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REPORT

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Title:
An introduction to hydrogeological and geochemical models and modelling.

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Summary:

This report presents an overview of programs that can be used for analytical and numerical hydrogeological modelling. The overview is not intended to be a complete list but an attempt has been made to include many of the most used and popular programs available today within hydrogeological and geochemical modelling.

The models listed include those falling into the categories of: groundwater flow models, particle tracking codes, pollution transport and geochemical models in addition to integrated modelling packages, pre- and post-processing programs, pumping test analysis programs and other miscellaneous programs of hydrogeological use.

The programs presented are particularly relevant for groundwater and reservoir simulation but should also be of use within soil chemistry, geotechnics, hazardous waste storage (including radioactive waste), domestic waste, acid rainfall and other related problems.

The theory behind the fundamental equations of groundwater flow is also presented together with the theory of the numerical finite-difference and finite-element approximations to these equations. An introduction to the practice of groundwater modelling is also presented in addition to references to more comprehensive works.

Key words: Hydrogeology	Groundwater	Modelling
Pollution	Groundwater quality	Geochemistry
Report		

1. INTRODUCTION

1.1 THE PURPOSE AND SCOPE OF THIS REPORT

The main purpose of this report is to provide an introduction to groundwater modelling and a single reference for modellers wishing to obtain more information on the models available today and their uses. It is hoped that the report will be of use to both users of models and to readers of project reports involving modelling.

This report presents an introduction to the fundamental equations of groundwater flow, the formulation of numerical models and an overview of available software that can be used to carry out hydrogeological modelling. No attempt has been made to compile a comprehensive list of available software but most of the popular commonly used programs available today within hydrogeological and geochemical modelling have been included. The programs presented are particularly relevant for groundwater and reservoir simulation but should also be of use within soil chemistry, geotechnics, hazardous waste storage (including radioactive waste), domestic waste, acid rainfall and other related problems.

Since modelling is a field involving continual development this report cannot represent a static document. Despite this, many numerical groundwater models often have a long useful life and the models presented in this report will be in mainstream use for many years to come.

Individual programs which have been extensively used earlier and/or have been important for the development of a particular genre of programs are included although no attempt has been made to present a complete historical overview. Depending on the problem more than one program may be applicable in any given situation. In this instance other factors will influence the choice of program. This report aims to provide potential users with information that will enable them to select the appropriate model for their use. A brief discussion of the factors involved in model selection is presented in Chapter 5 of this report.

Common geostatistical and general graphical packages are included in this report as they are often useful tools in groundwater modelling, particularly in terms of data file construction and output data analysis. A chapter covering many of the principal programs used for the analysis of pumping test and slug test data has also been incorporated. These programs are often used prior to model construction to obtain reliable estimates of the aquifer's hydraulic parameters.

An overview of integrated pre- and post-processing packages designed to speed-up and ease the process of model creation, execution and output analysis and presentation has also been included. This is a rapidly expanding field within groundwater modelling as commercial pressures result in an effort to shorten the time-consuming process of modelling and to reduce the amount of specialist computing knowledge required to construct and execute groundwater models.

GIS programs are not included even though the potential exists for the use of GIS databases together with a number of the groundwater models included in this report. They are not included as they are considered to represent a separate subject area and are seen as fulfilling a more specialised support function. It is recognised however that such programs can be of considerable assistance. Probably the best and most up-to-date source of information on GIS systems and their applications in geology and hydrogeology can be found on the Internet. In particular, the reader is referred to the site 'http://bordeaux.uwaterloo.ca/info/sites.html'. This site contains information on the application of GIS systems in hydrology and hydrogeology (including examples) in addition to GIS shareware and lists of commercial GIS providers (both software suppliers and consultants). Use of one of the many search machines on the Internet will undoubtedly locate other similar sites.

The various models have been classified into the following groups:

-Groundwater flow and particle tracking models: have two sub-groups - analytical and numerical models that solve the groundwater flow equation. The terms 'analytical' and 'numerical' refer to the method of solving the flow equations. Particle tracking models which track particles introduced into the groundwater flow field created by numerical models are also included in this section, though strictly speaking these are advection-only transport models.

-Pollution transport models: also have two sub-groups - analytical and numerical pollution transport models. These models combine the groundwater flow equation with advection, dispersion, retardation and/or degradation of single component pollution.

-Geochemical models: have three sub-groups for models which describe geochemical reactions - programs which include chemical mass balance and conservation of electrons; programs for speciation and determination of thermodynamic constants and programs which include chemical mass transfer (based on kinetics/sorption).

-Pollution transport models combined with geochemical models: these are the most complex models that combine multi-component geochemical transport with groundwater flow.

-Integrated modelling packages: This chapter reviews commercially available modelling packages combining flow, pollution transport and pre- and post-processing programs.

-Pre- and post-processing programs: Programs for the handling and presentation of data in connection with numerical and analytical modelling.

-Programs for pumping test analysis: This chapter presents a selection of the most commonly used programs for pumping test and slug test analysis. Only user-friendly menu-driven programs offering a wide variety of analytical methods are considered.

-Other hydrogeological models: A group that includes geostatistical programs and other miscellaneous programs for the analysis of hydrochemical data.

For each program the following aspects are presented:

Developed by: The developers of the program.
Program language: The programming language the program is written in.
Documentation: The original user documentation and/or any relevant articles.
Description: A summary of the model's characteristics and the flow and/or physical conditions to which the model can be applied.
Use: A brief description of the subject areas to which the model may be applied.
Solution method: The physical and chemical laws that apply to the method and the solution method used.
Special characteristics: Simulation possibilities and model characteristics not common with other similar programs.
Input-output data format: Type and ease of data input and output (text file, graphical, etc.). An indication is also given of the extent to which pre- and post-processing data handling packages are available.
Availability: Known program suppliers. Most programs are also available from the author.
System requirements: Computational resources necessary to run the program including variants designed to run on different operating systems.

'*' denotes that information is either lacking or irrelevant.

Considerable effort was put into tracing references (i.e. the name of the author(s) and the associated documentation) for as many models as possible. This was unfortunately not possible in all cases and some records may therefore be incomplete or missing.

The majority of the programs presented in this report are PC-based programs that are executed using DOS or WINDOWS operating systems. Many of these programs are however also available for UNIX users. A limited number of programs are available only for UNIX-operating systems. Two programs have been specially developed for Macintosh users (PROFILE. SAFE) whilst INTERGRAPH-SRS/ERMA was originally developed for INTERGRAPH workstations but is now available as a PC-based version.

A table is enclosed listing the programs in alphabetical order (Enclosure 1). The table includes information useful to those wishing to trace a program for a particular task.

1.2 MATHEMATICAL MODELLING

1.2.1 What is a mathematical model?

A mathematical model consists of a set of differential equations that are known to govern groundwater flow. An introduction to the theory behind these equations is presented in Chapter 2. In a limited number of cases analytical expressions can be derived by direct integration of these differential equations. In order to do this a number of simplifications and assumptions must be made.

The most commonly used assumptions are that:

- the flow is 1- or 2-dimensional (horizontal, radial, vertical, etc.)
- the aquifer is homogeneous, isotropic and of infinite extent
- the borehole is of negligible diameter

There are many analytical solutions to the equations governing the flow of groundwater. The simplest and most well known are those of Jacob, Theis and Theim. Many of these solutions are used in the pumping test analysis programs described in Chapter 12.

Nevertheless, many situations cannot be analysed using analytical methods due to the presence of non-linear features that cannot be incorporated in an analytical solution. An aquifer is for example rarely, if ever, homogeneous and isotropic and will often consist of more than one layer. Permeability values and aquifer thickness will vary spatially and vertical components of groundwater flow can often be significant. In these cases it is necessary to solve the equations numerically. The emphasis in this report is consequently placed on numerical models although a number of analytical models are included in the program listings for the sake of completeness.

There are essentially two types of numerical solutions to the groundwater flow equations. The first of these is the finite-difference approximation to the differential groundwater flow equations. This method involves the division of the aquifer into rectangular blocks. Finite-difference approximations are then made of the equations governing the flow between each block. A wide variety of finite-difference techniques have been developed. An alternative to the finite-difference approach is the finite-element formulation. This formulation makes extensive use of matrix techniques. With the finite-element formulation the aquifer can be divided into irregularly shaped blocks although triangular blocks are the most commonly used. A variation of the finite-element method is the boundary integral equation method. In this method solutions to the groundwater flow equations are derived in terms of the functions at certain positions on the boundary of the model domain. This type of formulation is however not extensively used at present in the groundwater industry.

1.2.2 The use of mathematical models

Numerical and analytical mathematical models can be powerful tools in investigating and assessing groundwater problems. The modelling of groundwater flow and in particular pollution transport is an active research field and with today's powerful computers and modelling programs the level of detail achievable in assessing problems is steadily increasing. Despite the already advanced modelling of complex environmental problems, further advances are constantly being made, particularly in the development of a more integrated approach to the simulation of hydrogeological problems through the use of packaged pre- and post-processing programs and larger models incorporating a greater number of processes.

More complex simulations require the use of parallel computer resources in addition to a team with specialist knowledge of the appropriate processes. Such a team will consist of specialists in fields such as hydrogeology, hydrology, porous media flow, geology, geochemistry, biology, physics, mathematics, programming, geostatistics, etc.. In many modelling projects such a team will not be financially viable and it is consequently important that modellers with suitable specialist subjects have the use of appropriate modelling software. Although this software will include simplifications and assumptions, observed phenomena can often be simulated with great precision. Such software can also be of great assistance in the prediction of future conditions.

There are many applications of groundwater modelling. Examples of these include:

- determination of the abstraction capacity of an aquifer and it's water sources
- enabling the prediction of the future behaviour of an aquifer under given conditions e.g. changes in groundwater levels during a proposed pumping regime at a well field or the behaviour of a pollution plume
- determination of the history of an aquifer e.g. tracing the movement of a pollution plume in order to determine it's origin
- determination of the physical and hydraulic properties of an aquifer
- determination of borehole catchment areas and groundwater protection zones
- determination of the groundwater pollution vulnerability of an area
- assessment of the physical, chemical and radioactive fate of a pollution plume
- assessment of the chemical impact of changes in the groundwater chemistry of recharge water e.g. the effect of acid rain on groundwater chemistry

These examples, although representing only a small selection of the possible uses of groundwater models, illustrate the wide variety of groundwater problems that can be solved using groundwater-modelling techniques.

When using modelling software it is important to be aware of the limitations inherent in any model, in particular the assumptions made by the model in formulating the problem. It would for example be of little use simulating the transport of hydrocarbons without taking into account the hydrocarbons' reaction with the porous media and their solubility. A multi-phase groundwater flow model incorporating geochemical reactions need not however be used. If the composition of the pollution is known, several single component models can be run each simulating a different component. One can for example then utilise linear isotherms to describe the retardation in the

porous media and microbial biological activity can be simulated using a degradation chain.

1.3 CHOICE OF SOLUTION FORMULATION

Finite-difference techniques are the most extensively used today. A number of reasons explain this wide use. Firstly, finite-difference techniques are fundamentally very simple as finite-difference approximation lead directly to simultaneous equations without the need for further mathematical treatment. Secondly, finite-difference equations require extensive mathematical computations to be carried out which are ideally suited to modern computers. Chapter 3 presents an introduction to the theory behind such methods. A wide variety of techniques have been developed with which to formulate and solve the finite-difference equations using computers and a brief discussion of these is also presented in Chapter 3.

Chapter 4 presents a summary of the principle methods involved in finite-element modelling together with a summary of the solution algorithms used to solve the groundwater equations. Due to the comparative complexity and variety of finite-element methods and the dominance of finite-difference methods in groundwater modelling, it is not considered appropriate to present a detailed description of the theory behind such methods in this report. References are provided for those who wish to find out more about the various techniques.

2. THE FUNDAMENTAL EQUATIONS OF GROUNDWATER FLOW

2.1 STEADY STATE CONDITIONS

Flow through porous media is governed by Darcy's law (Darcy, 1856). We can first define the specific discharge, $v = Q/A$. In the limit as the head loss $h_1 - h_2$ occurs over a small interval $l_2 - l_1$, we can write the differential form of Darcy's law as:

$$v = - K . \frac{\partial h}{\partial l} \qquad (1.1)$$

where K is the aquifer's hydraulic conductivity.

The specific discharge has units of velocity and is also known as the Darcy velocity. It should be noted that the Darcy velocity is an artificial velocity as it corresponds to the total quantity of water flowing divided by the cross-sectional area. The average velocity, v_w of the water can therefore be calculated as the Darcy velocity divided by the effective porosity, n_e.

$$v_w = v / n_e \qquad (1.2)$$

The three-dimensional generalisation of Darcy's law assumes that the one-dimensional form (Equation 1.1) is true for the three principal components of flow *x*, *y* and *z*:

$$v_x = - K_x \frac{\partial h}{\partial x} \qquad v_y = - K_y \frac{\partial h}{\partial y} \qquad v_z = -K_z \frac{\partial h}{\partial z} \qquad (1.3)$$

Let us consider the flow into and out of the elemental cube shown in Figure 1.

We can derive a mass balance for the cube by summing the results from each component direction.

The flow rate through each face is the product of the flow rate through the face per unit area and the area of the face. If we consider the cube in Figure 1, the flow through the right face can be expressed as:

$$\left(v_x - \frac{\partial v_x}{\partial x} \frac{dx}{2} \right) dy\, dz \qquad (1.4)$$

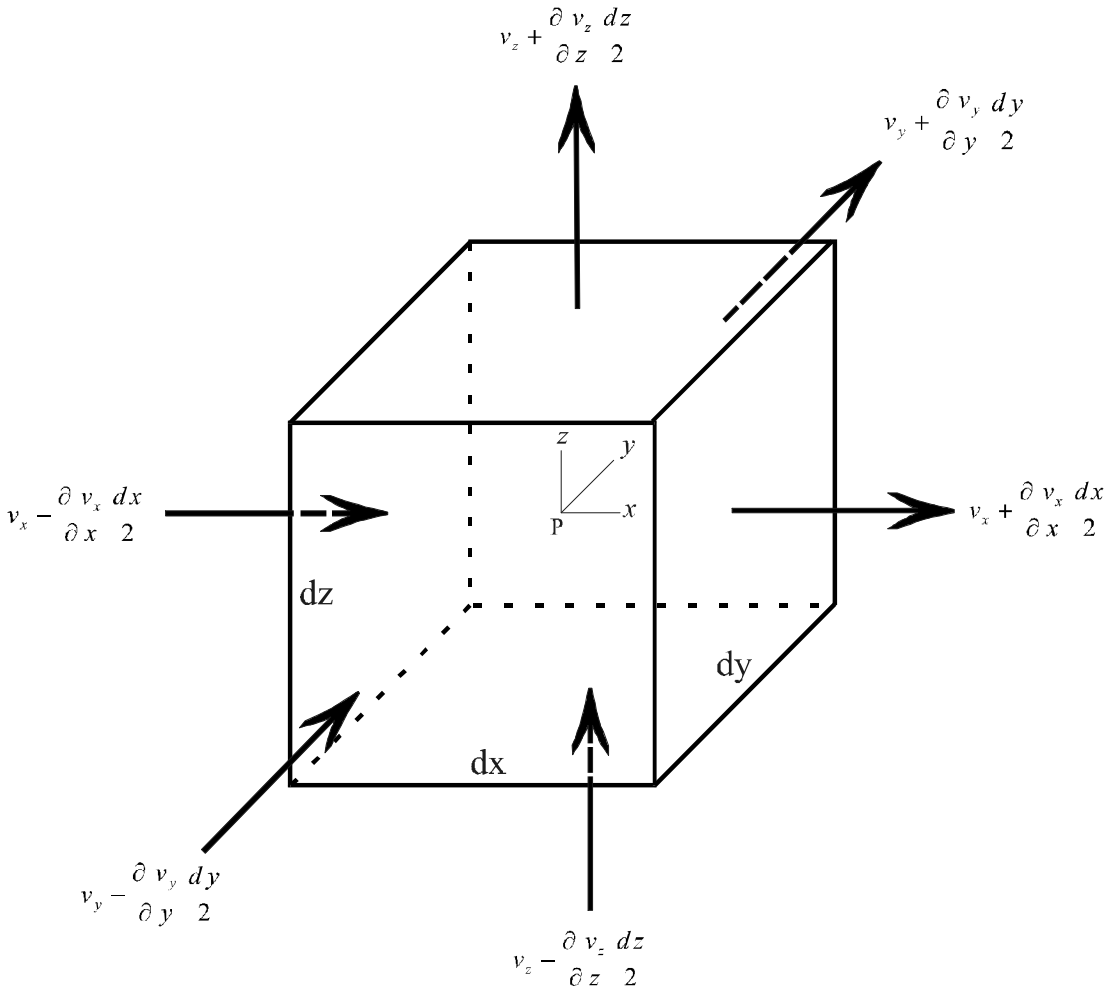

Figure 1. Flow for an elementary volume of fluid (after Rushton & Redshaw, 1977)

Similarly, the rate of flow leaving the element across the same face is given by the expression:

$$\left(v_x + \frac{\partial v_x}{\partial x}\frac{dx}{2}\right)dy\,dz \qquad (1.5)$$

The net volume of flow entering the element due to flow in the x-direction can therefore be expressed as:

$$\left(\frac{\partial v_x}{\partial x}\right)dx\,dy\,dz \qquad (1.6)$$

Similar expressions can be derived for the other principle directions, y and z so that an expression for the total volume of water entering the element can be expressed as:

$$\left(\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}\right)dx\,dy\,dz \qquad (1.7)$$

Under steady state conditions this equation must equal zero:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \qquad (1.8)$$

This is the *continuity equation for steady state conditions.*

By differentiating Darcy's law (Equations 1.3) with respect to *x*, *y* and *z* and adding in accordance with the continuity equation (Equation 1.8) we obtain a single second-order partial differential equation:

$$\frac{\partial}{\partial x}\left(-K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(-K_z \frac{\partial h}{\partial z}\right) = 0 \qquad (1.9)$$

Equation (1.9) is the general equation for three-dimensional steady state flow.

If the aquifer is assumed to be homogenous and isotropic, then K becomes independent of x, y and z. Equation (1.9) can then be simplified to:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial^2 h}{\partial z^2} = 0 \qquad (1.10)$$

This equation is known as Laplace's equation and is the governing equation for groundwater flow through an isotropic, homogenous equation under steady state conditions. This equation can be solved using analytical methods. However, if the aquifer is assumed to be heterogeneous and isotropic then Equation (1.9) cannot be reduced to Laplace's equation and numerical approximation methods are required to solve Equation (1.9).

2.2 TRANSIENT FLOW CONDITIONS

Under transient flow conditions the sum of the components of flow in the *x, y* and *z* are not equal to zero. In order to formulate the groundwater flow equations for transient conditions we must therefore introduce an expression to represent the net change in volume over a period of time.

The expression derived is dependent on whether the flow conditions existing in the aquifer are confined or unconfined.

2.2.1 Confined conditions

For a confined aquifer a net change in volume entering or leaving an element will result in a change of groundwater potential due to the compressibility of the water and the aquifer. The volume of water released per unit volume of aquifer due to a unit decrease in head is termed the *specific storage coefficient*, S_s [L^{-1}]. A further aquifer coefficient, which is sometimes used, is *storativity*, S [ ]. Storativity is defined as:

$$S = S_s \, . \, b$$

where b = aquifer thickness

However in this section we will only consider the specific storage coefficient.

If we consider the cube in Figure 1, the total volume of water entering an element *during a time dt* due to the changing groundwater velocities can be written as:

$$dx\,dy\,dz\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)dt \qquad (1.11)$$

During the time increment *dt*, the groundwater potential at the centre of the element increases by *dh*. The volume of water taken into storage due to the increase in the groundwater potential is:

$$dx\,dy\,dz\,S_s\,dh$$

From the principle of continuity these two quantities must be equal, hence

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = - S_s \frac{\partial h}{\partial t}$$

Substituting for v_x, v_y and v_z from Equation (1.3) we obtain the governing differential equation for transient flow in a confined aquifer:

$$\frac{\partial}{\partial x}\left(-K_x\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K_y\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(-K_z\frac{\partial h}{\partial z}\right) = S_s\frac{\partial h}{\partial t} \qquad (1.12)$$

Adding a term, $q(x,y,t)$, to account for inflows and outflows to/from the aquifer to as a result of external stresses on the aquifer (such as point and areal recharge, abstraction, etc.), we obtain the governing equation for three dimensional groundwater flow in a confined aquifer:

$$\frac{\partial}{\partial x}\left(-K_x\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K_y\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(-K_z\frac{\partial h}{\partial z}\right) = S_s\frac{\partial h}{\partial t} - q(x,y,t) \qquad (1.13)$$

2.2.2 Unconfined conditions

Two separate processes occur in an unconfined aquifer. Firstly, the compressibility of the aquifer and the water result in a change in the groundwater potential. The specific storage coefficient thus also applies to all elements within an unconfined aquifer. In addition, however, the fall of the free water surface leads to a dewatering of the aquifer. A unit fall in the free surface position will result in a release of water from storage equal to S_y per unit plan area of the aquifer, where S_y is the *specific yield* [ ]. The specific yield is often assumed to be approximately the same as effective porosity, n_e, particularly when dealing with groundwater flow velocities as in Equation (1.2). The release of the specific yield occurs at the free surface unlike the specific storage that occurs throughout the saturated volume of the aquifer.

