PRECISION      1.0E-4
               END

      >> GENERALISED FLUX LAW
         VARIABLES                 'CONC'
         ZERO DISPERSIVE FLUX
         END

         >> SELECT LINE
            START POINT    0.0    0.0
            END POINT      0.0  -20.0
            PRECISION      1.0E-4
            END


>> OUTPUT DATA

   >> PAGE SETUP
      LANDSCAPE
      END

   >> SET PLOT OPTIONS
      HEADING         'HENRY1'
      BOUNDARY COLOUR 'BLACK'
      GRID COLOUR     'BLACK'
      END

   >> PLOT BOUNDARY
      END
```

```
   >> PLOT GRID
      END


/* SOLVE PRESSURE EQUATION TO SET UP INITIAL CONDITION FOR COUPLED SOLVE */
>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH     50
      NUMBER OF ITERATIONS    2
      END

      >> SALT TRANSPORT
         PRES CONC FORMULATION
         END

         >> CHANGE EQUATION DICTIONARIES
            VARIABLE SELECT 'PRES' 'CONC'
            EQUATION SELECT 'PRES'
            END


>> OUTPUT DATA

   >> PLOT CONTOURS
      VARIABLE            'PRES'
      NUMBER OF CONTOURS  11
      CAPTION             'INITIAL PRESSURE'
      KEY TITLE           'RESIDUAL PRESSURE'
      END


/* FULL COUPLED SOLVE  */
>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH    100
      NUMBER OF ITERATIONS   25
      END

      >> SALT TRANSPORT
         PRES CONC FORMULATION
         END


>> OUTPUT DATA

   >> PLOT CONTOURS
      VARIABLE            'PRES'
      NUMBER OF CONTOURS  11
      CAPTION             'PRESSURE'
      KEY TITLE           'RESIDUAL PRESSURE'
      END
```

```
>> PLOT CONTOURS
   VARIABLE            'CONC'
   CONTOUR VALUES      -0.1 TO 1.0 BY 0.1
   COLOURS             'RED' 'BLACK' 'BLUE' 'BLUE' 'BLUE' 'BLUE' 'BLUE' +
                                     'BLUE' 'BLUE' 'BLUE' 'BLUE' 'BLUE'
   CAPTION             'SALT CONCENTRATION'
   KEY TITLE           'CONCENTRATION'
   END

>> PLOT CONTOURS
   FLUID DENSITY
   NUMBER OF CONTOURS  11
   CAPTION             'FLUID DENSITY'
   KEY TITLE           'DENSITY (KG/M3)'

>> DRAW LINE GRAPH
   VARIABLE            'PRES'
   START POINT           0.0  -85.0
   END POINT           200.0  -85.0
   NUMBER OF POINTS    200
   X AXIS LABEL RANGE    0.0  200.0
   X AXIS TITLE        'DISTANCE'
   Y AXIS TITLE        'PRESSURE'
   NO SYMBOLS
   JOIN POINTS
   CAPTION             'PRESSURE PROFILE AT Z=-85M'
   END

>> CALCULATE LINE INTEGRAL
   FLUID MASS FLUX
   NORMAL COMPONENT
   NUMBER OF POINTS PER SEGMENT 100
   NUMBER OF SEGMENTS 5

   SEGMENTS
   SEGMENT END POINTS
   <   0.0     0.0 >
   <  200.0    0.0 >
   <  200.0 -100.0 >
   <    0.0 -100.0 >
   <    0.0  -20.0 >
   <    0.0    0.0 >

>> CALCULATE LINE INTEGRAL
   ADVECTIVE FLUX OF SALT
   NORMAL COMPONENT
   NUMBER OF POINTS PER SEGMENT 100
   NUMBER OF SEGMENTS 5

   SEGMENTS
   SEGMENT END POINTS
   <   0.0     0.0 >
   <  200.0    0.0 >
   <  200.0 -100.0 >
```

```
      <    0.0 -100.0 >
      <    0.0  -20.0 >
      <    0.0    0.0 >

   >> CALCULATE LINE INTEGRAL
      DISPERSIVE FLUX OF SALT
      NORMAL COMPONENT
      NUMBER OF POINTS PER SEGMENT 100
      NUMBER OF SEGMENTS 5

      SEGMENTS
      SEGMENT END POINTS
      <   0.0     0.0 >
      <  200.0    0.0 >
      <  200.0 -100.0 >
      <    0.0 -100.0 >
      <    0.0  -20.0 >
      <    0.0    0.0 >

   >> CALCULATE LINE INTEGRAL
      TOTAL FLUX OF SALT
      NORMAL COMPONENT
      NUMBER OF POINTS PER SEGMENT 100
      NUMBER OF SEGMENTS 5

      SEGMENTS
      SEGMENT END POINTS
      <   0.0     0.0 >
      <  200.0    0.0 >
      <  200.0 -100.0 >
      <    0.0 -100.0 >
      <    0.0  -20.0 >
      <    0.0    0.0 >


>> STOP
```

10 EXAMPLE 8: ADJOINT SENSITIVITY ANALYSIS (2D PACOMA FLOW AND TRANSPORT MODELS)

10.1 Motivation for Calculating Sensitivities

Often there is uncertainty about the values of parameters, such as the hydrogeological properties and boundary conditions, used in numerical models. This naturally leads to uncertainty in the quantities (termed "performance measures" in this Section) predicted by a numerical model e.g. pressure or Darcy velocity at a point. In the context of the safety assessment of underground repositories for radioactive waste, performance measures of interest include the specific discharge in the vicinity of the repository, groundwater transit-times, and fluxes of radionuclides to the environment. The uncertainty in performance measures implied by the uncertainty in the parameters may only be one contribution to the overall uncertainty, others being uncertainties in the conceptual model, surface and subsurface geologies, and the description of the physics. However, it is useful to be able to quantify the uncertainty arising from the uncertainty in these parameters, and to identify those parameters which contribute most to the uncertainty. A first-order estimate of uncertainty can be obtained from the sensitivities of the performance measure to parameter variations, together with the mean and variance of the input parameters.

The calculation of sensitivities is often an important stage in methods used to solve inverse problems. In such cases, performance measures of a model are defined as some norm of the discrepancy between quantities predicted by the model and those measured in the field. For example, if piezometric head has been measured at several monitoring locations, a performance measure can be defined as the average of the square of the difference between the predicted and observed heads. Inverse methods, such as Gauss-Newton, use sensitivities in an iterative approach to minimize the performance measure, and so identify the range of parameters which give the best fit to the observed data.

10.2 Advantages of the Adjoint Method

To calculate sensitivities by explicitly varying each parameter in turn can be laborious and sometimes impractical for numerical models because of the large number of parameters involved. Typically, there will be a permeability tensor, porosity, and perhaps transport parameters specified for each rock stratum, and there may be ten or more strata. In addition, there are the boundary conditions. Hence, it may require several tens or even hundreds of simulations of the numerical model to compute all the sensitivities by explicit variation.

In contrast, adjoint sensitivity theory [21] offers a numerical method (the "adjoint method") which has the advantage that one can compute the sensitivities to all the parameters for a cost comparable with that of a single simulation of the numerical model. Generally, the adjoint method is an efficient way to calculate sensitivities provided that the number of parameters is larger than the number of performance measures of interest.

10.3 Methodology

In the adjoint method a set of adjoint equations are derived from the original model equations (e.g the groundwater flow equations). The derivation of the adjoint equations for the NAMMU groundwater flow, nuclide transport, and salt transport equations is detailed in [22]. The solutions of the adjoint equations are termed the "adjoint state variables". Sensitivity coefficients are evaluated from integrals of functions of both the adjoint state and original variables over the domain and boundary of the model. The sensitivity coefficients are exact derivatives (except for numerical round-off) of the performance measure with respect to the parameters, taken about the specified parameter values.

In the discrete form, the adjoint equations define a discrete system matrix which depends only on the original model and equations, and not on the user-defined performance measure. The performance measure only affects the right-hand-side, or residual, vector. This is an important point to note for the numerical implementation. If the sensitivities of a number of performance measures are required, then the most efficient way of carrying out the adjoint sensitivity calculations is to compute the factorization of the adjoint system matrix once, and reuse it to calculate the adjoint state variables for each performance measure. The procedure for doing this in NAMMU is described in the following sections.

10.4 Implementation of the Adjoint Method in NAMMU

The adjoint method has been implemented in NAMMU for standard and mixed-element formulations of the steady-state groundwater flow equations, and the standard formulation of the steady-state nuclide transport equations.

The computation of the sensitivity coefficients using the adjoint method in NAMMU typically involves the following stages:

1. define the model, including the finite-element grid and boundary conditions (e.g. a model of groundwater flow);
2. solve the model equations (e.g. solve the groundwater flow equations);
3. specify the performance measure of interest (e.g. the velocity at a point);
4. solve the adjoint equations;
5. compute the sensitivity coefficients.

The first two stages in this sequence are carried out in the usual way.

10.4.1 Defining the Performance Measure

For stage 3, the user has to return to the MODEL DATA phase and specify a performance measure (the various option are described in Sections 10.5.1 and 10.6.1, and in the NAMMU

Reference Manual [7]). The type of performance measure required is specified using the

```
>> MODIFY BOUNDARY CONDITIONS
```

command together with the subcommand

```
>> DEFINE PERFORMANCE MEASURE.
```

In the discrete system, a performance measure can always be expressed as the sum of a function of the variables evaluated at a set of discrete points (the "measure points"). The above commands automatically set up the correct right-hand-side for the discrete adjoint equations for later use in the solver stage.

10.4.2 Solving the Adjoint Equations

In stage 4, the adjoint equations corresponding to the original model equations are solved for the adjoint state variables. Generally, an adjoint state variable is introduced for each of the variables used in the original model equations. The adjoint state variables are stored in the same positions as the original variables, except they are on the second level of the global freedom vector. For example, in the standard formulation of the groundwater flow equations, residual pressure is the only variable used and is stored in the first variable position, so a single adjoint state variable is introduced in the first variable position on the second level.

Two SOLVER DATA options have been created for the adjoint method. The correct solver option to choose depends on whether a factorization (also known as a "LU-decomposition") of the discrete adjoint system matrix is available, and whether the discrete system matrix for the original problem is the same as for the adjoint problem. In the latter case, the original problem is said to be "self-adjoint". The first option does not rely on the original equations being self-adjoint or on a factorization of the discrete adjoint system matrix being available. This option takes an existing solution of the original model equations and solves the adjoint equations by full Newton-Raphson iteration (i.e. no use is made of an existing LU-decomposition). This is intended for cases where either the LU-decomposition from the original solution is not available, or for physics such as solute transport, where the equations are not self-adjoint. This solver option is invoked by the command

```
>> STEADY STATE ADJOINT ANALYSIS
```

The second solver option was primarily designed for use on the groundwater flow equations, which are self-adjoint. However, it can also be used when an LU-decomposition of the adjoint system matrix has been calculated in an earlier run and restored from disk. For the groundwater flow equations the same LU-decomposition is used to solve for both pressure and the adjoint state variable. This option is invoked by the command

```
>> SELF ADJOINT ANALYSIS
```

For the performance measures that involve the evaluation of pressure or velocity at points specified by the user, it is most efficient to reverse stages 2 and 3 in the sequence above. That is, the user can specify the performance measure along with the pressure boundary conditions, and then solve for pressure and the adjoint state variable simultaneously using the same LU-decomposition (see Section 10.5.2). Alternatively, the user may solve the groundwater flow calculations, saving the LU-decomposition, and then reuse the LU-decomposition to solve the adjoint equation by a single quasi Newton-Raphson iteration later on. This is useful if the travel time performance measure is selected, since the measure points correspond to discrete points on a particle path, which can only be calculated from the results of a previous groundwater flow calculation (see Dataset 10.1). In this case the following keywords should be included to reduce time spent in solving the adjoint problem:

```
USE SAVED LU DECOMPOSITION
NUMBER OF QUASI ITERATIONS 1
```

For general physics, this option is also useful when the sensitivities are required for a number of performance measures. In such cases the model (Fortran stream 4) and global freedoms (Fortran stream 50) should be saved after solving the original problem. In addition, the LU-decomposition of the adjoint system matrix (Fortran streams 11, 12, 13 and 14) should be saved after solving the adjoint problem for the first performance measure. It is then necessary to create a dataset for each additional performance measure. Each dataset should contain instructions to restore the model, global freedoms and LU-decomposition, define the performance measure, solve the adjoint equation and calculate the sensitivity coefficients.

10.4.3 Calculating Sensitivities

Having obtained solutions for the original and adjoint model equations, various sensitivities can then be computed by selecting the command

```
>> CALCULATE SENSITIVITY COEFFICIENTS
```

in the OUTPUT DATA phase. Three different sets of sensitivity coefficients are given for each parameter, these are the “direct”, “marginal” and “normalised” sensitivity coefficients. The direct sensitivity is defined as the derivative of the performance measure with respect to a parameter holding the variables fixed. For example, if the performance measure is the total specific discharge at a point in some one-dimensional problem, then from equation (x.x) in Reference [8] the direct sensitivity to the permeability k is

$$\frac{\partial q}{\partial k} = -\frac{1}{\mu}\frac{\partial P^{\mathrm{R}}}{\partial x} \tag{10.1}$$

The marginal sensitivity combines the direct sensitivity with any indirect sensitivity that arises from a change in the variables as the parameter varies. The marginal sensitivity represents a local derivative in the performance measure, taken at the specified parameter value. That is, it describes the change in the performance measure for a unit change in the parameter. Thus, in the above simple example the marginal sensitivity would be dq/dk and would include a term in the rate of change of pressure with respect to permeability. By multiplying the marginal sensitivity by the ratio of the parameter value to the value of the performance measure, the normalised sensitivity is obtained. One way of regarding the normalised sensitivity is that it represents the percentage change in the performance measure for a 1% change in the parameter. All of the sensitivity coefficients are written in the output file in a tabular format.

For groundwater flow calculations, sensitivities are given for each permeability parameter, and each porosity. For nuclide transport, sensitivities are also given for each dispersion length, tortuosity, and for the molecular diffusion.

Sensitivities to rock properties are calculated for each rock unit rather than for each element. This involves an integration of various functions of the original and adjoint state variables over all the elements with the appropriate rock type. The sensitivity to a sub-region of any particular rock strata can be obtained by restricting the domain of integration using the keyword `USE PLOT CRITERION`. Shaded plots of the normalised sensitivity to the parameters as defined on each element can also be obtained. For example the sensitivities to the horizontal permeability are obtained by specifying the command

```
>> PLOT GRID
   KXX SENSITIVITY
```

along with the required colours and interval values.

For groundwater flow in two dimensions, the sensitivities to the boundary conditions specified at each node are also calculated. Sensitivities to boundary conditions are calculated at each node for which a ≫ `SPECIFIED VALUE`, ≫ `SPECIFIED FLUX` or ≫ `NODAL DELTA FUNCTION` type boundary condition has been set. For prescribed pressure boundary conditions it is necessary to compute the normal to the boundary. Since this normal is not well defined at the corners of elements, it was necessary to adopt a suitable convention. The convention chosen was to take the boundary condition sensitivities at a corner node to be the average of the values obtained on each of the adjoining edges. At present, the calculation of sensitivities to boundary conditions has only been implemented in two dimensions.

10.5 Steady-State Groundwater Flow Sensitivities

The implementation of the adjoint method for steady-state groundwater flow is described in greater detail in [23]. The performance measures that are available for calculations of steady-state groundwater flow are described in Section 10.5.1. An example of the input

data structure required to compute the sensitivities of the velocity at a point is given in Section 10.5.2. An example of how the adjoint sensitivity method in NAMMU can be used to estimate the sensitivities of the travel time along a pathline is presented in Section 10.5.3.

10.5.1 Performance Measures

The performance measures available within NAMMU for groundwater flow are as follows:

1. the total specific discharge at a point. This could be used to quantify the uncertainties in the flow rates in the vicinity of a repository;
2. the x-component of specific discharge squared at a point.
3. the y-component of specific discharge squared at a point.
4. the z-component of specific discharge squared at a point.
5. an area-weighted velocity magnitude at a point. If each velocity component is weighted by an effective length (cross-sectional area in three-dimensions) of a repository, then this performance measure can be used to estimate the uncertainty in the groundwater flux out of the repository;
6. the pressure at a point.
7. a weighted average pressure error over a set of points. This is useful in calibration exercises where measurements of pressure are available. The adjoint sensitivity method may then be used as a part of an optimization method to obtain ranges of parameters that best fit the measurements;
8. the travel time along a pathline or portion of a pathline. This could be used in an assessment to quantify the uncertainties in groundwater travel times from the repository.

10.5.2 Velocity Sensitivities

Here is a schematic example of the input data structure required to compute the sensitivity of the total specific discharge at a point. The input data structure for any of the first seven performance measures given in Section 10.5.1 would be very similar to this. In the cases of the area-weighted velocity and weighted average pressure error performance measures, the user needs to specify extra information in order to define the performance measure (see the NAMMU Reference Manual [7]). The computation of velocity sensitivities using NAMMU follows a definite sequence:

1. define the model for groundwater flow;
2. specify the velocity performance measure;

3. solve groundwater flow and adjoint equations;

4. compute the sensitivity coefficients.

As an example, the sequence of commands and keywords used in a NAMMU input data set to perform an adjoint sensitivity analysis of the velocity at the point $(3500, -10)$ would be of the following form (only the more important commands are listed).

Stage 2:

```
>> MODIFY BOUNDARY CONDITIONS
   >> DEFINE PERFORMANCE MEASURE
      >> VELOCITY PERFORMANCE MEASURE
         COORDINATES   3500. -10.
         VARIABLES      'PRES'
```

Stage 3:

```
>> SOLVER DATA
   >> SELF ADJOINT ANALYSIS
      >> GROUNDWATER FLOW
```

Stage 4:

```
>> OUTPUT DATA
   >> CALCULATE SENSITIVITY COEFFICIENTS
```

10.5.3 Travel Time Sensitivities (Dataset 10.1)

In order to apply the adjoint method to the travel time along a path, the performance measure is expressed as a function of the parameters and the pressures at a set of discrete measure points along the path. The set of measure points is in fact a subset of the points used to calculate the path in the pathline algorithm. The rediscretisation of the path (i.e the number of measure points) can be controlled by the user as described below. In more precise terms, the travel time can then be written as a sum over the measure points of increments in the path length divided by the pore water velocity

$$\sum_{k=1}^{N} s_k/(|q(\mathbf{x}_k)|/\phi), \tag{10.2}$$

where N is the number of points $\mathbf{x}_k$ used to discretize the path, s_k is the pathlength between points, q is the specific discharge, and ϕ is the porosity. This estimate of the travel time along a path improves as the spacing between the selected points decreases.

The groundwater travel time sensitivities are computed by holding the position of the path fixed and letting the magnitude of the velocities at the measure points vary with the system parameters. That is, it is assumed that a perturbation of a system parameter does not result in a change in the increments of the displacement s_k, but does change the magnitude of the pore water velocity $|q(\mathbf{x_k})|/\phi$. Thus, the performance measure is in effect a sum of the inverse of the pore water velocity at the measure points with a weighting s_k. The value of s_k is taken as the mean of the distances between the measure point $\mathbf{x}_k$ and its two neighbouring measure points.

The fact that the positions of the measure points depend on the results of the groundwater flow calculation means that it may be difficult to predict how the travel times will change in response to large perturbations in the system parameters. For small perturbations in the system parameters the pathline may change little, and the variation in travel time will be largely due to changes in the magnitude of the velocity at the measure points. This is because small changes (say 10%) in permeability will result in a similar change in the specific discharge and hence in the travel time over a pathline segment. By contrast, a small deviation from the original position of the path will have much less effect on the overall path length. If the positions of the end of a straight path segment moves by a distance equal to 10%, say, of the original length of the segment, perpendicular to the original path, then the change in the path length is about 0.5%. The corresponding change in the travel time is then also about 0.5%.

The computation of travel time sensitivities using NAMMU follows a definite sequence of operations:

1. define the model for groundwater flow;
2. solve for groundwater flow and save the LU decomposition;
3. calculate and save a pathline;
4. specify the travel time performance measure;
5. solve for the adjoint state variable;
6. compute the sensitivity coefficients.

The first two stages in this sequence are specified as they would be for a solution of the steady state groundwater flow alone, with the exception that the `SAVE L` option must be included to save the complete LU-decomposition of the discrete coefficient matrix. In stage 3 the pathline that is to be analysed is specified using the usual ≫ `PATHLINES` command, except the extra keyword `SAVE PATH FOR SENSITIVITY ANALYSIS` is required to specify that the path is to be saved. If more than one path has been calculated, only the first will be saved for an adjoint analysis. The user may also specify how fine a discretisation of the pathline is required for the adjoint analysis using the keyword `MAXIMUM NUMBER`

OF EXTRA GAUSS POINTS. The discretisation used for the adjoint analysis is allowed to differ from that used to initially compute the pathline. Thus, the path itself may be calculated very accurately, using a fine discretisation of the path (by specifying a low value for the ACCURACY PARAMETER keyword), but then the path may be restricted to a coarser rediscretisation for the adjoint analysis. The advantages of this are that the the number of operations performed in the solver phase is reduced. Of course, if the rediscretisation of the pathline is very coarse then the approximation of the travel time is likely to be inaccurate.

It should be noted that the number of Gauss points set in the ≫ SET LIMITS command should be at least the sum of the number of extra Gauss points used for the adjoint analysis and the standard number of Gauss points required by the finite-element integration scheme.

The travel time performance measure is specified in stage 4 in a similar manner to pressure and velocity performance measures. For stage 5, ≫ SELF ADJOINT ANALYSIS is the most efficient solver option since it makes use of the LU-decomposition already carried out in the groundwater flow solve. Finally the sensitivity coefficients are calculated in stage 6.

Thus, the sequence of commands and keywords used in a NAMMU input data set to perform an adjoint analysis for travel time would be of the form shown in the following example (only the more important commands are listed).

Stage 2:

```
>> SOLVER DATA
   >> STEADY STATE
      SAVE L
      >> GROUNDWATER FLOW
```

Stage 3:

```
>> OUTPUT DATA
   >> PATHLINES
      SAVE PATH FOR SENSITIVITY ANALYSIS
      ROCK TYPES FOR SENSITIVITY ANALYSIS  2  5
      MAXIMUM NUMBER OF EXTRA GAUSS POINTS  5
```

Stage 4:

```
>> MODEL DATA
   >> MODIFY BOUNDARY CONDITIONS
      >> DEFINE PERFORMANCE MEASURE
         >> TRAVEL TIME PERFORMANCE MEASURE
```

Stage 5:

```
>> SOLVER DATA
   >> SELF ADJOINT ANALYSIS
      USE SAVED LU DECOMPOSITION
      NUMBER OF QUASI ITERATIONS 1
      >> GROUNDWATER FLOW
```

Stage 6:

```
>> OUTPUT DATA
   >> CALCULATE SENSITIVITY COEFFICIENTS
```

The keyword ROCK TYPES FOR SENSITIVITY ANALYSIS may be used if the sensitivities of the travel times in a restricted number of layers is required. For example, in this case only the travel time through the regions with property types 2 and 5 will be the performance measure. By setting the MAXIMUM NUMBER OF EXTRA GAUSS POINTS to 5 the number of path points saved within any element is restricted to being not greater than 5. If the number of points used by the pathline algorithm exceeds 5 in any element, then the first and last path points are saved together three more points selected uniformly from the points in between.

An example of a calculation of travel time sensitivities is provided in Dataset 10.1. The example corresponds to the PACOMA two-dimensional groundwater flow calculation already described in Section 6. Sensitivities are calculated for the travel time along a pathline that originates in the repository region, as shown in Figure 10.1. A sample of the sensitivity coefficient information produced in the output file is given below.

The approximation to the travel time created by the rediscretisation of the pathline is printed first. This is followed by the direct, marginal and normalised sensitivities to each permeability component and the porosity for each rock type. Rock type 1 corresponds to the first rock in the ROCK TYPE table, which is the Chalk in this case. Next, the sensitivities to specified value type boundary conditions are given for each node at which a Dirichlet condition has been set. Finally, if the grid has been shaded according to the sensitivity of a given parameter, the approximation to the travel time is printed again and a table of the normalised sensitivities to each element is printed. The last column in the table gives the approximation to the travel time created by the rediscretization of the pathline.

```
APPROXIMATION OF TRAVEL TIME USED IN SENSITIVITY ANALYSIS  6.6398064E+05


 ROCK TYPE SENSITIVITY COEFFICIENTS
 ----------------------------------



DIRECT SENSITIVITY COEFFICIENTS W.R.T PERMEABILITIES
```

TYPE	KXX	KYY	KZZ	KXY	KYZ	KZX
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	-8.3568E+20	-4.8460E+23	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	-4.9175E+17	-6.4714E+13	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

MARGINAL SENSITIVITY COEFFICIENTS W.R.T PERMEABILITIES

TYPE	KXX	KYY	KZZ	KXY	KYZ	KZX
1	-4.0472E+13	3.8374E+13	0.0000E+00	1.2505E+16	0.0000E+00	0.0000E+00
2	-8.3202E+20	-7.8540E+23	0.0000E+00	2.1269E+21	0.0000E+00	0.0000E+00
3	-1.7587E+16	1.7173E+13	0.0000E+00	1.0187E+16	0.0000E+00	0.0000E+00

NORMALISED SENSITIVITY COEFFICIENTS W.R.T PERMEABILITIES

TYPE	KXX	KYY	KZZ	KXY	KYZ	KZX
1	-2.0114E-05	1.9072E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	-1.6290E-02	-9.6995E-01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	-1.3773E-02	1.3449E-05	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

DIRECT SENSITIVITY COEFFICIENTS W.R.T POROSITIES

TYPE	PHI
1	0.0000E+00
2	1.3169E+06
3	7.5218E+05

MARGINAL SENSITIVITY COEFFICIENTS W.R.T POROSITIES

TYPE	PHI
1	0.0000E+00
2	1.3169E+06
3	7.5218E+05

NORMALISED SENSITIVITY COEFFICIENTS W.R.T POROSITIES

TYPE	PHI
1	0.0000E+00
2	6.1484E-01
3	3.8516E-01

BOUNDARY CONDITION SENSITIVITY COEFFICIENTS

SENSITIVITY COEFFICIENTS W.R.T BOUNDARY CONDITIONS

TYPE	NODE	COORDINATES		MARGINAL	NORMALISED
SPECIFIED VALUE	1	0.0000E+00	1.0937E+02	2.6272E-08	4.2114E-08
SPECIFIED VALUE	6	4.1435E+00	1.0937E+02	-9.0495E-05	-1.4506E-04
SPECIFIED VALUE	11	8.2869E+00	1.0936E+02	-6.7938E-05	-1.0890E-04

```
     .            .      .          .          .            .
     .            .      .          .          .            .
     .            .      .          .          .            .


ELEMENT  ROCK TYPE   NORMALISED SENSITIVITY
-----------------------------------------

APPROXIMATION OF TRAVEL TIME USED IN SENSITIVITY ANALYSIS  6.6398064E+05
     1       1         -3.650833E-11          6.639806E+05
     2       1          2.691099E-10          6.639806E+05
     3       1          4.717701E-09          6.639806E+05
     .       .               .                     .
     .       .               .                     .
     .       .               .                     .
```

Amongst the normalised sensitivities to permeability it can be seen that the travel time is most sensitive to the vertical permeability of rock type 2 (the Clay), and a 1% change in this parameter will cause the travel time to decrease by 0.97%. In contrast, the travel time is relatively insensitive to the permeabilities of the Chalk, and the vertical permeability of the Corallian.

The calculated pathline and the normalised sensitivity of the travel time to the horizontal permeability as defined on each finite element are shown in Figure 10.2. The normalised sensitivity of the travel time to the vertical permeability is shown in Figure 10.3. The sensitivity to a parameter defined on an element depends upon the size of the element as well as the parameter value. Each element is shaded according to the sign and magnitude of the normalised sensitivity. Elements shaded yellow-red indicate that increasing the parameter in that element will increase the performance measure, with yellow indicating a small sensitivity and red a large sensitivity. Elements shaded cyan-blue indicate that increasing the parameter in that element will decrease the performance measure, with cyan indicating a small sensitivity and blue a large sensitivity. From this type of picture it can be seen how a parameter within different parts of a stratum affects the performance measure by differing degree and sign.

Figures 10.2 and 10.3 reveal that the travel time is most sensitive to the horizontal permeability in a vertical column near the repository and in the underlying Corallian, and also to the vertical permeability of the Clay. Figure 10.3 shows that increasing the vertical permeability in the middle section of Clay will significantly increase the travel time, whereas increasing the vertical permeability in the upstream and downstream sections of Clay will significantly decrease the travel time. Thus, such plots can identify variations in the dependence on parameters within a defined rock type.

10.6 Steady-State Nuclide Transport Sensitivities

The implementation of the adjoint method for steady-state nuclide transport is described in greater detail in [24].

In order that the adjoint equations for nuclide transport are solved accurately in the discrete system it is necessary to firstly obtain numerical solutions for both the pressure and nuclide on the transport grid. If, for example, a pressure solution for a more extensive regional model is simply interpolated on to the transport grid, then the pressure will not exactly satisfy the groundwater flow equations on the transport grid. In such cases, it cannot be guaranteed that the adjoint sensitivities will accurately reproduce the derivatives of the performance measure with respect to the system parameters. However, a pressure solution from a regional flow model can be used in setting up a groundwater flow problem on the transport grid, the interpolate of the regional flow solution being used to set the pressure boundary conditions and as an initial guess on the transport grid.

The performance measures that are available for calculations of steady-state nuclide transport are described in Section 10.6.1. An example of the input data structure required to compute the sensitivities of the flux of nuclide integrated along a segment of the top surface boundary is given in Section 10.6.2.

10.6.1 Performance Measures

Performance measures of interest related to solute concentration include:

1. a weighted average of solute concentrations at a set of points. This could be used to quantify the uncertainties in predictions of solute concentration in a sub-domain, e.g. one of the geological strata;

2. a weighted average difference between measured and predicted solute concentration. This is useful in model calibration exercises where measurements of solute concentration are available. The adjoint sensitivity method may then be used as part of an optimisation method to obtain ranges of parameters that best fit the measurements;

3. a weighted average of solute fluxes at a set of points. This could be used in an assessment to estimate uncertainties in the radionuclide flux out of a repository zone, or through surrounding geological formations;

4. integrated flux of solute through a surface. This could be used in an assessment to quantify uncertainties in the discharge of radionuclides to the environment.

10.6.2 Integrated Nuclide Surface Flux Sensitivities (Dataset 10.2)

The computation of adjoint sensitivities for nuclide transport using NAMMU follows a definite sequence of operations:

1. define the model for groundwater flow;

2. solve for groundwater flow;

3. define the model for nuclide transport;

4. solve for groundwater flow on the transport grid (if necessary);

5. solve for nuclide transport;

6. specify the nuclide performance measure;

7. set the adjoint boundary conditions;

8. solve for the adjoint state variable;

9. compute the sensitivity coefficients.

The first five stages in this sequence are specified as they would be for a solution of the steady state groundwater flow and nuclide transport equations. The performance measure of the nuclide transport is specified in stage 6. There are four performance measures available, and they correspond to those detailed in Section 10.6.1. The boundary conditions for the adjoint equations must then be set in stage 7. The adjoint boundary conditions are a simplification of the boundary conditions for pressure and nuclide concentration. Where a specified value (Dirichlet) type condition has been set, the corresponding adjoint variable is set to zero. For a specified flux (Neumann) type condition, the discrete finite-element equations in NAMMU have been defined such that it is appropriate to set the flux in the corresponding adjoint system to zero. The command

```
>> ADJOINT ANALYSIS BOUNDARY CONDITION
```

has been introduced to set the adjoint boundary conditions automatically. This command should be included in the dataset along with a list of the relevant variables. For nuclide transport, the relevant variables are pressure and nuclide. For stage 8, the appropriate solver option is ≫ `STEADY STATE ADJOINT ANALYSIS`. If the sensitivities to permeability are not required, then the keyword `NO SENSITIVITIES TO FLOW` should be included. In this case, the solution to only one of the adjoint equations is computed, since this is sufficient to evaluate the sensitivities to the transport parameters (e.g. porosity, dispersion lengths, and molecular diffusion). Since only a single uncoupled equation is solved in this case, the computational cost is significantly less than in the default case when sensitivities to permeability are also computed. Finally the sensitivity coefficients are calculated in stage 9.

Thus, the sequence of commands and keywords used in a NAMMU input data set to perform an adjoint analysis for an integrated nuclide surface flux performance measure would be of the form shown in the following example (only the more important commands are listed).

Stage 2:

```
>> SOLVER DATA
   >> STEADY STATE
      >> GROUNDWATER FLOW
```

Stage 5:

```
>> SOLVER DATA
   >> STEADY STATE
      >> NUCLIDE TRANSPORT
```

Stage 6:

```
>> MODEL DATA
   >> MODIFY BOUNDARY CONDITIONS
      >> DEFINE PERFORMANCE MEASURE
         >> INTEGRATED NUCLIDE SURFACE FLUX
            >> SELECT BOUNDARY SEGMENT
```

Stage 7:

```
>> MODIFY BOUNDARY CONDITIONS
   >> ADJOINT ANALYSIS BOUNDARY CONDITION
      VARIABLES 'PRES'  'NUC1'
```

Stage 8:

```
>> SOLVER DATA
   >> STEADY STATE ADJOINT ANALYSIS
      NUMBER OF ITERATIONS 1
      >> NUCLIDE TRANSPORT
```

Stage 9:

```
>> CALCULATE SENSITIVITY COEFFICIENTS
```

An example of an adjoint sensitivity calculation for nuclide transport is given in Dataset 10.2. The nuclide transport calculation is a simplification of the PACOMA nuclide transport example described in Section 6.2. Here the plume of the notional contaminant is computed for steady-state conditions, and zero concentration rather than zero-dispersive flux is specified on the top surface. Contours of the contaminant concentration are shown in Figure 10.4.

The performance measure was specified to be the integrated nuclide surface flux out of the segment AB of the top surface.

In Figure 10.5 the normalised sensitivities to the horizontal permeability as defined on each finite element is shown. This figure shows that an increase in the horizontal permeability in the Clay or Corallian upstream of the repository increases the discharge of radionuclide across the line segment AB, while an increase in this parameter for most of Clay and Corallian downstream of the repository decreases the discharge. The sensitivity to the horizontal permeability of the chalk downstream of the repository is mainly large and positive. The normalised sensitivities to the longitudinal dispersion length as defined on each finite-element is shown in Figure 10.6. It can be seen that an increase in the longitudinal dispersion length for the downstream portion of the Corallian aquifer would significantly decrease the radionuclide flux through AB. The longitudinal dispersion length in the Clay is zero and so the normalised sensitivity is also zero.

Figures for Section 10

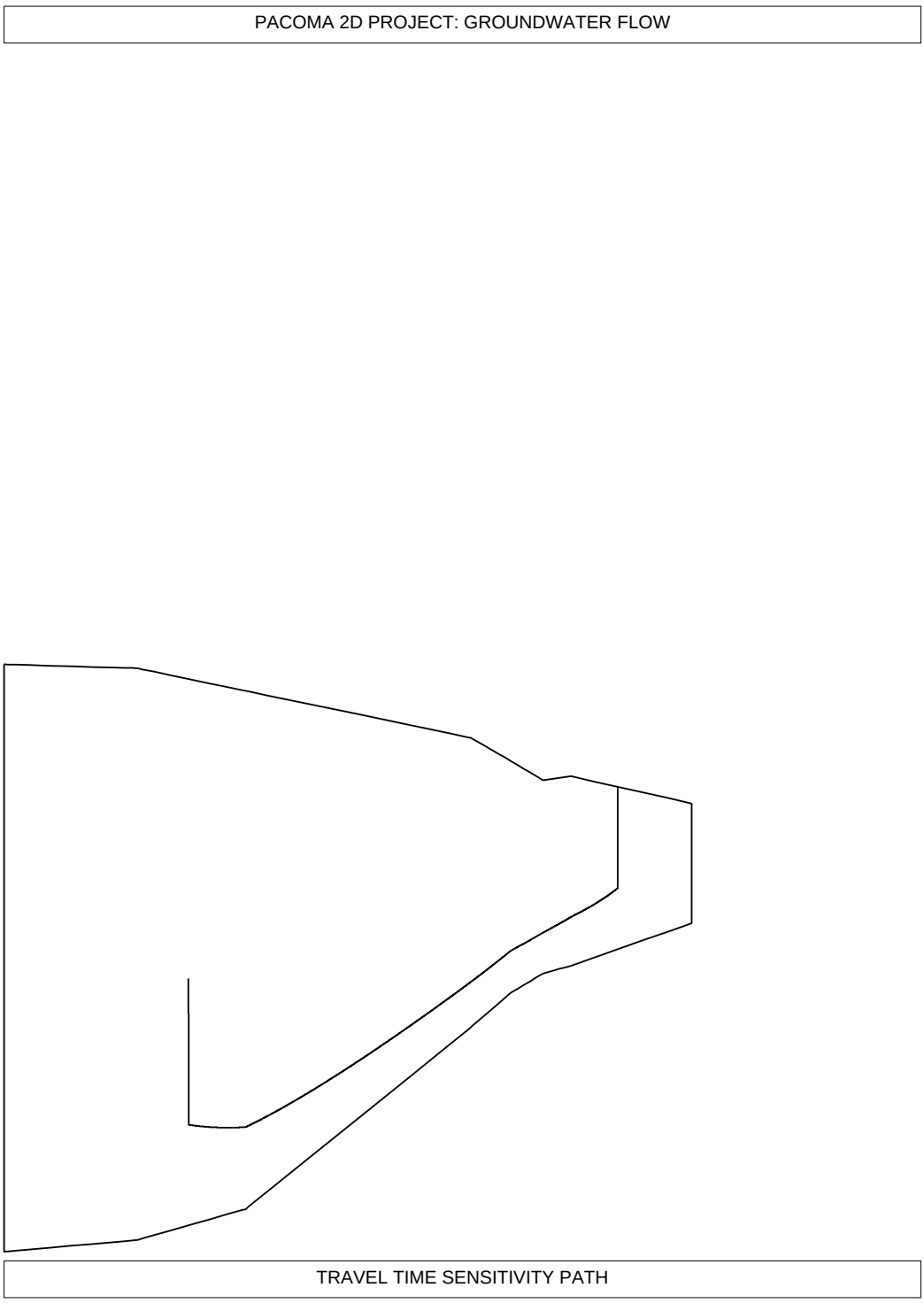


Figure 10.1 The pathline originating in the hypothetical repository used to calculate travel time sensitivities by the adjoint method.

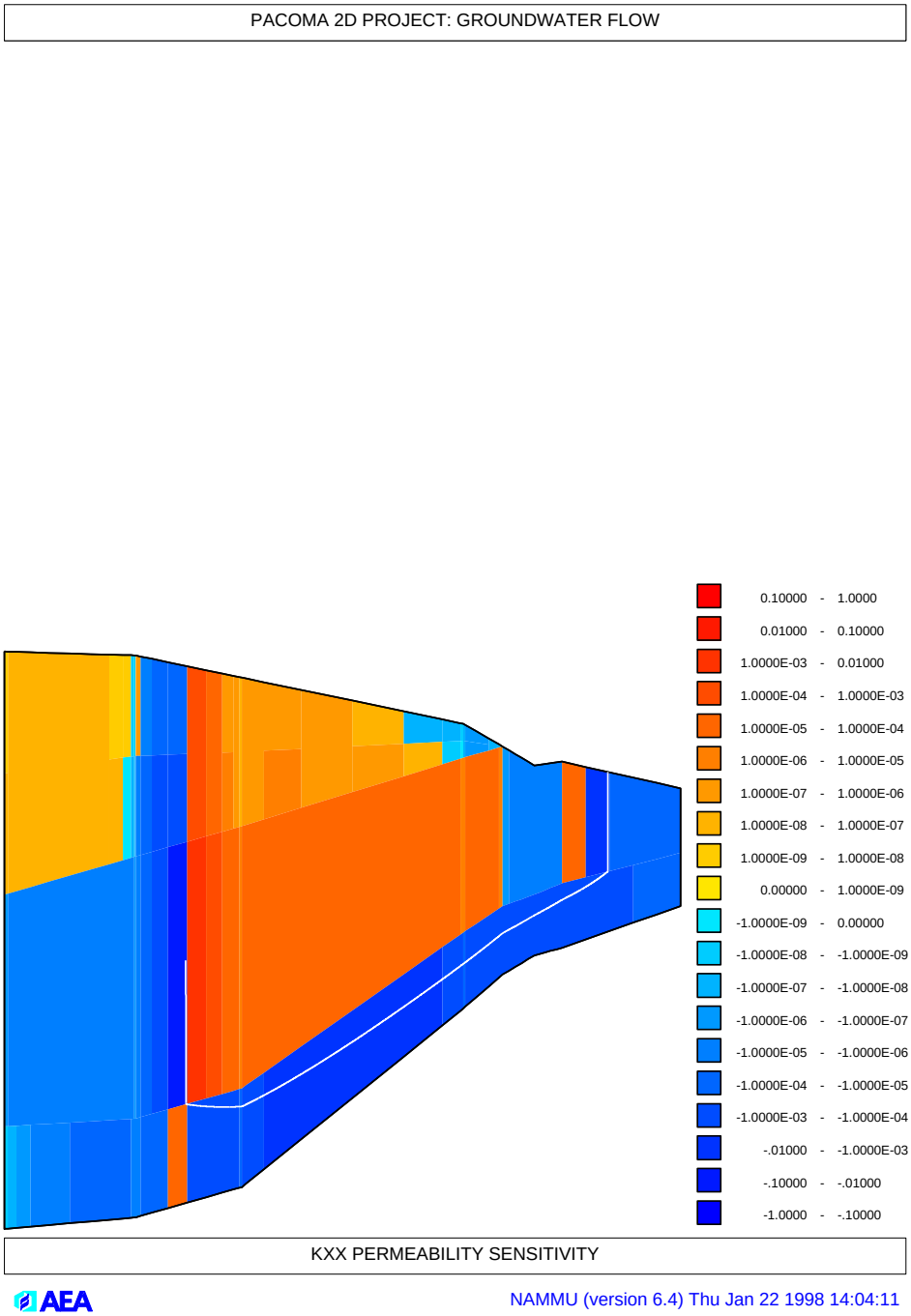


Figure 10.2 **Normalised sensitivities of travel time to the horizontal permeability as defined on each element. Elements shaded on a scale between yellow and red indicate that increasing the parameter in that element will increase the performance measure, with yellow indicating a small sensitivity ($< 10^{-9}$) and red a large sensitivity ($> 10^{-1}$). Elements shaded on a scale between cyan and blue indicate that increasing the parameter in that element will decrease the performance measure, with cyan indicating a small sensitivity ($> -10^{-9}$) and blue a large sensitivity $< -10^{-1}$). The pathline that was analysed is superimposed.**

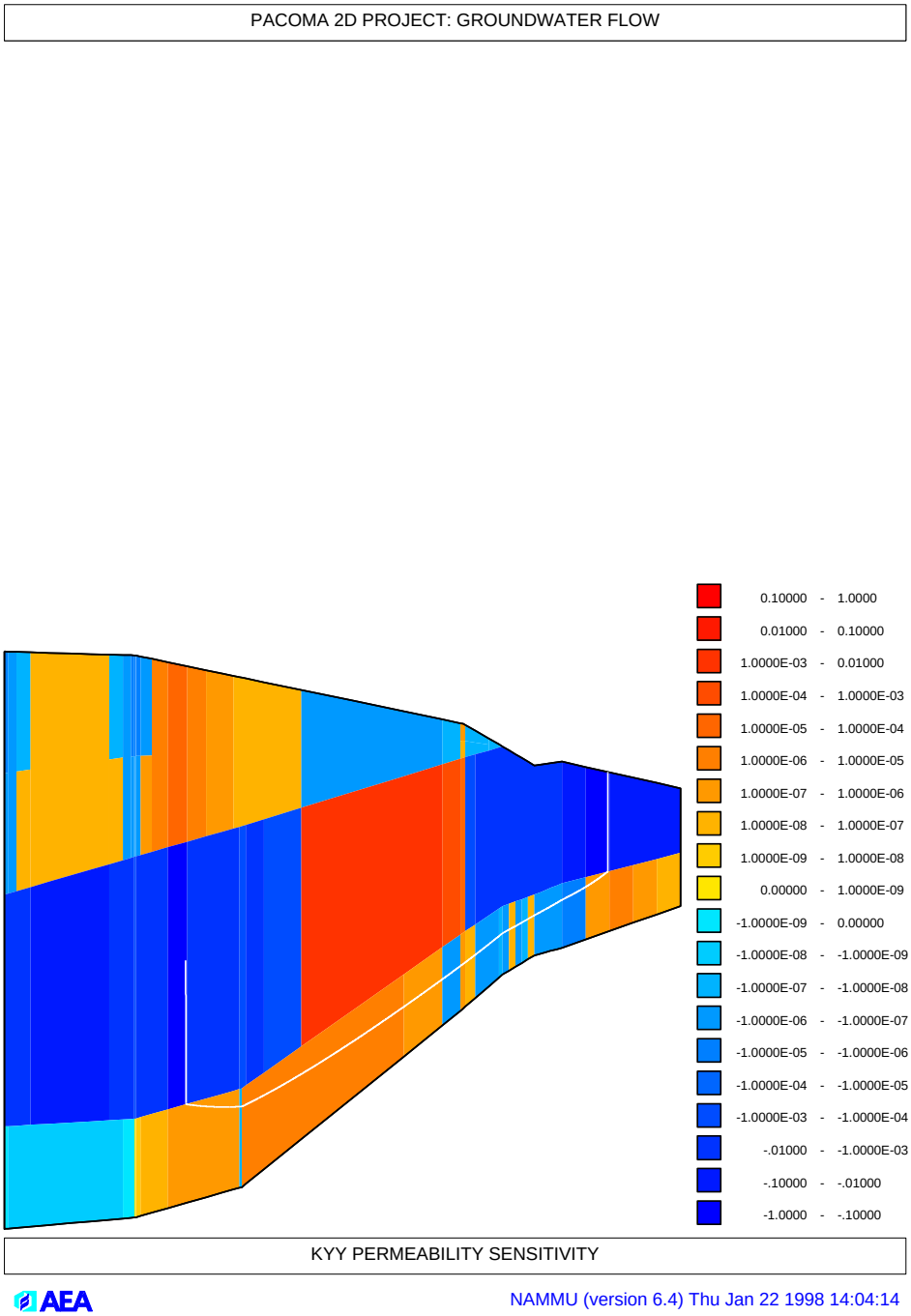


Figure 10.3 **Normalised sensitivities of travel time to the vertical permeability as defined on each element. Elements shaded on a scale between yellow and red indicate that increasing the parameter in that element will increase the performance measure, with yellow indicating a small sensitivity ($< 10^{-9}$) and red a large sensitivity ($> 10^{-1}$). Elements shaded on a scale between cyan and blue indicate that increasing the parameter in that element will decrease the performance measure, with cyan indicating a small sensitivity ($> -10^{-9}$) and blue a large sensitivity $< -10^{-1}$). The pathline that was analysed is superimposed.**

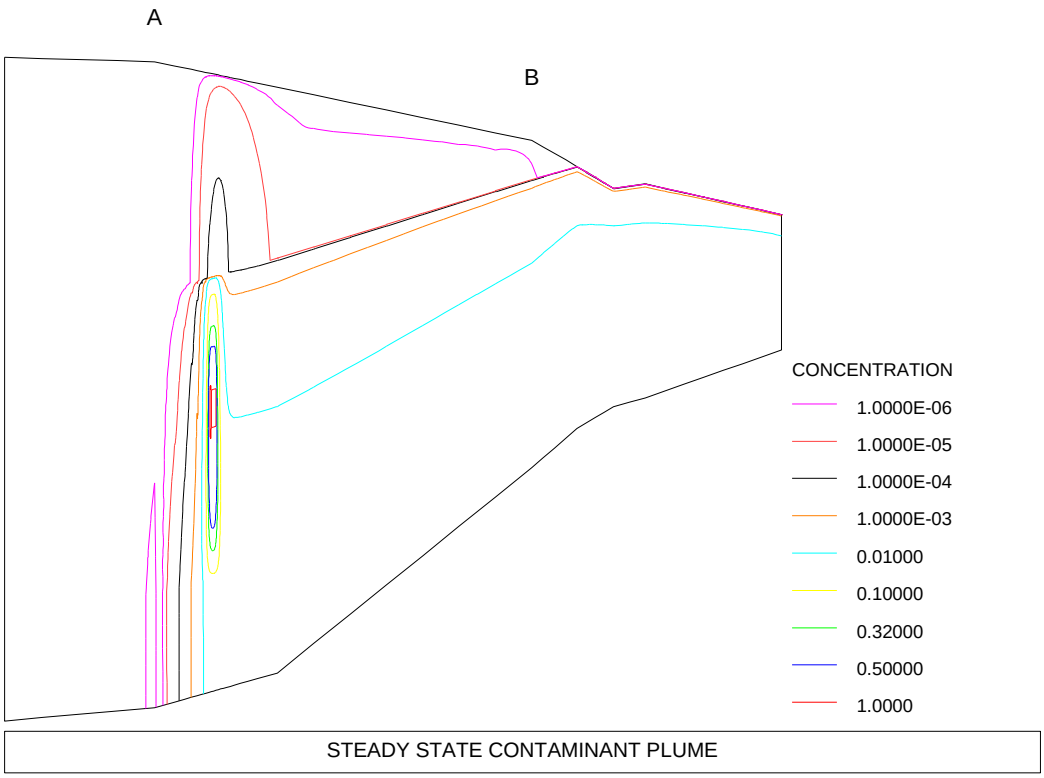


Figure 10.4 **Steady-State contours of contaminant concentration. Contours are plotted at concentrations of** $1, 0.3, 0.1, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}$. **The boundary segment AB denotes the line segment used in calculating the integrated surface flux performance measure.**

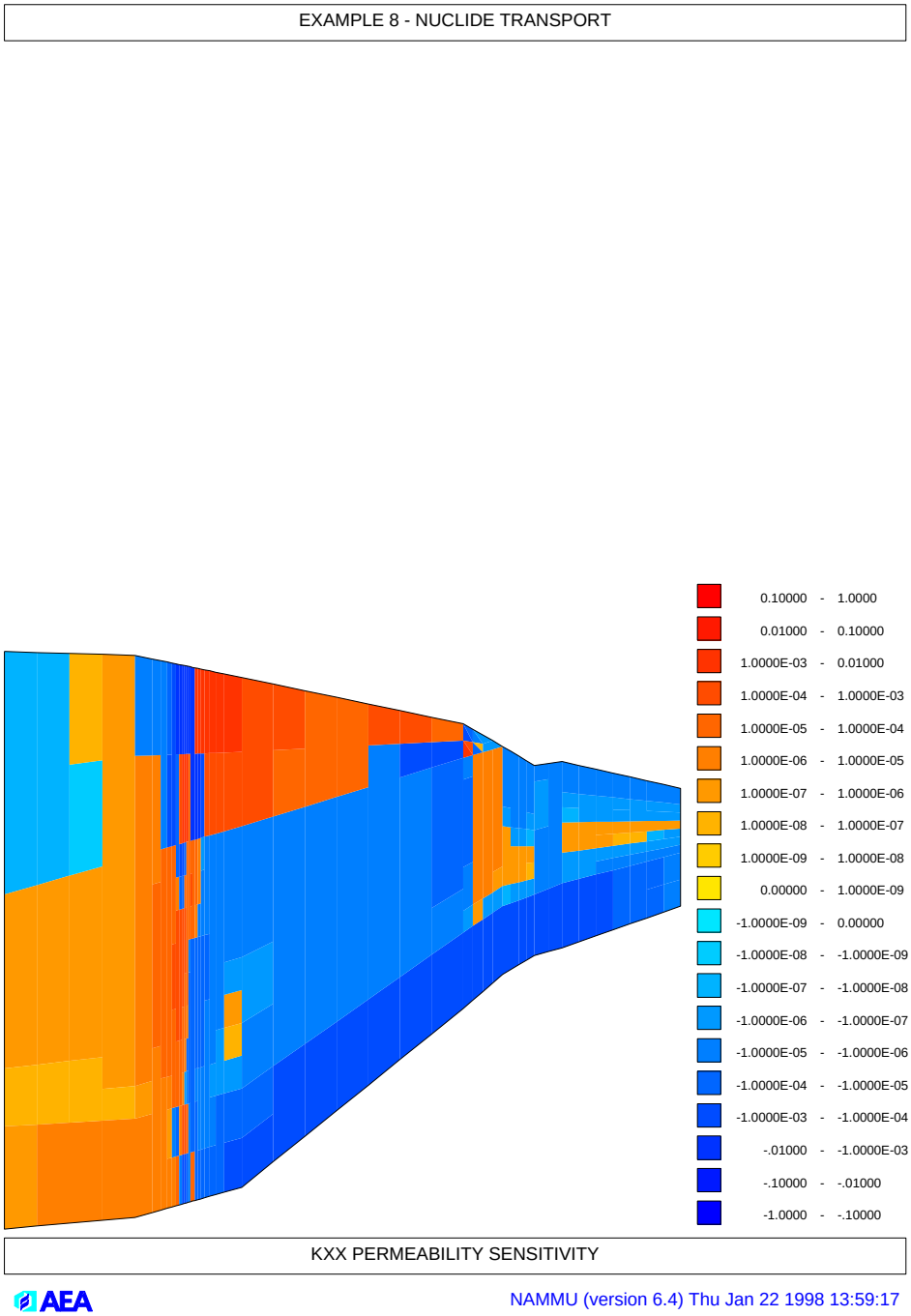


Figure 10.5 **Normalised sensitivities of the integrated nuclide surface flux along the segment AB to the horizontal permeability as defined on each element. Elements shaded on a scale between yellow and red indicate that increasing the parameter in that element will increase the performance measure, with yellow indicating a small sensitivity** $(< 10^{-9})$ **and red a large sensitivity** $(> 10^{-1})$**. Elements shaded on a scale between cyan and blue indicate that increasing the parameter in that element will decrease the performance measure, with cyan indicating a small sensitivity** $(> -10^{-9})$ **and blue a large sensitivity** $< -10^{-1})$**.**

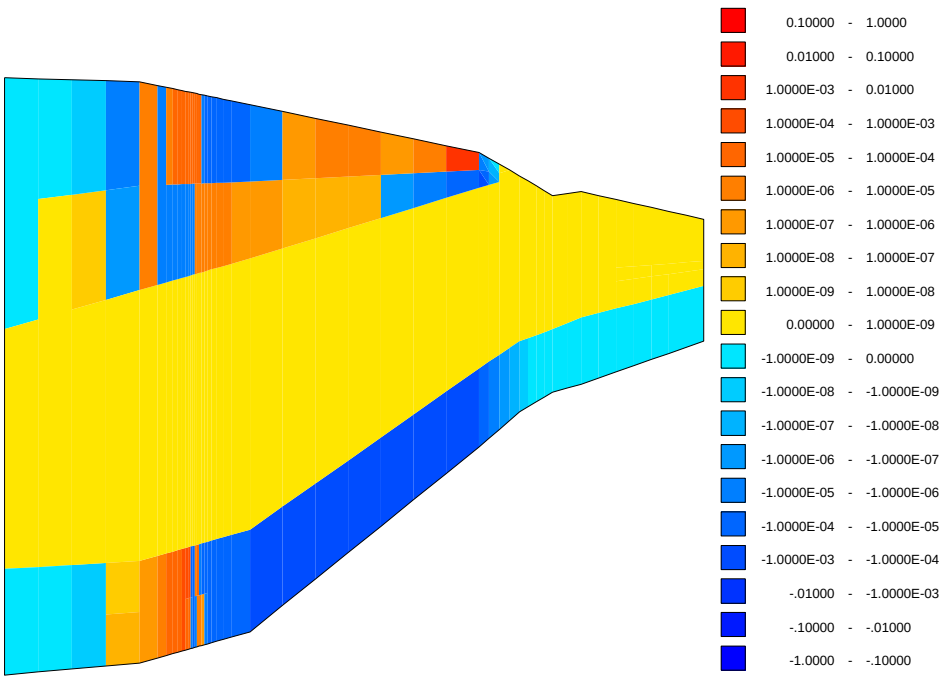


Figure 10.6 **Normalised sensitivities of the integrated nuclide surface flux along the segment AB to the longitudinal dispersion length as defined on each element. Elements shaded on a scale between yellow and red indicate that increasing the parameter in that element will increase the performance measure, with yellow indicating a small sensitivity ($< 10^{-9}$) and red a large sensitivity ($> 10^{-1}$). Elements shaded on a scale between cyan and blue indicate that increasing the parameter in that element will decrease the performance measure, with cyan indicating a small sensitivity ($> -10^{-9}$) and blue a large sensitivity $< -10^{-1}$).**

Dataset 10.1

```
   /* NAMMU TEST CASE PACOMA_TRT                                    */
   /*                                                               */
   /* INPUT DATA FILE FOR PACOMA PROJECT                            */
   /* GROUNDWATER FLOW CALCULATION                                  */
   /* TRAVEL TIME SENSITIVITY TEST CASE SOLVE USING THE             */
   /*  OLD MATRIX DECOMPOSITION                                     */

   /* SPACE ALLOCATION                                              */
   /* INTEGER WORKSPACE  300000                                     */
   /* REAL WORKSPACE     250000                                     */

   /* SOURCE FILES                                                  */
   /* COMPILED FILES                                                */
   /* LIBRARY FILES                                                 */

   /* INPUT DATA FILES                                              */
   /* OUTPUT DATA FILES                                             */
   /* 6        nammu/output/pacoma_trt.out                          */
   /* GRAPHICS nammu/output/pacoma_trt.ps                           */

   /* END JOB INFORMATION                                           */


>> NAMMU

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
      END

   >> SET LIMITS
      ELEMENTS                       200
      NODES                         1200
      NODES PER ELEMENT                9
      FRONTWIDTH                     400
      GAUSS POINTS                    38
      INTEGER BC WORKSPACE          7000
      REAL BC WORKSPACE             5000
      PARAMETERS PER FUNCTION TYPE     9
      FUNCTION TYPES PER ELEMENT       3
      VARIABLES                        1
      END

   >> SET VARIABLES
      VARIABLE NAMES  'PRES'
      END


>> INITIAL DATA

   >> PHYSICAL PROPERTIES
      FLUID DENSITY  992.0
```

```
      ROCK TYPE PERMEABILITIES
      ROCK NUMBER,    KXX,     KYY
           1        3.3E-13  3.3E-13
           2        1.3E-17  8.2E-19
           3        5.2E-13  5.2E-13

      ROCK TYPE PROPERTIES
      ROCK NUMBER,  POROSITY
           1          0.37
           2          0.31
           3          0.34

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NUMBER,  TORTUOSITIES,  LONGITUDINAL DISPERSION LENGTHS
           1           100.0                   82.0
           2             2.73                   0.0
           3           100.0                   88.0

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NUMBER,  TRANSVERSE DISPERSION LENGTHS
           1                    8.2
           2                    0.0
           3                    8.8
      END


>> MODEL DATA

   >> CREATE GRID

      >> GENERATE A GRID OF PATCHES
         PATCH SPACING IN FIRST DIRECTION
         SIZE,  GRADE POWERS
           1    < 1.0 1.0 >
           5    < 2.5 1.5 >
           2    < 1.0 1.0 >

         PATCH SPACING IN SECOND DIRECTION
         SIZE,  GRADE POWERS
          12    < 2.5 2.2 >
          10    < 2.4 1.7 >
           8    < 2.0 2.5 >
           5    < 2.5 1.5 >
           5    < 1.0 1.0 >
           1    < 1.0 1.0 >
           2    < 1.0 1.0 >


         PATCH POSITIONS
         CORNER NUMBER,   COORDINATES
              11       <  0.0  15.2   >
              12       <  3.3  15.1   >
              13       <  6.0  14.515 >
```

```
          14       < 11.6  13.3   >
          21       <  0.0   8.8   >
          22       <  3.3   9.8   >
          23       <  6.0  10.6   >
          24       < 11.6  12.4   >
          25       < 12.6  12.7   >
          26       < 13.4  12.2   >
          27       < 14.1  12.3   >
          28       < 17.1  11.6   >
          31       <  0.0   2.7   >
          32       <  3.3   2.9   >
          33       <  6.0   3.7   >
          34       < 11.6   7.8   >
          35       < 12.6   8.5   >
          36       < 13.4   8.8   >
          37       < 14.1   9.1   >
          38       < 17.1   9.9   >
          41       <  0.0   0.0   >
          42       <  3.3   0.3   >
          43       <  6.0   1.1   >
          44       < 11.6   5.8   >
          45       < 12.6   6.7   >
          46       < 13.4   7.2   >
          47       < 14.1   7.4   >
          48       < 17.1   8.5   >

