Appareil destiné a déterminer la loi
de l'écoulement de l'eau à travers le sable.

Summary of Selected Computer Programs
Produced by the U.S. Geological Survey for
Simulation of Ground-Water Flow and Quality
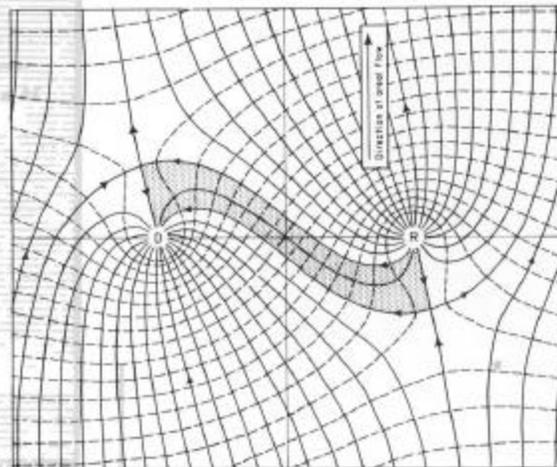
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U.S. GEOLOGICAL SURVEY CIRCULAR 1104

SUMMARY OF SELECTED COMPUTER PROGRAMS PRODUCED BY THE U.S. GEOLOGICAL SURVEY FOR SIMULATION OF GROUND-WATER FLOW AND QUALITY, 1994

By Charles A. Appel and Thomas E. Reilly

U.S. GEOLOGICAL SURVEY CIRCULAR 1104

U.S. DEPARTMENT OF THE INTERIOR
BRUCE BABBITT, Secretary

U.S. GEOLOGICAL SURVEY
Gordon P. Eaton, Director

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> Foreground – A two-dimensional flow net (DaCosta and Bennett, 1960).

> Artwork by Joan Rubin and Leslie Robinson

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ABSTRACT

A summary list of computer models that simulate ground-water flow and quality is presented. The list contains a brief description of each model program, its numerical features, a qualitative expression of the number of past applications, the reference for the report documenting the program, and where to obtain a copy. Reports included in the list have been published or developed by the U.S. Geological Survey, and contain listings of the computer programs, although in a few cases, the program is so long that a listing was not included in the report, but a copy of the program is available on request.

INTRODUCTION

Numerical models provide a powerful aid in understanding and assessing ground-water systems. The U.S. Geological Survey (USGS) has contributed significantly to the development and use of models for the analysis of ground-water problems. Two reports had previously documented the status of ground-water modeling in the USGS, Appel and Bredehoeft (1976) and Appel and Reilly (1988). Because developments in the field have taken place since that time, additional computer programs have been published. This report gives information on selected computer programs published or developed by the USGS or by the USGS in cooperation with Federal, State, and local agencies for modeling flow, quality, and solute or heat transport in ground-water systems. The information for each program includes the reference, a brief description of the field conditions that the program can simulate, the numerical approximation procedures used, an indication of the extent of past field applications of the program by USGS personnel, and where to obtain copies of the report and, in some cases, the computer code.

The list of programs is organized by general modeling category. Information on each program is separated by one solid horizontal line. In many cases a program is based on or related to another program. The parent program is listed first and followed by the related programs. Three solid lines mark the end of the list of those programs related to a parent computer program. In a few cases, however, a program listed under one category was derived from a program in another category; for example, some of the programs listed in the "Freshwater-Saltwater" category are modifications to ground-water flow programs described in the category "Flow-Saturated." Also, some programs could be included under other categories; for example, the programs by Grove and Stollenwerk (1984) and Lewis, Voss, and Rubin (1986) are models for the transport of fluids that are affected by physical and chemical processes. Both of those programs could have been included in the "Chemical Mass Transfer" category instead of the category of "Solute Transport" in which they are contained in this report. Although several flow models that account for surface-water interaction

are listed as having been derived from some parent flow model, we have listed the coupled ground- and surface-water flow model of Swain and Wexler (1993) separately even through it represents a coupling of the ground-water flow model of McDonald and Harbaugh (1988) and a surface-water flow model of Schaffranek, Baltzer, and Goldberg (1981). This choice was made to bring attention to the fact that it is the only case in which the surface-water formulation is based on a comprehensive set of unsteady flow equations, which are subject only to the limitations inherent in a one-dimensional formulation of streamflow. The intent of these examples is to indicate that a potential user should thoroughly evaluate the programs in all related categories to choose the most appropriate numerical tool. The category titles are generalized and are not intended to be all-inclusive.

Depending on the nature of the problem, more than one computer program may apply. In some cases, the choice of program may reflect more the individual's familiarity with a particular approach than the superiority of the approach. In other cases, the choice of program may definitely reflect the level of approximation required; for example, if field data indicate a thick zone of brackish water that separates strictly fresh water from strictly salt water, then the choice of a program that assumes the zone is an interface may result in a lesser level of approximation than would a solute-transport program that includes consideration of the density variations in the zone.

Many computer programs for the simulation of ground-water flow and quality are listed herein. Some of these programs are listed for historical reasons or because they represent specialized aspects of either physics or chemistry. Additionally, many areas of ground-water flow and chemistry are the subjects of multiple investigations, in which related programs are developed in an attempt to refine and (or) perfect the methods currently available; therefore, some aspects of ground water can be simulated by more than one model listed in this report. Although the reports that document the programs have been reviewed and approved, not all parts of every program have necessarily been thoroughly tested, and a user bears the ultimate responsibility for assuring that a program does, in fact, what is claimed. Confidence in a program increases with good agreement between program results and known solutions to problems closely related to those for which the program is intended to solve.