Water contributed to the aquifer due to specific yield is effectively an inflow or recharge, q_s. If we assume that the water table is approximately horizontal, the water derived from the specific yield can be written as:

$$q_s = -S_y \frac{\partial h}{\partial t} \tag{1.14}$$

Thus the equation for an unconfined aquifer is:

$$\frac{\partial}{\partial x}\left(-K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(-K_z \frac{\partial h}{\partial z}\right) = S_s \frac{\partial h}{\partial t} + S_y \frac{\partial h}{\partial t} \tag{1.15}$$

Adding the external stress term, $q(x,y,t)$, we obtain the governing equation for three dimensional groundwater flow in an unconfined aquifer:

$$\frac{\partial}{\partial x}\left(-K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(-K_z \frac{\partial h}{\partial z}\right) = S_s \frac{\partial h}{\partial t} + S_y \frac{\partial h}{\partial t} - q(x,y,t) \tag{1.16}$$

In practice the confined storage coefficient is very much smaller than the specific yield and is consequently often ignored.

3. FINITE-DIFFERENCE APPROXIMATION METHODS

3.1 INTRODUCTION

Solutions to the governing equations described in Section 1.3 can often be obtained by numerical means. One of the first numerical techniques to be developed is that of the finite-difference approximation (Richardson, 1911). Though other approaches have been developed, notably the finite-difference and the boundary-difference methods, the finite difference methods remain the most popular principally because of the relative simplicity and flexibility of its construction. There are many approaches to the finite-difference approximation. However, this introductory chapter is intended only as an introduction to the theory behind groundwater models and presentation of the technique will consequently be restricted to basic considerations.

3.2 STEADY STATE FINITE-DIFFERENCE APPROXIMATIONS

To introduce the fundamental idea behind the finite-difference approximation, we will consider the case of a one-dimensional constant transmissivity aquifer fed from recharge. The appropriate equation derived from Equation (1.16) is:

$$T\frac{\partial^2 h}{\partial x^2} = -q \qquad (1.17)$$

where: h is the groundwater potential [L]
T is the uniform aquifer transmissivity [L^2/T]
q is inflow per unit length [$L^3/L/T$]

There are many methods that can be used to approximate the groundwater head over a section of an aquifer. We will consider here the simplest of these methods - the straight-line approximation. Other methods such as the Taylor's series or other mathematical functions provide more accurate approximations but for our purposes, the straight-line method provides a good illustration of the fundamentals of finite-difference approximation.

Finite-difference approximations using straight lines are made by defining the groundwater heads at certain discrete points rather than by a continuous function. These points are positioned at intervals of Δx. The unknown groundwater potentials are written as h_{-1}, h_0, h_1, etc..

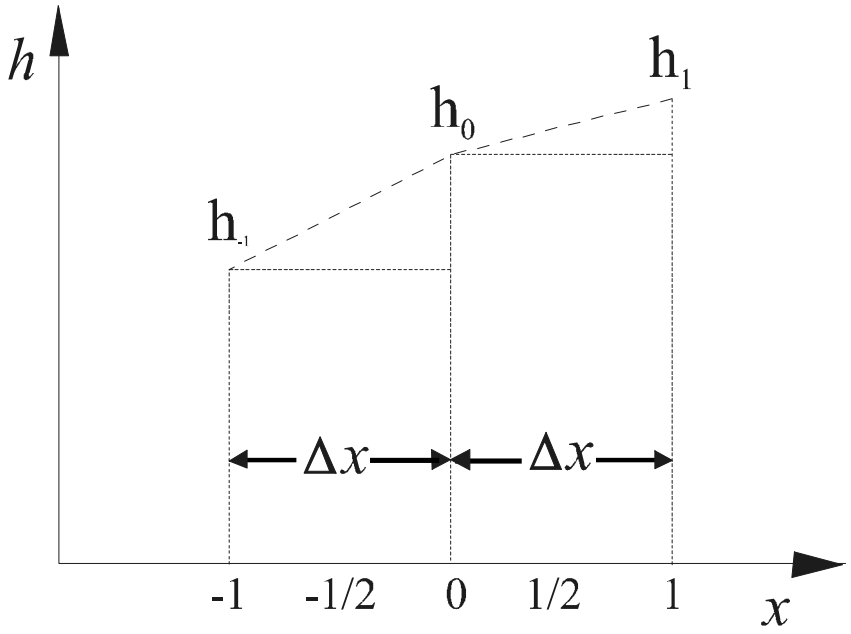

Figure 2. The straight-line finite-difference approximation to the groundwater head gradient between three points, h_{-1}, h_0 and h_1 (after Rushton & Redshaw, 1979).

Approximate values of the slopes at intermediate points can be calculated as:

$$\left(\frac{dh}{dx}\right)_{+\frac{1}{2}} = \frac{h_1 - h_0}{\Delta x}, \left(\frac{dh}{dx}\right)_{-\frac{1}{2}} = \frac{h_0 - h_{-1}}{\Delta x} \qquad (1.18)$$

where the suffices +1/2 and -1/2 signify distances ½ Δx on either side of node 0.

The second differential can be written as:

$$\left(\frac{d^2h}{dx^2}\right)_0 = \frac{d}{dx}\left(\frac{dh}{dx}\right) = \left[\left(\frac{dh}{dx}\right)_{+\frac{1}{2}} - \left(\frac{dh}{dx}\right)_{-\frac{1}{2}}\right] \Big/ \Delta x = \frac{\left(h_{-1} - 2h_0 + h_1\right)}{\Delta x^2} \qquad (1.19)$$

Therefore the differential equation (1.17) can be written as an algebraic equation:

$$h_{-1} - 2h_0 + h_1 = \frac{-\Delta x^2 q_0}{T} \qquad (1.20)$$

To apply this approach in a practical situation a finite-difference mesh is superimposed on the aquifer. An algebraic equation such as (1.20) is written for each node in the mesh.

Nodes that lie on the boundary of the mesh and those with special hydraulic properties (such as those representing impermeable boundaries, lakes, constant head boreholes, etc) are assigned appropriate values. For example, at an impermeable boundary node, dh/dx = 0 and therefore $q_0 = 0$ whilst at a fixed head node, n the value of h_n = H.

This produces a series of simultaneous equations that can then be solved. In each case the recharge and the transmissivity of the aquifer will be known. There will consequently never be more unknown variables than simultaneous equations enabling the equations to be solved through a variety of techniques.

Although obviously more complex, the above approximation methods can be applied to two- and three-dimensions and, by redefining the governing differential equation in terms of radial co-ordinates, radial flow.

3.3 TIME VARIANT FINITE-DIFFERENCE APPROXIMATIONS

When groundwater flow is time-variant, the equation is usually of the form

$$\tilde{N}^2 h = c\ \P h/\P t \qquad (1.21)$$

where c may be a function of space and the groundwater head, h. This is an elliptic differential equation (Smith, 1965).

Many alternative approaches are possible when representing the time dimension. One approach particularly suited to the use of computers is to divide the continuous time into discrete time steps at certain predetermined times in a similar manner to the discrete representation of continuous space.

Since in a discrete-time solution, the function is only defined at particular times, discrete time steps can be represented pictorially as a series of horizontal lines (see Figure 3).

If we consider the simplest finite-difference approximation:

$$c\frac{\P h}{\P t} = c\frac{h_{0,t+\Delta t} - h_{0,t}}{\Delta t} \qquad (1.22)$$

where the first suffix refers to the position in space and the second suffix refers to the time.

The various finite-difference approximations depend on the time at which $\tilde{N}^2 h$ is defined.

3.3.1 Forward-difference approximation

In the case where $\tilde{N}^2 h$ is defined at time t, this is called a forward-difference approximation. Taking the one-dimensional case where

$$\left(\frac{\P^{\ 2} h}{\P x^2}\right) = c\frac{dh}{dt}$$

the forward-difference finite-difference approximation in the space dimension with regular intervals Δx is:

$$h_{-1,t} - 2h_{0,t} + h_{1,t} = \left(c\Delta x^2/\Delta t\right)\left(h_{0,t+\Delta t} - h_{0,t}\right)$$

or

$$h_{0,t+\Delta t} = \frac{\Delta t}{c\Delta x^2}\left[h_{-1,t} - \left(2 - \frac{cx^2}{\Delta t}\right)h_{0,t} + h_{1,t}\right] \qquad (1.23)$$

Since the function at time $t+Dt$ can be expressed explicitly in terms of the known values of the function at time t, this is termed an explicit formulation.

3.3.2 Backward-difference formulation

When the term $\tilde{N}^2h$ is defined at time $t+Dt$, the approximation is termed backward-difference. The unknown functions at time $t+Dt$ are calculated from:

$$h_{-1,t+\Delta t} - \left(2 + c\Delta x^2/\Delta t\right)h_{0,t+\Delta t} + h_{1,t+\Delta t} = -\left(c\Delta x^2/\Delta t\right)h_{0,t} \quad (1.24)$$

This leads to simultaneous equations and is therefore said to be implicit.

3.3.3 Central-difference approximation

When the term $\tilde{N}^2h$ is defined both at times t and $t+Dt$,

$$0.5\left(\nabla^2 h\right)_t + 0.5\left(\nabla^2 h\right)_{t+\Delta t} = \left(c\Delta x^2/\Delta t\right)\left(h_{0,t+\Delta t} - h_{0,t}\right) \qquad (1.25)$$

This is a central-difference approximation often known as the Crank-Nicholson method. This method is also an implicit approximation.

3.3.4 Choice of method

From the above description the forward-difference approximation would seem to be the most advantageous as the solution of simultaneous equations is not required. However, the stability criteria of this method seriously limit its application. There are no stability criteria for backward-difference methods. Furthermore, errors resulting from the spatial discretisation, present in any numerical model are more serious in forward-difference models as the value of the function depends only of the behaviour at the previous time-step. These errors can be quite serious and the convergence of the forward-difference method is generally inferior to the backward-difference

approximation. For these reasons most commercially available finite-difference models use the backward-difference approximation.

3.4 SOLUTION OF THE FINITE-DIFFERENCE EQUATIONS

A large number of different methods have been developed to solve the simultaneous equations resulting from finite-difference models.

3.4.1 Direct solutions

For all but the simplest problems, the direct solution of the simultaneous equation is uneconomical even with the availability of modern high-speed computers. However, for one-dimensional problems efficient direct solutions can be obtained by using Gaussian elimination of the tri-diagonal matrix. Considering the two-dimensional grid as a series of interconnected one-dimensional grids can provide a feasible approach to two-dimensional problems. The grid is solved by solving the one-dimensional grid, row-by-row in one direction. This leads to a series of one-dimensional equations each with a tri-diagonal matrix. The equations are then solved in the other direction. This alternating direction implicit procedure was first introduced by Peaceman and Rachford (1955) and is suitable for certain types of problem.

3.4.2 Iterative solutions

Most iterative solutions are developments of the relaxation method developed by Southwell (1940). Iterative methods have the major advantage that non-linearities can easily be incorporated. The simplest technique is the point successive over-relaxation method (SOR). This method has the advantage that the speed of convergence is not particularly sensitive to the choice of the over-relaxation parameter. There are many variations of the SOR approach in addition to many other iterative procedures such as Jacobi iteration and Gauss-Seidel iteration. Readers wishing to find out more about such methods are referred to Wang & Anderson (1982) and Huyakorn & Pinder (1983) in addition to the literature for the appropriate model.

4. FINITE-ELEMENT APPROXIMATION METHODS

4.1 INTRODUCTION

The introduction of the finite-element method to groundwater problems is a relatively recent development compared with the finite-difference method. Each method leads to a series of algebraic equations in which the unknowns are the heads at a finite number of nodal points. Unlike the finite-difference method, which is usually implemented with rectangular cells, finite-element methods can be implemented with a variety of element types. Triangular elements are probably the most commonly used, being defined by three nodes - one at each corner. These nodes are the equivalent of the finite-difference nodes discussed in Chapter 3, i.e. they are the points at which the groundwater heads are computed.

The use of triangular elements gives finite-element methods a significant advantage over finite-difference methods. Irregular boundaries and heterogeneities can be much more accurately simulated without excessively increasing the number of elements. The comparatively complex formulation of finite-element and related methods has however restricted their widespread application.

Due to the complexity and variety of finite-element methods and the dominance of finite-difference methods in groundwater modelling, it is not considered appropriate to present a description of the theory behind such methods here. Given below is a summary of the principle methods involved in finite-element modelling together with a brief summary of the solution algorithms used to solve the groundwater equations. References are provided for readers who wish to find out more about the various techniques.

4.2 FINITE-ELEMENT METHODS

The finite-element analysis of a physical problem can be described as follows:

a) Following the discretisation of the model domain into elements, a matrix expression is developed to relate the nodal variables of each element. The resulting matrix is often referred to as an ‘element matrix’.

b) The element matrices are then combined to form a set of algebraic equations, which describes the entire model domain. The coefficient matrix of this final set of equations is known as the ‘global matrix’.

c) Prescribed boundary conditions are incorporated into the assembled global matrix equation.

d) The resulting set of equations is then solved using a variety of solution algorithms.

Many different solution algorithms can be used to solve the finite-element equations. Among the most widely used algorithms are the Gauss elimination and Choleski decomposition algorithms that take into account the banded and symmetric feature of the coefficient matrix (Bathe & Wilson, 1976).

For more detailed descriptions of these techniques, the reader is referred to Wang & Andersen (1982) and Huyakorn & Pinder (1983).

4.3 THE BOUNDARY-ELEMENT METHOD

The boundary-element method exploits the efficiencies associated with the reduction of the dimensionality of the problem. Specifically, it reduces a two- or three-dimensional problem to one defined in one or two dimensions, respectively.

For more information on the boundary element method the reader is referred to Huyakorn & Pinder (1983), Lennon et al (1980) and Ligget & Liu (1983).

4.4 THE POINT & SUBDOMAIN METHODS

The point collocation method is a conceptually simple and computationally efficient scheme for the solution of many groundwater flow problems. In its most sophisticated form it can be used with isoparametric elements so that irregular geometry is readily accommodated. For a detailed theoretical development of the point collocation method the reader is referred to Finlayson (1972) and Frind & Pinder (1979). A shorter presentation of the fundamental basis of the method can be found in Huyakorn & Pinder (1983).

The point collocation method has the advantage of avoiding the integration and assembly steps normally encountered in finite-element formulations. This is of particular significance in non-linear problems.

5. THE PROCESS OF GROUNDWATER MODELLING

5.1 MODEL SELECTION

The factors that influence the selection of a model will vary according to individual needs and circumstances. However the user should consider the following features of a model:

- Relevance to the hydrogeological problem (type of model, dimensionality, etc.). A model must for example be able to simulate three-dimensional pollution transport in an unconfined aquifer under transient flow conditions if that is what the problem dictates.
- Operating system compatibility (DOS, WINDOWS, UNIX, etc.) - the model must be able to run on the user's computer if finance is not available to purchase hardware for a particular problem.
- User friendliness - this will govern how easy the program is to set up and operate and will for example affect the speed with a model can be established. This is particularly important if project deadlines are tight.
- Model simplicity - as above
- The user's familiarity with the model - as above
- The level of detail required in the solution of the problem. For example: is a simplified 2-dimensional particle-tracking model sufficient or is a detailed 3-dimensional pollution transport model necessary?
- Solution method - this will determine whether the model will converge under the given conditions
- Capability in relation to other similar models - are other applicable models more suited to the problem?
- Price - are sufficient funds available to purchase the model?

5.2 DATA REQUIREMENTS

In order to construct a groundwater flow model the modeller must first have an understanding for the aquifer's physical characteristics (areal distribution, thickness, lithology, etc.) and hydraulic boundaries (constant head, impermeable, known infiltration rate, etc.). Data on the aquifer's hydraulic properties must also be obtained. Geological and hydrogeological data required by steady state groundwater models include:

- aquifer hydraulic boundaries
- aquifer physical characteristics (areal distribution, thickness, lithology)
- aquifer permeability
- recharge
- point and distributed sources and sinks
- groundwater level observations from observation boreholes
- surface water level observations

Transient models also require data on:

- any variation of the above parameters with time
- aquifer storage coefficients
- aquifer effective porosity

For particle tracking simulations observed data on groundwater travel times are also of particular value as they enable the model to be calibrated in terms of groundwater flow rates as well as head values.

These data are entered into data files in a format that can be read by the model (the format will vary from model to model). Data can be entered directly into text files using a text editor or graphically using a graphics program or a complete graphical modelling package such as Visual MODFLOW or ERMA.

5.3 MODEL CONSTRUCTION

The construction of a groundwater flow/particle-tracking model involves the following stages:

- Collation of field data
- Interpretation of field data
- Definition of the model grid and division of the aquifer(s) into layers
- Definition of the aquifer's hydraulic boundaries
- Definition of sources and sinks (lakes, rivers, abstraction boreholes, recharge basins, etc) within the model domain
- Definition of the aquifer's hydraulic properties (permeability/transmissivity, specific yield, etc.)
- Definition of other hydraulic parameters (recharge rate, river bed conductivities, surface water levels, borehole abstraction rates, etc.)
- Preliminary running of the model in order to check the data files have the correct format and that the correct data have been entered
- Calibration of the model against observed data (groundwater levels, drawdowns, travel times, etc.)
- Sensitivity analysis
- Execution of the model under the required hydraulic conditions to achieve the objective of the modelling process e.g. predicting future changes in groundwater level during a proposed groundwater abstraction regime.

5.4 MODEL CALIBRATION

A model must be calibrated before it can be used to simulate groundwater flow or pollution in an aquifer. The calibration of a numerical model involves the

demonstration of the model's ability to simulate observed groundwater data in a satisfactory way. Observed groundwater levels from a pumping test or other stress on the aquifer are the most suitable data for use in model calibration.
Calibrations carried out using groundwater level data obtained when the aquifer is not being subjected to a stress (such as during no abstraction or when significant water level changes are not taking place) often do not provide reliable calibrations. Generally, the greater the stress being applied to the aquifer, the more reliable the calibration will be. A model can often be 'satisfactorily' calibrated using one set of data only for the calibration to be proved inadequate following testing of the model under other more severe conditions. This situation is often unavoidable but the need to calibrate a model using hydraulic data measured during the application of a stress on the aquifer should be emphasised. Similar considerations apply to the length of time over which the field data was collected. Calibrations performed using data measured over a long time period will generally be more reliable than those carried out using data measured over a shorter period.

No attempt is made here to present a detailed description of the various methods of model calibration as the subject is covered adequately elsewhere in the literature (e.g. Anderson & Woessner, 1992). However, calibration is generally carried out by altering the input field data until the model simulates observed data in a satisfactory way. The data to be modified during model calibration should be determined on the basis of an assessment of the reliability of the input data. Data that is considered to be less reliable or accurate can be modified to a greater extent than data considered as reliable. When modifying data it should be remembered that the model is not an exact representation of the aquifer and that data will generally only be available from a relatively limited part of the aquifer. Deviations from the observed aquifer properties will consequently almost certainly be necessary.

The calibration of a transient model is a somewhat more complicated process than that of a steady state model. In order to calibrate a transient model, a steady state version of the model must first be calibrated in order to provide the initial starting heads for the transient calibration. The transient calibration is then carried out using the data derived from the steady state calibration. During this process the data from the steady state calibration is further modified until the model is capable of simulating a transient event in the aquifer.

Following the completion of this process a steady state version of the model is then run using the parameters derived from the transient calibration. If this steady state model is no longer satisfactorily calibrated, the steady state model must be re-calibrated and the process repeated until the same data set is capable of simulating both the steady state and the transient data sets. This process means that the calibration of a transient model is a considerably more time-consuming task than the calibration of a steady state model. A calibrated transient model is however much more reliable than a calibrated steady state model.

An important point to note is that a calibrated model does not represent a unique solution to the observed groundwater data. Other combinations of the physical and hydraulic properties of the aquifer will almost certainly be able to give as good or possibly better simulation of the observed data.

Numerical models can be used without calibration (for example due to the lack of field data or time to calibrate the model). In this case however the results from the model will be much less reliable and this situation should be avoided wherever possible.

5.5 SOURCES OF ERROR

When using a groundwater model, the modeller must be aware of the inherent limitations involved in the modelling process. Simulated and observed data will never precisely coincide due to the fact that:

- A numerical model is a simplification of reality. The objective of modelling is to adjust a model to real data without it being more complicated than necessary.

- The model is no more reliable than the data on which it is based.

- A calibrated model does not represent a unique solution to an observed data set. Other combinations of data can give equally good or better simulations of the observed data.

There are a number of limitations and assumptions inherent in groundwater modelling techniques both in the formulation of the approximations to the groundwater equations and in the execution of the actual modelling. For example, groundwater levels in a finite-difference model represent the average groundwater level within each block. In the case of a block or node representing an abstraction borehole, the value for groundwater head or drawdown will represent the average drawdown in that node and not the drawdown in the well itself. The average drawdown must therefore be corrected to account for this discrepancy. Many other examples of such discrepancies could be given but for more information on this aspect of groundwater modelling the reader is referred to Wang and Anderson (1983).

Provided a model is constructed in a way which takes account of these limitations and that these considerations are borne in mind when analysing model results, mathematical modelling can nevertheless provide answers to groundwater problems with a far greater reliability and accuracy than other conventional methods.

5.6 DEALING WITH UNCERTAINTY - SENSITIVITY ANALYSIS

A sensitivity analysis can be carried out in order to determine which of the aquifer's properties have the greatest importance to the groundwater flow in the aquifer. This involves the variation of the model's calibrated hydraulic properties and a subsequent analysis of the changes in the groundwater head distribution and flows in the aquifer. Parameters are typically increased or decreased by 5-10%. The greater the resulting variation in groundwater head or flows, the greater the importance of the parameter

concerned. Such an analysis also gives an indication of how much the model's parameters can be changed without altering the results of the model. This in turn gives an indication of the accuracy of the model's hydraulic parameters. For example, if the modelled horizontal permeability of the aquifer is increased by 10% without significantly altering the groundwater head distribution or flows in the aquifer, then the determination of the aquifer permeability is subject to an uncertainty of at least 10%. Similarly, if in two separate tests, the horizontal and vertical aquifer permeabilities are increased by 10% and the alteration of the vertical permeability produces a far greater change in aquifer flows or heads then it can be stated that the vertical permeability is of considerably greater importance to the groundwater flows in the aquifer.