      PATCH TOPOLOGY
      PATCH TYPE,      CORNERS,        INDICES, ROCK NUMBER
        'SQQ9'    < 11  21  22  12 >   <3 1>        1
        'SQQ9'    < 12  22  23  13 >   <3 2>        1
        'SQQ9'    < 13  23  24  14 >   <3 3>        1
        'TR69'    < 24  25  14     >   <2 7>        1
        'SQQ9'    < 21  31  32  22 >   <1 1>        2
        'SQQ9'    < 22  32  33  23 >   <1 2>        2
        'SQQ9'    < 23  33  34  24 >   <1 3>        2
        'SQQ9'    < 24  34  35  25 >   <1 4>        2
        'SQQ9'    < 25  35  36  26 >   <1 5>        2
        'SQQ9'    < 26  36  37  27 >   <1 5>        2
        'SQQ9'    < 27  37  38  28 >   <1 5>        2
        'SQQ9'    < 31  41  42  32 >   <1 1>        3
        'SQQ9'    < 32  42  43  33 >   <1 2>        3
        'SQQ9'    < 33  43  44  34 >   <1 3>        3
        'SQQ9'    < 34  44  45  35 >   <1 4>        3
        'SQQ9'    < 35  45  46  36 >   <1 5>        3
        'SQQ9'    < 36  46  47  37 >   <1 5>        3
        'SQQ9'    < 37  47  48  38 >   <1 5>        3
      END

>> SET BOUNDARY CONDITIONS

/*   ************ PRESSURE BOUNDARY SPECIFICATION **********   */
/*   ********************* TOP BOUNDARY ********************   */
   >> SPECIFIED VALUE
```

```
         >> VALUE VARYING LINEARLY WITH POSITION
            VARIABLES    'PRES'
            BASE VALUES  -1096082.3
            Y FACTORS      142132.4
            END

            >> SELECT BOUNDARY SEGMENT
               START POINT   0.0  15.2
               MID POINT    13.4  12.2
               END POINT    17.1  11.6
               PRECISION     1.0E-4
               END

   >> MAP GRID

      >> CHANGE ORIGIN
         MOVE TO  0.0  7.7117
         END

      >> SCALE COORDINATES
         DIVIDE X BY  1.3154E-3
         DIVIDE Y BY  6.8468E-2
         END


/*** SOLVE FOR PRESSURE ***/
>> SOLVER DATA

   >> STEADY STATE
      MAXIMUM FRONTWIDTH  250
      SAVE L
      END

      >> GROUNDWATER FLOW
         END


>> OUTPUT DATA

   >> SET OUTPUT OPTIONS
      HEADING                   'PACOMA 2D PROJECT: GROUNDWATER FLOW'
      BOUNDARY COLOUR           'BLACK'
      GRID COLOUR               'BLACK'
      COORDINATE SCALE FACTORS  1.0  50.0
      LINE THICKNESS            0.3
      END

   >> SET ROCK STYLES
      ROCK STYLES
      ROCK NUMBERS,  COLOUR,     GROUP NAME
         < 1 >      'RED'        'CHALK'
         < 2 >      'YELLOW'     'CLAY'
         < 3 >      'BLUE'       'CORALLIAN'
      END
```

```
   >> PLOT GRID
      SHADE
      CAPTION  'ROCK STRATA'
      END

   /*** CALCULATE AND SAVE A PATHLINE FOR ANAYSIS ***/
   >> PATHLINES
      NUMBER OF PATHS                1
      X COORDINATES OF PATHS       3483.7
      Y COORDINATES OF PATHS         -9.3
      SAVE PATH FOR SENSITIVITY ANALYSIS
      MAXIMUM EXTRA GAUSS POINTS     15
      TIMES IN YEARS
      MAXIMUM NUMBER OF TIMESTEPS  1000
      ACCURACY PARAMETER              0.05
      NO KEY
      COLOURS                      'BLACK'
      CAPTION                      'TRAVEL TIME SENSITIVITY PATH'
      END


>> MODEL DATA

   /*** SET THE PERFORMANCE MEASURE ***/
   >> MODIFY BOUNDARY CONDITIONS

     >> DEFINE PERFORMANCE MEASURE

        >> TRAVEL TIME PERFORMANCE MEASURE
           VARIABLES  'PRES'
           END

   >> SET INITIAL GUESS

      >> INITIAL VALUES
         LEVEL NUMBER  2
         VARIABLES     'PRES'
         VALUES        0.0
         END


/*** DO AN EFFICIENT SOLVE FOR THE ADJOINT STATE ***/
>> SOLVER DATA

   >> SELF ADJOINT ANALYSIS
      USE SAVED LU DECOMPOSITION
      MAXIMUM FRONTWIDTH          250
      NUMBER OF QUASI ITERATIONS    1
      END

      >> GROUNDWATER FLOW
         END
```

```
>> OUTPUT DATA

   >> SET COLOUR TABLE
      COLOUR DEFINITIONS
      COLOUR NAMES,   R,   G,   B
      'COL1'         0.0  0.0  1.0
      'COL2'         0.0  0.1  1.0
      'COL3'         0.0  0.2  1.0
      'COL4'         0.0  0.3  1.0
      'COL5'         0.0  0.4  1.0
      'COL6'         0.0  0.5  1.0
      'COL7'         0.0  0.6  1.0
      'COL8'         0.0  0.7  1.0
      'COL9'         0.0  0.8  1.0
      'COL10'        0.0  0.9  1.0
      'COL11'        1.0  0.9  0.0
      'COL12'        1.0  0.8  0.0
      'COL13'        1.0  0.7  0.0
      'COL14'        1.0  0.6  0.0
      'COL15'        1.0  0.5  0.0
      'COL16'        1.0  0.4  0.0
      'COL17'        1.0  0.3  0.0
      'COL18'        1.0  0.2  0.0
      'COL19'        1.0  0.1  0.0
      'COL20'        1.0  0.0  0.0
      END

   >> PLOT CONTOURS
      VARIABLE            'PRES'
      LEVEL NUMBER             1
      CONTOUR VALUES      500000.0 TO 1100000.0  BY  20000.0
      COLOURS             'RED' 'BLUE'
      CAPTION             'PRESSURE CONTOURS'
      KEY TITLE           'RESIDUAL PRESSURE'
      END

   >> PATHLINES
      NUMBER OF PATHS                 1
      X COORDINATES OF PATHS       3483.7
      Y COORDINATES OF PATHS         -9.3
      TIMES IN YEARS
      MAXIMUM NUMBER OF TIMESTEPS  1000
      ACCURACY PARAMETER              0.05
      NO KEY
      COLOURS                      'BLACK'
      NO CAPTION
      END

   >> PLOT CONTOURS
      VARIABLE            'PRES'
      LEVEL NUMBER         2
      CONTOUR VALUES       1.0E3  1.0E4  1.0E5  1.0E6  1.0E7  1.0E8  1.0E9 0.0 +
                          -1.0E3 -1.0E4 -1.0E5 -1.0E6 -1.0E7 -1.0E8 -1.0E9
```

```
   COLOURS             'RED' 'BLUE' 'RED' 'BLUE' 'RED' 'BLUE' 'RED' 'VIOLET'+
                       'ORANGE' 'CYAN' 'ORANGE' 'CYAN' 'ORANGE' 'CYAN' +
                                                                 'ORANGE'
   SUPERIMPOSE,  NO HEADING,  NO FOOTER
   CAPTION             'CONTOURS OF THE ADJOINT STATE'
   END

>> PRINT GLOBAL FREEDOMS
   LEVEL NUMBER 1
   END

>> PRINT GLOBAL FREEDOMS
   LEVEL NUMBER 2
   END

>> CALCULATE SENSITIVITY COEFFICIENTS
   END

/*** PLOT ELEMENTWISE SENSITIVITIES ***/
>> PLOT GRID
   SHADE
   KXX SENSITIVITY
   INTERVALS  -1.0    -1.0E-1 -1.0E-2 -1.0E-3 -1.0E-4 -1.0E-5 +
              -1.0E-6 -1.0E-7 -1.0E-8 -1.0E-9  0.0 +
               1.0E-9  1.0E-8  1.0E-7  1.0E-6  1.0E-5  1.0E-4 +
               1.0E-3  1.0E-2  1.0E-1  1.0
   COLOURS    'COL1'  'COL2'  'COL3'  'COL4'  'COL5'  'COL6'  'COL7'  +
              'COL8'  'COL9'  'COL10' 'COL11' 'COL12' 'COL13' 'COL14' +
              'COL15' 'COL16' 'COL17' 'COL18' 'COL19' 'COL20'
   CAPTION  'KXX PERMEABILITY SENSITIVITY'
   END

>> PATHLINES
   NUMBER OF PATHS                1
   X COORDINATES OF PATHS       3483.7
   Y COORDINATES OF PATHS         -9.3
   TIMES IN YEARS
   MAXIMUM NUMBER OF TIMESTEPS  1000
   ACCURACY PARAMETER              0.05
   NO KEY
   COLOURS                      'WHITE'
   NO CAPTION
   SUPERIMPOSE
   END


>> PLOT GRID
   SHADE
   KYY SENSITIVITY
   INTERVALS  -1.0    -1.0E-1 -1.0E-2 -1.0E-3 -1.0E-4 -1.0E-5 +
              -1.0E-6 -1.0E-7 -1.0E-8 -1.0E-9  0.0 +
               1.0E-9  1.0E-8  1.0E-7  1.0E-6  1.0E-5  1.0E-4 +
               1.0E-3  1.0E-2  1.0E-1  1.0
   COLOURS    'COL1'  'COL2'  'COL3'  'COL4'  'COL5'  'COL6'  'COL7'  +
```

```
                'COL8'  'COL9'  'COL10' 'COL11' 'COL12' 'COL13' 'COL14' +
                'COL15' 'COL16' 'COL17' 'COL18' 'COL19' 'COL20'
      CAPTION  'KYY PERMEABILITY SENSITIVITY'
      END

   >> PATHLINES
      NUMBER OF PATHS                1
      X COORDINATES OF PATHS       3483.7
      Y COORDINATES OF PATHS         -9.3
      TIMES IN YEARS
      MAXIMUM NUMBER OF TIMESTEPS  1000
      ACCURACY PARAMETER              0.05
      NO KEY
      COLOURS                      'WHITE'
      NO CAPTION
      SUPERIMPOSE
      END

   >> PLOT GRID
      SHADE
      POROSITY SENSITIVITY
      INTERVALS  -1.0    -1.0E-1 -1.0E-2 -1.0E-3 -1.0E-4 -1.0E-5 +
                 -1.0E-6 -1.0E-7 -1.0E-8 -1.0E-9  0.0 +
                  1.0E-9  1.0E-8  1.0E-7  1.0E-6  1.0E-5  1.0E-4 +
                  1.0E-3  1.0E-2  1.0E-1  1.0
      COLOURS    'COL1'  'COL2'  'COL3'  'COL4'  'COL5'  'COL6'  'COL7'  +
                 'COL8'  'COL9'  'COL10' 'COL11' 'COL12' 'COL13' 'COL14' +
                 'COL15' 'COL16' 'COL17' 'COL18' 'COL19' 'COL20'
      CAPTION  'POROSITY SENSITIVITY'
      END

   >> PATHLINES
      NUMBER OF PATHS                1
      X COORDINATES OF PATHS       3483.7
      Y COORDINATES OF PATHS         -9.3
      TIMES IN YEARS
      MAXIMUM NUMBER OF TIMESTEPS  1000
      ACCURACY PARAMETER              0.05
      NO KEY
      COLOURS                      'WHITE'
      NO CAPTION
      SUPERIMPOSE
      END

>> STOP
```

Dataset 10.2

```
     /* INPUT DATA FILE FOR PACOMA PROJECT                          */
     /* GROUNDWATER FLOW CALCULATION                                */
     /* AND STEADY-STATE NUCLIDE TRANSPORT                          */
     /* ADJOINT TRANSPORT CALCULATION FOR PERFORMANCE MEASURE       */
     /* INTEGRATED NUCLIDE SURFACE FLUX FOR A SELECTED SEGMENT      */
     /* OF THE BOUNDARY                                             */
     /* ZERO CONCENTRATION B.C. ON TOP SURFACE                      */

     /* SPACE ALLOCATION                                            */
     /* REAL WORKSPACE   1000000                                    */
     /* INTEGER WORKSPACE 350000                                    */

     /* SOURCE FILES                                                */
     /* INLINE FORTRAN
C  +-----------------------------------------------------------------+
C  | THIS ROUTINE DEFINES THE EXTENT OF REPOSITORY                   |
C  +-----------------------------------------------------------------+
      SUBROUTINE USLECT(XX,NSD,IIN)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION XX(NSD)
C
      IIN = 0
      EPSY=3.0
      EPSX=15.0
      IF (XX(1) .GT. 3432.4D0 - EPSX  .AND.
     >    XX(1) .LT. 3535.0D0 + EPSX  .AND.
     >    XX(2) .GT. -14.63D0 - EPSY  .AND.
     >    XX(2) .LT. -3.968D0 + EPSY)  IIN = 1
C
      RETURN
      END
                                                                    */
     /* COMPILED FILES                                              */
     /* LIBRARY  FILES                                              */
     /* INPUT DATA FILES                                            */
     /* OUTPUT DATA FILES                                           */
     /* 6        nammu/output/pacoma.nucadj.out                     */
     /* GFOUT    nammu/output/pacoma.nucadj.gf                      */
     /* GRAPHICS nammu/output/pacoma.nucadj.ps                      */

     /* END JOB INFORMATION                                         */

>> NAMMU

   >> SET NAMMU OPTIONS
      VARIABLE NUMBER OF FIRST NUCLIDE 6
      NUMBER OF NUCLIDES 1
      END

   >> SET OPTIONS
      TWO DIMENSIONS
      RECTANGULAR GEOMETRY
```

```
      END

   >> SET LIMITS
      ELEMENTS                      1000
      NODES                         9000
      FRONTWIDTH                     400
      INTEGER BC WORKSPACE          5000
      REAL BC WORKSPACE             1000
      PARAMETERS PER FUNCTION TYPE     9
      FUNCTION TYPES PER ELEMENT       3
      GAUSS POINTS                    16
      END


    >> SET VARIABLES
       VARIABLE NAMES 'PRES' 'TEMP' 'UVEL' 'VVEL' 'STFN' 'NUC1'
       END

>> INITIAL DATA
   >> PHYSICAL PROPERTIES
      FLUID DENSITY                     992.0
      GRAVITATIONAL ACCELERATION        9.81
      VISCOSITY                         1.0E-3
      MOLECULAR DIFFUSION COEFFICIENTS 6.0E-10
      ROCK TYPE PERMEABILITIES
      ROCK NAME,      KXX,     KYY
       'CHALK'      3.3E-13  3.3E-13
       'CLAY'       1.3E-17  8.2E-19
       'CORALLIAN'  5.2E-13  5.2E-13

      ROCK TYPE PROPERTIES
      ROCK NAME,    POROSITY
       'CHALK'        0.37
       'CLAY'         0.31
       'CORALLIAN'    0.34

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TORTUOSITIES,  LONGITUDINAL DISPERSION LENGTHS
       'CHALK'         100.0                    82.0
       'CLAY'           2.73                     0.0
       'CORALLIAN'     100.0                    88.0

      ROCK TYPE NUCLIDE PROPERTIES
      ROCK NAME,    TRANSVERSE DISPERSION LENGTHS
       'CHALK'                   8.2
       'CLAY'                    0.0
       'CORALLIAN'               8.8
      END

>> MODEL DATA
     >> CREATE GRID

        >> GENERATE A GRID OF PATCHES
           PATCH SPACING IN FIRST DIRECTION
```

```
FIRST SIZE, FIRST GRADE POWERS
    2       <1.0 1.0>
    8       <1.0 1.0>
    4       <1.0 1.0>
PATCH SPACING IN SECOND DIRECTION
SECOND SIZE, SECOND GRADE POWERS
   20       <0.6 0.6>
    7       <1.0 1.0>
    4       <1.0 1.0>
    2       <1.0 1.0>
    4       <1.0 1.0>

PATCH POSITIONS
CORNER NUMBER,    COORDINATES
     11          <  0.0    15.2   >
     12          <  3.3    15.1   >
     13          <  6.0    14.515 >
     14          < 11.6    13.3   >
     21          <  0.0     8.8   >
     22          <  3.3     9.8   >
     23          <  6.0    10.6   >
     24          < 11.6    12.4   >
     25          < 12.6    12.7   >
     26          < 13.4    12.2   >
     27          < 14.1    12.3   >
     28          < 17.1    11.6   >
     31          <  0.0     2.7   >
     32          <  3.3     2.9   >
     33          <  6.0     3.7   >
     34          < 11.6     7.8   >
     35          < 12.6     8.5   >
     36          < 13.4     8.8   >
     37          < 14.1     9.1   >
     38          < 17.1     9.9   >
     41          <  0.0     0.0   >
     42          <  3.3     0.3   >
     43          <  6.0     1.1   >
     44          < 11.6     5.8   >
     45          < 12.6     6.7   >
     46          < 13.4     7.2   >
     47          < 14.1     7.4   >
     48          < 17.1     8.5   >

PATCH TOPOLOGY
PATCH TYPE,   CORNERS,      INDICES, ROCK NAME
'SQQ9'  < 11  21  22  12>     <1 5>   'CHALK'
'SQQ9'  < 12  22  23  13>     <1 1>   'CHALK'
'SQQ9'  < 13  23  24  14>     <1 2>   'CHALK'
'TRT6'  < 24  25  14    >     <3 4>   'CHALK'
'SQQ9'  < 21  31  32  22>     <2 5>   'CLAY'
'SQQ9'  < 22  32  33  23>     <2 1>   'CLAY'
'SQQ9'  < 23  33  34  24>     <2 2>   'CLAY'
'SQQ9'  < 24  34  35  25>     <2 3>   'CLAY'
'SQQ9'  < 25  35  36  26>     <2 3>   'CLAY'
```

```
          'SQQ9'  < 26  36  37  27>      <2 4>   'CLAY'
          'SQQ9'  < 27  37  38  28>      <2 2>   'CLAY'
          'SQQ9'  < 31  41  42  32>      <1 5>   'CORALLIAN'
          'SQQ9'  < 32  42  43  33>      <1 1>   'CORALLIAN'
          'SQQ9'  < 33  43  44  34>      <1 2>   'CORALLIAN'
          'SQQ9'  < 34  44  45  35>      <1 3>   'CORALLIAN'
          'SQQ9'  < 35  45  46  36>      <1 3>   'CORALLIAN'
          'SQQ9'  < 36  46  47  37>      <1 4>   'CORALLIAN'
          'SQQ9'  < 37  47  48  38>      <1 2>   'CORALLIAN'

  >> SET BOUNDARY CONDITIONS
  /*   ************ PRESSURE BOUNDARY SPECIFICATION **********   */
  /*   ******************** TOP BOUNDARY ********************   */

      >> SPECIFIED VALUE
         >> VALUE VARYING LINEARLY WITH POSITION
            VARIABLES      'PRES'
            BASE VALUES    -1096082.3
            Y FACTORS        142132.4
            END

         >> SELECT BOUNDARY SEGMENT
            START POINT        0.0      15.2
            MID POINT         13.4      12.2
            END POINT         17.1      11.6
            PRECISION         1.0E-4
            END

      >> MAP GRID
         >> CHANGE ORIGIN
            MOVE TO  0.0  7.7117
            END
         >> SCALE COORDINATES
            DIVIDE X BY 1.3154E-3
            DIVIDE Y BY 6.8468E-2
            END

>> MODIFY GRID

  >> RENUMBER ELEMENTS
      >> SLOAN ALGORITHM

>> SOLVER DATA
   >> STEADY STATE
      MAXIMUM FRONT WIDTH   280
      NUMBER OF ITERATIONS  1
      >> GROUNDWATER FLOW

>> OUTPUT DATA

  >> SET OUTPUT OPTIONS
     COORDINATE SCALE FACTORS  1.0  50.0
     HEADING                   'EXAMPLE 8 - NUCLIDE TRANSPORT'
     BOUNDARY COLOUR           'BLACK'
```

```
      GRID COLOUR               'BLACK'
      END

   >> SET ROCK STYLES
      ROCK STYLES
      ROCK NAME,  COLOUR
       'CHALK'      'RED'
       'CLAY'       'YELLOW'
       'CORALLIAN'  'BLUE'
      END


    >> PLOT GRID
       CAPTION 'FINITE ELEMENT GRID'
       PLOT BOUNDARY
       END

    >> PLOT GRID
       SHADE
       CAPTION 'ROCK STRATA'
       END

    >> PLOT CONTOURS
       NUMBER OF CONTOURS 31
       VARIABLE 'PRES'
       CONTOUR VALUES  500000. TO 1100000. BY 20000.
       COLOURS  'RED' 'BLUE'
       CAPTION 'PRESSURE CONTOURS'
       KEY TITLE 'RESIDUAL PRESSURE'
       END