As an indication of models that are currently "popular," a poll was made in late 1992 of model usage in the U.S. Geological Survey's operational program. The models being used at that time are listed in table1. This listing provides general information on usage. However, new codes or specialty codes may not be included (or may be under represented) in this table simply because of the available utility of the codes at the start of these projects and the scope of the current projects being undertaken. Associated with many of the computer programs discussed in this report are acronyms. Appendix 1 gives a list of those acronyms and the full name of the corresponding program and the appropriate reference(s).

TABLE 1. *Summary table of use of U.S. Geological Survey Models for simulation of ground-water flow and water quality in the U.S. Geological Survey operational program (as of late 1992)*

Model Name	Number of Projects Using the Model
AQUIFEM-SALT (Voss, 1984b)	4
AX (Rutledge, 1991)	1
BALANCE (Parkhurst and others, 1982)	10
HST3D (Kipp, 1987)	8
INTERCOMP (INTERCOMP, 1976; INTERA, 1979)	2
MOC (Konikow and Bredehoeft, 1978; Goode and Konikow, 1989)	8
MODFE (Torak, 1993a, b; Cooley, 1992)	4
MODFLOW (McDonald and Harbaugh, 1988)	165
MODFLOWP (Hill, 1992)	8
MODPATH (Pollock, 1989)	54
NETPATH (Plummer and others, 1991)	29
PHREEQE (Parkhurst and others, 1980; revised, 1990)	36
PHRQPITZ (Plummer and others, 1988)	2
SHARP (Essaid, 1990)	8
SOLMINEQ (Kharaka and others, 1988)	3
SUTRA (Voss, 1984a)	12
TRACY (Dunlap and others, 1984)	2
Trescott-3D (Trescott, 1975)	1
Variable Density Flow (Kuiper, 1985)	1
VS2D (Lappala and others, 1987)	8
WATEQF (Plummer and others, 1976; revised, 1984)	11
WATEQ4F (Ball and Nordstrom, 1991)	20

Purpose and Scope

This report makes available a moderately comprehensive list of computer programs that have been produced by the U.S. Geological Survey for simulation of ground-water flow and quality. The main criterion used in compiling the list is that the program must be documented in a published report that includes a listing of the computer program, although in a few cases, the program is so long that a listing was not included in the report, but a copy of the program is available on request.

Sources of Reports and Computer Programs

For those reports not available from a cooperating State agency, an indication is given from which of the following Federal sources the report and computer program can be obtained:

> U.S. Geological Survey
> NWIS Program Office
> 437 National Center
> Reston, VA 22092
> (703) 648-5695
>
> NTIS, U.S. Department of Commerce
> 5285 Port Royal Road
> Springfield, VA 22161
> 703) 487-4650
>
> U.S. Geological Survey Open-File Reports and Water-Resources Investigations Reports, can be purchased from:
>
> USGS ESIC--Open-File Report Section
> Box 25286, MS 517
> Denver Federal Center
> Denver, CO 80225-0046
> (303) 236-7476
>
> U.S. Geological Survey Water-Supply Papers, Professional Papers, Bulletins, Circulars, and Techniques of Water-Resources Investigations, can be purchased from:
>
> USGS Map Distribution
> Box 25286, MS 306
> Denver Federal Center
> Denver, CO 80225
> (303) 236-7477

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INDIVIDUAL DESCRIPTIONS OF COMPUTER PROGRAMS

FLOW—SATURATED

Two-Dimensional Finite Difference

Program Documentation:

Trescott, P.C., Pinder, G.F., and Larson, S.P., 1976, Finite-difference model for aquifer simulation in two dimensions with results of numerical experiments: Techniques of Water-Resources Investigations of the United States Geological Survey, book 7, chap. C1, 116 p.

Description:

This model simulates steady and nonsteady ground-water flow in an irregularly shaped aquifer that can be a confined or unconfined aquifer or both. The transmissive properties of the aquifer may be heterogeneous and anisotropic, although the principal directions of anisotropy must be aligned with the grid and the anisotropy ratio must be constant, and the storage coefficient may be heterogeneous. The model simulates well discharge; recharge that can differ spatially, but not with time; leakage from a confining bed or streambed in which the effects of storage are considered; and evapotranspiration as a linear function of depth to water. Specified head and specified flux boundaries can be simulated.

Numerical features:

The grid is block centered and rectangular with variable spacing in each direction. Finite difference numerical approximations are used. The resulting matrix problem is solved by an iterative procedure; the user has a choice of selecting one of three solution algorithms: line successive overrelaxation, iterative alternating direction implicit, and the strongly implicit procedure. Mass balances are computed for each time step and as a cumulative volume of water from each source and each type of discharge.

Past applications:

Up to a few years ago, this was one of the most-used flow models for two-dimensional problems. See McDonald and Harbaugh (1988), which is one of the reports listed as "Flow-Saturated--Three-dimensional finite difference," for a newer code that contains most of the capabilities of this program.

Availability:

Report is available from the USGS Map Distribution. Computer program and report are available from NWIS.

Related program:

Larson, S.P., 1978, Direct solution algorithm for the two-dimensional ground-water flow model: U.S. Geological Survey Open-File Report 79-202, 22 p.

Most significant change to original program:

A direct-matrix-solver program that assumes the D4 (alternating diagonal) node-ordering scheme is presented. For moderate-sized grids, this solver can be computationally more efficient than iterative matrix methods.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Manteuffel, T.A., Grove, D.B., and Konikow, L.F., 1983, Application of the conjugate-gradient method to ground-water models: U.S. Geological Survey Water-Resources Investigations Report 83-4009, 24 p.