Examples of parameters that should be included in a sensitivity analysis are:

i) recharge rate/evapotranspiration
ii) horizontal permeability of each model layer
iii) vertical permeability of each model layer
iv) aquifer thickness
v) river bed thickness/permeability
vi) infiltration from a lake or other constant head boundary

Any other parameters that are not known with any great certainty should also be included in the analysis. It should be noted that the alteration of each parameter should be made from the original version of the model and not the version from the last sensitivity analysis.

The results of a sensitivity analysis can be used to improve the results of a model by enabling a concentration on the determination of the most important hydraulic parameters of the aquifer. The indication of the sensitivity of a model to changes in the aquifer's hydraulic parameters is also an important factor to be taken into consideration when assessing the results of the model.

6. GROUNDWATER FLOW AND PARTICLE TRACKING MODELS

6.1 NUMERICAL MODELS

Numerical flow models enable the user to simulate complex problems. The limitation in the degree of detail is theoretically only dependent on time and available computational resources. Even though the numerical solutions of the relevant differential equations are conceptually simple, considerations such as the definition of a model's boundary conditions and the execution of transient simulations require a thorough understanding of the principals of numerical modelling techniques.

MODFLOW is an extremely popular groundwater model that is based on the finite-difference model. Finite-element models, such as FEMWATER, are also useful tools for groundwater flow modellers. Both finite-difference and finite-element methods have clear advantages that make them applicable to particular problems. The method the modeller is most familiar with should be an important factor in the selection of a model. The factors involved in the choice between finite-difference and finite-element methods are well-discussed (Anderson & Woessner, 1992).

All numerical groundwater models require considerable time and effort and data output can be difficult to interpret because of the large quantities of data involved. This process has relatively recently become much easier with the advent of integrated graphical pre- and post-processing packages which are now available. Visual MODFLOW, GMS and PM are programs that are completely integrated with the numerical model. These programs are described in Chapter 6. ModelCad, MODLMAKR and Surfer and Grafer are commercially available pre- and post-processing packages that allow the user to utilise the same tool with several hydrogeological models. These programs are described in Chapter 7.

6.1.1 ASM

Developed by: Kinzelbach, W. and Rausch, R.

Program language: FORTRAN, VISUAL BASIC

Documentation: Kinzelbach, W. and Rausch, R., 1995, ASM-Aquifer Simulation Model, Manual, Heidelberg/Stuttgart, Germany, 56p.

Description: ASM (Aquifer Simulation Model) is a finite-difference 2-dimentional vertical or horizontal flow model which includes the calculation of flow lines, 'isochrone' and 'random walk' transport simulations of steady state flows. The model size is limited to 80x80 cells where each cell can be of variable size in the x- and y-directions.

Use: The program is capable of simulating a series of different situations:

- Steady-state and transient flow

- Simulation of heterogeneous aquifers, confined, unconfined and semi-confined aquifers.
- Anisotropy in the aquifer's hydraulic conductivity or transmissivity where the anisotropy is limited to the model's principal axes
- Abstraction and injection boreholes with continual or variable pumping
- Precipitation which can vary both spatially and temporally
- Water balances can be calculated for the entire model and for pre-defined areas within the model
- The program can compare measured and calculated piezometer pressure
- Generation of stochastic distribution of hydraulic conductivity or transmissivity
- Calculation of groundwater flow lines
- Calculation of isochrones around boreholes
- Simulation of pollution plumes occurring as a result of continual or short lived pollution
- Plotting of breakthrough curves in selected pumping and observation boreholes

Although initially developed as an educational tool ASM incorporates many features of more complex models and may be used for initial evaluations of hydrogeological problems.

Solution method: The groundwater flow equation is solved using a node-centred finite-difference method employing either a PCG (Preconditioned Conjugate Gradient) or an IADI (Iterative Alternating Direction Implicit Procedure) scheme. If measured values of piezometric head are available an automatic calibration procedure based on Marquardt-Levenberg for steady state flows can be used.

For the computation of flow lines and isochrones two different schemes of velocity interpolation are different. These are the scheme by Prickett (Random Walk) and the scheme by Pollock (MODPATH model).

The program can simulate steady state and transient flow conditions in addition to unconfined, confined and leaky-confined aquifer conditions. Options are available for time-varying pumping rates, temporally and spatially varying recharge, permanent or instantaneous solute injection and mass balance calculations.

The calculation of flow lines, isochrones and pollution transport is only possible for steady state flows.

Special characteristics: A package is included which incorporates pre- and post-processing data handling packages. The data are input using an interactive interface and the grid is generated after the dimensions have been specified. A user-friendly program which, although originally intended as a tool for use in teaching, includes so many advanced features that it can be used to simulate a wide variety of field situations.

Input-output data format: The program is menu-driven and includes an interactive user interface which enable the user to edit data in addition to a series of routines for the graphical presentation of the data.

Availability: IGWMC

System requirements: IBM PC, XT, AT or equivalent, 640K RAM, DOS 3.1 or higher, CGA or EGA graphics, Math coprocessor.

6.1.2 FEMWATER

Developed by: Yeh, G.T. Penn State University

Program language: *

Documentation: Yeh, G.T., 1987, FEMWATER: A finite-element model of water flow through saturated-unsaturated porous media: First revision, Rep. ORNL5567/R1, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Description: A 3-dimensional finite-element program for simulating unsaturated and saturated flow and transport. It provides density-driven, coupled flow and contaminant transport in both saturated and unsaturated conditions.

Use: Simulating flow in both the unsaturated and saturated zone. FEMWATER also includes a pollution transport module.

Solution method: Solves Richards's equation in heterogeneous, anisotropic porous media.

Special properties: FEMWATER is delivered as a part of the GMS pre- and post-processing package. There are currently problems with the modelling package (GMS/FEMWATER) but the supplier is working to correct these problems. Potential users are referred to EGCL for updated versions of the program and to check on the situation regarding the correction of the above mentioned problems.

Input-output data format: GMS provides for the integrated use of pre-processor, analysis and solution programs.

Availability: EGCL, SSG

System requirements: The Windows version of the GMS/FEMWATER package requires a PC386/486/Pentium running Microsoft Windows 3.1/NT/95 with 16Mb RAM (32Mb recommended) and math coprocessor. The UNIX X-Windows version runs on AIX, HP-UX, IRIX, OSF, Sun OS and SPARC Solaris.

6.1.3 FLOWPATH

Developed by: Waterloo Hydrologic Software

Program language: *

Documentation: *

Description: FLOWPATH is an integrated 2-dimensional groundwater flow and pathline analysis package. The flow model is based on the finite-difference formulation allowing for the simulation of confined, leaky or unconfined flow in heterogeneous and anisotropic porous media. The model can account for:

- wells
- spatially variable groundwater and evapotranspiration
- variable leakage characteristics of under- and overlying aquitards
- interaction between groundwater and surface water bodies can be simulated

Use: FLOWPATH can be used for 2-dimensional groundwater flow modelling and calculation of pathlines and travel times.

Solution method: FLOWPATH is a finite-difference model. Groundwater pathlines, travel times and groundwater velocities are calculated using the particle tracking method.

Special properties: *

Input-output data format: FLOWPATH has an interactive data input by menu/graphics. Results can be displayed as equipotential contours, velocity vectors and pathlines. The program includes on-line help and a user's manual.

Availability: RW, SSG

System requirements: PC386/486/Pentium with a minimum of 4 MB RAM, EGA or VGA display and a math co-processor. A mouse is also recommended. Most printers are supported as well as HP plotters and compatibles.

6.1.4 MICRO-FEM

Developed by: Hemker, C.J., van Eldurg, H.

Program language: *

Documentation: *

Description: MICRO-FEM is an integrated high capacity finite-element program for simulating steady state and transient flow in a multi-system aquifer. A 3-dimensional particle tracking program enables visualisation of flow lines in 3-dimensions in addition to normal plotting capabilities such as groundwater head contours.

The MICRO-FEM package consists of six programs. FEMGRID is a mesh generation program that builds and visualises regular or irregular element networks. FEMODEL, the pre- and post processing package, is the user interface program. FEMCALC or FEDCALC calculates the head values. Calculation is based on the finite-element method or on a hybrid finite-element difference scheme respectively. FEMPLOT is the post-processing program and can be used to plot the network, the head distribution, and the aquifer and aquitard model parameters on a HP plotter. The fifth program, MEMMERGE, is a utility to compile a new model based on existing and new network data.

Use: The model can simulate heterogeneous aquifer, semi-permeable layers and anisotropy and allows time dependent sources and sinks in addition to movable, temporary and time variable boundary conditions.

Solution method: *

Special properties: The program can handle large problems with up to 12500 nodes and 16 aquifers. The large capacity and geometric flexibility combined with a user-friendly interface has made the program the most used in Holland. A complete program package includes the sub-routines FemMesh, F3Model and FemCat.

Input-output data format: The program includes a number of modules. One modules is used for generating the element mesh, model construction, data input, solution, post-processing, graphical presentation and plotting. Data manipulation and grid design is carried out using an interactive graphic design menu. The program also has a good interface with other standard support tools such as a spreadsheet, GIS, databases and CAD programs.

The presentation of model results includes water balance calculations, flow lines and travel.

Availability: IGWMC

System requirements: IBM PC, XT, AT or equivalent, 640K RAM, DOS 3.3. or higher, CGA graphics. Math coprocessor optional.

6.1.5 MODFE

Developed by: Cooley, R.L., Torak, L.J., USGS

Program language: *

Documentation: Torak, L.J., (1993a). Model description and user's manual: Part 1 of a MODular Finite Element model (MODFE) for areal and axisymmetric ground-water flow problems: U.S. Geological Survey Techniques of Water-Resources Investigations, Book 6, Chapter A3, 136pp.

Description: MODFE (MODular Finite Element Model) is a modular finite-element model for areal and axisymmetric flow problems. The model can simulate confined or unconfined, steady state and transient conditions two-dimensional or axisymmetric groundwater flow in a heterogeneous anisotropic aquifer.

MODFE uses triangular elements to represent the aquifer's geometry, hydraulic boundaries and variations in groundwater head. One-dimensional elements are used to describe head changes over time. Linear co-ordinate functions are approximate the head distributions in the elements.

Use: MODFE was developed to solve flow problems based on the appropriate equations for axisymmetric radial flow in the aquifer. MODFE can simulate steady state and transient flow in heterogeneous, anisotropic aquifers. The anisotropic direction can vary in the different modelling zones. Other aspects of MODFE's potential include:

- Switch between unconfined and confined conditions with partial desiccation/re-wetting of unconfined aquifer nodes
- Decrease of aquifer thickness to zero under dewatering and increase of aquifer thickness from zone under water table rise and head-dependent fluxes from spring
- Drainage wells, leakage across river-beds or confining beds combined with aquifer dewatering and evapotranspiration
- Elastic storage coefficients, localised and distributed sources and sinks
- Possible boundary conditions include: constant head, constant flow and head dependent boundaries
- Vertical sections and radially symmetric flow
- Non-linear head dependent flow for the simulation of line, point or distributed sources and sinks
- Boundary conditions and other hydraulic influences can vary with the time steps
- The aquifers hydraulic parameters and boundary conditions can be varied within the model's zones.

Solution method: The finite element matrix is solved either with a direct symmetric Doolittle method with a triangular imperfect Cholesky iteration procedure or a conjugate gradient method. The iteration procedure is preferable for problems consisting of more than 500 nodes.

Special properties: The program is run in batch mode.

Input-output data format: The output file has a tabulated format and the program comes complete with examples of how to construct an input file.

Availability: USGS-NWIS, IGWMC, SSG, RWE

System requirements: PC 386/486/Pentium with 2Mb RAM and math coprocessor.

6.1.6 MODFLOW

Developed by: McDonald, M.G. and Harbaugh, A.W.. 1984, Modified 1988.

Program language: FORTRAN 77

Documentation: McDonald, M.G., Harbaugh, A.W., 1988. A modular three-dimensional finite-difference ground-water flow model: Techniques of Water Resources Investigations of the United States geological Survey. Book 6, Chapter A1, 586pp.

Description: MODFLOW is the USGS modular three-dimensional groundwater flow model. MODFLOWEM is able to represent flow in 1-, 2- and 3-dimensions in confined and unconfined aquifers under steady state or transient conditions.

Hydraulic conductivity or transmissivity can be varied within and between layers. Anisotropy can be simulated providing the principal direction is along the one of the model's grid axes and the anisotropy ratio is constant for each layer. MODFLOW requires that the value of vertical hydraulic conductivity divided by the vertical distance between adjacent nodes be input into the model.

The boundary conditions can be a fixed head or fixed flow. It is also possible to simulate a variable head-dependent flow. Flow from an external area to the model is dependent on the calculated head difference between the boundary node and the external area for each time step. The modelled area is divided into blocks within which the aquifer's hydraulic properties are assumed to be constant.

It is not intended to present a description of all the packages available with the latest version of MODFLOW here. There are however many such packages enabling the simulation of an extremely wide variety of flow conditions. A number of these packages are listed under 'special properties'.

Use: MODFLOW can be used to simulate steady state and transient flow in aquifers with irregular form. The model can be divided into up to 60 layers that represent unconfined and/or confined aquifers. External sources and sinks such as boreholes, variable precipitation distribution, flow to trenches and influent and effluent rivers can be simulated.

Solution method: The finite-difference matrix is solved using SIP (Strongly Implicit Procedure) or SSOR (Slice Successive Over Relaxation). The mass balance is calculated as a volume from all sources and sinks for each time step.

Special properties: The program is constructed of modules that are included in the model only when relevant for a given situation. Routines that are not applicable are thereby avoided.

A series of programs have been developed which can be used with MODFLOW enabling a wide variety of problems to be simulated. Many of these programs have been included in later versions of MODFLOW. These include:

- PCG, Preconditioned Gradient Method - an alternative solution for the finite-difference equations including three types: Choleski, point Jacobi and block Jacobi.
- MMSP, Modular Model Statistical Processor - handles input and output data from MODFLOW which assists in the handling and assessment of large data sets.
- MODFLOWARC - a version of MODFLOW which can utilise data from ARC/INFO systems
- ZONEBUDGET - calculates water balances for sub-areas within the simulated area
- AQUIFER COMPACTION - simulates changes in storage coefficients occurring as a result of elastic and inelastic compaction
- MODPATH-PLOT - calculates and graphically presents flow lines derived from steady state flow calculations by MODFLOW
- PCG2, Preconjugated Conjugate Gradient 2 - an effective and much used solution method for linear equations resulting from the solution of MODFLOW
- MODFLOWP - a version of MODFLOW which incorporates a routine for estimating relevant hydraulic parameters
- HFB, Horizontal flow barriers - is used to simulate thin vertical geological or artificial layers with low hydraulic conductivity which restricts horizontal groundwater flow
- TLK1, Transient Leakage from confining layers - enables the simulation of transient flow in low permeability layers. The programs avoids treating such a layer as an individual layer and thereby makes MODFLOW's computations more effective
- MODBRANCH - is a program which links MODFLOW with the surface hydrology model BRANCH. BRANCH is a program that solves flow equations for multi-canal/river systems. The program is limited by a 1-dimensional description of flow in the canal/river
- STREAMLINK - links MODFLOW with surface hydrology models such as RIVER and BRANCH

MOD2DFD and MOD3DFD are Microcode's enhanced implementation of the U.S.G.S. 2- and 3-dimensional finite-difference groundwater flow models respectively. These versions include:

- a graphical pre-processor to design models on-screen with a mouse or digitizer
- the production of graphics input files enabling graphical output of model results in a facility to produce very large models

Input-output data format: Constructing the data files required by MODFLOW is a time consuming task. There are however a number of pre- and post-processing programs available which ease this task. MODGRAF provides graphics for MODFLOW including groundwater velocity and vector capability. MODGRAF

contours heads and drawdowns from each layer, stress period and time step of each simulation and can generate and superimpose groundwater velocity vectors on the head contour plots. An interface to MODGRAF is included in the MODFLOW^{EM} version in addition to interface with Lotus 1-2-3 and SURFER and other compatible graphics packages.

Visual MODFLOW and MODFLOW^{win32}/CONTOUR^{win32} are two data handling packages specifically intended for this task of data input, editing and presentation for MODFLOW, MODPATH and MT3D. These programs consist of graphic routines for data handling, interpretation and presentation. Modelcad, Meshmaker and GMS are other examples of pre- and post-processing programs which can support a number of programs.

Availability: USGS-NWIS, IGWC, SSG, RWE

System requirements: PC386/486/Pentium with 2Mb RAM.

6.1.7 MODFLOWwin32/CONTOURwin32

Developed by: Environmental Simulations Inc., Rumbaugh, D. and Rumbaugh, J.

Program language: MODFLOW^{win32}/CONTOUR^{win32} is run as a 32-bit DLL program in Windows v3.1.1, Windows NT and Windows95

Documentation: The help menu includes the entire MODFLOW^{win32} manual in addition to the MODFLOW manuals

Description: MODFLOW^{win32} is ESI's version of the USGS 3-dimensional groundwater flow model MODFLOW. MODFLOW^{win32} was specifically developed for use with Windows (Win32s) and Windows NT.

The program includes the most popular MODFLOW sub-routines such as BCF2, BCF3, PCG2, STREAM routing and Aquifer Compaction. All the MODFLOW manuals are available on the help menu. CONTOUR^{win32} can plot the results from MODFLOW directly. MODFLOW^{win32}/CONTOUR^{win32} offers the possibility of working with several windows.

The program package includes CONTOUR^{win32}, which is a post-processor that can be used for contouring MODFLOW results and displaying particle trace pathlines computed by MODPATH.

Use: Intended for WINDOWS users who wish to use MODFLOW. A pre-processing program for this program was released in 1996.

Solution method: See MODFLOW.

Special properties: MODFLOW^{win32} was specifically developed for use with Windows. Both MODFLOW^{win32} and CONTOUR^{win32} have an on-line context-sensitive help based on re-formatted MODFLOW manuals.

Input-output data format: MODFLOW^{win32}/CONTOUR^{win32} requires the use of other pre-processing programs. Graphical presentation of the results from MODFLOW and MODPATH is carried out through the use of CONTOUR^{win32}.

Availability: ESI

System requirements: PC 486/Pentium running Windows 3.1/95/NT, math co-processor and 8 MB RAM.

6.1.8 MODPATH386

Developed by: Pollack, D.W. (1990)

Program language: FORTRAN 77

Documentation: Pollack, D.W. (1990). Documentation of computer programs to compute and display pathlines using results from the U.S. Geological Survey Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. U.S. Geological Survey, Open File Report 89-381.

Description: MODPATH is a particle tracking post-processing package for computing three-dimensional pathlines using output from steady state simulations obtained from the U.S. Geological Survey modular three-dimensional finite-difference groundwater flow model (MODFLOW).

Use: Particle tracking for the determination of groundwater flow and non-reactive transport flow rates and directions.

Solution method: MODPATH uses a semi-analytical particle-tracking scheme. The method is based on the assumption that each directional velocity component varies linearly within a grid cell in its own co-ordinate direction. This assumption allows an analytical expression to be obtained describing the flow path within a grid cell. Given the initial position of a particle anywhere in a cell, the co-ordinates of any other point along its pathline within the cell, and the travel time between them, can be computed between them.

Special properties: Program dimensions have been increased with the ability to address all available RAM on an 80386-based computer.

Input-output data format: Data is input to MODPATH and MODPATH-PLOT through a combination of files and interactive dialogue. The program MODPATH-PLOT^{EM} is available for the graphical presentation and analysis of the output from MODPATH.

Availability: RW (not MODPATH-PLOT), SSG

System requirements: PC386/486/Pentium with 2 Mb RAM, math co-processor, hard disk, EGA or VGA graphics card and display and a printer or plotter for hardcopy output.

6.2 ANALYTICAL MODELS

Analytical flow models give exact solutions of the groundwater flow equations. The solutions can be utilised for verifying numerical models and simulating situations where more work-intensive numerical models are unsuitable. Even though the mathematical solution of the partial differential equations is no simple task, the use of intricate mathematical methods can be avoided. The models are conceptually simple for users with a hydrogeological background and can be easily and rapidly constructed. The results are also easy to interpret.

The exact solution demands strict boundary conditions and this limits the application of this type of model. It is important that the user is aware of the limitations and assumptions involved before the modelling process is started. The aquifer must be assumed to be homogenous and of infinite lateral extent and the aquifer's catchment area of infinite lateral extent

The three programs listed below are based on the same solution method and generally have very similar characteristics. For DOS-users Quickflow or TWODAN are preferable, whilst WINDOWS-users will find WinFlow more suitable.

6.2.1 QUICKFLOW

Developed by: Rumbaugh, J., Geraghty and Miller Modelling Group

Program language: *

Documentation: *

Description: Quickflow is an interactive analytical 2-dimensional steady state/transient groundwater flow model. The model can therefore only simulate 2-dimensional problems and requires a uniform aquifer with a given hydraulic gradient, flow direction, hydraulic conductivity, elevation of the top and bottom of the aquifer and a reference level for total head.

Quickflow has the following features:

- Simulation of steady state and transient flow
- Simulation of unconfined and confined conditions
- Functions for wells, line sinks, recharge and regional gradients

- Head contours, streamlines and particle tracking
- Importation of DXF files for base maps

The program includes the calculation of flowlines and has an interactive menu. The output files are in DXF format compatible with SURFER (Golden Software Inc.).

Use: Preliminary studies, storage tanks, landfill sites and other related problems where limited data is available.

Solution method: The program calculates the analytical function using the 'principle of superposition' to solve the groundwater flow equations summing the effect of individual elements affecting the hydraulic conditions within the aquifer. The solution for flow lines is based on analytical functions from Strack (1988). For transient modelling the solution is limited to boreholes with a single regional hydraulic gradient and a leaky aquifer response based on Theis (1935) and Jacob (1950).

Special properties: Relatively little data is required to run the program.