>> MODEL DATA

    >> MODIFY BOUNDARY CONDITIONS
/* ****** ZERO CONCENTRATION CONDITION ON TOP SURFACE ********* */
      >> SPECIFIED VALUE
         >> CONSTANT VALUE
            VARIABLES 'NUC1'
            VALUES    0.0
         >> SELECT BOUNDARY SEGMENT
            START POINT          0.0     109.37
            MID POINT        10187.0      65.55
            END POINT        13000.0      56.8
            PRECISION         1.0
            END

/*   ********* SPECIFY THE CONTAMINANT SOURCE ***********   */

      >> SPECIFIED VALUE
         >> CONSTANT VALUE
            VARIABLES 'NUC1'
            VALUES    1.0
         >> CALL SUBROUTINE USLECT
```

```
 >> SOLVER DATA
    >> STEADY STATE
       NUMBER OF ITERATIONS 1
       MAXIMUM FRONT WIDTH              280
       >> NUCLIDE TRANSPORT
          NUCLIDE NUMBER 1
          NUCLIDE 'NUC1'

 >> OUTPUT DATA

   >> SET OUTPUT OPTIONS
      COORDINATE SCALE FACTORS  1.0  50.0
      HEADING                   'EXAMPLE 8 - NUCLIDE TRANSPORT'
      BOUNDARY COLOUR           'BLACK'
      GRID COLOUR               'BLACK'
      END

    >> PLOT CONTOURS
       NUMBER OF CONTOURS 9
       CONTOUR VALUES 1.0 0.5 0.32 0.1 1.0E-2 1.0E-3 1.0E-4 +
                      1.0E-5 1.0E-6
       VARIABLE 'NUC1'
       COLOURS 'RED' 'BLUE' 'GREEN' 'YELLOW' 'CYAN' 'ORANGE' +
                'BLACK' 'BROWN' 'VIOLET'
       KEY TITLE 'CONCENTRATION'
       CAPTION 'STEADY STATE CONTAMINANT PLUME'

    >> PLOT TEXT
       ALIGN CENTRE
       TEXT  'A'
       POSITION 2508.7  120.0

    >> PLOT TEXT
       ALIGN CENTRE
       TEXT  'B'
       POSITION 8818.6 100.0

>> MODEL DATA
   >> MODIFY BOUNDARY CONDITIONS
/* ****** SET A NUCLIDE PERFORMANCE MEASURE ********* */

   >> DEFINE PERFORMANCE MEASURE
   >> INTEGRATED NUCLIDE SURFACE FLUX
      VARIABLES 'NUC1'
      >> SELECT BOUNDARY SEGMENT
         START POINT    2508.7      107.91
         MID POINT      4561.4       99.15
         END POINT      8818.6       81.61
         PRECISION      1.0
         END

  >> ADJOINT ANALYSIS BOUNDARY CONDITION
     VARIABLES 'PRES'  'NUC1'
```

```
 >> SOLVER DATA
    >> STEADY STATE ADJOINT ANALYSIS
       NUMBER OF ITERATIONS 1
       MAXIMUM FRONT WIDTH              280
       >> NUCLIDE TRANSPORT
          NUCLIDE 'NUC1'

>> OUTPUT DATA

   >> SET COLOUR TABLE
      COLOUR DEFINITIONS
      COLOUR NAMES,   R,   G,   B
      'COL1'        0.0  0.0  1.0
      'COL2'        0.0  0.1  1.0
      'COL3'        0.0  0.2  1.0
      'COL4'        0.0  0.3  1.0
      'COL5'        0.0  0.4  1.0
      'COL6'        0.0  0.5  1.0
      'COL7'        0.0  0.6  1.0
      'COL8'        0.0  0.7  1.0
      'COL9'        0.0  0.8  1.0
      'COL10'       0.0  0.9  1.0
      'COL11'       1.0  0.9  0.0
      'COL12'       1.0  0.8  0.0
      'COL13'       1.0  0.7  0.0
      'COL14'       1.0  0.6  0.0
      'COL15'       1.0  0.5  0.0
      'COL16'       1.0  0.4  0.0
      'COL17'       1.0  0.3  0.0
      'COL18'       1.0  0.2  0.0
      'COL19'       1.0  0.1  0.0
      'COL20'       1.0  0.0  0.0

   >> SET OUTPUT OPTIONS
      COORDINATE SCALE FACTORS  1.0  50.0
      HEADING                   'EXAMPLE 8 - NUCLIDE TRANSPORT'
      BOUNDARY COLOUR           'BLACK'
      GRID COLOUR               'BLACK'
      END


   >> CALCULATE SENSITIVITY COEFFICIENTS
      ROCK PROPERTY SENSITIVITIES

   >> PLOT GRID
      SHADE
      COLOURS 'COL1' 'COL2' 'COL3' 'COL4' 'COL5' 'COL6' 'COL7' +
              'COL8' 'COL9' 'COL10' 'COL11' 'COL12' 'COL13'    +
              'COL14' 'COL15' 'COL16' 'COL17' 'COL18' 'COL19' 'COL20'
      KXX SENSITIVITY
      INTERVALS -1.0 -1.0E-1 -1.0E-2 -1.0E-3 -1.0E-4 -1.0E-5 +
                -1.0E-6 -1.0E-7 -1.0E-8 -1.0E-9 0.0 +
                1.0E-9 1.0E-8 1.0E-7 1.0E-6 1.0E-5 1.0E-4 +
                1.0E-3 1.0E-2 1.0E-1 1.0
```

```
      CAPTION 'KXX PERMEABILITY SENSITIVITY'
      END

   >> PLOT GRID
      SHADE
      COLOURS 'COL1' 'COL2' 'COL3' 'COL4' 'COL5' 'COL6' 'COL7' +
              'COL8' 'COL9' 'COL10' 'COL11' 'COL12' 'COL13'    +
              'COL14' 'COL15' 'COL16' 'COL17' 'COL18' 'COL19' 'COL20'
      LONGITUDINAL DISPERSION SENSITIVITY
      INTERVALS -1.0 -1.0E-1 -1.0E-2 -1.0E-3 -1.0E-4 -1.0E-5 +
                -1.0E-6 -1.0E-7 -1.0E-8 -1.0E-9 0.0 +
                1.0E-9 1.0E-8 1.0E-7 1.0E-6 1.0E-5 1.0E-4 +
                1.0E-3 1.0E-2 1.0E-1 1.0
      CAPTION 'LONGITUDINAL DISPERSION SENSITIVITY'
      END

>> STOP
```

11 USER ROUTINES

Most of the processing of a finite-element model that a user normally requires can be specified directly through the input data. However, sometimes the facilities available in NAMMU may not meet the precise requirements of a user. Therefore, interfaces to user-supplied subroutines have been defined at suitable places so that by supplying appropriate versions of these subroutines the user can get exactly the required facility.

User routines may be used in each of the main input phases, and used to define:

1. Material properties (NAMMU commands), such as:
    - the fluid density;
    - the fluid viscosity;
    - the rock permeability;
    - the rock porosity;
    - the source of heat, fluid mass, or nuclide;
    - the dispersion tensor.
2. Features of the model (MODEL DATA commands), such as:
    - a user defined flux for a generalised flux boundary condition;
    - a mapping of the grid;
    - an initial guess;
    - nodes at which a boundary condition is set.
3. Post-processing (OUTPUT DATA commands), such as:
    - a scalar, vector, tensor or generalised function to be plotted;
    - a criterion for plotting.

To decide which user routines are appropriate to the particular facility required, the user should consult the NAMMU Reference Manual [7]. The user routines are described with the commands in which they are used. A description of the arguments for each routine is also included to aid the user in creating these source files.

Details of how to include these FORTRAN source files in a NAMMU run are given in the Installation and Running Guide [11]. When NAMMU is run, these routines are compiled

and checked for any errors. If errors are detected, the job will terminate before any of the TGIN commands in the input file are executed.

To make these user subroutines flexible and easy to use, a simple facility has been provided for communicating to them values read from the input data. This can be done using the COMMON blocks:

```
COMMON/CUIDNO/ IDNO
COMMON/CURPAR/ RUP(10),NRUP
COMMON/CUIPAR/ IUP(10),NIUP
```

where

`IDNO` – is the identification number;
`RUP` – the real parameter list;
`IUP` – the integer parameter list;
`NRUP` – the number of real parameters set;
`NIUP` – the number of integer parameters set.

The values in these COMMON blocks can be set through the input data as follows:

`IDNO` is set using the keyword `IDENTIFICATION NUMBER`;
`RUP` is set using the keyword `REAL PARAMETERS`;
`IUP` is set using the keyword `INTEGER PARAMETERS`;
`NRUP` is set to the number of real parameters read from the input;
`NIUP` is set to the number of integer parameters read from the input.

Within a user subroutine any of the TGSL utility routines may be called and values from any of the TGSL COMMON blocks may be used, although values in such COMMON blocks should **not** be changed. Useful COMMON blocks are documented in subsection 11.2.3. The utility routines are not documented, however.

11.1 User-specified Material Properties

As an illustration, we shall give a few examples of user-supplied routines that define non-standard behaviour of the material properties.

11.1.1 Density (DENUSR)

The user may specify the variation of density with temperature and pressure by means of the subroutine DENUSR. This has the argument list:

1. RHO is the density;
2. DRHODV is an array which contains the derivatives of density with respect to the variables;
3. VAR is an array which contains the variables ('PRES', 'TEMP' and so on);
4. NVAR is the number of variables;
5. R is the position vector;
6. NSD is the number of space dimensions.

If the user wishes to take advantage of this facility the keyword CALL SUBROUTINE DENUSR must be specified for the command ≫ PHYSICAL PROPERTIES and a version of the subroutine DENUSR provided. In the routine, RHO and DRHODV must be calculated given the variables and the position. Furthermore, DRHODV must be consistent with RHO else poor (or no) convergence will occur. An example is given below. This version calculates the density as a quadratic function of temperature.

```
      SUBROUTINE DENUSR(RHO,DRHODV,VAR,NVAR,R,NSD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      DIMENSION R(NSD),VAR(NVAR),DRHODV(NVAR)
      A=0.0
      B=1.0E3
      C=1.0E1
      D=1.0E-1
C
      P=VAR(1)
      T=VAR(2)+A
      RHO=B+C*T+D*T*T
      DRHODV(1)=0.0
      DRHODV(2)=C+2.0*D*T
C
      RETURN
      END
```

11.1.2 Permeability (PERUSR)

The user may specify the rock permeability by means of the subroutine PERUSR. This has the argument list:

1. AKR is a (3×3) array which contains the permeabilities;
2. R is the position vector;
3. NSD is the number of space dimensions.

If the user wishes to take advantage of this facility the keyword CALL SUBROUTINE PERUSR must be specified for the command ≫ PHYSICAL PROPERTIES and a version of the subroutine PERUSR provided. In the routine, AKR must be calculated given the variables and the position. An example is given below.

This version calculates an anisotropic depth-dependent permeability. This example also demonstrates the use of the communication COMMON blocks. The quantities AL, AKX, AKY, AKZ and Z0 are set from the information passed down in the COMMON block CURPAR, which is set up in the input data by the keyword REAL PARAMETERS.

```
      SUBROUTINE PERUSR(AKR,R,NSD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      DIMENSION R(NSD),AKR(3,3)
C
      COMMON/CUIDNO/ IDNO
      COMMON/CURPAR/ RUP(10),NRUP
      COMMON/CUIPAR/ IUP(10),NIUP
C
      AL=RUP(1)
      AKX=RUP(2)
      AKY=RUP(3)
      AKZ=RUP(4)
C
      Z0=RUP(5)
      Z=R(3)
C
     AKR(1,1)=AKX*EXP(-(Z-Z0)/AL)
     AKR(1,2)=0.0
     AKR(1,3)=0.0
     AKR(2,1)=0.0
     AKR(2,2)=AKY*EXP(-(Z-Z0)/AL)
     AKR(2,3)=0.0
     AKR(3,1)=0.0
     AKR(3,2)=0.0
     AKR(3,3)=AKZ*EXP(-(Z-Z0)/AL)
C
     RETURN
     END
```

11.1.3 Nuclide Source (SRCXY and SRCT)

The user may specify a nuclide source as a function of position and time by means of the subroutines SRCXY and SRCT. These routines specify the nuclide source as the product of a function of space and a function of time. For convenience, the temporal factor is specified by giving the integrated source over time rather than the instantaneous rate. This process of separating the temporal and spatial behaviours is identical to that described for a heat source in subsection 5.1.3. SRCXY has the argument list:

1. INUC is the nuclide number;
2. R is the position vector;
3. NSD is the number of space dimensions;
4. SOURCE is the spatial factor of the nuclide source.

SRCT has the argument list:

1. INUC is the nuclide number;
2. TIME is the current value of time;
3. SCN is the integrated nuclide source over time, expressed as a function of time.

If the user wishes to use this facility, the keyword USER NUCLIDE SOURCE must be specified for the command ≫ PHYSICAL PROPERTIES and versions of subroutines SRCXY and SRCT provided. In these subroutines, SOURCE and SCN are calculated for nuclide number INUC, position R and time TIME. An example is given below.

```
      SUBROUTINE SRCXY(INUC,R,NSD,SOURCE)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      DIMENSION R(NSD)
C
      SOURCE=0.0
      IF(R(1).GT.150.0.OR.R(1).LT.125.0) RETURN
      IF(R(2).GT.-40.0.OR.R(2).LT.-66.0) RETURN
      SOURCE=0.1
      RETURN
      END

      SUBROUTINE SRCT(INUC,TIME,SCN)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      SCN=1.0E8*(1.0-EXP(-TIME*1.0E-8))
      RETURN
      END
```

This version gives a nuclide concentration which is zero except in the region where 125m$<$R(1)$<$150m, $-$66m$<$R(2)$<$ $-$40m and decays in time so that the integrated source tends to a constant.

11.2 User-specified Boundary Conditions

11.2.1 Generalised Flux (GF... and GJ...)

The keyword `USER DEFINED FLUX` of the subcommand >> `GENERALISED FLUX LAW` allows the user to specify a flux over the boundary for any of the variables as a function of the variables as well as their spatial derivatives. This flux is integrated over elements having sides/faces on the part of the boundary selected and used together with the equations defined within the domain to form the appropriate discrete matrix system for the vector of dependent variables. The integral of the flux over the side/face of an element is evaluated using gaussian quadrature. For a variable i the flux f_i may be written in the discrete system as

$$f_i = \sum_{g=1}^{NGS} w_g \left[E N_i + \sum_{j=1}^{NSD} E R_j \frac{\partial N_i}{\partial x_j} \right] \Bigg|_{x=x_g} \tag{11.1}$$

where NGS is the number of gauss points on the side/face of the element, w_g is the gauss weight for the g-th gauss point and x_g is the position of the g-th gauss point, N_i is the finite element basis function associated with variable i, E and ER are functions of the variables and their derivatives. The gauss points used to evaluate this integral are positioned as appropriate to an interpolation over the side/face of an element for a dimension one less than that of the model. Thus for two-dimensional elements with quadratic interpolation, the flux is sampled at three extra gauss points. The user supplies E, ER and derivatives of E and ER with respect to the spatial derivatives of the variables. For the types of problems solved using NAMMU, the derivatives of the basis functions rarely appear in the flux term, and so normally

$$ER = 0 \tag{11.2}$$

As an example of how E and ER are set, the flux of a nuclide species α is considered with concentration N_α. From [8], the standard form for the flux F_{N_α} for the nuclide is

$$F_{N_\alpha} = (\mathbf{q} N_\alpha - \phi \mathbf{D}_\alpha \nabla N_\alpha) \cdot \mathbf{n} \tag{11.3}$$

where ϕ is the porosity, $\mathbf{D}_\alpha$ the dispersion tensor, and $\mathbf{n}$ is a unit outward normal across the boundary. If a zero-diffusive flux were set then

$$F_{N_\alpha} = \mathbf{q} \cdot \mathbf{n} N_\alpha \tag{11.4}$$

on the boundary, and so the appropriate functional form for E and ER is

$$E = \mathbf{q} \cdot \mathbf{n} N_\alpha \tag{11.5}$$

$$ER = 0 \tag{11.6}$$

In most cases a zero-dispersive flux boundary condition is set by specifying the keyword `ZERO DISPERSIVE FLUX` and no user routines are required.

For a zero-advective flux then

$$F_{N_\alpha} = -\phi \mathbf{D}_\alpha \nabla N_\alpha \cdot \mathbf{n} \tag{11.7}$$

would be set on the boundary and so the appropriate functional forms for E and ER are

$$E = -\phi \mathbf{D}_\alpha \nabla N_\alpha \cdot \mathbf{n} \tag{11.8}$$

and

$$ER = 0. \tag{11.9}$$

In the case of nuclide transport using standard elements for the flow E and ER are supplied in the routine GFR2NU and their spatial derivatives are supplied in the routine GJR2NU. A full list of the generalised flux law user routines may be found in the NAMMU Reference Manual [7].

The argument lists of GFR2NU and GJR2NU contain the following:

1. `V` is the real array of variable values at the extra gauss point;
2. `DVDR` is the real array of spatial derivatives of the variables at the gauss point;
3. `R` is the position vector of the extra gauss point;
4. `E` is the term E in Equation (11.1) (GFR2NU only);
5. `ER` is the term ER in Equation (11.1) (GFR2NU only);
6. `DEDV` is the array of derivatives of E with respect to the variables (GJR2NU only);
7. `DERDV` is the array of derivatives of ER with respect to the variables (GJR2NU only);
8. `DEDVR` is the array of derivatives of E with respect to the spatial derivatives of the variables (GJR2NU only);
9. `DERDVR` is the array of derivatives of ER with respect to the spatial derivatives of the variables (GJR2NU only);
10. `NVAR` is the number of variables;
11. `NDIM` is the actual number of dimensions;
12. `LSP` is the maximum number of dimensions;
13. `MXLVEL` is the maximum number of levels of the global freedom vector;
14. `MXRHS` is the maximum number of right hand sides (GFR2NU only);
15. `MMAT` is the maximum number of equation matrices (GJR2NU only);

16. IPAR is an integer parameter passed from the input file;
17. NIP is the number of integer parameters;
18. VPAR is a real parameter passed from the input file;
19. NVP is the number of real parameters;
20. XN is the unit outward normal calculated at the point when the boundary condition is set;
21. BFLD is an array of user-specified boundary values.

If the user wishes to use this facility the keyword USER DEFINED FLUX of the command ≫ GENERALISED FLUX LAW must be specified as part of the ≫ SET BOUNDARY CONDITIONS phase and appropriate subroutines must be provided with the arrays E, ER DEDV, DERDV, DEDVR and DERDVR specified. The unit outward facing normal is calculated at the point when the boundary condition is set. If the grid is subsequently mapped it will be necessary to calculate this normal within routines GFR2NU and GJR2NU. An example is given below for a case where the boundary condition is set to no-flow for the nuclide if the groundwater flow is into the model and to zero diffusive flux if the groundwater flow is out of the model.