Most significant change to original program:

A conjugate-gradient matrix solution procedure is presented for the two-dimensional ground-water flow problem. Application to a field problem of this method as compared with the iterative alternating direction implicit procedure (IADIP) and the strongly implicit procedure (SIP) methods showed the conjugate gradient method to compare favorably with IADIP but less satisfactorily with SIP. The main advantage of the conjugate gradient method is that it does not require the use of iteration parameters.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

Related program:

Ozbilgin, M.M., and Dickerman, D.C., 1984, A modification of the finite-difference model for simulation of two-dimensional ground-water flow to include surface-ground water relationships: U.S. Geological Survey Water-Resources Investigations Report 83-4251,   98 p.

Most significant change to original program:

The Trescott, Pinder, and Larson (1976) two-dimensional finite-difference program is based on the assumption that the water level in streams that are in hydraulic connection with an aquifer are not appreciably affected by the flow between those streams and the aquifer. Because the Ozbiligin and Dickerman (1984) program related stream discharge to the depth of water in the stream at that place (by using the Manning formula), it accounts for changes in stream-water level associated with changes in stream discharge resulting from flows between the aquifer and the stream.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Related program:

Hutchinson, C.B., Johnson, D.M., and Gerhart, J.M., 1981, Hydrogeology of well-field areas near Tampa, Florida, Phase 1--Development and documentation of a two-dimensional finite-difference model for simulation of steady-state ground-water flow: U.S. Geological Survey Open-File Report 81-630, 129 p.

Most significant change to original program:

The original program assumed that model-grid boundaries are places where either the head or the fluxes across the boundary are specified. This report described a head-controlled flux condition for the model grid boundary that allows both head and flux to change. Two assumptions are made — that at some distance beyond the model grid, the head is constant and equals the head in an overlying source zone and that the transmissivity, confining-bed leakance, and source-zone head are constants in the strip between the model-grid and the constant-head boundaries. The storage properties of the aquifer and the confining bed in the strip are neglected.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Two-Dimensional Finite Element

Program Documentation:

Kuniansky, E.L., 1990, A finite-element model for simulation of two-dimensional steady-state ground-water flow in confined aquifers: U.S. Geological Survey Open-File Report 90-187, 77 p.

Description:

This report described a finite-element model that can be used to simulate two-dimensional steady-state ground-water flow in either isotropic or anisotropic aquifers. The principal axes of anisotropy can vary in direction over the modeled area, and the transmissivity can vary spatially, but not with changes in head. Constant head, constant flux, and head-dependent flux boundary conditions can be simulated.

Numerical features:

The computer program is based on the Galerkin finite-element technique and it uses triangular elements.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Two-Dimensional Finite-Element Galerkin

Program Documentation:

Dunlap, L.E., Lindgren, R.J., and Carr, J.E., 1984, Projected effects of ground-water withdrawals in the Arkansas River Valley, 1980-99, Hamilton and Kearny Counties, southwestern Kansas: U.S. Geological Survey Water-Resources Investigations Report 84-4082, 168 p. (Pages 27 to 168 contain documentation for the program developed by J. V. Tracy.)

Description:

This model simulates steady and nonsteady two-dimensional ground-water flow in an irregularly shaped confined or unconfined aquifer. The transmissive and storage properties of the aquifer may be heterogeneous. The model accounts for gains and losses from the river flow in each reach based on the incoming river and tributary flows and the gain from or loss to the aquifer in the reach. With an estimate of river discharge,

the river stage is computed for each reach by using an input stage-discharge relation given for each reach. The river/aquifer gains and losses are calculated as a function of streambed area, riverbed leakance values, and the head gradient between the river and the aquifer. Evapotranspiration from ground water is estimated by using monthly values of precipitation, applied water rate, evapotranspiration demand, the moisture capacity of the soil zone, and depth of root zone. Well discharges can vary monthly. Specified flux and specified head boundaries can be simulated.

Numerical features:

A "regular" finite-element grid is used in the simulation. A "regular" grid is defined as a region subdivided by a given number of columns that do not have to be parallel or the same length but that have an equal number of elements. The effect is of a deformed rectangular grid. Applying the Galerkin method results in an associated matrix problem that is solved by using a direct method. Mass balances from all sources are computed for each time step and as a cumulative volume for each source from the start of the simulation.

Past applications:

Several field problems.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Two-Dimensional Finite Element (kinematic equation representing river flows)

Program Documentation:

Glover, K.C., 1988, A finite-element model for simulating hydraulic interchange of surface and ground water: U.S. Geological Survey Water-Resources Investigations Report 86-4319, 90 p.

Description:

This model couples the equation of two-dimensional ground-water flow with the kinematic equation approximation for one-dimensional open-channel flow. Darcy's law for vertical flow through a semipermeable streambed is used to couple the ground-water flow and streamflow equations. The transmissive and storage properties and distributed recharge/discharge of the aquifer can vary by element, as can the stream-channel properties. Elements can be grouped together into user-defined property zones for ease of varying the magnitudes of those properties. The program can simulate perched streams, streamflow diversions, springs, recharge from irrigated acreage, and evapotranspiration.

Numerical features:

Triangular elements are used to approximate the aquifer, and one-dimensional linear elements located along the sides of the aquifer elements are used to approximate the stream network. The stream depth, stream velocity, and aquifer head are approximated throughout the stream/aquifer system as varying linearly within elements and are continuous between adjacent elements. The program assumes that the changes in hydraulic head are small and that the aquifer transmissivity does not change. Modifications to the program are outlined for the case where the aquifer transmissivity changes with hydraulic head.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Two-Dimensional Finite Element (including transient leakage effects)

Program 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, chap. A3,   136 p.

Cooley, R.L., 1992, Derivation of finite-element equations and comparisons with analytical solutions; Part 2 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, chap. A4, 108 p.