Input-output data format: Quickflow has a dedicated graphical menu enabling the interactive input of data and the presentation of output data and the export of data files to other programs. QUICKFLOW can be used to produce report quality graphics using HP plotters, laser printers and dot-matrix printers. QUICKFLOW can also import map files in a number of different formats.

Availability: RWE

System requirements: PC 386/486/Pentium running DOS.

6.2.2 TWODAN

Developed by: Fitts, C.R.

Program language: *

Documentation: *

Description: TWODAN is a two-dimensional groundwater flow model. TWODAN has the following capabilities:

- 2-layer aquifers
- Confined and/or unconfined conditions
- Heterogeneous, polygonal regions inside which the aquifer can have varying elevations and/or hydraulic conductivities
- Global infiltration or leakage
- Local infiltration or leakage areas
- Uniform regional flow
- Wells, discharge or head-specified

- Line-sinks, discharge or head-specified
- Transient wells
- Resistant elements for modelling thin, resistant boundaries such as slurry walls in open polylines or closed irregular polygon shapes
- Pathline tracing
- Calibration

Use: An effective tool for simulating regional groundwater flow.

Solution method: The program is based on the analytical element method described by Strack (1988).

Special properties: Quickflow and TWODAN are two programs with very similar characteristics but with a number of minor differences.

Input-output data format: The program uses a menu-driven graphical input and output. DXF format maps can be imported. Output can be produced as text files, plotted model components, base map, stream function contours, potential function contours and flow pathlines.

Availability: IGWMC, SSG, RWE

System requirements: PC 386/486/Pentium with 4 MB RAM running DOS under Windows and OS/2.

6.2.3 WINFLOW

Developed by: Environmental Simulations Inc.

Program language: Windows MDI

Documentation: Dedicated help menu includes the entire manual.

Description: WinFlow is an analytical model that simulates 2-dimensional steady state and transient flow.

WinFlow includes:

- steady state and transient flow in unconfined and confined aquifers;
- incorporation of features such as boreholes, infiltration basins, springs, dams, recharge, drainage ditches and regional hydraulic gradients;
- importing of DXF and ModelCad format map files in Quickflow and ModelCad format;
- calibration targets and calibration statistics.

Use: Preliminary studies, storage tanks, landfills where little data is available.

Solution method: The steady state module simulates groundwater flow in a horizontal plane using analytical functions developed by Strack (1988). The solution for transient simulations uses equations developed by Theis (1935) and by Hantush and Jacob (1955) for confined and leaky aquifers.

Special properties: In contrast to Quickflow and TWODAN, Winflow is a WINDOWS-based program. The entire WinFlow manual is incorporated in the help menu in the program.

Simulations involving steady state flow can incorporate features such as boreholes, springs, infiltration basins, line sources and sinks and regional flow and use the 'principal of superposition'. For transient modelling only regional boreholes, uniform hydraulic gradients and leaky aquifer response can be incorporated.

Input-output data format: WINDOWS characteristics such as: double click on elements for editing, click and drag for moving of boreholes and drainage ditches. Several windows can be run simultaneously and data can be cut, copied and pasted to and from clipboards and a keyword-based help menu (including the entire manual).

Output may be exported to a variety of file types including SURFER, Geosoft, Spyglass, Windows Metafiles and AutoCAD DXF files.

Availability: SSG, RWE

System requirements: PC 386/486/Pentium running Windows 3.1 or higher and 2.5Mb hard disk space. A math coprocessor is recommended.

7. POLLUTION TRANSPORT MODELS

7.1 NUMERICAL POLLUTION MODELS

Numerical pollution transport models include advection, dispersion, retardation and/or degradation with the groundwater flow equation. Numerical pollution models use numerical solution methods to solve the relevant equations. Common to all numerical models however is the fact that they treat each individual component of the pollution separately. The modeller therefore must decide which components should be simulated.

There are distinct differences in terms of the transport mechanisms that each model incorporates. Some of the mechanisms, which can be included, are:

- Langmuir and Fruendlich sorption isotherms
- biological degradation
- retardation
- mechanical dispersion
- diffusion

These programs are not geochemical models in that they do not incorporate detailed geochemical modelling methods. They attempt to simulate the processes occurring in the ground with approximations that are often combinations of several chemical processes. Some programs are specifically designed for simulation of the saturated or unsaturated zone. The most fundamental difference between these programs is that some include the effect of density and temperature on the pollution transport whilst others assume that these do not significantly affect the transport mechanisms.

7.1.1 BIOPLUME II

Developed by: Rifai, H.S., Bendient, P.B., Borden, R.C. and Hassbeek, J.F. (1988)

Program language: *

Documentation: BIOPLUME II, Computer model of two-dimensional contaminant transport under the influence of oxygen limited biodegradation in ground water, User's Manual - Version 1.0, National Center for Ground Water Research, Rice University, P.O. Box 1892, Houston, Texas 77251, USA.

Description: BIOPLUME II is a U.S. EPA computer model of two-dimensional transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. The model is based on the USGS model MOC that calculates changes in concentration as a function of advection, dispersion, mixing and biological degradation.

Use: A 2-dimensional model for the simulation of transport of dissolved hydrocarbons under biological degradation limited by oxygen supply. BIOPLUME II enables the simulation of an oxygen supply to a former anærobic system. It is also possible to simulate the anærobic first-order degradation of hydrocarbons.

The model is extremely user-friendly and can be used to simulate natural processes in addition to biological clean-up procedures. Injection boreholes for oxygen supply can also be simulated enabling the optimisation of a clean-up process. The boundary conditions can also act as oxygen supply sources.

Solution method: The BIOPLUME II algorithm solves for the same conditions as MOC but it solves for two pollution plumes - one for oxygen and one for hydrocarbons. It is assumed that instantaneous mixing occurs between the oxygen and hydrocarbons and that two plumes are combined on order to calculate the biological degradation.

Special properties: *

Input-output data format: A menu-driven program incorporating pre- and post-processing functions is included. The output files produced are compatible for use with SURFER, which enables plotting of groundwater heads and hydrocarbon and oxygen concentrations. An optional graphics

Availability: IGWMC, SSG

System requirements: IBM PC, AT, XT or equivalent, 640 K RAM, minimum of 500 K free RAM, DOS 2.01 or higher, CGA, EGA or VGA graphics, math co-processor.

7.1.2 HST3D

Developed by: Kipp, K.L., Jr., (1987), adapted from other models.

Program language: FORTRAN

Documentation: U.S. Geological Survey Water Resources Investigation Report 86-4095, 517pp.

Description: A 3-dimensional groundwater flow, heat and solute transport model. The model is based on the simulation of flow through pores dependent on the fluid's density and viscosity in relation to pressure, temperature and the solute's concentration. The equation for the transport of dissolved components only applies to single dissolved components with linear equilibrium sorption and linear degradation.

Use: HST3D is primarily intended for three-dimensional analysis of flow, heat and solute transport in the saturated zone of a groundwater system with variable or constant density and viscosity.

HST3D can be used for the analysis of problems such as:

- Infiltration of pollution into the ground/Waste injection
- Landfill contaminant movement
- Salt water/freshwater intrusions
- Brine disposal
- Radioactive waste disposal sites
- Geothermal systems
- Storage of heat energy in the ground
- Liquid phase geothermal systems
- Single component contaminant transport in a complex aquifer system

Solution method: A finite-difference technique is used to discretise the simulated area. The flow, heat and pollution equations are solved in series after reduction using a Gaussian reduction scheme. The reduced equation set is more stable and better suited to numerical solution. Two methods for solving the equation set are available, a direct elimination method and an SOR method.

Special properties: The program is a development of a program written by INTERCOMP Resource Development and Engineering Inc. (1976) which was later revised by INTERA Environmental Consultants Inc. (1979).

This is a program that demands a good understanding of modelling techniques.

Input-output data format: The SSG version of HST3D includes the pre- and post-processing routines PREHST and HSTPOST allowing input/editing of the complex data input required for the model.

A graphical interface for HST3D, HST3D-ANE, is also available from SSG. HST3D-ANE is a user-friendly interface integrated within the Argus Numerical Environments (ANE) modelling environment. ANE integrates CAD, GIS, DataBase, Conceptual Modelling, Automatic Grid and Mesh Generation, and Scientific Visualisation within a single graphical user interface.

Availability: USGS-NWIS, IGWMC, SSG

System requirements: PC 386/486/Pentium, Three executable versions are available requiring 4, 8 and 16 MB RAM and a math co-processor. Optional FORTRAN extended memory compiler. Mainframe version: FORTRAN 77 compiler.

7.1.3 MOC

Developed by: Konikow, L.F. and Goode, D.J. (1989).

Program language: FORTRAN

Documentation: Techniques of Water-Resources Investigations of the United States Geological Survey, Book 7, Chapter C2. 90pp and U.S. Geological Survey Water-Resources Investigations Report 89-4030, 65pp.

Description: MOC (Method-Of-Characteristics) is the USGS 1- and 2-dimensional finite-difference pollution transport model for steady state and transient saturated flow. MOC solves the groundwater flow equation for the saturated zone with advection, dispersion, dilution and mixing of water from different sources (e.g. rain). It includes a number of chemical processes linked to the solution of the groundwater flow equation.

MOC has the following features:

- Solute transport in groundwater
- 1- and 2-dimensional problems involving steady state or transient flow
- Computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion and mixing from fluid sources
- Heterogeneous and/or anisotropic aquifers
- Rectangular block-centred finite-difference grid
- Specification of injection or abstraction wells and of spatially varying diffuse recharge or discharge, saturated thickness, transmissivity, boundary conditions and initial heads and concentrations

The model incorporates:

- First-order irreversible rate-reaction
- Reversible equilibrium-controlled sorption with linear, Freundlich or Langmuir isotherms
- Reversible equilibrium-controlled ion exchange for monovalent and divalent ions.

It is assumed that variations in density, viscosity and temperature have no effect on groundwater flow. The model can simulate heterogeneity and anisotropy and injection and abstraction boreholes. The injection or abstraction of water from diffuse sources can also be included. It is also possible to vary the depth of the saturated zone, transmissivity, boundary conditions and the starting values of groundwater head and concentrations.

Use: MOC can be used to simulate the 1- and 2-dimensional transport of pollution in the saturated zone under steady state and transient flow conditions. MOC is particularly suitable for investigation of problems involving changes in concentrations over an area with time as a result of convection, dispersion, mixing, dilution and chemical reactions.

Solution method: The model links the solution of the groundwater flow equation with the equation for pollution transport. IADIP is used to solve the finite-difference approximation, IADIP whilst the method of characteristics is used to solve for pollution transport. Pollution transport resulting from convection is described using a particle tracking procedure and a two-step explicit procedure is used to describe dispersion, water sources and sinks and velocity divergence. The explicit procedure

has a number of stability criteria but the model incorporates limitations in the time-steps to overcome this problem.

Special properties: This is a much-used program for pollution transport. The model is generalised and flexible in design and can be used for a variety of problems. There is also a variant of the program called MOCDENSE that includes the effect of variable density.

Input-output data format: PREMOC is an interactive program for the preparation of MOC input files and is available from USGS-NWIS and IGWMC. The program has four main functions: preparation of new data sets, modification of new data sets, reading of data from files and saving to file. SSG also has a series of pre- and post-processing programs for the handling of data files specially designed for MOC.

Availability: USGS-NWIS, IGWMC, SSG

System requirements: PC 386/486/Pentium and math co-processor.

7.1.4 MT3D96 (New version of MT3D)

Developed by: Geeing, C. (1994)

Program language: FORTRAN 77

Documentation: MT3D A Modulation Three-Dimensional Transport Model for simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems, S.S. Papadopulos & Associates Inc., Environmental & Water Resources Consultants, 7944 Wisconsin Avenue Bethesda, Maryland 20814, USA.

Description: MT3D is a 3-dimensional solute transport model for the simulation of advection, dispersion, groundwater sinks and sources, mixing and the chemical reaction of dissolved components in the groundwater system. MT3D is capable of simulating equilibrium controlled linear and non-linear sorption and first-order irreversible degradation.

The program has the same modular construction as MODFLOW, which enables the simulation of individual processes without the unnecessary use of computational resources. A main module is linked with a series of sub-routines for the simulation of each process. The model is compatible with MODFLOW.

The model is capable of simulating:

- Finite confined, unconfined or variably confined/unconfined aquifers
- Sloping model layers and variable cell thickness within the same layer
- Boundary conditions with a specified concentration/mass flux
- Pollution transport from external sources such as boreholes, drains, rivers, diffuse sources and evapotranspiration

Use: MT3D is an extensively used popular program which can be used to simulate 3-dimensional pollution transport involving advection, dispersion, groundwater sinks and sources, mixing and the chemical reaction of dissolved components in the groundwater system.

Solution method: The MT3D transport uses a mixed Euler-Lagrange solution method for the 3-dimensional advection/dispersion equation. There are three basic solution options: the basic MOC method, a modified version (MMOC) and a hybrid version (HMOC). HMOC uses the MOC method to eliminate numerical dispersion and the MMOC method to increase the efficiency of the calculations. All of these solution methods are available and mean that MT3D is a versatile tool for the simulation of pollution transport problems.

Special properties: MT3D is designed to be used with a block-centred finite-difference groundwater flow model such as MODFLOW and assumes that changes in concentrations do not affect flow. The groundwater flow model is first run and calibrated independent of MT3D. MT3D then uses the results from the flow model and it's own data input files.

MT3D is incorporated in the modelling packages Visual MODFLOW and Groundwater Vistas and is available as an option with GMS.

Input-output data format: MT3D uses the total head, sources and sinks and the various hydraulic parameters for the aquifer output from the groundwater flow model. Boundary conditions are automatically transferred to MODFLOW. MT3D should be able to be used with any block-centred finite-difference groundwater flow model but the documentation is produced with the assumption that MODFLOW is used. More work will consequently be required should another flow model be used.

MT3D includes a post-processing program to assist the plotting of concentration breakthrough curves and contour maps using SURFER and other graphics packages.

MT3D is also supported by many pre- and post-processing packages including ModIME, ModelCad, PROCESSING MODFLOW (PMWIN), Visual MODFLOW, GMS and Groundwater Vistas.

Availability: IGWMC-NWIS, EGCL, SSG, RWE

System requirements: PC 386/486/Pentium with 2 MB RAM. The source code is included for incorporation on Macintoshes, workstations or mainframes.

7.1.5 SHARP

Developed by: Essaid, H.L. (1990)

Program language: FORTRAN

Documentation: U.S. Geological Survey Water-Resources Investigation Report 90-4130, 181pp.

Description: A quasi 3-dimensional numerical finite-difference model for simulating fresh/salt water flow in layered coastal aquifers. SHARP simulates regional flow in confined/unconfined aquifers where salt and fresh water is separated by a sharp boundary. The effect of salt water on fresh water flow is incorporated. Multi-layer aquifers separated by aquicludes can also be simulated. The aquifer's hydraulic conductivity and any flow through the aquitards can be varied within each of the layers. The uppermost aquifer can be unconfined or confined and distributed sources can be incorporated. Variations in pumping rates and sources and sinks are possible. The boundary conditions can be flux, constant salt/fresh water or head dependent.

Use: Simulating 3-dimensional flow involving for salt-water intrusion in coastal aquifers with a sharp boundary between salt and fresh water.

Solution method: A finite-difference program.

Special properties: SHARP is driven in batch mode.

Input-output data format: Text editor for the input of data. Output stored in text files.

Availability: USGS-NWIC, IGWMC

System requirements: *

7.1.6 SUTRA/SUTRA-PLOT

Developed by: Voss, C.I. (1984) and Souza, W.R. (1987)

Program language: FORTRAN

Documentation: U.S. Geological Survey Water Resources Investigations Report 84-434369, 409pp. and U.S. Geological Survey Water Resources Investigations Report 87-4245, 122pp.

Description: SUTRA is a Saturated-Unsaturated, fluid-density dependent groundwater flow model with energy transport or chemically reactive single-species solute transport. The model is a 2-dimensional finite-element model for the simulation of saturated and unsaturated flow dependent on density. SUTRA includes heat transport and chemical reactions. In the saturated zone vertical and horizontal sections can be simulated whilst in the unsaturated zone only vertical sections can be simulated.

Chemical processes include both natural and anthropogenic processes. Processes such as sorption, degradation and reaction of the pollution can be simulated.

Use: SUTRA can be used to analyse density-dependent pollution transport in the unsaturated and saturated zone. Examples include:

- the planning of clean-up projects
- assessment of well performance and pumping test data
- density-dependent flow or constant-density flow analysis
- analyses of chemical species transport including processes of solute sorption, production and decay
- prediction of hazardous waste migration from landfill disposal sites
- analysis of aquifer, thermal regimes, subsurface heat conduction, aquifer thermal energy storage systems, geothermal reservoirs, thermal pollution of aquifers and natural hydrogeological convection systems
- salt water intrusion in cross-sectional sections in aquifers at near-well or regional scales with either dispersed or relatively sharp transition zones between freshwater and saltwater

Solution method: SUTRA uses a 2-dimensional hybrid finite-element and integrated finite-difference method to approximate groundwater flow equations. Changes in density and transport of pollution where adsorption, first-order degradation or transport of thermal energy are factors can be simulated.

Special properties: SUTRA is a comprehensive model that has been used for simulation of salt water and thermal zones.

Input-output data format: SUTRA is run in batch mode. Input files can be edited in text editor whilst SUTRA-PLOT uses input and output files from SUTRA for the graphical presentation of results. SUTRA-PLOT can calculate contours of pressure, degree of saturation, concentration and temperature. It is also possible to use other programs to create contour of these variables. SSG have produced a special program, Data manager, which enables the user to run SUTRA from WINDOWS.

A new program has been added to SUTRA, the Data Manager, a Windows-based product which includes LADE (Large Array Data Entry) and GMSL (Groundwater Math Science Library). A pre-processor is also included to assist in the creation of the two input files required.

An interface for Sutra, SUTRA-ANE, is available from SSG. SUTRA-ANE is a user-friendly interface integrated within the Argus Numerical Environments (ANE) modelling environment. SUTRA-ANE allows graphical data input, the execution of the model and the visualisation of the results. ANE integrates CAD, GIS, DataBase, Conceptual Modelling, Geostatistics, Automatic Grid and Mesh Generation and Scientific Visualization within a single graphical user interface.

Availability: USGS-NWIS, IGWMC, SSG

System requirements: PC386/486/Pentium with 4MB RAM, math co-processor, 2.5MB hard disk space, EGA or VGA graphics card and display and printer or plotter for hard copy output.

7.1.7 VS2D and VS2DT

VS2D, Variable Saturation 2-dimensions

Developed by: Laapala, E.G., Healy, R.W. and Weeks, E.P.

Program language: FORTRAN 77

Documentation: Laapala, E.G., Healy, R.W. and Weeks, E.P. (1987). Documentation of computer program VS2D to solve the equations of fluid flow in a variably saturated porous media: U.S. Geological Survey Water-Resources Investigations Report 83-4099, 184pp.

Description: VSD is a program for calculating 2-dimensional flow in an aquifer with variable saturation. Standard 2-dimensional axes or radially symmetric co-ordinates can be used.

Use: Calculation of isothermal 2-dimensional flow in an aquifer with variable saturation.

Solution method: The models use a non-linear form of Darcy's equation combined with the law of conservation of mass. The final equations are expressed with total head as the independent variable. This simplifies the treatment of the conditions in the saturated and unsaturated zones.

VS2D uses central differences based on a grid system with block boundaries to approximate the spatial derivatives of the groundwater equation. The time derivative is approximated with a backward implicit scheme. Non-linear storage coefficients, conductance boundary conditions are made linear using an implicit procedure. The relative hydraulic conductivity is evaluated using the arithmetic or geometric mean value based on adjacent cells with an upstream-weighted scheme. The finite linear matrix is solved using SIP (Strongly Implicit Procedure).

Special properties: VS2DT is a development of VSD that contains four new sub-routines.

VS2DT, Variable Saturation 2-Dimensional Transport

Developed by: Healy, R.W. (1990)

Program language: FORTRAN 77

Documentation: Healy, R.W. (1990). Simulation of solute transport in variably saturated porous media with supplemental information on modifications to the U.S. Geological Survey's computer program VS2D. U.S. Geological Survey Water-Resources Investigations Report 90-4025, 125pp.

Description: VS2DT uses a finite-difference approximation to the advection/dispersion equation with a non-linear flow expression. Boundary conditions for the pollution are first-order degradation, Langmuir and Freundlich isotherms and ion exchange.

Program options include:

- Backward or central approximations for both space and time derivatives
- First-order decay
- Equilibrium adsorption (Freundlich or Langmuir) isotherms
- Ion exchange

Use: VS2DT can be used for studies of water quality, groundwater pollution, waste disposal or groundwater recharge.

Solution method: See VS2D.

Special properties: The program has a modular construction so that the user can easily carry out modifications on the source code.

Input-output data format: The program package from IGWMC includes a pre- and post-processing package which can be used to prepare files for plotting with commercially available graphical presentation packages.

Availability: USGS-NWIS, IGWMC, SSG

System requirements: PC 386/486/Pentium, 4Mb RAM and math co-processor.

7.1.8 AQUA (2D and 3D)

Developed by: *

Program language: *

Documentation: A user's manual is provided with the program.

Description: AQUA 3D is a 3-dimensional groundwater flow and contaminant transport model. Its structure is similar to the existing AQUA 2D software. It is a multi-layered model where variable-thickness layers are connected by leakage between them.

AQUA 3D solves the transient groundwater flow with heterogeneous and anisotropic flow conditions. The model can have a large number of pumping and injection wells and spatial variation of all parameters. Time variation of pumping/injection is allowed. Boundary conditions may be specified as fixed head, time-dependent flow and head-dependent flow.

The program solves the transient transport of contaminants and heat with convection, decay, adsorption and velocity dependent dispersion. Boundary conditions may be specified as fixed concentration (temperature) or fixed dispersive mass (heat) flux.