```
      SUBROUTINE GFR2NU(V,DVDR,R,
     >                  E,ER,
     >                  NVAR,NDIM,LSP,MXLVEL,MXRHS,
     >                  IPAR,NIP,RPAR,NVP,XN,BFLD)
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION V(NVAR,MXLVEL),DVDR(NVAR,NDIM,MXLVEL),
     >          R(NDIM),E(NVAR,MXRHS),ER(NVAR,NDIM,MXRHS)
      DIMENSION QR(3),DQRDV(3,2),DQRDDP(3,3)
      DIMENSION DRHODV(2),DPORDV(2)
      DIMENSION XN(NDIM)
      DIMENSION IPAR(NIP),RPAR(NVP),BFLD(8,5)
C
      DATA IP/1/,IN/3/,IN1/4/
      DATA IX/1/,IY/2/
      DATA ZERO/0.0D0/
C
      ANUC=V(IN,1)
C
      CALL GWVEL1(RHOF,POROS,QR,DRHODV,DPORDV,
     >                  DQRDV,DQRDDP,S,DSDP,
     >                  V,DVDR,R,NVAR,NDIM,LSP)
C
      QDOTN = QR(IX)*XN(IX) + QR(IY)*XN(IY)
```

```
C
      IF (QDOTN .GT. ZERO) THEN
        E(IN,1) = ANUC*QDOTN
        ER(IN,IX,1) = ZERO
        ER(IN,IY,1) = ZERO
      ELSE
        E(IN,1) = ZERO
        ER(IN,IX,1) =ZERO
        ER(IN,IY,1) =ZERO
      END IF
C
      RETURN
      END

      SUBROUTINE GJR2NU(V,DVDR,R,
     >               DEDV,DERDV,DEDVR,DERDVR,
     >               NVAR,NDIM,LSP,MXLVEL,MMAT,
     >               IPAR,NIP,RPAR,NVP,XN,BFLD)
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION V(NVAR,MXLVEL),DVDR(NVAR,NDIM,MXLVEL),
     >          R(NDIM),DEDV(NVAR,NVAR,MMAT),
     >          DERDV(NVAR,NDIM,NVAR,MMAT),
     >          DEDVR(NVAR,NVAR,NDIM,MMAT),
      DIMENSION QR(3),DQRDV(3,2),DQRDDP(3,3)
      DIMENSION DRHODV(2),DPORDV(2)
      DIMENSION XN(NDIM)
      DIMENSION IPAR(NIP),RPAR(NVP),BFLD(8,5)
C
      DATA IP/1/,IN/3/,IN1/4/
      DATA IX/1/,IY/2/
      DATA ZERO/0.0D0/
C
      ANUC=V(IN,1)
C
      CALL GWVEL1(RHOF,POROS,QR,DRHODV,DPORDV,
     >                  DQRDV,DQRDDP,S,DSDP,
     >                  V,DVDR,R,NVAR,NDIM,LSP)
C
      QDOTN = QR(IX)*XN(IX) + QR(IY)*XN(IY)
C
      IF (QDOTN .GT. ZERO) THEN
        DEDV(IN,IN,1) = QDOTN
        DEDVR(IN,IN,IX,1) = ZERO
        DEDVR(IN,IN,IY,1) = ZERO
        DERDV(IN,IX,IN,1) = ZERO
        DERDV(IN,IY,IN,1) = ZERO
        DERDVR(IN,IX,IN,IX,1) = ZERO
```

```
          DERDVR(IN,IX,IN,IY,1) = ZERO
          DERDVR(IN,IY,IN,IX,1) = ZERO
          DERDVR(IN,IY,IN,IY,1) = ZERO
        ELSE
          DEDV(IN,IN,1) = ZERO
          DEDVR(IN,IN,IX,1) = ZERO
          DEDVR(IN,IN,IY,1) = ZERO
          DERDV(IN,IX,IN,1) = ZERO
          DERDV(IN,IY,IN,1) = ZERO
          DERDVR(IN,IX,IN,IX,1) = ZERO
          DERDVR(IN,IX,IN,IY,1) = ZERO
          DERDVR(IN,IY,IN,IX,1) = ZERO
          DERDVR(IN,IY,IN,IY,1) = ZERO
        END IF
C
        RETURN
        END
```

11.2.2 Mixed Elements

Section 8.1.3 described the subcommand ≫ `SPECIFIED VALUE FOR MIXED ELEMENTS` which is used to set a Dirichlet boundary condition on the pressure when solving the flow equation using mixed elements. This boundary condition actually sets a generalised flux law type boundary condition on the flux variables. If the components of the mass flux are variable numbers IFX and IFY the boundary condition set is:

$$E(IFX) = n_x P^{\mathrm{R}} \tag{11.10}$$

$$E(IFY) = n_y P^{\mathrm{R}} \tag{11.11}$$

where n_x and n_y are the x and y components of the unit outward facing normal and P^{R} is the specified value of the residual pressure that was given in the ≫ `SPECIFIED VALUE FOR MIXED ELEMENTS` subcommand. The ER terms are all zero, as are the spatial derivatives since P^{R} is a constant at the point.

11.2.3 Useful Common Blocks

In some instances the user may wish to access the values of the physical properties that are stored by the code in common blocks. An example is given in subsection 11.3.1, where values for gravitational acceleration and fluid density are obtained from common blocks so that contours of the hydrostatic head may be plotted. The main common blocks holding the values of physical properties are as follows:

```
      COMMON/GRAVIT/G
      COMMON/REFST/P0,T0
      COMMON/REFZ/Z0
      COMMON/REFDEN/RHOF0
      COMMON/FPVIS/AMU0,DELTA
      COMMON/FPDEN/ALPHAF,BETAF
      COMMON/ELTINF/IREG(10)
      COMMON/RPPORL/POR0L(500),DPORL(500)
      COMMON/RPPERL/PERML(6,500)
      COMMON/ROKDEL/RHORL(500)
      COMMON/FPSALT/RHOBRN,ALPHAS,BETAS
```

where

G	– is the gravitational acceleration;
P0	– is the reference pressure;
T0	– is the reference temperature;
Z0	– is the reference depth;
RHOF0	– is the reference fluid density;
AMU0	– is the reference fluid viscosity;
DELTA	– is the viscosibility;
ALPHAF	– is the fluid compressibility for fresh water;
BETAF	– is the thermal expansion coefficient for fresh water;
IREG(3)	– is the current rock type;
POR0L	– is the rock porosity, dimensioned by the rock layer;
DPORL	– is the derivative of the rock porosity with respect to pressure, dimensioned by the rock layer;
PERML	– is the rock permeability, dimensioned by the components KXX, KYY, KZZ, KXY, KYZ, KZX and then by the rock layer;
RHORL	– is the rock density, dimensioned by the rock layer;
RHOBRN	– is the reference density of the concentrated salt solution;
ALPHAS	– is the compressibility of the concentrated salt solution;
BETAS	– is the thermal expansion coefficient of the concentrated salt solution;

11.3 User-specified Post-processing

Sometimes the user may wish to present output that cannot be produced directly through the input data. An example of a subroutine that generates non-standard output is provided below.

11.3.1 Scalar Functions (SCLUSR)

The user may specify a scalar function to be plotted by means of the subroutine SCLUSR. This has the argument list:

1. VAL is the value of the scalar at a particular point, returned by the subroutine;
2. X is the position vector;
3. NSD is the number of spatial dimensions;
4. V is the array of values of the variables at the point;
5. NVAR is the number of variables;
6. DVDR is the array of spatial derivatives of the variables at the point.

If the user wishes to use this facility the keyword CALL SUBROUTINE SCLUSR must be specified for the required PLOT command and a version of the subroutine SCLUSR provided. An example is given below.

```
      SUBROUTINE SCLUSR(VAL,X,NSD,V,NVAR,DVDR)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(NSD),V(NVAR),DVDR(NSD,8)
      COMMON /CUIDNO/ IDNO
      PI = ATAN( 1.0D0 ) * 4.0D0
      A  = 1000.0D0
      B  = 200.0D0
      CH = COSH( PI * X(2) * SQRT( A / B ) / A )
      TH = TANH( PI * B * SQRT( A / B ) / A )
      SH = SINH( PI * X(2) * SQRT( A / B ) / A )
      C  = COS( PI * X(1) / A )
      S  = SIN( PI * X(1) / A )
      IF ( IDNO .EQ. 1 ) THEN
        VAL = -( CH + TH * SH ) * C
      ELSE IF ( IDNO .EQ. 2 ) THEN
        VAL = -2.0D-12 * 992.0D0 * PI * ( CH + TH * SH ) * S
      ELSE IF ( IDNO .EQ. 3 ) THEN
        VAL = 1.0D-12 * 992.0D0 * PI * SQRT( 2.0D0 )
     >        * ( SH + TH * CH ) * C
      END IF
      RETURN
      END
```

In this version, we have chosen to plot three scalar functions, which are selected by the value assigned to the identification COMMON block CUIDNO. If we chose to plot the analytic solution to the Toth testcase (see Section 8) for the residual pressure, then the input data would include the commands

```
>> DRAW LINE GRAPH
   CALL SUBROUTINE SCLUSR
   IDENTIFICATION NUMBER  1
```

Alternatively, if we selected `IDENTIFICATION NUMBER` 2 then the x-component of the analytic solution for the darcy velocity would be plotted.

12 TREATMENT OF ERRORS

NAMMU checks for errors such as incorrect syntax, insufficient parameter ranges and limits, and structural singularity of the frontal matrix. If an error is trapped by the program, an appropriate error message is written to the output file (see the Installation and Running Guide [11] for the organisation of files) as soon as it is detected. Most of these messages should be self explanatory.

NAMMU issues both error messages and warning messages. Some, but not all, error messages are fatal.

Errors in the syntax of the TGIN language are amongst the simplest mistakes that can occur in preparing an input dataset. These may be errors in the spelling of a TGIN instruction or in the order in which options are invoked. However the consequences of such errors vary considerably. Generally, if the fault occurred in an instruction that is high up in the command structure, then the program is more likely to issue an error message and terminate the job, but for erroneous keywords or low-level commands the program will usually issue a warning and continue as best it can.

All of the user routines are checked for syntax errors by the local FORTRAN compiler before the processing of the TGIN commands. If any errors are detected, the job is terminated as soon as all the user routines have been checked by the compiler. Particular care should be taken in checking the dimensioning of arrays in these routines. The dimensions of arrays included in the argument list of routines should agree with those specified in the Reference Manual. Care should also be taken to declare double precision variables as appropriate.

A successful compilation of a user routine does not imply that no further errors will arise from this routine. In fact, user-supplied routines can give rise to errors that are quite difficult to diagnose, since it is hard for the NAMMU package to anticipate the kind of errors that may occur. The user should carefully check each routine to ensure that there is no possibility of an overwrite or a division by zero.

Error and warning messages generally have the format

```
****** ERROR ******
ERROR MESSAGE
```

or

```
****** ERROR IN SUBROUTINE NAME ******
ERROR MESSAGE
```

and

```
****** WARNING ******
WARNING MESSAGE
```

or

```
****** WARNING FROM SUBROUTINE NAME ******
WARNING MESSAGE
```

One common error message is:

```
THE FOLLOWING KEYWORD HAS NOT BEEN PROCESSED ...
```

This means that a TGIN instruction has been mis-spelt or is not a valid option for the preceding command. NAMMU will usually continue as best it can. Many commands require essential keyword values, which if not supplied will acquire the default values that may not be sensible for the problem of interest. This may lead to unexpected results. This can be easily avoided by checking which keywords are required by a command in the Reference Manual [7].

Other common error messages relate to the workspace allocation. If the following error messages are encountered, the appropriate workspace allocation should be increased in ≫ `SET LIMITS`:

```
INTEGER BC WORKSPACE TOO SMALL

REAL BC WORKSPACE TOO SMALL
```

If the following error messages are encountered, the appropriate workspace allocation in the JOB INFORMATION at the start of the dataset should be increased by at least the specified amount:

```
EXTRA INTEGER SPACE OF .... NEEDED FOR SUBROUTINE ....
  VARIABLE ....

EXTRA REAL SPACE OF .... NEEDED FOR SUBROUTINE ....
  VARIABLE ....
```

The following common warning messages are advisory:

```
****** WARNING FROM BCNPRT ******
BOUNDARY CONDITIONS IGNORED AT .... NODES BECAUSE VARIABLES WERE NOT PRESENT
```

In this case, the user is advised to check that the variables concerned should not have been set at the nodes concerned.

```
****** WARNING FROM ROUTINE PHS2BY ******
THE MAXIMUM OF .. ITERATION AND .. QUASI-ITERATIONS HAS BEEN COMPLETED
THE MAXIMUM RELATIVE CHANGE FOR THE ABOVE ITERATION
HAS NOT MET THE CONVERGENCE CRITERION: 1.0000E-06
IF EQUATIONS ARE NON-LINEAR, THE SOLUTION MAY NOT HAVE CONVERGED SUFFICIENTLY
```

If the equations being solved are linear, the user does not need to take any action. If the equations are non-linear, the solution may not be properly converged.

Error messages relating to the solver will normally be trapped by the Harwell subroutine library routine MA42 [9, 10]. The following warning and error messages are fairly common:

```
***** Error return from MA42B/BD *****  INFO(1) =  4
      NFRONT not large enough, currently equals  ....
  *** Error return from MA42B/BD *****  INFO(1) = -12
      Size of NFRONT required is   ...
```

This message indicates that insufficient space has been allocated for the in-core frontal matrix. The user should increase the value for the keyword MAXIMUM FRONTWIDTH of the current solver option (e.g. ≫ STEADY STATE). If this new frontwidth now exceeds the value of FRONTWIDTH specified in ≫ SET LIMITS it will also be necessary to change that limit.

```
***** Error return from MA42B/BD *****  INFO(1) =  -14
      Matrix found to be singular
  *** Error return from MA42B/BD *****  INFO(1) = ...
***** Error discovered after input of elt/eqn ***** ....
```

This message indicates that a singularity was detected in the frontal matrix during decomposition. This error may arise for a number of reasons. Some of the more likely causes are that the model has been specified incorrectly, the problem is ill-posed or the initial condition may be inadequate in the case of non-linear equations. The user should carefully check the INITIAL DATA and MODEL DATA phases of the input file for any mistakes in the physical properties, grid, boundary conditions or initial guess. By systematically varying the model data, such as the specification of the boundary conditions and grid, the user may be able to locate the cause of the singularity.

The following warning message is often seen for mixed-element calculations.

```
***** Warning from MA42B/BD *****  INFO(1) = 2
Numerical criterion not satisfied by ... pivots
```

The solver used a number of pivots that did not satisfy the pivot criterion. It is possible that the solution may be inaccurate. This message is very common when the matrix is badly scaled e.g. when using mixed-elements. Increasing the frontwidth will remove the message with the penalty of greatly increased time being required in the solver.

REFERENCES

1. A.W. Herbert, *The verification of NAMMU using HYDROCOIN Level 1 Cases 1 and 7: Transient flow from a borehole and saturated flow through a shallow land disposal facility*, UKAEA Report AERE-R. 11944, 1985.

2. A.W. Herbert, *The verification of NAMMU using HYDROCOIN Level 1 Case 2: Steady state flow in a rock mass interspersed by permeable fracture zones*, UKAEA Report AERE-R. 11636, 1985.

3. T.P Cherill and A.W. Herbert, *The verification of NAMMU using HYDROCOIN Level 1 Case 4: Transient convection in a saturated permeable medium*, UKAEA Report AERE-R. 11952, 1985.

4. A.W. Herbert and C.P. Jackson, *A study of salt transport in a porous medium: The application of NAMMU to HYDROCOIN Level 1 Case 5*, UKAEA Report AERE-R. 12147, 1986.

5. R. Atkinson, T.P. Cherill, A.W. Herbert, D.P. Hodgkinson, C.P. Jackson, J. Rae and P.C. Robinson, *Review of the groundwater flow and radionuclide transport modelling in KBS-3*, UKAEA Report AERE-R. 11140, 1984.

6. P.C. Robinson, C.P. Jackson, A.W. Herbert and R. Atkinson, *Review of the groundwater flow modelling of the Swiss Project Gewähr*, UKAEA Report AERE-R. 11929, 1986.

7. S.T. Morris and S.P. Watson, *NAMMU (Release 6.4) Reference Manual*, AEA Technology Report AEAT-2842, 1998.

8. S.T. Morris, *NAMMU (Release 6.4) Technical Overview*, AEA Technology Report AEAT-2987, 1998.

9. I.S. Duff and J.A. Scott, *MA42–A new frontal code for solving sparse unsymmetric systems using the frontal method*, Rutherford Appleton Laboratory Report RAL-93-064, 1993.

10. Harwell Subroutine Library, *A catalogue of subroutines (11th Ed.)*, AEA/SERC, 1993.

11. K.A. Cliffe and S.T. Morris, *NAMMU (Release 6.4) Installation and Running Guide*, AEA Technology Report AEA-ESD-0287, 1998.

12. K.H. Winters and C.P. Jackson, *A Guide to Finite-element Grid Generation using TGIN (Release 1)*, UKAEA Report AERE-R. 11530, 1984.

13. O.C. Zienkiewicz, *The Finite Element Method*, McGraw-Hill, 1977.

14. J. Bear, *Dynamics of Fluids in Porous Media*, Elsevier, 1972.

15. NEA/SKI, *The International HYDROCOIN Project, Level 1: code verification*, OECD Publications, 1988.

16. O.C. Zienkiewicz and J.Z. Zhu, *A Simple Error Estimator and Adaptive Procedure for Practical Engineering Analysis*, Int. J. Num. Meth Eng **24**, 337–357, 1989.

17. K.H. Winters, C.M. Clark and C.P. Jackson, *The UK Contribution to the CEC PACOMA Project: Far-field Modelling of Radioactive Waste Disposal in Clay*, Nirex Safety Studies Report NSS/R185, AEA D&R Report 0063, 1990.

18. M.A. Brightman and D.J. Noy, *Finite-element modelling of the Harwell regional groundwater flow regime*, IGS–NERC Report FLPU 84-1, 1984.

19. J.A Toth, *A theoretical analysis of groundwater flow in a small drainage basin*, J.Geophys. Res. **68**, 4795–4812, 1963.

20. P.S. Huyakorn, P.F. Andersen, J.W. Mercer and H.O. White Jr., *Saltwater intrusion in aquifers: development and testing of a three dimensional finite element model*, Water Resources Res. **23**, 293–312, 1987.

21. D.G. Cacuci, C.F. Weber, E.M. Oblow and J.H. Marable, *Sensitivity Theory for General Systems of Nonlinear Equations*, Nucl. Sci. Eng. **75**, 88–110, 1980.

22. L.J Hartley, *A Summary of the Adjoint Equations and Sensitivities Corresponding to the Groundwater Flow and Transport Equations used in the Groundwater Flow Code NAMMU*, AEA ESD-0447, 1994.

23. L.J. Hartley and J.D. Porter, *A Study of an Adjoint Sensitivity Technique using the Groundwater Flow Code NAMMU*, Nirex Safety Series Report NSS/R364, 1994.

24. L.J. Hartley and J.D. Porter, *Adjoint Sensitivity Analysis of Steady-state Solute Transport*, Computational Methods in Water Resources, volume X, Kluwer Academic Publishers, 1994.

25. R.J. Greathead, A.W. Herbert and C.P. Jackson, *A three-dimensional finite element model of a hypothetical repository site using the NAMMU groundwater flow computer code*, UKAEA Report AERE-R. 13143, 1988.

26. D.P. Hodgkinson, *A mathematical model for thermal convection around a radioactive waste repository in a hard rock*, Annals of Nuclear Energy **7**, 313–334, 1980.

27. D.P. Hodgkinson, *Specification of a test problem for HYDROCOIN Level 1 Case 4: transient thermal convection in a saturated permeable medium*, UKAEA Report AERE-R. 11566, 1985.

28. D.P. Hodgkinson, *Analytical models for thermal mechanics*, UKAEA Report AERE-R. 10341, 1982.

A THE FINITE-ELEMENT METHOD

NAMMU uses a standard Galerkin formulation of the finite-element method. This is briefly described in the Appendix of 'A Guide to Finite-Element Grid Generation Using the TGIN Language' [12] and is summarised below. Those interested in more detail should consult one of the many excellent books on the subject, e.g. Reference [13]. The discretisation is approached via a weak form of the equations. This is derived by multiplying the equations by an arbitrary test-function, integrating over the domain of interest, and integrating by parts the terms involving second derivatives. The weak form is not unique: an arbitrary weight-function may be used, and some of the terms involving first derivatives may also be integrated by parts.

The equations are then discretised by approximating the domain by finite elements, approximating the field variables by expansions in terms of the finite-element basis functions, and using the set of finite-element basis functions as the test functions in the weak form.

The integration by parts which is carried out in obtaining the weak formulation produces a boundary integral for each equation. The domain of integration is the part of the boundary for which a specified value is *not* set for the appropriate variable. The integrand consists of a normal flux. This flux is the quantity that can be specified as a boundary condition using the command ≫ `SPECIFIED FLUX`.

If a Dirichlet boundary condition is specified for the variable then the finite-element equations for nodes on that section of the boundary are replaced by the Dirichlet boundary condition.

If no boundary condition is specified explicitly on part of the boundary then the boundary integral on that part of the boundary is assumed to be zero. This is known as the *natural boundary condition.*

The equations used to characterise each of the physical processes are given in the Technical Overview [8]. The form of the flux for each of the variables and equations is also given.

The finite-element method is used for the spatial discretisation of the equations. In the time-dependent case the time step may be constant or a version of Gear's method may be used to determine the size of the time step. Gear's method is a predictor-corrector algorithm, based on several low-order backward-difference schemes, that automatically chooses both the order of the scheme and the size of the time step so that the time step is as large as possible subject to a constraint upon the error in each step, which is estimated from the difference between the predictor and corrector.

The result of spatial and temporal discretisation is a set of coupled algebraic equations, which is usually non-linear. The nonlinearities are handled by Newton-Raphson iterations or by quasi-Newton-Raphson iterations. These lead to a set of linear equations, which is solved using a very fast direct frontal solver.

B THE NAMMU ELEMENT LIBRARY

This Appendix catalogues all the one-, two-, and three-dimensional elements available to the NAMMU user. A brief description of each element, and its associated basis functions are also given.

B.1 The One-dimensional Elements

ELEMENT			BASIS FUNCTIONS	
NAME	DESCRIPTION	GAUSS SCHEME	TYPE	DESCRIPTION
'LIN2'	2 node line	3 point	1	2 node linear
'LIN3'	3 node line	3 point	1	3 node quadratic
'L3/1'	3 node line	3 point	1	3 node quadratic
			2	1 node constant
'L3/2'	3 node line	3 point	1	3 node quadratic
			2	2 node linear

B.2 The Two-dimensional Elements

ELEMENT			BASIS FUNCTIONS	
NAME	DESCRIPTION	GAUSS SCHEME	TYPE	DESCRIPTION
'QAD4'	4 node quadrilateral	13 point	1	4 node linear
'QAD8'	8 node quadrilateral	13 point	1	8 node quadratic
'QAD9'	9 node quadrilateral	13 point	1	9 node quadratic
'Q984'	9 node quadrilateral	13 point	1	9 node quadratic
			2	8 node quadratic
			3	4 node linear
'Q4/1'	5 node quadrilateral	2×2 product	1	4 node linear
			2	1 node constant discontinuous
'Q8/4'	8 node quadrilateral	13 point	1	8 node quadratic
			2	4 node linear
'Q9/1'	9 node quadrilateral	13 point	1	9 node quadratic
			2	1 node constant discontinuous
			3	4 node linear

ELEMENT			BASIS FUNCTIONS	
NAME	DESCRIPTION	GAUSS SCHEME	TYPE	DESCRIPTION
’Q9/4’	9 node quadrilateral	3×3 product	1	9 node quadratic
			2	4 node linear
’QMX2’	9 node quadrilateral	2×2 product	1	4 node linear
			2	1 node constant discontinuous
			3,4	x, and y components of 4 node linear vector valued function with continuous normal components across element boundaries
’TRI3’	3 node triangle	7 point	1	3 node linear
’TRI6’	6 node triangle	7 point	1	6 node quadratic
’T6/3’	6 node triangle	7 point	1	6 node quadratic
			2	3 node linear
’TDIS’	7 node triangle	7 point	1	7 node quadratic
			2	7 node linear
			3	3 node linear
’T763’	7 node triangle	7 point	1	7 node quadratic
			2	6 node quadratic
			3	3 node linear
’TMX2’	7 node triangle	7 point	1	3 node linear
			2	1 node constant discontinuous
			3,4	x, and y components of 3 node linear vector valued function with continuous normal components across element boundaries

B.3 The Three-dimensional Elements

ELEMENT			BASIS FUNCTIONS	
NAME	DESCRIPTION	GAUSS SCHEME	TYPE	DESCRIPTION
’CQ3L’	27 node cuboid	27 point	1	27 node quadratic
			2	26 node quadratic
			3	20 node quadratic
			4	8 node linear
’C271’	27 node cuboid	27 point	1	27 node quadratic
			2	1 node constant discontinuous
’CB27’	27 node cuboid	27 point	1	27 node quadratic
’CB08’	8 node cuboid	8 point	1	8 node linear
’CBQL’	27 node cuboid	27 point	1	27 node quadratic
			2	8 node linear
’CQ20’	20 node cuboid	27 point	1	20 node quadratic
’CQ26’	26 node cuboid	27 point	1	26 node quadratic
’CBMX’	15 node cuboid	8 point	1	8 node linear
			2	1 node constant discontinuous
			3,4,5	x, y and z components of 6 node trilinear vector valued function with continuous normal components across element boundaries
’PRI6’	6 node prism	21 point	1	6 node linear
’PR15’	15 node prism	21 point	1	15 node quadratic
’PR18’	18 node prism	21 point	1	18 node quadratic
’PRQL’	18 node prism	21 point	1	18 node quadratic
			2	6 node linear
’PRMX’	12 node prism	21 point	1	8 node linear
			2	1 node constant discontinuous
			3,4,5	x, y and z components of 5 node trilinear vector valued function with continuous normal components across element boundaries

ELEMENT			BASIS FUNCTIONS	
NAME	DESCRIPTION	GAUSS SCHEME	TYPE	DESCRIPTION
’TTMX’	9 node tetrahedron	15 point	1	4 node linear
			2	1 node constant discontinuous
			3,4,5	x, y and z components of 4 node trilinear vector valued function with continuous normal components across element boundaries

C OUTPUT INFORMATION FOR EXAMPLE 1

This Appendix contains a description of the information that is printed in the output file. Diagnostic information is printed automatically for each major phase of a NAMMU run, together with other information relating to the execution of specific TGIN instructions. An echo of the input data is also written to the output file, with each command being echoed as soon as it is read. This input echo is interspersed by the diagnostic information relating to the current command being executed.

In this Section, an explanation is given of the meaning of the more important information written to the output files; the output file corresponding to Example 1 is used as illustration. Each phase of the output is described in the sequence in which it is printed.

C.1 Initial Data Information

A list of all the standard physical parameters within the program is printed together with the value assigned to each parameter. Some of these parameters may have been set by the user, but others will not be relevant to the current problem and will have been set to the default values. The default value for each physical property is given in the NAMMU Reference Manual [7].

Here is the output list of physical properties used in Example 1:

```
PHYSICAL PROPERTIES
===================

FLUID DENSITY IN REFERENCE STATE                9.9225E+02
REFERENCE PRESSURE                              0.0000E+00
REFERENCE TEMPERATURE                           0.0000E+00
REFERENCE DEPTH                                 0.0000E+00
GRAVITATIONAL ACCELERATION                      9.8100E+00
VISCOSITY                                       1.0000E-03
DELTA                                           1.6710E-02
FLUID COMPRESSIBILITY                           0.0000E+00
FLUID THERMAL EXPANSION COEFFICIENT             3.8536E-04
DENSITY OF SALT SOLUTION                        1.2000E+03
COMPRESSIBILITY OF SALT SOLUTION                0.0000E+00
THERMAL EXPANSION COEFFICIENT OF SALT SOLUTION  3.8536E-04
FLUID HEAT CAPACITY                             4.1786E+03
AIR SPECIFIC HEAT                               0.0000E+00
AIR HEAT CONDUCTIVITY                           0.0000E+00
FLUID HEAT CONDUCTIVITY                         0.0000E+00
DECAY CONSTANTS                                 0.0000E+00
MOLECULAR DIFFUSION COEFFICIENTS                1.0000E-06
SALT DIFFUSION COEFFICIENT                      1.0000E-06


ROCK PROPERTIES
---------------

          PERMEABILITIES
    ROCK                                        KXX         KYY         KZZ
-------------------------------------------------------------------------------
  1 ROCK   1                                1.0000E-16  1.0000E-16  1.0000E-16

          PERMEABILITIES
```

```
    ROCK                                          KXY         KYZ         KZX
-------------------------------------------------------------------------------
  1 ROCK   1                                  0.0000E+00  0.0000E+00  0.0000E+00

          PROPERTIES
    ROCK                                      DENSITY     POROSITY    D(POR)/DP
-------------------------------------------------------------------------------
  1 ROCK   1                                  2.6000E+03  1.0000E-04  0.0000E+00

          PROPERTIES
    ROCK                                      TORTUOSITY    SALT DISP LENGTHS
-------------------------------------------------------------------------------
  1 ROCK   1                                  1.0000E+00  1.0000E+00  1.0000E+00

          PROPERTIES
    ROCK                                      SPEC HEAT   CONDUCT'Y     TEMP DISP LENGTHS
-------------------------------------------------------------------------------------------
  1 ROCK   1                                  8.7900E+02  2.5100E+00  0.0000E+00  0.0000E+00

          PROPERTIES
    ROCK                                      SPECIFIC STORAGE COEFFICIENT
-------------------------------------------------------------------------------------------
  1 ROCK   1                                  0.0000E+00

          NUCLIDE PROPERTIES
    ROCK                                      LONGITUDINAL DISPERSION LENGTHS
-------------------------------------------------------------------------------
  1 ROCK   1                                  1.0000E+00

          NUCLIDE PROPERTIES
    ROCK                                      TRANSVERSE DISPERSION LENGTHS
-------------------------------------------------------------------------------
  1 ROCK   1                                  1.0000E+00

          NUCLIDE PROPERTIES
    ROCK                                      SORPTION COEFFICIENTS
-------------------------------------------------------------------------------
  1 ROCK   1                                  0.0000E+00

          UNSATURATED PROPERTIES
    ROCK                                         AKR         BKR         SKR
-------------------------------------------------------------------------------
  1 ROCK   1                                  1.0000E+00  1.0000E+00  1.0000E+00

          UNSATURATED PROPERTIES
    ROCK                                         APC         BPC         SPC
-------------------------------------------------------------------------------
  1 ROCK   1                                  1.0000E+00  1.0000E+00  1.0000E+00

===============================================================================
```

Other information is given concerning physical properties that are required for such problems as radionuclide transport. Where appropriate, this information is printed in an easily readable tabular format. Finally, the total time spent in the ≫ `INITIAL DATA` phase is given in seconds.

C.2 Model Information

Information concerning the grid and boundary conditions is automatically printed out during the ≫ `MODEL DATA` phase, as described below.

C.2.1 General Grid Information

```
MODEL INFORMATION
-----------------

      1 VARIABLES PRESENT: PRES

      4 ELEMENTS USED OF TYPE  8  QAD9
      4 ELEMENTS PRESENT

ELEMENT ELEMENT                                                                 GAUSS
NUMBER   TYPE                          NODE NUMBERS                             SCHEME REGION PROPERTY PATCH SUBDOMAIN
------- ------- ------------------------------------------------------------- ------ ------ -------- ----- ---------
     1   QAD9       1     3    13    11     2     8    12     6     7    0      0       1       1      1
     2   QAD9       3     5    15    13     4    10    14     8     9    0      0       1       1      1
     3   QAD9      11    13    23    21    12    18    22    16    17    0      0       1       1      1
     4   QAD9      13    15    25    23    14    20    24    18    19    0      0       1       1      1


     25 FREEDOMS PRESENT

     25 NODES PRESENT

 NODE  FREEDOM       COORDINATES              FREEDOMS
        COUNT
------ -------       -----------              --------
     1       1   0.0000E+00  1.0000E+00    PRES
     2       2   0.0000E+00  7.5000E-01    PRES
     3       3   0.0000E+00  5.0000E-01    PRES
     4       4   0.0000E+00  2.5000E-01    PRES
     5       5   0.0000E+00  0.0000E+00    PRES
     6       6   2.5000E-01  1.0000E+00    PRES
     7       7   2.5000E-01  7.5000E-01    PRES
     8       8   2.5000E-01  5.0000E-01    PRES
     9       9   2.5000E-01  2.5000E-01    PRES
    10      10   2.5000E-01  0.0000E+00    PRES
    11      11   5.0000E-01  1.0000E+00    PRES
    12      12   5.0000E-01  7.5000E-01    PRES
    13      13   5.0000E-01  5.0000E-01    PRES
    14      14   5.0000E-01  2.5000E-01    PRES
    15      15   5.0000E-01  0.0000E+00    PRES
    16      16   7.5000E-01  1.0000E+00    PRES
    17      17   7.5000E-01  7.5000E-01    PRES
    18      18   7.5000E-01  5.0000E-01    PRES
    19      19   7.5000E-01  2.5000E-01    PRES
    20      20   7.5000E-01  0.0000E+00    PRES
    21      21   1.0000E+00  1.0000E+00    PRES
    22      22   1.0000E+00  7.5000E-01    PRES
    23      23   1.0000E+00  5.0000E-01    PRES
    24      24   1.0000E+00  2.5000E-01    PRES
    25      25   1.0000E+00  0.0000E+00    PRES

MODEL INFORMATION SUMMARY
-------------------------
NUMBER OF ELEMENTS        4
NUMBER OF NODES          25
NUMBER OF FREEDOMS       25
NUMBER OF VARIABLES       1
```

For each element, the element number, the element type, the nodes, the gauss scheme, the region number, the property type, the patch number and the subdomain number are printed. Note that a gauss scheme of type 0 indicates that the default gauss scheme for the element type is to be used (see Appendix B).

For each node, the node number, the number of global freedoms (that is, the number of unknowns) up to and including that node, the x and y coordinates, and the freedoms at that node are printed out.

C.2.2 Boundary Condition Information

```
DIRICHLET BC FOR VARIABLE PRES AT NODE     21 WITH VALUE  1.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE     22 WITH VALUE  1.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE     23 WITH VALUE  1.0000E+00
```

```
DIRICHLET BC FOR VARIABLE PRES AT NODE     24 WITH VALUE  1.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE     25 WITH VALUE  1.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE      1 WITH VALUE  0.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE      2 WITH VALUE  0.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE      3 WITH VALUE  0.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE      4 WITH VALUE  0.0000E+00
DIRICHLET BC FOR VARIABLE PRES AT NODE      5 WITH VALUE  0.0000E+00
TIME SPENT IN EXECUTING MODEL PHASE:      .23 SECONDS
```

Information is printed out for each node at which a boundary condition has been set, including the type of condition, the variable, the node and the value. In this particular case, DIRICHLET BC denotes a Dirichlet type boundary condition, that is one for which a value has been specified. It should be noted that no information is given on the default (natural) boundary conditions assumed by the program. Finally, the total time spent in the ≫ MODEL DATA phase is given in seconds.

C.3 Solver Information

Certain information is also printed automatically during the ≫ SOLVER DATA phase. The time to assemble the element information into a suitable format for the solver is given in seconds. There is then a summary of what the solver is going to do followed by a summary for each iteration:

```
CALCULATING ELEMENT INFORMATION TOOK      .00 SECONDS


   >> STEADY STATE
      END

      >> GROUNDWATER FLOW
         END


>> OUTPUT DATA

MAXIMUM NUMBER OF NEWTON-RAPHSON ITERATIONS      :  1
MAXIMUM NUMBER OF QUASI-NEWTON-RAPHSON ITERATIONS:  0
SOLVER METHOD: FRONTAL METHOD

CALCULATING ARRAY "LAST" TOOK      .02 SECONDS


------ NEWTON-RAPHSON ITERATION NUMBER  1 ------

ASSEMBLY TOOK             .00 SECONDS
LU DECOMPOSITION TOOK     .01 SECONDS
TOTAL SOLUTION TOOK       .01 SECONDS

FREEDOMS                            15
FLOATING POINT OPERATIONS          582   (        .001 MILLION OPERATIONS)
MAXIMUM FRONTWIDTH                   9
NON-ZEROS IN U                      82
NON-ZEROS IN L                      82
REAL STORAGE FOR U                  97
REAL STORAGE FOR L                  82
INTEGER STORAGE                    111
BUFFERS FOR U                        1
BUFFERS FOR L                        0
```

```
BUFFERS FOR INTEGERS                 1

PIVOT INFORMATION
COLUMNS SEARCHED                    15
NON-ZEROS TESTED                     8
NON-ZEROS ACCESSED                  72
PIVOT CRITERION BROKEN               0
STATIC CONDENSATIONS                 8
POTENTIAL STATIC CONDS               8

NATURAL LOG OF DETERMINANT OF JACOBIAN MATRIX = -3.3121E+02
SIGN OF DETERMINANT OF JACOBIAN MATRIX: POSITIVE

PRES: MAX. CHANGE = 7.5000E-01 AT FREEDOM     20  MAX. ABS(GF) = 0.0000E+00
MAXIMUM RELATIVE CHANGE = 7.5000E-01 AT FREEDOM     20

RSTEP =  7.5000E-01 (MAXIMUM RELATIVE CHANGE IN SOLUTION)

****** WARNING FROM ROUTINE PHS2BY ******
THE MAXIMUM OF 1 ITERATION AND  0 QUASI-ITERATIONS HAS BEEN COMPLETED
THE MAXIMUM RELATIVE CHANGE FOR THE ABOVE ITERATION
HAS NOT MET THE CONVERGENCE CRITERION: 1.0000E-06
IF EQUATIONS ARE NON-LINEAR, THE SOLUTION MAY NOT HAVE CONVERGED SUFFICIENTLY

TIME SPENT IN EXECUTING SOLVER PHASE:      .04 SECONDS
```

In addition to the diagnostic messages the following quantities are printed out for each iteration:

- ASSEMBLY time is the time spent assembling the equations, in seconds;
- LU DECOMPOSITION time is the time spent in the frontal solver, in seconds;
- The sign of the Jacobian determinant, for use in stability analyses;
- The natural logarithm of the absolute value of the Jacobian determinant;
- RSTEP is the largest relative change in any freedom from its value on the previous iteration if the same basis functions are used for different variables and the largest absolute change in any freedom from its value on the previous iteration if different basis functions are used for different variables – the integer printed immediately after the value of RSTEP is the freedom number.

The groundwater flow equations are linear so in this case the warning from routine PHS2BY may be ignored. Finally, the total time spent in the ≫ SOLVER DATA phase is given in seconds.

C.4 Output Data Information

The information printed out as part of the ≫ OUTPUT DATA phase is a mixture of output specifically requested and that which is printed automatically.

C.4.1 Global freedom information

```
   >> PRINT GLOBAL FREEDOMS
      END
       1  0.0000E+00
       2  0.0000E+00
       3  0.0000E+00
       4  0.0000E+00
       5  0.0000E+00
       6  2.5000E-01
       7  2.5000E-01
       8  2.5000E-01
       9  2.5000E-01
      10  2.5000E-01
      11  5.0000E-01
      12  5.0000E-01
      13  5.0000E-01
      14  5.0000E-01
      15  5.0000E-01
      16  7.5000E-01
      17  7.5000E-01
      18  7.5000E-01
      19  7.5000E-01
      20  7.5000E-01
      21  1.0000E+00
      22  1.0000E+00
      23  1.0000E+00
      24  1.0000E+00
      25  1.0000E+00
```

The above output results from the command ≫ `PRINT GLOBAL FREEDOMS`. For each node, the node number and the values of the global freedoms at that node are printed out. The global freedoms are in the order in which they appear in the node information given previously.

C.4.2 Contour Plot Information

```
NUMBER OF CONTOURS:  11
CONTOUR VALUES:  0.0000E+00  1.0000E-01  2.0000E-01  3.0000E-01  4.0000E-01
                 5.0000E-01  6.0000E-01  7.0000E-01  8.0000E-01  9.0000E-01
                 1.0000E+00

MINIMUM IS  0.0000E+00, FOUND AT POINT  0.0000E+00  7.5000E-01
 IN ELEMENT     1 LOCAL COORDINATES   .0000 -1.0000
MAXIMUM IS  1.0000E+00, FOUND AT POINT  1.0000E+00  1.0000E+00
 IN ELEMENT     3 LOCAL COORDINATES -1.0000  1.0000
```

The actual contour levels which were chosen by the program as a result of the command ≫ `PLOT CONTOURS` are printed out, and these are followed by information on the location of the maximum and minimum values.

C.4.3 Draw Line Graph Information

```
MINIMUM VALUE =  0.0000E+00  MAXIMUM VALUE =  1.0000E+00

POINT         COORDINATES          ROCK NUMBER    VALUE
    1    0.0000E+00  5.0000E-01              1  0.0000E+00
```

```
    2    1.0000E-01  5.0000E-01             1  1.0000E-01
    3    2.0000E-01  5.0000E-01             1  2.0000E-01
    4    3.0000E-01  5.0000E-01             1  3.0000E-01
    5    4.0000E-01  5.0000E-01             1  4.0000E-01
    6    5.0000E-01  5.0000E-01             1  5.0000E-01
    7    6.0000E-01  5.0000E-01             1  6.0000E-01
    8    7.0000E-01  5.0000E-01             1  7.0000E-01
    9    8.0000E-01  5.0000E-01             1  8.0000E-01
   10    9.0000E-01  5.0000E-01             1  9.0000E-01
   11    1.0000E+00  5.0000E-01             1  1.0000E+00
AVERAGE VALUE OVER PROFILE =  5.0000E-01
```

The ≫ DRAW LINE GRAPH command automatically produces a list of the values of the specified variable or scalar at equally spaced points along the specified line. The rock number at each point is also printed. In addition, the average value along the line is given. This is calculated by a simple trapezoidal rule, based on the points specified, and its accuracy depends on both the number of points and the behaviour of the variable or scalar along the line.