Torak, L.J., 1993b, Design philosophy and programming details; Part 3 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, chap. A5, 243 p.

Description:

MODFE was developed to provide solutions to ground-water flow problems based on the governing equations that describe two-dimensional and axisymmetric-radial flow in porous media. The documentation is divided into three parts.

Part 1 is the user's manual in which the hydrologic features and simulation capabilities of MODFE are described. Descriptions are given for preparing hydrologic data to characterize aquifer properties and boundary conditions by zone. Examples of data input and model output are provided to demonstrate the different types of ground-water problems that are solved by using the simulation capabilities of MODFE. Guidelines for designing the finite-element mesh and for node numbering and determining bandwidths are given to instruct users in the appropriate application of MODFE to ground-water problems.

In Part 2, the finite-element equations are derived by minimizing a functional of the difference between the true and approximate hydraulic head, which produces equations that are equivalent to those obtained by either classical variational or Galerkin techniques. Spatial finite elements are triangular with linear basis functions, and temporal finite elements are one dimensional with linear basis functions. Comparisons of finite-element solutions with analytical solutions are given for five example problems.

Part 3 contains descriptions of subroutines, programming details and program structure diagrams. Descriptions of subroutines that execute the computational steps of the modular-program structure are given in tables that cross-reference the subroutines with particular versions of MODFE. Programming details of linear and nonlinear hydrologic terms are provided. Structure diagrams for the main programs show the order in which subroutines are executed for each version and illustrate some of the linear and nonlinear versions of MODFE that are possible. Computational aspects of changing stresses and boundary conditions with time and of mass balance and error terms are given for each hydrologic feature. Program variables are listed and defined according to their occurrence in the main programs and subroutines. Listings of the main programs and subroutines are given.

Numerical features:

Aquifer geometry, flow boundaries, and variations in hydraulic properties are represented by triangular elements or element sides in a finite-element mesh. Time variations in hydraulic response are represented by one-dimensional elements. Linear coordinate functions are used to approximate the head distribution within elements. The finite-element matrix equations are solved by using either a direct symmetric Doolittle method of triangular decomposition or an iterative method that uses the modified, incomplete Cholesky, conjugate-gradient method. The direct method can be efficient for small- to medium-sized problems (less than about 500 nodes), and the iterative method generally is more efficient for larger-sized problems.

Simulation capabilities and uses of MODFE are transient or steady-state conditions, nonhomogeneous and anisotropic flow where directions of anisotropy change within the model region; vertical leakage from a semiconfining layer that contains laterally nonhomogeneous properties and elastic storage effects; point and areally distributed sources and sinks; specified head (Dirichlet), specified flow (Neumann), and head-

dependent (Cauchy-type) boundary conditions; vertical cross-section and axisymmetric cylindrical flow; confined and unconfined (water-table) conditions; partial drying and resaturation of a water-table aquifer; conversion between confined- and unconfined-aquifer conditions; and nonlinear head-dependent fluxes (for simulating line, point, or areally distributed sources and sinks). Aquifer stresses and boundary conditions can be changed on a time-step basis, or a stress-period basis or both. Hydraulic properties and boundary conditions can be input by zone.

Past applications:

This is a new program that has been used in a few field studies.

Availability:

Reports are available from the USGS Map Distribution. Computer program and reports are available from NWIS.

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Cylindrical Coordinates

Program Documentation:

Reilly, T.E., 1984, A Galerkin finite-element flow model to predict the transient response of a radially symmetric aquifer: U.S. Geological Survey Water-Supply Paper 2198, 33 p.

Description:

This computer program was developed to evaluate radial flow of ground water at a pumping well, a recharge basin, or an injection well. It is capable of simulating anisotropic, inhomogenous, confined, or pseudounconfined (constant saturated thickness) conditions.

Numerical features:

The program is based on the Galerkin finite-element technique. It uses linear triangular elements and a backwards finite difference in time.

Past applications:

Several.

Availability:

Report is available from the USGS Map Distribution. Computer program and report are available from NWIS.

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Related program:

Pucci, A.A., Jr., and Pope, D.A., 1987, Preprocessor and postprocessor computer programs for a radial-flow, finite-element model: U.S. Geological Survey Open-File Report 87-680, 69 p.

Most significant change to original program:

This program serves as a preprocessor by: generating a triangular finite-element mesh from minimal data input, producing graphical displays and tabulations of data for the mesh, and preparing an input data file. The postprocessor has the ability to produce graphical output for simulation and field results and to generate statistics for comparing the simulation results with observed data.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Axisymmetric Finite-Difference (well bore/aquifer)

Program Documentation:

Rutledge, A.T., 1991, An axisymmetric finite-difference flow model to simulate drawdown in and around a pumped well: U.S. Geological Survey Water-Resources Investigations Report 90-4098, 33 p.

Description:

This computer program was developed to simulate drawdown in and around a pumped well. It provides a tool that is useful for analyzing some aquifer test data that are complicated by features not handled by analytical methods. Aquifer properties that can be simulated include confined (leaky or nonleaky) conditions, unconfined conditions, vertical-horizontal anisotropy, and vertical variation in hydraulic conductivity and specific storage. The model requires horizontal uniformity of hydraulic conductivity, specific yield, and specific storage. Well properties that can be simulated include well-casing storage, hydraulic head loss across the well screen, and hydraulic head variation along the length of the well bore that results from pipe-flow friction and nonuniform velocity. The program allows for partial well penetration and for multiple screened intervals.