Use: AQUA 3D has been developed for use in situations where there are a number of interacting aquifers, each with different characteristics. AQUA 3D is also suited to modelling situations with a large difference in horizontal and vertical permeabilities.

Solution method: The equations are solved by the finite-element method in each layer followed by the necessary number of vertical iterations to obtain the desired accuracy.

Special properties: AQUA 2D and 3D can handle up to 10,000 nodes and 100 layers. A version is available from SSG that is capable of handling in excess of 10,000 nodes.

Input-output data format: AQUA 3D features a menu-driven, user-friendly interface for data entry and editing by digitizer, mouse or keyboard entry. Mesh generation and condensation is done automatically. A variety of pointing devices such as mice, digitizers, etc.) are supported through the use of the HALO Professional Graphics Library. AQUA 3D supports the graphical output of results (contours, flow arrows and time series) on screen, printer and plotter.

Availability: SSG

System requirements: PC386/486 or Pentium with 4 Mb RAM, math coprocessor, hard disk and EGA or VGA graphics card and display. Optional hardware supported includes mouse, digitizer, dot matrix and laser printers and Hewlett Packard or compatible plotters for hardcopy output.

7.2 ANALYTICAL POLLUTION MODELS

Analytical pollution transport models consider pollution as a single inert component in the same way as numerical transport models. A number of the models include the same processes as the numerical models. Due to the strict boundary conditions for the analytical solution the use of analytical models is limited. They are however of use in situations where rapid calculations of a pollution plume's lateral extent is required. They can also be used to verify a numerical model.

7.2.1 KYSPILL

Developed by: Sergio, S., HydroScience Inc.

Program language: *

Documentation: KYSPILL Version 1.0 (1994). A Groundwater Pollution Forecasting System, User Manual, HydroScience Inc., 101 Deer Crossing Way, Lexington, Kentucky 40509, USA, 47pp.

Description: KYSPILL is a 3-dimensional groundwater pollution model capable of simulating 3-dimensional dispersion in unsaturated soils and the subsequent 2-dimensional propagation in unconfined heterogeneous aquifers.

Use: KYSPILL is an effective tool for modelling pollution plumes from storage tanks, waste disposal sites, chemical spillages, and point and distributed pollution sources both in the saturated and unsaturated zone.

Solution method: KYSPILL uses a half-analytical solution for the stochastic differential equations that apply to groundwater flow and pollution transport in the ground. The aquifer's heterogeneity is handled statistically and the dispersion factor is scaled according to the aquifer's physical parameters. Pollution transport in both the saturated and unsaturated zone can be simulated using a retardation factor.

Special properties: The dispersion factor is given as a function of the regional hydrogeological parameters and is calculated using stochastic methods. This enables KYSPILL to simulate a dispersion factor that is dependent on the distance from source to which the pollution has spread (scale-dependent dispersion factor). KYSPILL is the only program that includes this possibility.

Input-output data format: A model can be rapidly constructed once the physical properties of the aquifer and the pollution are known. The output file can be shown graphically using the program and hard copy can be produced.

Availability: SSG

System requirements: IBM PC or compatible with 640 K RAM and math co-processor.

7.2.2 PESTAN

Developed by: Enfield, C., Ravi, V. and Johnson, J. (USEPA/RSKERL-CSMoS)

Program language: *

Documentation: PESTAN Pesticide Analytical Model Version 4.0, The United States Environmental Protection Agency Office of Research and Development, Robert S. Kerr Environmental Research Laboratory Center for Subsurface Modelling Support, P.O. Box 1198 Ada, Oklahoma 74820.

Description: PESTAN (PESTicide ANalytical model) is a U.S. EPA program for evaluating the transport of organic solutes through the vadose zone to groundwater. Active pollution can be added up to ten times in the course of a simulation.

The calculated values include predicted degree of water saturation, groundwater flow rate, pollution flow rate, size of the pollution plume. Values for dissolved, precipitated and total pollutant concentration are also calculated for up to four time steps and seven depths.

Input values are required for solubility, precipitation, sorption, degree of saturation, degradation, coefficient for the characteristic curve, saturated hydraulic conductivity, bulk density, dispersion factor, minimum and maximum depth and minimum and maximum time.

Use: Evaluation of 1-dimensional transport of organic pollution through a homogenous unsaturated soil layer. Suitable for preliminary studies where it is wished to determine parameters that need to be investigated further.

Solution method: PESTAN uses an analytical solution to calculate organic movement based on a linear isotherm, first-order degradation and hydrodynamic dispersion.

Special properties: The program was first written as a selection tool for insecticides and their movement in the groundwater and was later developed for use with organic compounds.

Input-output data format: The program is menu-driven and the input file is prepared in a DOS editor. The output is written to a text file and to a graphics file for presentation using a commercial package.

Availability: IGWMCS, SSG, CSMoS

System requirements: Intel 80i86 based computer, at least 256 Kb free conventional RAM, DOS 3.1 or higher; math coprocessor optional.

7.2.3 PRINCE

Developed by: Waterloo Hydrogeologic Software Inc.

Program language: C

Documentation: *

Description: A program package which consists of seven sub-modules which include: 1-, 2- and 3-dimensional analytical mass transport models and 2- and 3-dimensional analytical flow models based on the 'Princeton Analytical Models' report. It is assumed that the aquifer is homogenous, isotropic and that the flow is in steady state. The mass transport models can be used for analysis of a uniform flow field with uniform dispersion. Linear retardation and degradation can be simulated. Pollution can be added to the aquifer as continual or time-dependent point or diffuse sources.

Use: The positioning of boreholes for the treatment of polluted soil and groundwater with simple boundary conditions, the investigation of a pollution plume's movement, biological degradation and dilution. Simulation of natural biological clean-up schemes and verification of numerical models.

Solution method: Ten different solutions for pollution transport. See the Principal Analytical Models report for details.

Special properties: Ten different methods for solution of the flow and transport equations.

Input-output data format: The program has an interactive menu that is very user-friendly. Model selection, data input and output is carried out through a graphical menu. The output file can be presented graphically, output to hard copy and/or exported to other graphics packages such as AutoCad.

Availability: IGWMC, SSG

System requirements: PC with 640 K RAM, math coprocessor, EGA or VGA graphics, card and display and dot matrix or Hewlett Packard laser printer.

7.2.4 RITZ

Developed by: Nofziger, D.L., Williams, J.R. and Short, T.E. (1988)

Program language: *

Documentation: Interactive simulation of the fate of hazardous chemicals during land treatment of oily wastes: Ritz user's guide, EPA/600/8-88/001, Robert S. Kerr Environmental Research Laboratory Office of Research and Development, U.S. Environmental Protection Agency ADA, Oklahoma 74820, USA, 56pp.

Description: RITZ (Regulatory and Investigative Treatment Zone model) is a U.S. EPA 1-dimensional transport model for the unsaturated zone. The program takes into account the effect of oil in polluted soil. The model incorporates the influence of oil in sludge, water movement, volatilisation and degradation upon the transport and fate of a hazardous chemical.

Use: A useful program for the investigation of hazardous chemicals in the ground.

Solution method: The model calculates the proportion of the organic compound which evaporates, forms other compounds, is retained or washed out of a zone defined by the modeller. Soil water content is related to hydraulic conductivity by the Clapp and Hornberger function.

Special properties: A database is available which contains information on organic and inorganic compounds and how they react in the soil. This database, STF (Soil Transport and Fate) is available from CSMoS and includes RITZ.

Input-output data format: Menu-driven program with an interactive input-menu. The results can output graphically or in tabulated format.

Availability: IGWMC, CSMoS, SSG

System requirements: Intel 80i86 based computer; 640 Kb RAM; about 1 Mb free disk space; DOS 2.0 or higher; CGA graphics; math co-processor recommended.

7.2.5 RessqM

Developed by: Javendal et al. (1984)

Program language: *

Documentation: *

Description: RessqM (Ressq Modified) is an enhanced version of the RESSQ model (Javendal et al., 1984). RESSQ is a computer program for the simulation of 2-dimensional contaminant transport and adsorption in a homogenous, isotropic confined or unconfined aquifer of uniform thickness where regional flow, sources and sinks create a steady-state flow field.

Use: RessqM can be used in the following areas:

- Capture zones and contaminant transport
- Groundwater remediation
- Well head protection area

Solution method: RessqM is a semi-analytical model, employing both analytical and numerical solution schemes.

Special properties: Simple 2-dimensional models can be rapidly constructed using RessqM.

Input-output data format: RessqM creates Surfer graphics files that automatically draw capture zone, well head protection area or contaminant front position.

RessqM is user-friendly with a menu-driven system and data pre-processor enabling data input.

Availability: RW

System requirements: RessqM is available as a DOS, Mac or Windows-based program. Mac 68020 or better with math co-processor (68881 FPU) and 2 MB RAM; Windows 3.1+; Surfer v.4.

7.2.6 WINTRAN

Developed by: Environmental Simulations Inc.

Program language: Windows MDI

Documentation: The entire manual is available as an interactive help menu.

Description: WinTRAN couples the steady state groundwater flow model from WinFLOW with a contaminant transport model. The transport model appears to be similar to an analytical model but is actually an embedded finite-element simulator. The transport model includes the effects of dispersion, linear sorption (retardation) and first-order decay. Contaminant mass may be injected or extracted using any of the analytic elements including wells, ponds and linesinks.

Some of the other features of WinTran include:

- Steady state and transient flow in confined or unconfined aquifers
- Concentration contours at user-specified time intervals
- Flow rates can be calculated analytically or using the finite-element pollution transport model
- Includes all the properties of WinFlow apart from the transient flow model

Use: Problems where a rapid preliminary analysis of the extent of a pollution plume is required.

Solution method: WinTran links the steady state flow module in WinFlow with a finite-element pollution transport model. The finite-element grid is automatically constructed and numerical criteria (the Peclet and Courant number) are shown so that numerical or mass balance problems can be avoided.

Special properties: A genuine Windows program which is supported by Windows 3.1, NT and 95. The entire user manual is available as a help menu. The program

constructs the finite-element grid automatically. This means that the program retains the advantages of an analytical model enabling a simulation to be rapidly constructed.

Input-output data format: Windows properties such as: double-click on the element for editing, click and drag for moving of boreholes, drainage ditches, etc., several windows/models can be run simultaneously, cut, copy and paste from a clipboard and drag and release input files in the WinTran window.

Availability: ESI

System requirements: 486/Pentium with Windows 3.1/NT or ’95 and 2.5 MB hard disk space.

8. GEOCHEMICAL MODELS

This group of programs includes models designed for the simulation of many different geochemical processes. Geochemical models are often used to simulate complex problems where individual processes are considered separately using separate solution methods. Common to all the programs listed in this chapter is that they can all be used to interpret and/or simulate chemical reactions between minerals, gasses and organic matter in aqueous solution in a water/rock system.

In both hydrogeological flow models and pollution transport models the matrix of the aquifer is considered inert. In nature this is not true and in certain cases, such as during water injection in petroleum reservoirs, modelling the interaction between water and rock is relevant and necessary.

Geochemical modelling is based on chemical and thermodynamic laws that are independent of the geological environment. The programs can therefore be used to simulate processes in many different environments. The principal methods used by geochemical models are inverse, forward and aqueous speciation. Inverse speciation uses observed compositions to identify and quantify geochemical reactions, whilst the forward method uses assumed geochemical reactions to predict future compositions. The aqueous speciation models use thermodynamic descriptions of the aqueous solutions. More information on geochemical modelling techniques can be obtained from Appelo & Postma (1993) and Plummer (1992).

The limitations and assumptions involved in the use of any model should be considered before modelling work is commenced. This is of particular relevance to geochemical modelling as it is important that a model is not used to simulate the course of a reaction for which it was not designed.

8.1 MODELS BASED ON CHEMICAL MASS BALANCES AND ELECTRON CONSERVATION

This group of programs includes models for the analysis of potential net reactions occurring along a flow line. Balance is the predecessor to Netpath.

8.1.1 BALANCE

Developed by: Parkhurst, D.L., Plummer, L.N. and Thorstenson, D.C. (1982)

Program language: FORTRAN 77

Documentation: Parkhurst, D.L., Plummer, L.N. and Thorstenson, D.C., (1982). BALANCE - A computer program for calculating mass transfers for geochemical

reactions in groundwater. U.S. Geological Survey Water-Resources Investigations Report 82-14, 29pp.

Description: BALANCE is a USGS computer program for calculating mass transfer for geochemical reactions in groundwater. The program is designed to define and quantity chemical reactions between groundwater and minerals.

Using the chemical compositions of water samples from two points along a flow path and a set of mineral phases hypothesised to be the reactive constituents in the system, the program calculates the mass transfer (i.e. the amounts of the phases entering or leaving the aqueous phase) necessary to account for the observed changes in composition between the two water samples.

The mixing of two water samples without mineral reactions, redox reactions and isotope composition in a simplified form can also be included.

Use: BALANCE can be used to define and quantity chemical reactions between the groundwater and soluble mineral reactions.

Solution method: BALANCE solves a set of linear equations that represent the conservation of mass for the selected elements, electrons and isotope composition. The number of potential reactants or product phases must be equal to the number of elements if situations other than mixing are to be considered.

Special properties: BALANCE defines and quantifies chemical equilibrium reactions between groundwater and minerals. The program uses two water samples along a hydrogeological flow line and the mineral phases that are assumed to be involved in the reactive components in the system. Dissolved and precipitated phases are calculated from the aqueous phase. The authors no longer maintain the program as they consider NETPATH as a development of and replacement for BALANCE.

BALANCE includes an external database file containing default data.

Input-output data format: BALANCE is run as a batch program where input files are constructed using BALNINPT or a text editor.

Availability: IGWMC, SSG, USGS-NWIS

System requirements: *

8.1.2 NETPATH

Developed by: Plummer, L.N., Prestemon, E.C. and Parkhurst, D.L. (1991)

Program language: FORTRAN 77

Documentation: Plummer, L.N., Prestemon, E.C. and Parkhurst, D.L. (1991). An interactive code (NETPATH) for modelling of net geochemical reactions along a flow path, U.S. Geological Survey Water-Resources Investigations Report 91-4078, 227pp.

Description: NETPATH is an interactive program for modelling NET geochemical mass balance reactions along a flow PATH. Data required for the program include the chemical and isotopic composition of two water samples along a groundwater flow line.

NETPATH will determine all geochemical mass balance possibilities that indicate several possible minerals and gasses that must be added or precipitated along a groundwater flow line in order to obtain the composition observed in a borehole downstream of the original sample.

NETPATH can also calculate the mixing fractions of two initial water samples and the final geochemical reactions that are responsible for the final water composition. All possible geochemical mass balance reactions that are mathematically possible are tested for the chemical composition of the initial and final water. Tests are also carried out for limitations on chemical composition, isotopes and the set of possible phases for the system.

Use: A model that can be used to assist in the interpretation of end-point geochemical mass balance reactions between two points along a hydrogeological flow line.

NETPATH is particularly useful for the interpretation of geochemical reactions, mixing relationships, evaporation/dilution of water and mineral mass balances in the chemical and isotopic development of natural waters.

Solution method: NETPATH combines saturation indices with the modelling of mass balances for the identification and quantification of mineral reactions in a given system. The program enables the user to input chemical and isotopic data for the samples and to run speciation using a modified version of the WATEQF model (Plummer, Jones and Truesdell, 1976). The output from the speciation is then linked to the chosen samples, chemical and isotope data, mass balance limitations and assumed reactions to calculate possible chemical development models.

Special properties: The model is best suited to the simulation of processes which occur in regional aquifers where steady state flow conditions can be assumed and the effect of hydrodynamic dispersion ignored. It is important that the samples are from the same flow line and that transient chemical conditions do not influence the composition to any significant degree.

Input-output data format: An interactive pre-processor is included in the program and the results are produced in text file format. All mathematically possible combinations from the given predictions are output. The program allows the user to specify which reactions will occur by forcing precipitation or dissolution of given minerals based on expected results. This procedure reduces the number of combinations that must assessed.

Availability: Report and diskette available from USGS ESIC Open File Report Section, the NWIS or the Internet. The diskette contains the source and executable code.

System requirements: PC 386/486/Pentium running DOS.

8.2 MODELS FOR THE SPECIATION AND CALCULATION OF THERMODYNAMIC CONSTANTS

This category includes programs for the determination of thermodynamic parameters and speciation of aqueous solutions. The programs are important for the analysis of individual samples and can be included as part of a larger geochemical analysis where past or future changes of groundwater composition are being studied. Both SUPCRT92 and WATEQ4F are included in other programs but they can also be used as independent programs.

8.2.1 SUPCRT92

Developed by: Johnson, J.W., Oelkers, E.H. and Helgeson, H.C. (1992)

Program language: FORTRAN 77

Documentation: Johnson, J.W., Oelkers, E.H. and Helgeson, H.C. (1992). A software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species and reactions from 1 to 5000 bars and 0 to 1000^0C, Computers and Geoscience, Vol. 18, p.899-947.

Description: The program calculates standard molal thermodynamic properties for minerals, gasses, aqueous species and chemical reactions where they occur.

Use: SUPCRT92 has been extensively used in geochemical research projects.

Solution method: *

Special properties: The program includes a thermodynamic database with 294 aqueous species.

Input-output data format: Text input and output files.

Availability: LTC

System requirements: *

8.2.2 WATQ4F

Developed by: Ball, J.W. and Nordstrom, D.K. (1991)

Program language: FORTRAN 77

Documentation: Ball, J.W. and Nordstrom, D.K. (1991). User's manual for WATQ4F with revised thermodynamic data base and test cases for calculating speciation of major, trace and redox elements in natural waters, U.S. Geological Survey Open-File Report 91-183, 189pp., diskette in pocket.

Description: WATQ4F is a program for the calculation of chemical equilibrium in natural waters. A mass balance is written for the analysed elements and related to the concentration of free ions, bound ions and the total measured concentration. The law of mass conservation is combined with the chemical activity of ion pairs and bonds involving the relevant element. The mass balance and equilibrium equations form a set of non-linear equations where the concentration of free ions and bonds are unknown. Debye-Hüekel or Davis equations are used to calculate ion activity.

Use: Calculating chemical equilibrium in natural waters. Modelling of thermodynamic speciation of the many inorganic ions and complex species for a given water analysis where temperature, pH and redox potential are known.

Solution method: Iteration procedure based on the activity coefficient calculated from ionic strength and updated following each iteration. When the mass balance for the anions is within 0.5% of the analytical value the program is terminated and the solution written to a text file.

Special properties: A popular program with a large catalogue of reactions and thermodynamic data.

Input-output data format: The output file is typical for a speciation program. It includes concentrations, thermodynamic activities for the aqueous species and ion-activity products that can be used to determine the water-mineral reactions leading to the solution. The mineral's saturation indices give the degree to which the aqueous solution is in equilibrium with the mineral phases.

Availability: USGS-NWIS, IGWMC

System requirements: IBM PC, XT, AT or equivalent, 640 K RAM, DOS 3.0 or higher. Optional: math co-processor.

8.3 MODELS WHICH INCLUDE CHEMICAL MASS TRANSFER (BASED ON KINETICS-SORPTION)

This group includes programs of the type described under 8.2, which are also designed for simulating geochemical processes that include kinetics or sorption. The programs can also be used for geochemical simulations that do not include kinetics or sorption as they include speciation as an integrated part of the program, and are often based on the speciation programs listed in this report (e.g. Section 8.2). The programs cover a wide spectrum of problems and have very different constructions. EQ3/6 and PHREEQ can be used for forward modelling where pH and pe can be calculated as a result of chemical reactions. MINTEQA2 and SOLMINEQ.88 are actually speciation programs for low pressure and temperature environments. SOLMINEQ.88 was enveloped for the simulation of reactions in deep sediment basins where petroleum and other organic components are found at high pressure, temperature and salinity. PROFILE was developed for studies of forest floors with a special emphasis on the nitrogen balance.

8.3.1 EQ3/6

Developed by: Wolery, T.J.

Program language: *

Documentation: EQ3/6 - Status and future, Proceedings Workshop on Geochemical modelling, September 1986, Fallen Leaf Lake, California, USA. Lawrence Livermore CONF-8609134, pp10-19.

Description: The program was first developed to study reactions between seawater and basalt in a Mid-Pacific Ocean ridge geothermal environment

Use: A program for modelling complex geochemical systems that occur as a result of the reaction between host-rock, radioactive waste, groundwater, air and pollutants. The program can also be used to evaluate whether pollution will remain dissolved or form other compounds over time.

Solution method: EQ3/6 consists of a series of program modules with attached databases. The databases are very comprehensive and include data on many organic and inorganic compounds.

Special properties: The program has also been used to study changes in petroleum reservoirs following the injection of water. It has also been used in the mining industry and in the investigation of many other pollution scenarios.

Input-output data format: The program is run on Sun SPARC terminals but it can also be run on UNIX-based terminals and PC’s with at least 16Mb RAM.

Availability: LLNL

System requirements: DOS and UNIX versions available.

8.3.2 PHREEQE

Developed by: Parkhurst, D.L., Thorstenson, and Plummer, L.N. (1980)

Program language: FORTRAN 77

Documentation: Parkhurst, D.L., Thorstenson, and Plummer, L.N. (1980). PHREEQE- A computer program for geochemical calculations, U.S. Geological Survey Water Resources Investigations Report, 195pp.

Description: PHREEQE (pH-Redox-EQuilibrium-Equations**)** is a USGS computer program designed to model geochemical reactions model based on aqueous ion pairs. PHREEQE can calculate pH, redox potential and mass transfer as a function of reaction process. The composition of solutions in equilibrium with multiple phases can be calculated. The aqueous model, including elements, aqueous species and mineral phases is exterior to the computer code and is completely user-definable.

PHREEQE can simulate several types of reaction including:

- Addition of reactants to a solution
- Mixing of two waters
- Titrating one solution with another

In each of these cases PHREEQE can simultaneously maintain the reacting solution at equilibrium with multiple phase boundaries.