```
TIME SPENT IN EXECUTING OUTPUT PHASE:      .59 SECONDS

AMOUNT OF INTEGER WORKSPACE SO FAR UNUSED IS    103325
AMOUNT OF REAL    WORKSPACE SO FAR UNUSED IS     41353
```

Finally, the total time in the ≫ OUTPUT DATA phase is given in seconds, and the amount of unused workspace is printed.

D DEFINITION OF HYDROCOIN LEVEL 1 TEST CASE 2 (EXAMPLE 2)

STEADY-STATE FLOW IN A ROCK MASS INTERSECTED BY PERMEABLE FRACTURE ZONES

D.1 Background

This test case concerns steady-state flow in a two-dimensional vertical slice of a fractured rock [15]. The region contains two inclined fracture zones, which have a higher permeability than the surrounding rock. The fracture zones intersect one another at depth.

The purpose of this test case was to test the capabilities of different programs (including NAMMU) to treat large permeability contrasts. In view of the complicated geometry, no attempt was made to find an analytical solution for this problem. Thus, the accuracy of the solutions was judged by examining the convergence with respect to spatial discretisation.

It was recognised that flow in crystalline rock systems is generally poorly described by two-dimensional models. However, a two-dimensional problem was chosen since it was deemed tractable by the majority of the participants, especially since convergence tests for a three-dimensional problem would have been extremely expensive and time consuming. The main point of this case, namely the solution convergence of a problem with large permeability contrasts, can still be appropriately tested in two dimensions.

D.2 Conceptual Model

A two-dimensional cross-section of a fractured rock mass is intersected by two fracture zones as shown in Figure D.1. The zones, which have different widths and inclinations, intersect at depth within the modelled region.

The topography has been made simple so that it consists of two valleys located where the fracture zones meet the surface. To simplify the problem definition, the shape of the surface is described by straight lines. It should be noticed that in order to define the horizontal derivative unambiguously at the top corners, the surface is taken to be horizontal for the first ten metres. Although the surface topography is symmetric, the flow is influenced by the asymmetry of the fracture zones.

This problem is based on an idealised version of the hydrogeological conditions encountered at a potential site for a deep repository in Swedish bedrock. A detailed three-dimensional model of this was made for the KBS 3 study [5].

D.3 Assumptions

It is assumed that Darcy's law is applicable to both the fracture zones and the rock matrix. Moreover, both units are assumed to be homogeneous and isotropic media with permeabilities k_{f} and k_{m} respectively.

The rainfall is assumed to be sufficient to cause the water table to be coincident with the surface. The remaining boundaries are assumed to be impermeable to water flow.

D.4 Mathematical Model

The basic entities to be compared are the pressure in the fracture zones and the matrix as a function of horizontal and vertical coordinates x and y. As this is a steady-state problem, pressure is described by Laplace's equation:

$$\frac{\partial^2 P^{\mathrm{R}}(x,\ y)}{\partial x^2} + \frac{\partial^2 P^{\mathrm{R}}(x,\ y)}{\partial y^2} = 0 \tag{D.1}$$

for $P^{\mathrm{R}} = P_{\mathrm{f}}^{\mathrm{R}}$ and $P_{\mathrm{m}}^{\mathrm{R}}$ in the fracture zones and the rock mass respectively. The Darcy flux is defined by

$$\mathbf{q}(x,\ y) = -K \nabla P^{\mathrm{R}} / \mu \tag{D.2}$$

where K has constant values in the fractures and matrix. At the interfaces between the fracture zones and the matrix, the pressure and the normal component of the Darcy flux are continuous. For the top boundary (ground surface) the boundary condition is

$$P^{\mathrm{R}}(x,\ y) = y \tag{D.3}$$

the values of y being obtained by linear interpolation between points 1 to 9 in Figure D.1. The coordinates of these points are listed in Table E.1. No-flow conditions are assumed at the vertical boundaries (x=0 m and x=1600 m) and the bottom boundary ($y = -1000$ m) and thus

$$\frac{\partial P^{\mathrm{R}}(0,\ y)}{\partial x} = \frac{\partial P^{\mathrm{R}}(1600,\ y)}{\partial x} = \frac{\partial P^{\mathrm{R}}(x,\ -1000)}{\partial y}. \tag{D.4}$$

The pathlines are defined by

$$\frac{d\mathbf{r}}{dt} = \frac{1}{\phi}\,\mathbf{q}. \tag{D.5}$$

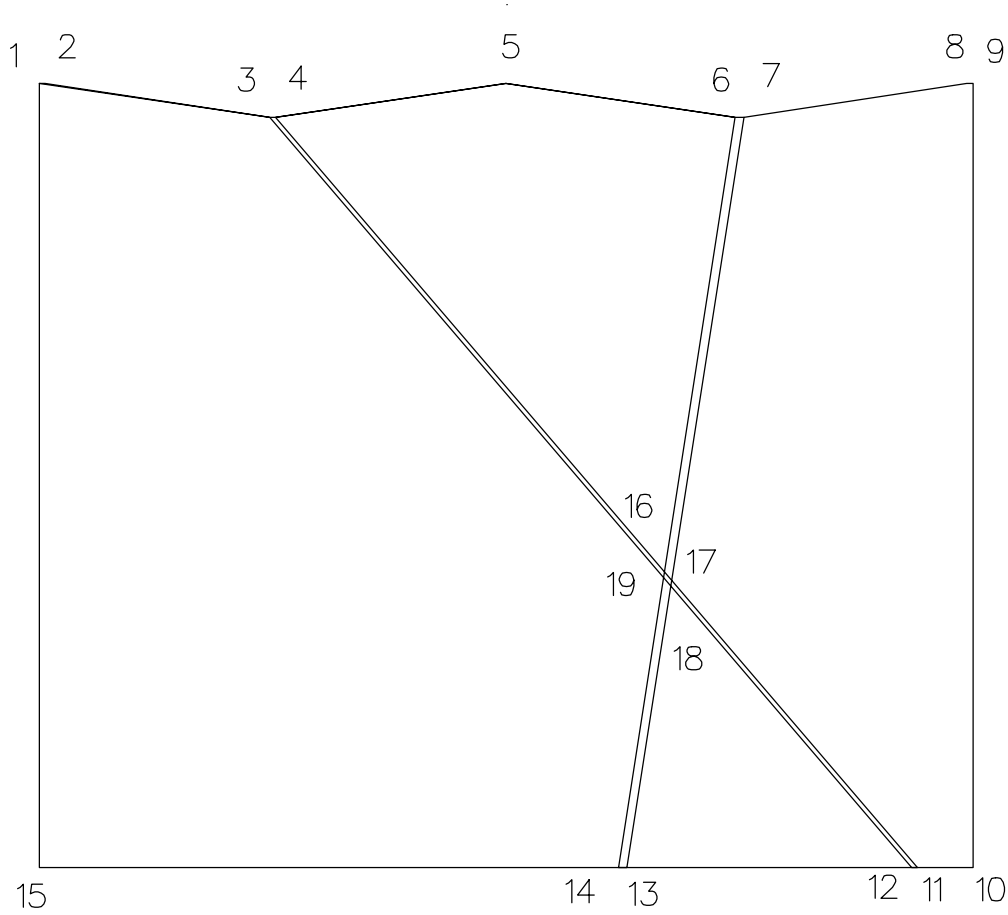


Figure D.1: Geometry of modelled domain in Example 2.

D.5 Input Parameters

The geometry of the modelled domain is defined by points 1 to 19 in Figure D.1. The coordinates of these points are listed in table D.1. The values of the hydraulic conductivities in the fracture zones and matrix are 10^{-6} ms^{-1} and 10^{-8} ms^{-1} respectively. The kinematic porosity, ϕ, which is required for pathline calculations, is taken to be 0.03 for both the fracture zones and rock mass.

Point no.	x (m)	y (m)
1	0.00	150.00
2	10.00	150.00
3	395.00	100.00
4	405.00	100.00
5	800.00	150.00
6	1192.50	100.00
7	1207.50	100.00
8	1590.00	150.00
9	1600.00	150.00
10	1600.00	-1000.00
11	1505.00	-1000.00
12	1495.00	-1000.00
13	1007.50	-1000.00
14	992.50	-1000.00
15	0.00	-1000.00
16	1071.35	-566.35
17	1084.04	-579.04
18	1082.50	-587.50
19	1069.81	-574.81

Table D.1: Coordinates of numbered points in the modelled domain.

E DEFINITION OF HYDROCOIN LEVEL 1 TEST CASE 4 (EXAMPLE 3)

TRANSIENT THERMAL CONVECTION IN A SATURATED PERMEABLE MEDIUM

E.1 Background

The heat output from a repository containing high-level waste can induce regional groundwater flows which last for thousands of years after burial. Since these flows are predominantly vertical they could shorten the leakage path and transit time of water-borne radionuclides. Safety assessments of radioactive waste disposal thus require an adequate quantification of this problem. The purpose of the present Example was to test the accuracy with which numerical codes can treat time-dependent buoyancy driven flows. This was achieved by comparing their results with an analytical solution for an idealised model of a repository in a homogeneous isotropic permeable medium. The solution is described in detail elsewhere [25, 26].

E.2 Conceptual Model

In the present example the rock-mass is assumed to be a homogeneous isotropic permeable medium of infinite extent. The repository is idealised as a uniform spherical heat source with the same physical properties as the surrounding rock, and a power output that decays exponentially with time. This geometry approximates repositories in which several waste blocks are placed in each deposition borehole.

The model considered here assumes that the dominant heat transfer mechanism is conduction through the rock rather than convective transfer due to the flow of groundwater. This is the most likely situation for low-permeability rocks envisaged for geological disposal.

E.3 Assumptions

The rock in and around the repository is assumed to be a saturated homogeneous isotropic permeable medium with constant physical properties e.g. permeability, thermal conductivity, and density. Flow transients arising from compressibility effects are neglected since they occur on a time-scale that is short compared to the time evolution of the regional temperature field. Thus the time-dependence of the flow field arises solely from the time-dependent heat output from the repository.

The Boussinesq approximation is made, which amounts to keeping variations of the water density in only the buoyancy term. Furthermore, the density of water is assumed to vary linearly with temperature and to be independent of pressure. The viscosity of water and the volumetric thermal expansion coefficient of water are assumed to be independent of temperature and pressure.

The flow is assumed to be governed by Darcy's law, and in the absence of the heat source there is no flow.

E.4 Mathematical Model

In this section the equations for temperature rise and dynamic pressure rise (i.e. the pressure causing flow), are written in terms of cylindrical polar coordinates $(r,\ z)$ whose origin is at the centre of the sphere. In [25] the equations are formulated in terms of the stream function, whereas in [26] a derivation is given in terms of the dynamic pressure.

With the assumptions outlined above, the dynamic pressure (i.e. the actual pressure minus the hydrostatic pressure) satisfies

$$\frac{\partial}{\partial r}\left[r\frac{\partial P^{\mathrm{R}}(r,\ z,\ t)}{\partial r}\right]+\frac{\partial^2 P^{\mathrm{R}}(r,\ z,\ t)}{\partial z^2}=g\beta\rho_0\frac{\partial T(r,\ z,\ t)}{\partial z}. \tag{E.1}$$

The Darcy velocity components (q_r and q_z) are related to $P^{\mathrm{R}}(r,\ z\,t)$ by

$$q_r(r,\ z,\ t)=-\frac{k}{\mu}\frac{\partial P^{\mathrm{R}}(r,\ z,\ t)}{\partial r} \tag{E.2}$$

and

$$q_z(r,\ z,\ t)=-\frac{k}{\mu}\left[\frac{\partial P^{\mathrm{R}}(r,\ z,\ t)}{\partial z}-g\beta\rho_0\theta(r,\ z,\ t)\right]. \tag{E.3}$$

In the low Rayleigh number regime assumed here, the temperature rise $\theta=T-T_0$, satisfies the heat conduction equation. Since it is unaffected by gravity in this limit, the temperature rise in an infinite medium will be spherically symmetric and thus

$$\theta(r,\ z,\ t)=\theta(R,\ t) \tag{E.4}$$

where

$$R=\left(r^2+z^2\right)^{\frac{1}{2}} \tag{E.5}$$

is the spherical radial coordinate.

For the present heat source, the temperature is given by

$$\rho_r c_r\frac{\partial\theta(R,\ t)}{\partial t}=\Gamma_a\frac{1}{R^2}\frac{\partial}{\partial R}\left[R^2\frac{\partial\theta(R,\ t)}{\partial R}\right]+\frac{3W_0}{4\pi A^3}\exp(-\lambda t)H(A-R). \tag{E.6}$$

The repository has a radius A, and a power W_0 at $t=0$ which subsequently falls off exponentially with a decay constant λ.

The initial conditions are

$$P^{\mathrm{R}}(r,\ z,\ 0)=\theta(r,\ z,\ 0)=0 \tag{E.7}$$

while the boundary conditions are that the rises in both dynamic pressure and temperature are finite at the centre of the sphere, and zero at infinity. In fact, the dynamic pressure at the centre of the sphere is zero for the present problem.

The analytical solution to this problem is described in the specification document [27]. The solution applies in an infinite medium, whereas the numerical models are limited to a finite

domain. It was therefore suggested that either the modelled region should be made large enough for the boundary conditions to have a negligible effect, or that the analytic solutions for a point source are specified on the boundary. These are much simpler than the full analytical solution, as discussed in the Appendix of [28].

E.5 Input Parameters

The input parameters for this case are given in Table E.1. They represent a typical repository containing high-level waste decaying with a half-life of 30 years, situated in a fractured hard rock.

Parameter	llllll	Value	Unit
Radius of sphere	A	250	m
Initial power output	W_0	10	MW
Decay constant†	λ	7.3215×10^{-10}	s^{-1}
Thermal conductivity of rock	Γ_a	2.51	$W\,m^{-1}k^{-1}$
Density of rock	ρ_r	2.6×10^{3}	$kg\,m^{-3}$
Specific heat of rock	c_r	8.79×10^{2}	$J\,kg^{-1}K^{-1}$
permeability of rock	k	1.0×10^{-16}	m^2
Density of water	ρ_0	9.922×10^{2}	$kg\,m^{-3}$
Expansion coefficient of water	β	3.85×10^{-4}	K^{-1}
Viscosity of water	μ	6.529×10^{-4}	$kg\,m^{-1}s^{-1)}$
Flowing porosity	ϕ	1.0×10^{-4}	–

†365.25 days per year is assumed

Table E.1: Input parameters for Example 3.

F TRANSPORT OF A NOTIONAL CONTAMINANT

In this Appendix, it is shown that the equation describing transport of a single nuclide may be simplified by exploiting its linearity. In particular, for a retention of unity (corresponding to zero sorption), it is shown that all dependence upon physical properties specific to a radionuclide can be removed. Further, this allows the spread of a single radionuclide for an arbitrary source to be deduced from the transport of a notional contaminant that is released at a constant rate.

For a single radionuclide of concentration denoted by N, Equation 49 in Reference [8] reduces to

$$\frac{\partial}{\partial t}(\phi RN) + \nabla \cdot (\mathbf{q}N) - \nabla \cdot (\phi \mathbf{D} \nabla N) = -\lambda \phi RN + \phi f. \tag{F.1}$$

where
- N is the concentration of the nuclide;
- ϕ is the porosity;
- R is the retardation;
- $\mathbf{q}$ is the darcy velocity;
- $\mathbf{D}$ is the dispersion tensor;
- λ is the half life of the nuclide;
- f is source of the nuclide (into the porewater).

It is convenient to transform this equation by changing to a new variable N^* defined by

$$N^* = N\mathrm{e}^{\lambda t}, \tag{F.2}$$

to give a new equation

$$\frac{\partial}{\partial t}\left(\phi RN^*\right) + \nabla \cdot \left(\mathbf{q}N^*\right) - \nabla \cdot \left(\phi \mathbf{D} \nabla N^*\right) = \phi f \mathrm{e}^{\lambda t}. \tag{F.3}$$

The effect of this transformation is to remove the term representing radioactive decay and to introduce a modified source term. The removal of decay allows greater flexibility in the choice of time-step in the numerical solution of (F.3), since the half-life of the radionuclide is no longer crucial in determining an appropriate time-step size.

The linearity of Equation (F.3) in N^* can be exploited to remove the dependence on the source term. We introduce the new function G' which represents the response to an impulse in source flux at $t = 0$ and which satisfies the equation

$$\frac{\partial}{\partial t}\left(\phi RG'\right) + \nabla \cdot \left(\mathbf{q}G'\right) - \nabla \cdot \left(\phi \mathbf{D} \nabla G'\right) = \delta(t). \tag{F.4}$$

This has the same physical constants and flow field as the left hand side of equation (F.3) but a delta function replaces the nuclide source term on the right hand side. Because of the linearity of these two equations, the nuclide concentration N^* resulting from a particular source function $\phi f \mathrm{e}^{\lambda t}$ is related to the response function G^* by the following convolution:

$$N^*(t) = \int G'\left(t - t'\right) \phi f\left(t'\right) \mathrm{e}^{\lambda t'} dt'. \tag{F.5}$$

Thus, the concentration of a particular nuclide may be derived from the concentration of a notional contaminant, G', using the convolution (F.5) and the transformation (F.2).

In practice, it is more convenient to compute the response function from a related equation

$$\frac{\partial}{\partial t}(\phi RG) + \nabla \cdot (\mathbf{q}G) - \nabla \cdot (\phi \mathbf{D} \nabla G) = H(t), \tag{F.6}$$

obtained by integrating Equation (F.4) with respect to time, where $H(t)$ is the Heaviside step function and

$$G' = \frac{d\,G}{dt}. \tag{F.7}$$

Hence, G represents the response of the system to a step change in contaminant concentration, and by differentiating the result with respect to time, the response of the system to a delta function or impulse source of contaminant is obtained.

Notes:

1. The formulation as described above applies only to cases with a source specified and with zero-concentration or flux boundary conditions, or with an imposed advective flux condition (zero diffusive flux);

2. Equation F.6 is also appropriate to the common case of transport away from a repository where the radionuclide is maintained at a solubility limit. In this case $G = 1$ would represent the solubility limit;

3. Equation F.6 is, in fact, the form of the equation solved in the example presented in Section 6. In this case the Heaviside function is distributed over a region specified using the user-supplied subroutine USLECT. The solution for this case could be differentiated with respect to time to give the response function G' appropriate to contaminant transport in this model.

G DEFINITION OF THE TOTH TESTCASE (EXAMPLE 6)

G.1 Model

The Toth test case is an example of regional constant-density groundwater flow for which an analytic solution is available [19]. The domain is 1000m in the x-direction ($0 \leq x \leq 1000$), 200m in the z-direction ($-200 \leq z \leq 0$) and is anisotropic but homogeneous. The permeability components are $k_x = 2.0 \times 10^{-12}\,\mathrm{m}^2$ and $k_z = 2.0 \times 10^{-12}\,\mathrm{m}^2$, the porosity is 10^{-4} and the viscosity, μ, is $10^{-3}\,\mathrm{kg\,m^{-1}\,s^{-1}}$.

The boundary conditions are

$$P = -\cos\left(\frac{\pi x}{1000}\right)$$

where x is the x-coordinate on the top boundary and no-flow on all of the other boundaries.

G.2 Analytic Solution

In the two-dimensional case the analytic solution for the residual pressure, P^{R}, is given by

$$P^{\mathrm{R}} = -\left[\cosh\left(\frac{\pi z\sqrt{\theta}}{a}\right) + \tanh\left(\frac{\pi b\sqrt{\theta}}{a}\right)\sinh\left(\frac{\pi z\sqrt{\theta}}{a}\right)\right]\cos\left(\frac{\pi x}{a}\right), \qquad \text{(G.1)}$$

where $\theta = k_x/k_z$, a is 1000 and b is 200.

The Darcy velocity in the x-direction is given by

$$u = -\frac{k_x\pi}{\mu a}\left[\cosh\left(\frac{\pi z\sqrt{\theta}}{a}\right) + \tanh\left(\frac{\pi b\sqrt{\theta}}{a}\right)\sinh\left(\frac{\pi z\sqrt{\theta}}{a}\right)\right]\sin\left(\frac{\pi x}{a}\right), \qquad \text{(G.2)}$$

where μ is the viscosity.

The Darcy velocity in the z-direction is given by

$$w = \frac{k_z\pi\sqrt{\theta}}{\mu a}\left[\sinh\left(\frac{\pi z\sqrt{\theta}}{a}\right) + \tanh\left(\frac{\pi b\sqrt{\theta}}{a}\right)\cosh\left(\frac{\pi z\sqrt{\theta}}{a}\right)\right]\cos\left(\frac{\pi x}{a}\right). \qquad \text{(G.3)}$$