Numerical features:

The program is based on the finite-difference technique. Because the time derivative approximation used is the forward-difference (explicit) in time, an upper limit on the time-step length is needed to assure numerical stability. The program allows an early time-step size and a larger later time-step size.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Two-Aquifer System

Program Documentation:

Mallory, M.J., 1979, Documentation of a finite-element two-layer model for simulation of ground-water flow: U.S. Geological Survey Water-Resources Investigations Report 79-18, 347 p.

Description:

Theoretical development of the model represented by this program is from Durbin (1978). The program simulates steady and nonsteady ground-water flow in an irregularly shaped two-aquifer system. The areal extent of the two aquifers does not have to be coincident. The transmissive and storage properties of the aquifer can differ spatially but are assumed to be isotropic. Discharge and recharge can be varied spatially and with time. Evapotranspiration is treated as a linear function of depth to water. The vertical hydraulic conductivity of the confining layer is assumed to be a constant, its thickness can differ spatially, and the changes in confining layer storage are assumed to be negligible.

Numerical features:

The program uses the Galerkin finite-element method and approximates the time derivative by backwards finite-difference formulation. The region to be modeled is subdivided into triangles, and the head is assumed to vary linearly in any one triangle. The associated matrix problem is solved by using the PSOR (point iterative successive over-relaxation method).

Past applications:

A few field applications.

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Quasi-Three-Dimensional Aquifer System (Finite Difference)

Program Documentation:

Weeks, J.B., 1978, Digital model of ground-water flow in the Piceance Basin, Rio
Blanco and Garfield Counties, Colorado: U.S. Geological Survey Water-Resources
Investigations 78-46, 108 p.

Description:

The computer program capability is "quasi-three-dimensional" in that it simulates a
three-dimensional multiaquifer system by assuming horizontal flow in the aquifers and
vertical flow through the confining layers that separate the aquifers. The program
simulates steady and nonsteady ground-water flow in an irregularly shaped flow system
that consists of aquifer layers and confining layers. Changes in storage in the confining
layers are assumed to be negligible. The transmissivity and storage coefficient of each
aquifer layer and the confining layer leakance values can differ spatially. Uniform
recharge to each layer and distributed discharge can be simulated. Specified head
boundaries can be simulated in the uppermost aquifer.

Numerical features:

The planar area of the irregularly shaped flow region is divided into a rectangular block-
centered grid that permits variable grid spacing. Finite-difference numerical
approximations reduce the equations of ground-water flow in each aquifer to a matrix
problem that can be solved by using IADIP (the iterative alternating-direction implicit
procedure). The computational procedure essentially is to treat the aquifer system as a
sequence of two-dimensional flow models coupled by terms that represent flow
(leakage) through intervening confining beds. The leakage at a node in a particular
layer is based on, among other things, the difference in head in the layer during the
current iteration and the most recently computed heads for the nodes in the overlying
and underlying layers vertically in line with the subject node. Outflows to the specified
head boundaries are computed for each time period and as a cumulative volume of
water.

Past applications:

Many.

Remarks:

This program is a revision and adaptation for the Piceance Basin of a program developed by J. D. Bredehoeft in 1969 and described in Bredehoeft and Pinder (1970); the latter program was used widely before about 1980. See McDonald and Harbaugh (1988) for a newer code that has more capabilities.

Availability:

Report is available from NTIS (PB–284–341).

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Three-Dimensional Finite-Difference

Program Documentation:

Bredehoeft, J.D., 1992, Microcomputer codes for simulating transient ground-water flow—In two and three space dimensions: U.S. Geological Survey Open-File Report 90-559, 73 p., diskette in pocket.

Description:

This report is the documentation for a code for solving two- and quasi-three-dimensional formulations of the general ground-water flow equation. The code is written in FORTRAN 77 and was developed to be a simple basic code that could run on a variety of small computer systems. Specified head and specified flux boundaries can be simulated. The transmissivity is assumed to be isotropic and not change with head, but it can vary spatially. One value is assumed to be representative of the storage coefficient of all aquifers, and the effects of storage in the confining layers are assumed to be negligible. The leakance values (vertical hydraulic conductivity divided by the thickness of the leaky confining layer) can vary spatially for each confining layer. Recharge/discharge can be simulated and can vary spatially.

Numerical features:

The flow region is considered to be divided into blocks in which the medium properties are assumed to be uniform. Block-centered finite-difference numerical formulations are used. The associated matrix problem is solved by using the SIP (strongly implicit procedure) iterative technique. A total mass balance and the rate of flow in the system are computed and printed at user selected times.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. The report includes a source diskette that contains the two- and three-dimensional programs and data sets that correspond to the test problems described in the report.

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Three-Dimensional Finite-Difference

Program Documentation:

Trescott, P.C., 1975, Documentation of finite-difference model for simulation of three-dimensional ground-water flow: U.S. Geological Survey Open-File Report 75-438, 32 p.,

Trescott, P. C., and Larson, S. P., 1976, supplement to Open-File Report 75-438—Documentation of finite-difference model for simulation of three-dimensional ground-water flow: U.S. Geological Survey Open-File Report 76-59l, 21 p.

Description:

Steady and nonsteady flow are simulated in an irregularly shaped three-dimensional flow region. The flow system can be fully confined, or the uppermost zone can be an unconfined aquifer. Hydraulic conductivities may be heterogeneous and anisotropic (restricted to having the principal directions alined with the grid axes and the anisotropy ratios fixed for each layer), and the storage coefficient may be heterogeneous. The model simulates well discharge from any layer and recharge to the uppermost layer that can vary spatially (but not with time). Specified head and specified flux boundaries can be handled. For some flow systems that are characterized by alternating layers of "high" and "low" hydraulic conductivities, a modified three-dimensional formulation is available that exploits essentially horizontal flow in "aquifer" layers and essentially vertical flow (assuming storage in confining beds is not significant) in "tight" layers to give approximate solutions for less computational effort.