PHREEQE calculates the following quantities during the reaction simulation:

- pH
- total concentration of elements
- amounts of minerals transferred into or out of the aqueous phase
- distribution of aqueous phase
- distribution of aqueous species
- saturation state of the aqueous phase with respect to specified mineral phases

Use: PHREEQE can be used for the analysis of irreversible reactions in a geochemical system. The extent of reaction can be determined from the intersection of the reaction line and possible phases for pre-specified minerals.

The program can be used for the determination of pH, relative electron activity, total elemental concentrations, mineral transferred to/from the aqueous phase, distribution

of aqueous species and the relative degree of saturation with regard to a given mineral phase. Many different types of reaction can be simulated and PHREEQE will maintain the equilibrium between dissolution and the mineral specified for several phases.

Solution method: PHREEQE solves a set of non-linear equations using a combination of a fractions scheme for solution of species concentrations and a modified Newton-Raphson iteration technique for pH, pe and mass transfer estimation.

Determination of the distribution of species that must maintain electrical neutrality and conserve mass and the number of electrons for each element is a non-linear problem. Convergence in such a problem can not be guaranteed particularly in problems involving systems that involve reduction/oxidation where there are large differences in the equilibrium concentrations for individual elements.

PHREEQE accesses an external thermodynamic database.

Special properties: The geochemical reaction model PHREEQE has been used with flow models and pollution transport models. It enables the simulation of complex geochemical processes together with the physical processes of advection and dispersion. Sanford and Konikow (1989) used PHREEQE with MOCDENSE.

PHREEQM is a variant of PHREEQE enabling the calculation of mass transport. It is best suited to batch simulations. PHREEQM includes a three-step process where advection is first analysed, followed by the determination of chemical equilibrium (by PHREEQE) and a dispersion process between adjacent cells.

Input-output data format: PHREEQE includes PHRQINPT is a menu-based input scheme that has a help menu and a check on the validity of the input data.

Availability: USGS-NWIS, IGWMC, SSG

System requirements: PC running DOS.

8.3.3 PHREEQC

Developed by: Parkhurst, D.L. (1995)

Program language: C.

Documentation: Parkhurst, D.L. (1995). User's guide to PHREEQC - A computer program for speciation, reaction-path, advective-transport, and inverse geochemical reactions. U.S. Geological Survey Water-Resources Investigations Report 95-4227, 143 p.

Description: PHREEQC retains the capabilities of PHREEQE but eliminates many of this model's deficiencies and limitations. Mole balances for speciation calculation can be defined for any oxidation state. Distribution of redox elements is based on the

specified pe of the redox couple. PHREEEQC allows the concentration of an element to be adjusted to attain equilibrium with a specified phase.

Reaction path calculations are orientated more towards system equilibrium than aqueous equilibrium.

Use: As for PHREEQE. However, PHREEQC has a number of new capabilities that extend the use of the program.

Solution method: As PHREEQE but with minor modifications.

Special properties: The geochemical reaction model PHREEQC is better suited for coupling with flow models and pollution transport models. It enables the simulation of complex geochemical processes together with the physical processes of advection and dispersion.

Input-output data format: PHREEQC is a program written in C with free-format data input and is consequently much more user friendly than PHREEQE.

Availability: USGS-NWIS.

System requirements: PC running DOS.

8.3.5 PHRQPITZ

Developed by: Plummer, L.N., Parkhurst, D.L., Fleming, G.W., and Dunkle, S.A., (1988).

Program language: C

Documentation: Plummer, L.N., Parkhurst, D.L., Fleming, G.W., and Dunkle, S.A., (1988). A computer program incorporating Pitzer's equations for calculation of geochemical reactions in brines: U.S. Geological Survey Water-Resources Investigations Report 88-4153, 310 pp.

Description: PHRQPITZ is a USGS computer program whose reaction modelling capabilities include calculation of (1) aqueous speciation and mineral-saturation index, (2) mineral solubility, (3) mixing and titration of aqueous solutions, (4) irreversible reactions and mineral-water mass transfer, and (5) reaction path.

Use: PHRQPITZ is designed to carry out geochemical calculations in brines and other electrolyte solutions to high concentrations.

Solution method: PHRQPITZ is a USGS computer program designed to make geochemical calculations in brines and other electrolyte solutions to high concentrations.

Special properties: PHRQPITZ uses the Pitzer virial coefficient approach for activity-coefficient calculations

Input-output data format: PHRQPITZ includes an external interactive program, PITZINPUT, to create/modify input data files. Help is available and the program checks for errors. PHRQINPUT reads an external Minerals Thermodynamic database and assesses an extensive external Thermodynamic database file (included).

Availability: SSG

System requirements: 386/486/Pentium with 2 MB RAM. Versions compiled for other operating systems are available.

8.3.5 MINTEQA2

Developed by: Allison, J.D., Brown, D.S and Novo-Gradec, K.J.

Program language: FORTRAN, Assembler, GSS/GKS, VP-Expert

Documentation: MINTEQA2/PRODEFA, A Geochemical Assessment Model for Environmental Systems: Version 3.00 User's Manual, EPA/600/3-91; NTIS:PB91-182-469.

Description: MINTEQA2 is a U.S. EPA geochemical equilibrium speciation model for simulating dilute aqueous systems. The model can be used to calculate mass distribution in dissolved, adsorbed, solid and gas phases under a variety of different environmental conditions. A given gas phase with a constant partial pressure can for example be simulated. Seven adsorption models are available in MINTEQA2.

The model requires a total concentration for the relevant components. Other parameters such as pH, pe and partial pressure for one or more gases can be entered as limiting factors on the reactions. Measured pH and pe values can be specified as equilibrium values. MINTEQA2 can also calculate equilibrium constants. Minerals can be specified as in equilibrium with the solution, that they dissolve under favourable conditions or that they dissolve incompletely.

Reported parameters include the concentration of all species in the system and saturation states of all solids.

A thermodynamic database including many components is included. The user can however modify this database.

Use: The program is often used to estimate the mobility of metals in the ground and groundwater.

Solution method: *

Special properties: MINTEQA2 can be used to calculate Kd, the distribution factor between adsorbed and dissolved concentrations. This factor is extremely important in transport models.

Input-output data format: PRODEFA2 is an interactive pre-processor that assists in the preparation of the input data files used by MINTEQA2.

Availability: IGWMC, SSG, CSMoS.

System requirements: PC 386/486/Pentium with 2 MB RAM and math co-processor.

8.3.6 PROFILE and SAFE

Developed by: Sverdrup, H. & Warfvinge, P. (1993). Department of Chemical Engineering II, University of Lund, Box 124, S-221 00, Lund, Sweden.

Program language: *

Documentation: Sverdrup, H. and Warfvinge, P. (1993). Calculating field weathering rates using a mechanistic geochemical model PROFILE, Applied Geochemistry, Vol. 8, pp.273-283

Kinetics of silicate mineral weathering and methods for estimating field rates, Sverdrup, H. and Warfvinge, P. (1993). Department of Chemical Engineering II, University of Lund, Box 124, S-221 00, Lund, Sweden.

Description: Both programs are based on a conceptual model of the soil layer in a forested area. This conceptual model can represent the entire catchment area or a single profile. PROFILE is a steady state version of SAFE and therefore ignores changes in the soil over time and calculates the final composition immediately. The program can be used to calculate starting values for use in SAFE.

The following chemical systems are including in SAFE:

- Deposition, formation and precipitation of chemical components
- Chemical weathering and reactions between mineral in the earth and solution
- Cation exchange reactions
- Net result of nitrogen compound reactions, complete nitrification
- Internal exchange of nitrogen and basic cations between different biomass components and net biological uptake of nitrogen and basic cations
- Equilibrium between solution and reactions which include CO_2, Al and organic acids

Use: SAFE has been developed to study the effect of acid rain on the soil and groundwater. The program calculates different chemical variables as a function of time and can therefore be used to study the effect of acidification as a function of acid supply, soil parameters and hydrological variations.

Solution method: *

Special properties: *

Input-output data format: The programs are developed for Macintosh computers and are very user friendly.

Availability: The programs and manuals are available from the authors.

System requirements: *

8.3.7 SOLMINEQ.88

Developed by: Karaka, Y., Gunter, W.D., Aggarwal, P.K., Perkins, E.H. and DeBraal, J.D. (1988).

Program language: FORTRAN 77

Documentation: U.S. Geological Survey Water-Resources Investigations Report 88-4227, 420pp.

Description: SOLMINEQ.88 (SOLution-MINeral-Equilibrium-computations**)** is a program for geochemical modelling of water-mineral reactions. The program calculates the equilibrium distribution of several inorganic aqueous components for given concentrations of measured ions found in waters with temperatures between 0-350^{o}C. Values of pH and Eh can be entered.

Use: Simulation possibilities include the geochemical modelling of water-mineral reactions and other processes such as the effect of boiling, mixing of solutions and calculation of fractions present in aqueous, oil and gas phases. There is the possibility of mass transfer analysis, which can be used for studies of ion exchange, adsorption/desorption and solution/precipitation of solid phases.

SOLMINEQ.88 includes a database that covers a wide temperature range, which makes it suitable for analysis of a wide range of thermal groundwaters.

Solution method: A repeated approximation method combined with a convergence criterion is used on the mass balance of anions for solution of the main program. The logical construction of the program is derived from WATEQ.

Special properties: The thermodynamic database includes 260 inorganic, 80 organic aqueous components, 220 minerals and calculated pH together with mineral solubility at relevant temperatures and pressures.

Input-output data format: An interactive program developed by DeBraal and Kharka (1989), SOLINPUT (U.S. Geological Survey Open-File Report 89-616,

140pp.), is available which assists the user to define the problem and construct the necessary data files.

Availability: USGS-ESIC

System requirements: *

9. LIGHT NON-AQUEOUS PHASE LIQUID MODELS

Groundwater contamination from hydrocarbon spills/leaks is a serious environmental problem. Non-aqueous phase liquids (NAPL's) are immiscible fluids that have insignificant solubility in water. Light NAPL's (LNAPL's) float and migrate on top of the water table posing a continuous source of contamination to the groundwater. Due to water table fluctuations, some of the NAPL gets trapped in the unsaturated and saturated zones. NAPL trapped in the soil and groundwater acts as a continuous source of groundwater contamination resulting in expensive restoration of these aquifers. The use of groundwater models in the simulation of the behaviour of LNAPL's is therefore an important aspect of any restoration project both in terms of maximising recovery and minimising costs.

9.1 MARS 2D/3D

Developed by: *

Program language: *

Documentation: *

Description: MARS (Multiphase Areal Remediation Simulator) models the flow of water and light non-aqueous phase liquid (LNAPL) and aqueous phase transport of up to five species in groundwater, with multiple pumping and/or injection wells. MARS is a finite-element model that allows accurate representation of highly irregular material and physical boundaries in a heterogeneous and anisotropic media. MARS writes input flow files for the BIOF&T model, which simulates multi-species dissolved phase transport in heterogeneous, anisotropic, fractured media, or unfractured granular porous media.

Use: MARS can be used to model the recovery and migration of light non-aqueous phase liquids in unconfined heterogeneous, anisotropic aquifers. MARS can also simulate NAPL recovery with skimmers and trenches and optimise the number, location and recovery rates for water and oil.

Solution method: *

Special properties: *

Input-output data format: The WindowsTM pre-processor for MARS is designed to help users create and edit input files for the MARS numerical model. There is also a mesh editor which can be used to create and edit finite-element meshes.

The DAEM post-processor is a data-parsing tool, graphing package and contour export tool for DAEM numerical models. The post-processor is designed to be a user-

friendly tool for quickly discerning model results. Users can also review model text output files for a more detailed view of the model results.

Availability: SSG

System requirements: (1,500 nodes) Windows 3.x/Windows 95/Windows NT and 4 MB RAM. MARS 3-D Transport requires Windows 95/NT and 16 MB RAM.

9.2 BIOSLURP

Developed by: *

Program language: *

Documentation: *

Description: BIOSLURP is an areal finite-element model for the simulation of three-phase (water, oil and gas) flow and multi-component transport in groundwater in the unsaturated zone. BIOSLURP simulates heterogeneous, anisotropic porous media or fractured media. BIOSLURP can also be used to simulate coupled flow of water and LNAPL with a static atmosphere gas phase, as well as the transport in groundwater.

Use: BIOSLURP can be used to optimise the recovery of LNAPL, water and gas by minimising NAPL entrapment in the saturated/unsaturated zones and simultaneously multi-species aqueous and gas phase transport in unconfined aquifers. BIOSLURP can be used to design NAPL recovery and hydraulic containment systems for the free phase hydrocarbon plume and dissolved phase plume under complex hydrogeological conditions.

Solution method: *

Special properties: Currently the most advanced model of its kind.

Input-output data format: Graphical user interface in Windows 3.x, Windows 95 and Windows NT. This interface includes a mesh generator/graphical editor that allows DXF site map import and highly irregular geometry.

Availability: SSG

System requirements: (1,500 nodes) Windows 3.x/Windows 95/Windows NT and 8 MB RAM.

9.3 BIOMOD 3-D

Developed by: *

Program language: *

Documentation: *

Description: BIOMOD 3-D (Bioremediation Fate and Transport Simulator) is a 2-D /3-D finite-element and multi-component transport model that is linked to the USGS finite-difference MODFLOW 3-D model. BIOMOD simulates convection, dispersion, diffusion, adsorption, desorption and microbial processes based on oxygen limited, first order, Monod, anaerobic biodegradation kinetics, as well as anaerobic or first order sequential degradation involving multiple daughter products.

Use: BIOMOD 3-D can be used to simulate heterogeneous and/or anisotropic porous media (includes cross derivative terms in dispersive tensor) with (or without) fractures. BIOMOD can be used to model contaminated sites that have complex heterogeneous and/or anisotropic hydrogeology and/or anisotropic hydrogeology.

Solution method: *

Special properties: *

Input-output data format: BIOMOD comes with a MODFLOW to BIOMOD data converter, a velocity calculation module, a pre-processor, a mesh-editor and a post-processor. The pre-processor and mesh editor can be used to create an input data file for BIOMOD.

The BIOMOD output file consists of a list of the input parameters, initial and boundary conditions, and the mesh geometry. It also includes the species (organic/inorganic) concentration of each node, total mass of species in water and in the residual hydrocarbon phase (if present).

Availability: SSG

System requirements: (1,500 nodes) Any version of MODFLOW which includes the BCF2 package, 486 or higher with 16 MB RAM and Windows 95/NT for pre-/post-processing.

9.4 ARMOS

Developed by: *

Program language: *

Documentation: *

Description: ARMOS is a numerical model for areal flow of water and/or separate phase light hydrocarbons in unconfined aquifers. The model considers non-uniform vertical hydrocarbon distributions governed by soil capillary characteristics and fluid table elevations. Residual hydrocarbons in the saturated and unsaturated zones associated with changing water and oil tables is also considered.

Use: ARMOS can be used to estimate immiscible plume movement under any hydraulic conditions or to optimise free product recovery systems.

Solution method: *

Special properties: *

Input-output data format: includes a user interface which can generate a flow field to model dissolved phase transport with BIOTRANS and imports isoparametric, quadrilateral and triangular meshes.

Availability: *

System requirements: 486 or higher with 8 MB RAM, 10 MB free disc space, DOS 3.3 or higher or Windows, math coprocessor, VGA graphic adapter and monitor, MS compatible mouse, not compatible with some AST computers or Macintosh computers.

10. COMBINED FLOW AND GEOCHEMICAL MODELS

This chapter describes models that combine flow in porous media with geochemical processes. The programs can simulate several components in a reactive pollution transport single or multi-phase flow system. These programs all attempt to simulate the complex and integrated environment where the simulation of hydrochemical and geochemical process must be combined with flow theory.

As combined flow and geochemical processes are so complex it is necessary to make many approximations and solution methods consequently vary. Users of these programs should have a good background within geochemistry and flow in porous media.

Combined flow and geochemical modelling is an active research field and there will certainly be programs released in the near future. OS3D/GIMRT and TBC are both new programs which have not yet been commercially released but can be obtained from the program's authors. Even though OS3D/GIMRT is available for PC use, like TBC it is a resource-demanding program and the use of UNIX terminals is advisable for the simulation of larger problems. MOFAT and PHREEQM are two programs which have a more restricted use but which can be run on a DOS operating system without capacity problems. These two problems are however quite different and are intended for use on widely differing intended problems.

10.1 OS3D/GINRT

Developed by: Steefel, C.I. and Yabusake, S.B. (1985)

Program language: FORTRAN

Documentation: Steefel, C.I. and Yakusaki, S.B., OS3D/GIMRT Software for modelling Multi-component – Multi-dimensional Reactive Transport, User Manual & Programmer's Guide, Battelle Memorial Institute, 1995, 58pp.

Description: OS3D/GINRT is an Operator Splitting 3-Dimensional reactive transport model/Global Implicit Multi-component Reactive Transport model. Chemical processes that can be simulated in OS3D/GIMRT include aqueous equilibrium speciation, kinetic controlled mineral precipitation and weathering and adsorption. The model is based on a continuum representation of transport and reaction in porous media. Steady state and transient conditions, advection, dispersion, diffusion or a combination of these can be simulated. There is also a kinetic formulation for mineral solubility and precipitation. It is therefore not necessary to assume local equilibrium even though this can be achieved where the rate of reaction is much higher than the rate of mass transport. The preliminary version of the program that is available from

the authors assumes that surface complexation is reversible but the authors hope to improve this aspect of the program in later versions.

Use: OS3D is designed for simulating transient concentration fronts particularly with a high Peclet number. GIMRT is suitable for modelling of chemical weathering where the aqueous concentration field is approximately steady state and the numerical errors are smaller. GIMRT is more applicable to the analysis of mineral/water reactions over geological time scales than OS3D, as longer time intervals can be used.

Solution method: A finite-difference method is used to solve the non-linear partial differential equations which describe coupled reactions and flow in a multi-component system. The two programs have different solution methods and they therefore have different simulation applications. GIMRT can simulate non-isothermal conditions in 0-, 1- and 2-dimensions (0-D represents the calculation of reaction lines or batch reactions). OS3D can simulate 0-, 1-, 2- and 3-dimensions.

Special properties: The thermodynamic database is based on that of EQ3/EQ6. If the problem involves of reactive transport at higher pressure than the EQ3/EQ6 database allows, then the necessary thermodynamic data must be obtained (SUPCRT92 can be used for this purpose).

Input-output data format: Data input is via text files that can be used by both GIMRT and OS3D. The output files can be used by various commercially available graphics programs.

Availability: The programs are not directly available yet as they are still under development. Copies can however be obtained from the authors.

System requirements: *

10.2 MODFLOW-SURFACT

Developed by: HydroGeoLogic Inc.

Program language: *

Documentation: *

Description: MODFLOW-SURFACT is a new flow and transport model based on the USGS 3-dimensional groundwater flow model MODFLOW. HydroGeoLogic has incorporated additional computational modules to enhance the simulation capabilities and robustness.

The flow module, MODFLOW-SURF incorporates the following features:

S - Solution Schemes with axisymmetric simulation options, adaptive time stepping and enhanced output control features

U - Treatment of Unconfined flow with complete wetting/drying capabilities, taking into account unsaturated flow and delayed yield effects

R - Treatment of non-ponding/limited-ponding Recharge and seepage face conditions

F - Fracture well package superimposing tubular fracture elements to the discretise system providing more rigorous treatment of wells.

HydroGeoLogic have integrated new transport modules into MODFLOW-SURFACT including:

- Advective-dispersive transport of up to five species
- Linear/non-linear retardation
- First-order biochemical degradation in soil and/or water, including generation of transformation products

Use: 3-dimensional groundwater flow and transport modelling.

Solution method: *

Special properties: MODFLOW-SURFACT is fully compatible with previous versions of MODFLOW and includes all additional packages included in later versions of MODFLOW.

MODFLOW-SURFACT overcomes several limitations of other available transport counterparts of the MODFLOW code. The limitations concern mass balance problems, excessive numerical dispersion and/or oscillations, and the impact of transient flow storage effects on transport.

Input-output data format: Input and output formats for MODFLOW-SURF are similar to MODFLOW. Input preparation for MODFLOW-SURFACT follows the MODFLOW format structure and makes use of all MODFLOW data sets. An additional data set, including all transport parameters, is required.

Availability: SSG

System requirements: PC486/Pentium with 16 MB RAM and Microsoft Windows 3.1 or later.

10.3 MOFAT

Developed by: Katyal, A.K., Kaluarachchi, J.J. and Parker, J.C. (1991)

Program language: *

Documentation: Katyal, A.K., Kalurachchu, J.J. and Parker, J.C. (1991). MOFAT: A two-dimensional finite-element program for multi-phase flow and multi-component transport, Program Documentation and User's Guide, U.S. Environmental Protection Agency, U.S. EPA-600-0291-020.

Description: A 2-dimensional finite-element program for simulating multiphase flow and pollution transport in vertical section. In order to run the program, the following parameters are required: van Genuchten parameters, fluid density, viscosity, surface tension, inter-surface tension, fluid composition, equilibrium constants for air/water, water/oil and water/solid phase. The program will then calculate changes in degree of saturation and concentration of a given compound.

Use: Simulation of multiphase flow and pollution transport in a vertical section.

Solution method: The equation set is solved using a mixture of linear and non-linear methods that are effective and precise.

Special properties: The program includes multiphase flow and several species in solution. MOTRANS is an earlier version of the program.

Input-output data format: Pre- and post- processing packages are available. Input files can also be constructed and edited in an editor. A contouring package can be used to plot the results.

Availability: CSMoS

System requirements: *

10.4 TBC

Developed by: Schäfer, D., Schäfer, W. and Therrien, R.

Program language: FORTRAN

Documentation: TBC, Transport, Biology and Chemistry, User's guide for TBC - Version 1.4, An Efficient Simulator for Three-Dimensional Saturated Groundwater Flow and Multi-species Transport Reactions in Porous Formations.

Description: TBC (Transport, Biology and Chemistry) is a program that solves the equation for saturated 3-dimensional groundwater transport, advection and dispersion using a finite-element method. Pollution transport is coupled with microbial degradation of organic carbon. Microbial growth and degradation is simulated using Monod kinetics. Solution consumption and metabolic products are connected to the growth of microbes using an output coefficient and stoichiometric connections. The effect of microbial activity on the inorganic composition in the groundwater is also taken into consideration. TBC allows the user to specify a series of possible biological and chemical reactions. This makes the program extremely flexible and able to simulate a wide variety of different situations. The program assumes that micro-organisms

remain in a biophase which is stationary and where all biochemical reactions occur. The volume of biomass is constant with time and areal extent and is not connected to the growth of microbes. It is therefore not possible to simulate changes in porosity.

Reactive transport is divided into five calculation stages:

- Flow calculations
- Advective and dispersive transport
- Biochemical reactions
- Chemical equilibrium reactions
- Chemical kinetic reactions

Use: Developed for the simulation of reactive processes involving organic species in connection with in-situ biological clean-up procedures but it can be used for modelling reduction and oxidation processes in column experiments related to the degradation of organic carbon, field problems which involve natural biological degradation and early sediment diagenesis.

Solution method: TBC uses a sequential solution method where the equations for advective-dispersive transport are solved first followed by the equations for biological and chemical reactions. The advantage with this method is that the correct solution method can be used for each set of equations and the program becomes simpler. A problem with this 'operator splitting' technique is that further numerical inaccuracies are introduced. Iterating between the different calculation stages can however reduce this. The program includes four phases: biophase, mobile porewater, NAPL ('non aqueous phase liquid'), chemical/biochemical matrices which are coupled together using linear isotherms.

Special properties: The program is under development and is only available for UNIX operating systems. The simulation of complex processes will require the use of powerful computational resources. It is therefore planned to modify the program for use with parallel computers.

Input-output data format: There are pre- and post-processing packages designed especially for the program but a number of programs are available to assist the user with graphical presentation of the data. It is a time consuming task to construct the text-input file required by TBC.

Availability: The program is available from Dirk Schäfer, Institute of Environmental Physics, University of Heidelberg, Germany who developed the program.

System requirements: *

10.5 PHAST

Developed by: Parkhurst, D.L., Kipp,K., Engesgaard P.

Program language: FORTRAN, C

Documentation: PHAST—A Program for simulating ground-water flow and multi-component geochemical reactions

Description PHAST is a 3 dimensional multi-component reaction-transport model that can be used to simulate transient groundwater flow with or without geochemical reactions. The transport reaction calculations are coupled using a sequential approach and there are no iterations between transport and reaction calculation. PHAST is a coupling of HST3D (solute/transport) and PHREEQC (geochemical) model.

Use: Combined reaction/transport calculation including flow and geochemical reactions.

Solution method: see PHREEQC & HST3D, The reaction transport equations are solved using the sequential approach (Yeh & Tripathi 1989)

Special properties: The program is under development and but will be available from USGS in the near future.

Input-output data format: Three data files similar to PHREEQC.

Availability: From USGS (no available yet)

System requirements: *

11. INTEGRATED MODELLING PACKAGES

This chapter reviews commercially available modelling packages combining flow, pollution transport and pre- and post-processing programs. Constructing a model often requires the processing of large quantities of data. This is particularly true for large numerical models. Pre- and post-processing programs have been developed for simplify the setting up of a problem and interpretation of the results. A current trend in the development of modelling software is the incorporation of these pre- and post-processing programs into integrated packages including the model. Each package therefore provides all the facilities needed for the construction, execution, calibration and output presentation and assessment of a groundwater model. This considerably eases the process of modelling and can result in significantly reduced model construction times.

Many different program packages are now available for the processing of modelling data in connection with hydrogeological investigations. The programs included in this chapter are generally available for different operating systems. Many of these packages have been specifically designed for popular programs such as MODFLOW and MT3D (Visual MODFLOW, VMS, ModIME, Groundwater Vistas and PMWIM) although a number are intended for use with any groundwater model. There are often demonstration versions of the program available at a token price. These demonstration programs can be useful aids for users who are looking to choose a program package, particularly as the packages tend to be considerably more expensive than purchasing the individual component programs.

In addition to the programs listed in this chapter an increasing number of programs with integrated graphical input and output interfaces are becoming available. Examples of these include SUTRA and HST3D. There is an inevitable overlap between these packages and the programs described in this chapter. To avoid excessive duplication however the majority of these packages are described in the ‘special properties’ category in each model description. The modelling packages described in this chapter include those that are considered to be more comprehensive and those that include more than one model e.g. MODFLOW, MODPATH and MT3D.

11.1 FEMSEEP

Developed by: *

Program language: *

Documentation: *

Description: A 2-dimensional finite element groundwater flow and contaminant transport model. FEMSEEP includes:

- Steady state and transient groundwater flow in a 2-dimensional horizontal plane, a vertical cross-section or a 3-dimensional axisymmetric system
- Advective transport
- Advective-dispersive transport
- Restart option with time-dependent boundary conditions

The model can also calculate changes in solute concentration caused by advection, dispersion, mixing, chemical adsorption and first-order decay.

Use: FEMSEEP is suitable for local groundwater investigations and aquifer remediation projects. It can be used for designing extraction, injection and recharge systems and for predicting system performance.

FEMSEEP can also be used for construction and geotechnical problems such as excavation, mining and seepage control. It can be used for simulating groundwater flow and seepage face through dams and embankments or into trenches, tunnels and wells.

Solution method: FEMSEEP is based on the Petrov-Galerkin finite-element with a particle-tracking algorithm.

Special properties: The model is able to handle a fine, detailed mesh around a single or multiple well system where water level and concentration information is critical and a coarser mesh to be used in areas far away from the pumping wells is an important advantage of this model.

Input-output data format: Model output can be sent to the screen and a large number of printers and plotters. HPGL, DXF, Postscript and CGM file formats can also be produced and imported directly into word processor and graphics packages (e.g. WordPerfect, Ventura and AutoCad).

Element mesh and aquifer properties can be presented and contour plots of head, drawdown, stream function and concentration can be produced. Velocity vectors, flowpaths and particle fronts can also be plotted.

Availability: SSG

System requirements: PC386/486 or higher with 4 MB RAM, math co-processor and a printer or plotter for hard copy output.

11.2 GFLOW

Developed by: *

Program language: *

Documentation: *

Description: GFLOW is a groundwater and surface water modelling system including digitizer program, data pre-processor, analytical element model and a graphics post-processor. The groundwater model is capable of simulating confined and/or unconfined conditions.

Use: GFLOW is well suited for remedial system design, wellhead protection studies and more generic local and regional modelling investigations.

Solution method: GFLOW is an analytical element conjunctive surface water and groundwater model.

Special properties: GFLOW integrates surface water and groundwater flow solutions allowing streams to lose water to the aquifer based on surface water availability, avoiding the problem of over-infiltrating streams which invalidate groundwater flow solutions.

Input-output data format: GFLOW includes GAEP, a pre-processor which uses a digital hydrography map for creation and modification of GFLOW input data files. Error checking and graphical calibration facilities are also included. GFPRINT, a graphical post-processor, is also included which is capable of producing report-ready colour graphics in DXF, PostScript and over 100 printers.

Availability: SSG

System requirements: PC386/486/Pentium with 4 MB RAM (3 Mb extended) and math co-processor.

11.3 GMS

Developed by: The US Department of Defense

Program language: *

Documentation: *

Description: GMS (Groundwater Modelling System) is a graphical modelling tool that integrates MODFLOW, MT3D and FEMWATER. The program is menu-driven so that assistance is given with managing the large number of files necessary for running these models.

GMS attempts to integrate and simplify the process of groundwater flow and transport modelling by bringing together the majority of the tools involved in such studies.

GMS includes the following features:

- Site characterisation
- 2- and 3-dimensional mesh generation
- Graphically-based model input for finite-element and finite-difference flow and transport codes
- Interpolation and geostatistics
- DXF input and output
- 3-dimensional visualisation

Use: GMS can be used where the simulation of flow or pollution transport is required. The code is general and can be modified to pre- and post-process data from any 2D/3D model.

Solution method: *

Special properties: A powerful tool that also includes a geostatistical module.

Input-output data format: User-friendly interface.

Availability: EGCL, SSG

System requirements: Windows version: PC 386/486/Pentium running Microsoft Windows 3.1, 16Mb RAM (32Mb RAM recommended) and math co-processor. UNIX X-Windows version: IBM RS6000, Sun SparcStation, HP9000 Series 700/800, Silicon Graphics and DEC Alpha.

11.4 Graphic Groundwater

Developed by: Micro-innovations, Inc.

Program language: *

Documentation: *

Description: Graphic Groundwater is a graphical computer program designed to enhance data input, output and analysis when using the U.S.G.S. Three-Dimensional Finite Difference Groundwater Flow Model MODFLOW.

Use: The program integrates grid development, data input, model execution and analysis of the results. The finite difference grid can be created using a mouse and simple dialog boxes. The grid can be superimposed and geo-referenced on a scanned or digitised map if required.

Solution method: *

Special properties: Graphic Groundwater is based on MODFLOW.

Input-output data format: Data entry is designed to be as simple as possible. Series of cells can be selected using the mouse and a value for a stress or other hydrogeological parameter entered. Stress periods and output are scheduled with dialog boxes. Graphic Groundwater can contour any grid parameter, including hydraulic head, drawdown, cell by cell budgets, or initial data such as hydraulic conductivity or bottom elevation. Data can be exported for analysis with other software. The program supports all Windows' features including a common clipboard, multi-tasking and all printer drivers.

Availability: RW

System requirements: PC 386/486/Pentium with at least 4 MB RAM and Windows 3.1.

11.5 Groundwater Vistas

Developed by: Geraghty and Miller Modelling Group

Program language: *

Documentation: *

Description: A graphical modelling environment for Microsoft Windows that includes both pre- and post-processing capabilities. Groundwater Vistas is a model-independent graphical design system supporting MODFLOW, MODPATH (both steady state and transient versions) MT3D, MODFLOWT and MODFLOW-SURFACT. Groundwater Vistas supports the use of the PEST model-independent calibration software.

Use: A pre- and post-processing package for the above models.

Solution method: *

Special properties: An interactive graphical pre- and post-processing package incorporating many user-friendly features. The program can be obtained bundled with MODFLOW^{win32}.

Full on-line context-sensitive help is provided.

Input-output data format: A graphical program enabling the creation and editing of input data. Model results are presented using contours, shaded contours, velocity vectors and detailed analysis of mass balance. MODPATH particle traces are also displayed in both plan and cross-sectional views.

Availability: SSG

System requirements: PC486+ running Microsoft Windows and 8 MB RAM.

11.6 Intergraph Site Restoration Solution Systems and ERMA

Developed by: INTERGRAPH

Program language: *

Documentation: *

Description: Intergraph Site Restoration Solution Systems and ERMA (Environmental Resources Management Application) together form a program package that includes a number of modules such as:

- Database management system
- CAD options
- Geographic Information Systems
- Technical information management system
- 3-dimensional modelling possibilities include flow modelling, pollution transport
- 2- and 3-dimensional geostatistical modelling
- Volume modelling and analysis.

Use: An extremely comprehensive package, which includes many advanced possibilities.

Solution method: *

Special properties: An Intergraph program providing an extremely comprehensive interface for 3-dimensional modelling using MODFLOW, MODPATH and AT123D. The program can be used in conjunction with other 3-dimensional volume modelling programs produced by Intergraph.

Input-output data format: User-friendly interface using menu-driven interactive data input and output.

Availability: IG

System requirements: Both UNIX and PC DOS-based versions are now available.

11.7 MIKE/SHE

Developed by: Danish Hydraulic Institute as a further development of SHE - European Hydrological System.

Program language: FORTRAN

Documentation: *

Description: A comprehensive program that includes many different aspects of the hydrological system. Use of the model therefore demands that the user has access to personnel with specialist knowledge in the different subject areas being modelled.

Use: A program for the simulation of the most important processes in the hydrogeological 'land' phase of the hydrological cycle. Typical modelling tasks the program has been used for include:

- Water supply studies
- River drainage studies
- Irrigation studies
- Landfill pollution studies
- Effects of agriculture
- Soil and water planning studies
- Modelling of possible effects from changes of land use
- Ecological assessments for wetland areas

Solution method: *

Special properties: An extremely comprehensive and powerful tool that is much used in Denmark.

Input-output data format: A UNIX program that includes several different modules in addition to pre- and post-processing modules.

Availability: DHI

System requirements: Workstation running UNIX operating system.

11.8 ModIME

Developed by: *

Program language: *

Documentation: *

Description: ModIME is a Modular Integrated Modelling Environment for MODFLOW, PATH3D and MT3D. ModIME allows the user to prepare input data, run the models and post-process the results of simulations interactively in a graphical environmental.

Use: Pre- and post-processing package for use with MODPATH, PATH3D and MT3D.

Solution method: *

Special properties: An interactive graphical pre- and post-processing package incorporating many user-friendly features. The models are available as options but ModIME is compatible with all versions of MODPATH, PATH3D and MT3D.

A full on-line help menu is included.

Input-output data format: The program consists of a series of intuitive menu-driven schemes for creating and editing input data for the above models and processing and presenting the results. Post-processing capabilities include displaying areal and cross-sectional water level and concentration-contour maps, pathlines, hydrographs, drawdown and concentration-breakthrough curves at selected locations. ModIME can be used to compare observed and simulated water levels and concentrations and produce detailed flow budgets.

Availability: SSG

System requirements: PC386 or higher, math co-processor, 4 MB RAM and 10 MB free memory (486 with 66 MHz recommended).

11.9 MS-VMS

Developed by: HydroGeoLogic Inc.

Program language: *

Documentation: *

Description: MS-VMS (MODFLOW-Surfact - Visual Modelling System) is a MODFLOW-based groundwater flow and contaminant transport modelling system incorporating Groundwater Vistas, an interactive graphical interface.

Use: MS-VMS can be used for the following:

- Fully and variably saturated flow modelling
- Parent and transformation product transport modelling
- Migration pathline and capture zone delineation
- Interactive input preparation and grid construction
- Visualisation of modelling results in 2- and 3-dimensions

Solution method: *

Special properties: The model uses the MODFLOW-SURFACT version of MODFLOW that is claimed to overcome the limitations of MODFLOW in its original form including

- re-wetting of drained cells
- handling of pumping wells
- solute mass balance problems
- numerical dispersion and oscillations
- implicit assumption of negligible impact of transient storage effects on transport

MS-VMS is fully compatible with any previously created MODFLOW model.

Input-output data format: MS-VMS uses the interactive, graphical interface Groundwater Vistas. The interface includes additional features such as importing AutoCAD DXF image files to facilitate the determination of the model boundaries. It also provides graphical input of pumping and observation well data.

Availability: SSG

System requirements: PC486/Pentium with 16 MB RAM and Microsoft Windows 3.0 or later.

11.10 PMWIM

Developed by: Chiang, W-H. and Kinzelbach, W.

Program language: FORTRAN 77

Documentation: Pre- and post-processors for simulation of Flow and Contaminant Transport in Groundwater Systems with MODFLOW, MODPATH and MT3D. Version 3.0, Wen-Hsing Chiang and Wolfgang Kinzelbach, Heidelburg, Germany.

Description: PMWIM (Processing MODFLOW for Windows) is a Windows-based graphical pre- and post-processing package for modelling groundwater flow and transport processes with the 3-dimensional finite-difference groundwater flow model MODFLOW, the particle tracking models PMPATH for Windows or MODPATH, the solute transport model MT3D and the parameter estimation program PEST. As supplied by SSG, PMWIN comes complete with MODFLOW, PMPATH for Windows, PMDIS and the educational versions of MT3D (MT3DLITE) and PEST (PESTLITE).

Use: Pre- and post- processing package for use with the programs listed above.

Solution method: *

Special properties: A number of different features are included: calculation of water balances, generation of isolines, plotting of flowlines, running of MODFLOW, PMPATH and MODPATH, plotting of head versus time and other graphical presentation features such as plotting of contour lines and the distribution of hydraulic parameters.

The Windows version includes an on-line help system with examples. A DOS-based version is also available.

Input-output data format: Graphical user interface with an interactive menu.

Availability: IGWMC, SSG

System requirements: PC 386/486/Pentium with 2 MB RAM (4Mb RAM and Windows for PMPATH), math co-processor and Microsoft Mouse. Windows version: PC running Microsoft Windows 3.1 or later or Windows'95 with 8 MB RAM (16 Mb recommended).

11.11 Visual MODFLOW

Developed by: Waterloo Hydrogeologic Inc., Guiguer, N. and Franz, T. (1996)

Program language: *

Documentation: Guiguer, N. and Franz, T.. (1996). User's Manual for Visual MODFLOW. Waterloo Hydrogeologic Inc..

Description: A program package incorporating MODFLOW, MODPATH and MT3D integrated in a graphical program so that the user has no need for other pre- and post-processor programs. Using Visual MODFLOW the user can graphically input data, run MODFLOW, MODPATH and MT3D and visualise the results. Visual MODFLOW uses a mouse-driven user interface and greatly reduces the time taken to construct a groundwater model.

Use: 3-dimensional groundwater flow simulation, the determination of groundwater flow lines, particle tracking and contaminant transport modelling using MODFLOW, MODPATH and MT3D.

Solution method: Visual MODFLOW incorporates Waterloo Hydrogeologic's own solver for MODFLOW in addition to SIP, PCG2 and SOR.

Special properties: It is possible to incorporate MODFLOW files constructed earlier making it compatible with virtually any of the older processors for MODFLOW available on the market. This enables the development or reassessment of older models constructed on older versions of MODFLOW.

The program can also visualise head versus time at specified points as well as time-variant observed versus calculated head plots. This facility eases the process of model calibration considerably.

Input-output data format: Menu-driven windows for the construction of input files and the graphical presentation of output results. The model results can be displayed as equipotential and drawdown contours, velocity vectors, pathlines and calibration residuals.

Availability: IGWC, SSG

System requirements: PC 386/486/Pentium with 8 MB RAM and 40Mb disk space. Most printers are supported including HP LaserJet, DeskJet and PostScript.

12. PRE- AND POST-PROCESSING PROGRAMS

The process of model creation, execution and output and analysis of data can be tedious and unrewarding tasks particularly in complex modelling situations where a large number of parameters are involved. Fortunately there are programs available which can ease these processes. A number of these programs are described below. The purchase of these programs can be considerably cheaper than the program packages detailed in Chapter 10. The disadvantage with using the programs individually is that it is more cumbersome and time-consuming to switch between the input and output programs and the model itself.

Model calibration can also be a demanding and time-consuming process. Three programs specifically designed to assist in this process are also described. These programs tend to be orientated towards use with the U.S.G.S. 3-dimensional groundwater flow model MODFLOW. This is because MODFLOW is by far the most widely used groundwater flow model. The program PEST can however be used with any model although a PEST Utilities package is also available which is specifically designed to interface PEST and MODFLOW/MT3D.

12.1 ModelCad 386

Developed by: Geraghty and Miller Modelling Group

Program language: *

Documentation: *

Description: ModelCad displays the finite-difference grid graphically and stores it in a format independent of the model being used. The user determines block size, boundary conditions and the aquifer physical properties using a graphical user menu.

Use: The program supports MODFLOW, MODPATH, MOC and MT3D directly. It has CAD-like characteristics, interactive graphical model construction, graphical presentation of the aquifer's physical properties and boundary conditions, import and export capability to Surfer (Golden Software) and import capability for map files in DXF format.

Solution method: *

Special properties: *

Input-output data format: User-friendly graphical interface.

Availability: RWE

System requirements: PC 386/486/Pentium with 3Mb extended memory.

12.2 MODFLOWP

Developed by: U.S. Geological Survey

Program language: FORTRAN 77

Documentation: *

Description: MODFLOWP is U.S.G.S. computer program for estimating the hydraulic parameters of a transient or steady state, 3-dimensional groundwater flow model using non-linear regression.

Data used to estimate parameters can include existing independent estimates of parameter values, observed hydraulic heads or temporal changes in hydraulic heads and observed gains and losses along head-dependent boundaries.

Use: Estimation of parameters including: transmissivity, hydraulic conductivity, vertical leakage, horizontal anisotropy, hydraulic conductance of the river, stream-flow routing, general-head boundary, drain packages, areal recharge rates, maximum evapotranspiration, pumping rates, hydraulic heads at constant head boundaries.

Solution method: Non-linear parameter estimation.

Special properties: The user can define any spatial variation in parameters. Model output includes statistics for analysing the parameter estimates and the model. These statistics can be used to quantity the reliability of the resulting model.

Input-output data format: *

Availability: SSG

System requirements: PC 386/486/Pentium with 2 MB RAM and math co-processor.

12.3 MODINV

Developed by: *

Program language: *

Documentation: *

Description: MODINV is a suite of programs that include and enhance MODFLOW. Each member of the suite carries out a particular function of MODFLOW pre-processing or post-processing including:

- grid construction
- construction and manipulation of 2-dimensional real and integer data arrays
- interpolation of MODFLOW head and drawdown arrays to borehole locations
- interpolation of MODFLOW head and drawdown arrays to an arbitrary transect through the finite-difference grid
- formatting of model data for input to spreadsheets, graphing and contouring software
- translation of grid parameter zonation to SURFER display format
- parameter optimisation

MODINV is able to adjust parameter values within the active part of the MODFLOW finite-difference grid until the fit between observed and calculated borehole heads is minimised in the least squares sense.

Use: MODINV is designed to assist the creation, execution of input data, model calibration and the analysis of output data from the U.S.G.S. 3-dimensional groundwater flow model MODFLOW.