Numerical features:

The flow region is considered to be divided into blocks in which the medium properties are assumed to be uniform. Block-centered finite-difference numerical approximations are used. In plan view, the discretization is formed by dividing the area by two sets of parallel lines that may be variably spaced and the sets of lines are mutually perpendicular. In the vertical direction, the real conditions are approximated by a set of parallel layers. The resulting matrix problem is solved by using the SIP (the Strongly Implicit Procedure) iterative scheme. Mass balances are computed for each time step and as a cumulative volume from each source and type of discharge.

Past applications:

Many field problems.

Remarks:

During the 1970's and early 1980's, one of the most-used models for three-dimensional flow problems. See McDonald and Harbaugh (1988) for a newer code that has more capabilities.

Availability:

Reports are available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Related program:

Torak, L. J., 1982, Modifications and corrections to the finite-difference model for simulation of three-dimensional ground-water flow: U.S. Geological Survey Water-Resources Investigations Report 82-4025, 30 p.

Most significant changes to original program:

This report describes corrections to be made and extends the application of the Trescott three-dimensional program to simulations that involve leaky rivers, evapotranspiration as a linear function of depth to water, and discharge to drains and springs.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Related program:

Helgesen, J.O., Larson, S.P., and Razem, A.C., 1982, Model modifications for simulation of flow through stratified rocks in eastern Ohio: U.S. Geological Survey Water-Resources Investigations Report 82-4019, 109 p.

Most significant changes to original program:

The changes are as follows: The calculation for vertical leakage between adjacent aquifer layers allows for the case in which a lower aquifer converts from confined to unconfined conditions; a head-dependent function was added to simulate spring discharge from the top layer and interaction between leaky streams and the aquifer layer immediately below the top layer; recharge from precipitation to any layer can be simulated; water-budget calculations are made for each layer; and spring flow from the top aquifer can recharge the next lower aquifer.

<u>Past Applications:</u>

Few.

<u>Availability:</u>

Report is available from the USGS ESIC--Open-File Report Section.

<u>Related program:</u>

Torak, L.J., and Whiteman, C.D., Jr., 1982, Applications of digital modeling for evaluating the ground-water resources of the "2,000-foot" sand of the Baton Rouge area, Louisiana: Louisiana Department of Transportation and Development, Office of Public Works Water Resources Technical Report 27, 87 p.

<u>Most significant change to original program:</u>

The most significant changes were the simulation of transient-leakage effects in confining layers, and the addition of a program to quantify the effect of making selected changes in aquifer-parameter values on computed heads. The program gives estimates of the percentage change in parameter values that would reduce the sum of the squares of the differences between observed and computed heads.

<u>Past applications:</u>

Few.

<u>Availability:</u>

Report is available from:

Louisiana Department of Transportation and Development
Water Resources Section
P.O. Box 94245
Baton Rouge, LA 70804-9245

<u>Related program:</u>

Leahy, P.P., 1982, A three-dimensional ground-water flow model modified to reduce computer-memory requirements and better simulate confining-bed and aquifer pinchouts: U.S. Geological Survey Water-Resources Investigations Report 82-4023, 59 p.

<u>Most significant changes to original program:</u>

Modifications are presented that permit the simulation of confining-bed and aquifer pinchouts without the use of artificial hydraulic parameters, reduce the computer-memory requirements for aquifer systems that have complex external boundary shapes, and include the capability to approximate transient leakage from confining layers.

Availability:

Report is available from the USGS ESIC--Open-File Report Section

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Related program:

Meyer, W.R., and Carr, J.E., 1979, A digital model for simulation of ground-water hydrology in the Houston area, Texas: Texas Department of Water Resources Report LP-103, 27 p. (Appendix, 107 p.)

Most significant change to original program:

Land subsidence induced by ground-water extraction can be approximated. Different storage coefficients are used for elastic and inelastic compression of two clay layers. The choice of storage coefficient depends on the current head relative to the "critical head" associated with the maximum effective stress to which the clays have been previously subjected.

Past applications:

Few.

Availability:

Report and computer program are available from:

Texas Water Development Board
TNRIS
P.O. Box 13231
Austin, TX 78711

Three-Dimensional Finite-Difference

Program Documentation:

Posson, D.R., Hearne, G.A., Tracy, J.V., and Frenzel, P.F., 1980, A computer program for simulating geohydrologic systems in three dimensions: U.S. Geological Survey Open-File Report 80-421, 795 p.

Description:

   This program has the same basic capabilities as Trescott's (1975) except that (1) this
   program uses "cube" input commands that allow the modeler to change aquifer
   parameters by zones that are believed to have uniform values and reinitialize the model
   with few input records; (2) a data-swapping procedure between the central memory and
   the peripheral storage devices exploits the nature of the SIP (strongly implicit
   procedure) matrix-solving technique by solving for heads at a subset of blocks at any
   one time, this data-swapping procedure allows simulations to be run that involve more
   blocks than can be handled by the approach of having all the problem variables in
   central memory at one time; and (3) in flow systems characterized by aquifer layers,
   separated by tight "confining" layers, the effects of storage in the confining layers is
   approximated.

Numerical features:

   They are the same as for Trescott's (1975) except that an analytical/numerical
   approximation is included for transient leakage from the confining beds.

Past applications:

   Few.

Availability:

   Report is available from the USGS ESIC--Open-File Report Section.

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Related program:

   Hearne, G.A., 1982, Supplement to the New Mexico three-dimensional model: U.S.
   Geological Survey Open-File Report 82-857, 90 p.