Solution method: The calibration program MODINV uses a non-linear weighed squares method to optimise MODFLOW parameters.

Special properties: MODINV can optimise parameter values for any model type that MODFOW can run. MODINV is compatible with Processing MODFLOW (PM).

Input-output data format: *

Availability: SSG

System requirements: PC 386/486/Pentium with 1 MB RAM. math co-processor and hard disk.

12.4 MODLMAKR

Developed by: MICROCODE Inc. Engineering/Software Scientific

Program language: *

Documentation: *

Description: The program is a pre-processing program for the construction of finite-difference and finite-element models for flow and pollution transport simulations. It has a generalised construction and can be used to produce input files for any model.

Use: Input files can be constructed using a menu-driven system and a mouse or a digitiser can be used if desired. Hydraulic boundary conditions are entered directly. The input files can be exported to a variety of different applications.

Solution method: *

Special properties: *

Input-output data format: User-friendly menu-driven interface.

Availability: MC

System requirements: PC 386/486/Pentium preferably with 4 MB RAM.

12.5 PEST

Developed by: *

Program language: FORTRAN 77

Documentation: *

Description: PEST (Parameter ESTimation) is a non-linear parameter estimator for use with any model.

Use: PEST is designed to assist in the calibration of any model. It can be used not only with hydrogeological models but also in hydrology, engineering, geophysics, biology and many other fields. Adjustable parameters can include virtually anything found in an input file including tabulated data such as drain and riverbed conductance as well as array-based data such as transmissivity, recharge and dispersivity.

Solution method: PEST implements a robust form of the Gauss-Marquardt-Levenberg method of parameter estimation.

Special properties: PEST can be used as a parameter estimator with any model. The model does not need to be re-compiled or re-cast as a subroutine. PEST MODFLOW/MT3D are an optional set of programs that automate construction of PEST interface files for use with MODFLOW and MT3D. Programs are also provided which interpolate MODFLOW and MT3D unformatted output files to borehole locations for direct comparison with field measurements.

Input-output data format: PEST reads its data from one or more text input files, writes its output to one or more text output files and can be run using a DOS command.

Availability: SSG

System requirements: IBM-PC or compatible with math co-processor. PEST can use extended memory for more complex cases.

12.6 SURFER/GRAPHER

Developed by: Golden Software

Program language: *

Documentation: *

Description: Graphical presentation tools:

SURFER can import data from a number of applications and a number of methods can be selected to generate contours. The program will generate contour maps of surface plots in user specified dimensions.

GRAPHER is a powerful tool for the presentation of large quantities of complex data graphically. A spreadsheet menu allows rapid and user friendly presentation of the graphs.

Use: *

Solution method: *

Special properties: A popular program that is very often used for the presentation of data from hydrogeological simulations. A completely generalised tool which can be used to generate contour plots and graphs.

Input-output data format: GRAPHER and SURFER can import files in a number of common formats. Output to hundreds of different printers or plotters is supported.

Availability: SSG

System requirements: DOS version: PC with 320 K RAM, Windows: PC running Microsoft Windows. These programs take advantage of extra RAM.

13. PROGRAMS FOR PUMPING TEST ANALYSIS

Groundwater models require initial estimates of an aquifer's properties, particularly aquifer transmissivity, permeability and storage coefficients. The analysis of pumping test data can lead to reliable estimates of these properties. Such reliable estimates can be invaluable during the construction and calibration of a groundwater model as they reduce the degree of freedom with which the input data can be modified during the calibration process. This can considerably shorten the time required for model calibration as more time can be spent concentrating on areas where less or no data is available.

The analysis and interpretation of data from pumping tests can however involve large quantities of data and can be a time consuming process particularly if large quantities of data are involved and more than one method is to be used. A number of programs are available which assist in this interpretation and the most important examples of these are described below.

13.1 ADEPT

Developed by: *

Program language: *

Documentation: *

Description: ADEPT is a program for aquifer data evaluation and contains over 40 solutions for the analysis of pumping test and slug test data. ADEPT includes solutions for:

- unconfined, confined, artesian and leaky aquifers with partial penetration corrections
- distance and time-drawdown analyses
- five slug test techniques
- safe yield, well efficiency
- capture zone
- recharge basin analyses
- drawdown analyses at constant head boundaries
- flowing well functions
- fractured aquifer analysis

Use: Analysis and interpretation of many different hydraulic aquifer tests.

Solution method: 40 different solutions for the analysis of pumping test data.

Special properties: A comprehensive pumping test analysis package.

Input-output data format: ADEPT uses the linked-object embedding programming and on-line hypertext features of Mathcad and Windows. The program is menu-driven using a spreadsheet format for data. Report-ready text output and graphics can be produced.

Availability: SSG

System requirements: PC386/486/Pentium with 4 Mb RAM, 4 Mb hard disk space, Microsoft Windows 3.1, Mathcad 5.0 and VGA graphics card and display.

13.2 Aqtesolv

Developed by: Modelling Group, Geraghty & Miller, Inc.

Program language: *

Documentation: Duffield, G. M. (1994). Aqtesolv, Aquifer Test Solver Version 2.0. Geraghty & Miller, Inc..

Description: Interactive visual type-curve matching software with automatic estimation of aquifer properties. The program includes the following solution methods:

Confined aquifer:
- Theis, constant and variable pumping rate (1935)
- Theis, variable rate with recovery (1935)
- Cooper-Jacob, constant and variable pumping rate (1946)
- Papadopulos-Cooper large-diameter well solution (1973)

Unconfined aquifer:
- Neuman and QuickNeuman (1974)
- Streltsova (1988)

Leaky aquifer:
- Hantush-Jacob (1955)
- Hantush (1960)
- Moench large-diameter well solution (1985)

Fractured aquifer:
- Moench solution for slab-shaped blocks (1984)

Slug tests:
- Bredehoeft-Papadopulos
- Bouwer-Rice

Use: Aqtesolv enables the user to apply the above analytical solutions for determining aquifer properties from pumping tests and slug tests.

Solution method: Aqtesolv enables the user to apply visual or automatic curve fitting methods using the above solution methods. The automatic curve fitting method uses a non-linear weighted least-squares parameter estimation algorithm to match type curves or straight lines to time-displacement data measured during an aquifer test.

Special properties: The program includes a wide variety of solution methods.

Input-output data format: Aqtesolv includes data set management tools for entering, editing and importing data. Error checking during data entry ensures that the data entered are consistent and complete. Data can also be imported. Compatible with HP and compatible plotters.

Availability: RW

System requirements: PC running DOS

13.3 Aquifer Test for Windows

Developed by: Waterloo Hydrogeologic Inc.

Program language: *

Documentation: Aquifer Test v2.0, Waterloo Hydrogeologic Inc.

Description: Aquifer Test for Windows is a graphically orientated package for estimating transmissivity, hydraulic conductivity and storage properties for a variety of aquifer conditions. The program contains analytical solutions for pumping and slug tests for confined, unconfined and leaky confined aquifers including the following:

- Theis (1935)
- Cooper & Jacob time-drawdown (1946)
- Cooper & Jacob distance-drawdown (1946)
- Theis & Jacob recovery test
- Neuman (1975)
- Hantush & Jacob (1955), no aquitard storage
- Well performance test
- Bouwer-Rice slug/bail test (1976)
- Hvorslev slug/bail test
- Step-wise pumping Cooper & Jacob (1946)
- Step-wise pumping Theis (1935)

Use: Analysis and pumping tests, slug tests and well performance tests.

Solution method: Automatic data fitting using least squares regression is included for all analysis methods.

Special properties: A wide variety of solution methods are included in the program.

Input-output data format: Aquifer Test provides a flexible, user-friendly environment. Pumping test data can be directly input into Aquifer Test, imported from a data logger file in ASCII format or inserted from any Windows-based test editor/spreadsheet/database by 'cutting and pasting' through the Windows clipboard.

Availability: Waterloo Hydrogeologic Inc.

System requirements: PC 386 or better with a hard drive with at least 5 Mb free, Windows 3.x, Windows 95 or Windows NT, math co-processor, Microsoft mouse or compatible.

13.4 AQUIX-4S

Developed by: EnviroTools Ltd.

Program language: *

Documentation: EnviroTools Ltd. (1993). User's Manual for Aquix-4S, Version 1.1.

Description: AQUIX-4S is a forward and inverse modelling program to aid in interpreting flow and slug test data sets.

Flow rate or drawdown curves are calculated using the methods described by:

- Theis (1935)
- Hantush (1960)
- Hantush (1964)
- Neuman (1975)
- Cooper et al. (1967)

Use: Analysing pumping test and slug test data.

Solution method: Inverse modelling allows the user to obtain a set of parameters that best fits the data in a least squares sense. Forward modelling allows the user to calculate synthetic (model) curves for the chosen model.

Special properties: The program includes a wide variety of solution methods.

Input-output data format: Data can be input to AQUIX either through the keyboard in a spreadsheet-style editor or from ASCII text files. Graphic displays are presented as bi-logarithmic, semi-logarithmic or linear plots versus time. Hardcopy output can be in

simple plot form or can utilise the plate plotting capability of AQUIX to produce report ready graphic displays.

Availability: RW

System requirements: PC running DOS.

13.5 GWAP

Developed by: Groundwater Graphics

Program language: *

Documentation: *

Description: GWAP (Graphical Well Analysis Package) is a program which uses data collected in connection with pumping tests and slug tests and presents logarithmic graphs for the drawdown cone against time or other parameter as required by the various analysis methods. The graph can then be superimposed on to a type curve. GWAP has a graphical module that allows the user to do this on the screen and to carry out the required calculations on completion of a good match between the two curves for transmissivity, storage coefficient, or other parameter as each method requires.

GWAP includes the following capabilities for the graphical analysis of:

- Standard pumping test where the well storage is negligible
- Well tests carried out with larger boreholes where well storage is included
- Slug and injection tests

Use: GWAP is designed to simplify the time consuming task of graphical interpretation of aquifer pumping tests and the determination of hydraulic parameters.

Solution method: *

Special properties: The program includes 73 different type curves for graphical matching to pumping test data for five different aquifer conditions: Confined aquifer with some leakage, unconfined aquifer with a fast response, unconfined aquifer with delayed yield, slug and injection tests and large diameter well tests.

Can plot up to 15 different observation boreholes which can each have up to 100 observations over time.

Input-output data format: GWAP is a DOS program with a dedicated menu system that includes an editing, output and help menu.

Availability: A number of similar programs for the determination of hydraulic parameters including AQTESOLV, ADEPT, PUMPTEST and TECTYPE are available from most suppliers.

System requirements: *

13.6 THE AQUIFER TEST TOOLBOX (ATT)

Developed by: *

Program language: *

Documentation: *

Description: ATT is a series of Excel 5.0 workbooks containing worksheets, charts and macros designed for the analysis of pumping test data.

ATT contains a number of commonly used test methods:

- Theis Confined Aquifer
- Cooper-Jacob (with Hantush's modification for leaky conditions)
- Walton Leaky Aquifer
- Hantush Inflection Point pumping tests
- Theis Recovery Line-Fit and Curve Match Method
- Hvorslev Slug Test Method
- Bouwer and Rice Slug Test Method
- Birsoy-Summers Variable Discharge Method
- Stallman Single-Boundary Method
- Biershenk Step Test Method
- Falling Head vertical hydraulic conductivity tests

Use: Analysis of pumping tests and slug tests under a wide variety of hydrogeological conditions.

Solution method: Automatic or interactive linear regression for straight-line analysis. Curve matching methods include data point weighting and partial fitting.

Special properties: ATT includes Stallman's Single-Boundary Method and a blank data entry form for use in the field.

Input-output data format: ATT uses Excel spreadsheet technology to ease data entry, analysis and presentation. ATT combines all the data, results and graphs in one report.

Availability: SSG

System requirements: Windows: Excel 5.0 or higher, 4 MB RAM (8 Mb and math coprocessor recommended). Macintosh: System 7.0 or later, Excel 5.0, at least 3.6 MB RAM available for Excel, 68020 or newer CPU (math coprocessor recommended). Power Macs require an additional megabyte of free RAM for best performance.

13.7 Infinite Extent

Developed by: *

Program language: *

Documentation: *

Description: Infinite Extent is a Windows-based pumping test analysis program with both on-screen type curve matching and automatic parameter estimation. Data is matched to the type curve visually with the keyboard or on-screen control panel.

Infinite Extent includes the following on-screen type curve matching or graphical methods:

- Theis Confined Aquifer
- Walton Leaky Aquifer
- Hantush Leaky Aquifer
- Neuman Unconfined Aquifer
- Hantush's Modification of Theis Method for Partial Penetration
- Distance-Drawdown
- Theis Recovery

Infinite Extent also includes the following automatic parameter-estimation methods:

- Specific Capacity
- Theis Confined Aquifer
- Hantush Leaky Aquifer Steady-State
- Theim Confined and Unconfined Steady-State
- Distance-Drawdown for Multiple Observation Well Tests

Use: Analysis of pumping tests and slug tests under a wide variety of hydrogeological conditions.

Solution method: Curve matching and automatic parameter-estimation.

Special properties: Infinite Extent can read or write Aqtesolv files and can accept up to 400 time and drawdown data pairs for up to five wells. In addition to graphical and type curve methods, Infinite Extent includes arithmetic, semi-logarithmic and double logarithmic graphs.

Also included are calculators for steady-state radius of influence, maximum well yield, steady-state drawdown, transmissivity estimation by specific capacity method with partial penetration, and Huisman partial penetration corrections (methods I and II).

Input-output data format: Data is entered via Windows-style dialog boxes. Automatic parameter estimation results are written to output files in column or tab-delineated format in a variety of units.

Availability: SSG

System requirements: PC386/486/pentium with 4 MB RAM and Microsoft Windows 3.1/Windows/Windows NT.

14. MISCELLANEOUS HYDROGEOLOGICAL PROGRAMS

This chapter details programs which do not fall into the main categories for modelling tasks listed in this report but are nevertheless important in hydrogeological analysis. These programs include geostatistical programs, programs for the analysis for hydrochemical data and graphical packages.

GEOEASE and VARIOWIN are programs for the geostatistical handling of parameters for hydrogeological modelling. GWAP is a program designed for the analysis and calculation of hydraulic parameters in connection with pumping tests. SURFER/GRAPHER are much-used general programs for the graphical presentation of model results and test data. There are many other similar programs available with similar capabilities and only a selection of the more commonly used programs are presented here.

14.1 GEO-EAS

Developed by: Englund, E. U.S.EPA, Sparks, A., Computer Science Corp.

Program language: *

Documentation: *

Description: GEO-EAS is a 2-dimensional geostatistical analytical tool for data distributed over an area. The program is actually a series of linked interactive programs. The program includes a hierarchical menu system with information messages, screen pictures for data entry, parameter files and a graphical post-processor for presentation of calculated data. Parameters can rapidly be edited and the results presented graphically. Programs which are incorporated in the GEO-EAS package include: data file handling, data transformation, univariant statistics, variogram analysis, cross-checking, kriging, contour mapping, post-plot, line and distribution graphs.

Use: A geostatistical analytical tool.

Solution method: *

Special properties: *

Input-output data format: Interactive graphical menu where parameters can be easily changed and presented graphically.

Availability: IGWMC

System requirements: IBM PC, XT, AT or equivalent, 640 K RAM, DOS 3.0 or higher, CGA or EGA graphics.

14.2 HYDROWIN

Developed by: Calmbach, L., Department of Earth Sciences, University of Lausanne

Program language: *

Documentation: Calmbach, L. Geochemistry and isotopic composition of mineral and thermal waters from the upper Rhine graben (Baden-Wurttenberg and Alsace), Thesis, ETH.

Description: A program which includes many of the most used methods for the interpretation of hydrochemical data from simple conversion of units, charge balances or definition of chemical facies to more complex equilibrium and geothermal calculations e.g. saturation indices, geothermometers. Hydrowin was originally developed for mineral/thermal waters but is also useful for more typical groundwaters. The program's main drawbacks include: i) lack of graphics export facilities and ii) a number of bugs e.g. errors in conversion of SiO_2, H_3BO_3 and NO_3^- from mg/l to meq/l or mmol/l during input.

Twelve different diagrams are available for the presentation of data. Many of these diagrams are specially designed for the analysis of hydrochemical data. Several diagrams can be presented simultaneously if desired. Clicking on a data point will identify the data registration number of that point.

Use: A program for the graphical and numerical analysis of hydrochemical data including a pre-processing package for PHREEQE, NETPATH and SOLMINEQ.88.

Solution method: *

Special properties: Includes a help menu.

Input-output data format: The program can import ASCII and EXCEL files or use files input directly. Export of data to PHREEQE, NETPATH and SOLMINQ.88 is possible.

Availability: A beta version of the program is available from the authors, ETH.

System requirements: PC 386/486/Pentium running Windows 3.1 or higher.

14.3 VARIOWIN

Developed by: Pannatier, Y. Department of Earth Sciences, University of Lausanne.

Program language: C++

Documentation: Pannatier, Y., (1995) 1) VARIOWIN: logiciel pour l'analyse spatiale de données en 2D. 2) Etude géostatistique du gîte de phosphates de Taïba (Sénégal), Theis, ETH.

Description: The program includes three separate modules for the analysis and graphical modelling of continuous 2-dimensional data. These three modules are:

- PREVAR2D allows large quantities of data to be compared.
- VARIO2DP is used to characterise and describe the simulated area.
- MODEL allows interactive modelling with experimental variograms produced by VARIO2DP includes a help menu that contains the entire user manual.

Use: A WINDOWS program with three separate modules for analysing variographs and variogram modelling in 2-dimensions.

Solution method: *

Special properties: *

Input-output data format: Interactive graphical user interface assists the user with data input and interpretation of the results.

Availability: ETH

System requirements: PC running Windows.

15. OTHER SOURCES OF INFORMATION ON GROUNDWATER MODELLING

The references provided in this report provide a valuable starting point for anyone wishing to obtain further information on any of the models listed in this report or groundwater modelling in general.

An enormous amount of information is also available on the Internet including relevant references, manuals, copies of public domain programs and other relevant information. As the Internet is constantly changing and being updated, a comprehensive list of sites would be inappropriate here. However, for the user with access to the Internet the following addresses represent particularly valuable sources of information on groundwater modelling:

Pages supported by	Internet address
Geotechnical and Geoenvironmental Software Directory Andrew.Piggott@CCIW.ca	http://www.ibmpcug.co.uk/~bedrock/gsd/ http://gwrp.cciw.ca/internet/software.html
Hydrosystems	http://hydrosystems.com/
Private page (R.B. Winston)	http://www.mindspring.com/˜rbwinston/rbwinsto.htm
Geological Survey of Norway (NGU)	http://www.ngu.no/iah/geo-l.html
United States Geological Survey	http://h20.usgs.gov/software/ground-water.html
United States Geological Survey	http://h20.usgs.gov/software/geochemical.html
US Environmental Protection Agency	http://www.epa.gov/ada/models.html
Environmental Systems & Technologies	http://www.esnt.com/napl.htm

These addresses contain information on an extremely comprehensive list of models and also include many links to other relevant addresses. Internet search machines such as ‘Infoseek’ and ‘Alta Vista’ can be of great assistance in finding information on modelling tools. Using more specific keywords during searches greatly enhances their efficiency as general searches can often find hundreds or even thousands of ‘relevant’ sites. In particular, including the model name will obviously target relevant sites most precisely.

The Institute for Geology and Rock Mechanics at the University of Trondheim (NTNU) is planning a WEB site dedicated to groundwater modelling. This site will include the program overview presented in this report and other relevant hydrogeological information.

For institutions and modellers wishing to utilise a large number of models, the program *Model Expert96 for Windows* may be worth considering. *Model Expert96* is an interface for Windows 3.x or higher that enables the user to search for an appropriate model based on a wide variety of criteria. These criteria include model availability (public domain, proprietary codes), medium type (fractured rock, porous media only, etc.), simulation type (flow, transport, etc), saturated/unsaturated and

confined/unconfined flow conditions, model cost, etc. The user is therefore able to rapidly select the model most appropriate to his or her needs.

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16. PROGRAM SUPPLIERS

CSMoS - The United States Environmental Protection Agency, Office of Research and Development, Robert S. Kerr Environmental Research Laboratory, Center for Subsurface Modelling Support, P.O.Box 1198, Ada Oklahoma 74820, USA.

DHI - Danish Hydraulic Institute, Agern Allé, DK 2970 Hørsholm, Denmark.

ECGL - Engineering Computer Graphics Lab., 300 CB, Birgham Young University, Provo, Utah 84602, USA.

ESI - Environmental Simulation Inc. 2997, Emerald Chase Drive, Herndon, Virginia 22071, USA.

ETH - Institut de Minéralogie et Pétrographie, Université de Lausanne, BFSH2, CH-1015 Lausanne, Switzerland.

HS - HydroScience Inc., 1021 Deer Crossing Way, Lexington, Ky 40509 USA.

IG - Intergraph Corporation, Huntsville, AL 35894-0001, USA.

IGWMC - International Ground Water Modeling Center, Colorado, School of Mines, Golden, CO 80401, USA.

LLNL - Lawrence Livermore National Laboratory, University of California, 7000 East Avenue Livermore, CA 94550, USA.

LTC - Laboratory of Theoretical Geochemistry Department of Geology, University of California, Berkeley, CA 94720, USA.

MC - MICROCODE INC., 12136 calle Zagal NE, Albuquerque, NM 87111, USA.

RWE - Rockware Europe, P.O.Box 621, 2501 CP The Hague, The Netherlands.

SSG - Scientific Software Group, P.O.Box 2304, Washington, D.C. 20023-3041, USA.

USGS-EISC - U.S. Geological Survey, Open File Report Section, Box 25286, MS 517, Denver Federal Center, Denver, CO80225-0046, USA.

USGS-NWIS - U.S. Geological Survey, NWIS Program Office 437 National Center, Reston, VA 22092, USA.

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