Most significant changes to original program:

   The computer program, which was discussed in Posson and others (1980), was changed
   to allow representation of more than one head-dependent flow boundary in each cell, to
   improve the program stability and convergence by making the calculation of flow at
   such boundaries more implicit, and to allow the program to execute on a CRAY-1
   computer.

Past applications:

   Few.

Availability:

   Report is available from the USGS ESIC--Open-File Report Section.

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Three-Dimensional Finite-Difference

Program Documentation:

McDonald, M.G., and 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, chap. A1, 586 p.

Description:

The model (referred to as MODFLOW) simulates steady and nonsteady flow in an irregularly shaped flow system in which aquifer layers can be confined or unconfined or both. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can be simulated. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotropic (restricted to having the principal directions aligned with the grid axes and the anisotropy ratio between horizontal coordinate directions is fixed in any one layer) and the storage coefficient may be heterogeneous. The model requires input of the ratio of vertical hydraulic conductivity to distance between vertically adjacent block centers. Specified head and specified flux boundaries can be simulated as can a head–dependent flux across the outer boundary of the model that allows water to be supplied to a boundary block in the modeled area at a rate proportional to the current head difference between a "source" of water outside the modeled area and the boundary block.

Numerical features:

The flow region is considered to be divided into blocks in which the medium properties are assumed to be uniform. The plan view rectangular discretization results from a grid of mutually perpendicular lines that may be variably spaced. In the vertical direction, zones of varying thickness are transformed into a set of parallel "layers." The associated matrix problem is solved by using either the SIP (Strongly Implicit Procedure) or the SSOR (slice-successive overrelaxation). Mass balances are computed for each time step and as a cumulative volume from each source and type of discharge.

Past applications:

Widely used.

Remarks:

This is the most-used numerical model in the U.S. Geological Survey for ground-water flow problems. An efficient contouring program is available (Harbaugh, 1990a) to visualize heads and drawdowns output by the model.

Availability:

Report is available from the USGS Map Distribution. Computer program and report are available from NWIS.

Related program:

Kuiper, L.K., 1987, Computer program for solving ground-water flow equations by the preconditioned conjugate gradient method: U.S. Geological Survey Water-Resources Investigations Report 87-4091, 24 p.

Most significant changes to original program:

A preconditioned conjugate-gradient method is given for the solution of the finite-difference approximating equations generated by the modular flow model. Five preconditioning types may be chosen—three different types of incomplete Choleski, point Jacobi, or block Jacobi. Either a head change or residual error criteria may be used as an indication of solution accuracy and iteration termination.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Scott, J.C., 1990, A statistical processor for analyzing simulations made using the modular finite-difference ground-water flow model: U.S. Geological Survey Water-Resources Investigations Report 89-4159, 218 p.

Most significant changes to original program:

The report described the computer program MMSP (Modular Model Statistical Processor). By using MMSP, data input or output from the modular model MODFLOW can be used to calculate descriptive statistics, generate histograms, make logical comparisons between data arrays, generate new data arrays by operating on specified data arrays, and prepare data files that can be used to graphically display some of the model results.

Past applications:

Several.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Orzol, L.L., and McGrath, T.S., 1992, Modifications of the U.S. Geological Survey modular, finite-difference, ground-water flow model to read and write geographical information system files: U.S. Geological Survey Open-File Report 92-50, 202 p.

Most significant changes to original program:

The report documented the design and use of the program MODFLOWARC which is an enhanced version of MODFLOW that can transfer data directly between ARC/INFO software and the ground-water flow model. ARC/INFO can be used to process data that is in a nongridded form into the gridded form required for input to the ground-water model, and to graphically display and edit the gridded data sets.

Past applications:

Several.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Harbaugh, A.W., 1990b, A computer program for calculating subregional water budgets using results from the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 90-392, 46 p.

Most significant changes to original program:

This report describes the computer program ZONEBUDGET that uses cell-by-cell flow data saved by the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model. ZONEBUDGET calculates water-budgets for subareas within the modeled region, as defined by the user.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available form NWIS.

Related program:

Leake, S.A., and Prudic, D.E., 1991, Documentation of a computer program to simulate aquifer-system compaction using the modular finite-difference ground-water flow model: Techniques of Water-Resources Investigations of the United States Geological Survey, book 6, chap. A2, 68 p.

Most significant changes to original program:

Removal of ground water by pumping from aquifers may result in compaction of compressible fine-grained beds that are within or adjacent to the aquifers. Compaction of the sediments and resulting land subsidence may be permanent if the head declines result in vertical stresses beyond the previous maximum stress. The process of permanent compaction is not routinely included in simulations of ground-water flow. This computer program was written for use with the U.S. Geological Survey modular finite-difference ground-water flow model, to simulate storage changes from elastic and inelastic compaction.

Past applications:

Limited.

Availability:

Report is available from the USGS Map Distribution. Computer program and report are available from NWIS.

Related program:

Miller, R.S., 1988, User's guide for RIV2—A package for routing and accounting of river discharge for a modular, three-dimensional, finite-difference, ground-water flow model: U.S. Geological Survey Open-File Report 88-435, 33 p.

Most significant changes to original program:

This computer program was developed to provide an accounting for river discharge by river reach. The program limits the maximum leakage from a river to the aquifer by considering the river discharge available and assuming that the maximum effective downward head difference is the difference in elevation between the stream stage and the streambed bottom. The user needs to specify the stream stage for each stream reach, and the stage is assumed to not vary with stream discharge.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

Related program:

Hansen, A.J., Jr., 1993, Modifications to the modular three-dimensional finite-difference ground-water flow model used for the Columbia Plateau regional aquifer-system analysis, Washington, Oregon, and Idaho: U.S. Geological Survey Open-File Report 91-532, 162 p.

Most significant changes to the original program:

Changes are described that permit flow between layers to be simulated without the use of artificial hydraulic parameters, and the simulation of canyons and other flow barriers (for example, faults) that are much narrower than a grid cell.

Past applications:

Recently published.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Related program:

Prudic, D.E., 1989, Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model: U.S. Geological Survey Open-File Report 88-729, 113 p.

Most significant changes to original program:

This computer program was written for use in the modular finite-difference ground-water flow model to account for the amount of flow in streams and to simulate the interaction between surface streams and ground water. This package is not a true surface-water flow model but rather is an accounting program that tracks the flow in one or more streams that interact with ground water. The program limits the amount of ground-water recharge to the available streamflow. The stream stage in each river reach is computed by using the Manning formula under the assumption that the stream channel is rectangular. The program permits two or more streams to merge into one with flow in the merged stream equal to the sum of the tributary flow and also permits diversions from streams.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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<u>Related programs:</u>

Pollock, D.W., 1989, 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, 188 p.

Pollock, D., W., 1990, A Graphical Kernel System (GKS) version of computer program MODPATH-PLOT for displaying path lines generated from the U.S. Geological Survey three-dimensional ground-water flow model: U.S. Geological Survey Open-File Report 89-622, 49 p.

<u>Most significant changes to original program:</u>

This particle-tracking program was developed to compute three-dimensional path lines on the basis of output from steady-state simulations obtained with the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model. The package consists of two FORTRAN 77 computer programs—MODPATH, which calculates pathlines, and MODPATH-PLOT, which presents results graphically.

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

<u>Past applications:</u>

Widely used.

<u>Remarks:</u>

This is a very powerful tool for determining pathlines in flow models.

<u>Availability:</u>

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

<u>Related program:</u>

Hill, M.C., 1990, <u>P</u>reconditioned <u>C</u>onjugate-<u>G</u>radient 2 (PCG2)—A computer program for solving ground-water flow equations: U.S. Geological Survey Water-Resources Investigations Report 90-4048, 43 p.

Most significant changes to original program:

This report described and documented two preconditioned conjugate-gradient methods
(a modified incomplete Choleski factorization and a least-squares polynomial
preconditioner) that can be used for the solution of the system of linear equations in the
U.S. Geological Survey modular three-dimensional finite-difference ground-water
flow model.

Past applications:

Many.

Remarks:

This efficient matrix solver is gaining acceptance as a good alternative to the standard
solvers as more people gain experience with it.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer
program and report are available from NWIS.

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Related program:

Hill, M.C., 1992, A computer program (MODFLOWP) for estimating parameters of a
transient, three-dimensional, ground-water flow model using nonlinear regression:
U.S. Geological Survey Open-File Report 91-484, 358 p.

Most significant changes to original program:

When this new version of the U.S. Geological Survey modular, three-dimensional,
finite-difference, ground-water flow model (MODFLOW) is combined with the new
Parameter-Estimation Package, which also is documented in Hill (1992), it can be used
to estimate parameters by nonlinear regression. The new version of MODFLOW is
called MODFLOWP and functions nearly identically to MODFLOW when the
Parameter-Estimation Package is not used. Parameters are estimated by minimizing a
weighted least-squares objective function by either the modified Gauss-Newton
method or a conjugate-direction method. The following MODFLOW model input
parameters can be estimated: transmissivity and storage coefficient of confined layers;
hydraulic conductivity and specific yield of unconfined layers; vertical leakance;
horizontal and vertical anisotropy; hydraulic conductance of the River, Streamflow-
Routing, General-Head Boundary, and Drain Packages; areal recharge rates; maximum
evapotranspiration; pumpage rates; and the hydraulic head at constant-head boundaries.
Any spatial variation in parameters can be defined by the user. Data used to estimate
parameters can include independent estimates of parameter values, observed hydraulic
heads or temporal changes in hydraulic heads, and observed gains and losses along

head-dependent boundaries (such as streams). Model output includes statistics for analyzing the parameter estimates and the model; these statistics can be used to quantify the reliability of the resulting model, to suggest changes in model construction, and to compare results of models constructed in different ways.

Past applications:

Recently published.

Remarks:

Hill (1994) describes five computer programs that use results from MODFLOWP to (1) produce data sets that can be used to create two graphs commonly used to test weighted residuals that are important in analyzing regression results, (2) calculate linear confidence and prediction intervals, (3) test the validity of one of the assumptions of the method used to calculate linear confidence and prediction intervals.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Harbaugh, A.W., 1992, A generalized finite-difference formulation for the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 91-494, 60 p.

Most significant changes to original program:

The U.S. Geological Survey's three-dimensional finite-difference modular ground-water flow model MODFLOW assumes that model nodes are in the center of cells and that transmissivity is constant within a cell. On the basis of these assumptions, the model calculates coefficients, called conductances, that are multiplied by head difference to determine flow between cells. Although these are common assumptions in finite-difference models, other assumptions are possible. This option to the model program allows conductance to be part of the input data rather than calculating it. This option allows the user to calculate conductance outside of the model. The user thus has the flexibility to define conductance by using any desired assumptions.

Past applications:

New program.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Reilly, T.E., and Harbaugh, A.W., 1993b, Source code for the computer program and sample data set for the simulation of cylindrical flow to a well using the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 92-659, 7 p., diskette in pocket.

Most significant changes to original program:

The computer program documented in this report serves as a preprocessor to the U.S. Geological Survey model MODFLOW by creating the input data file needed to implement an axisymmetric conceptualization for simulation of flow to a well. The theory involves the conceptualization of a system of concentric shells that are capable of reproducing the large variations in gradient in the vicinity of the well by decreasing their area in the direction of the well. The theory and logic of the computer program, as well as an example of the use of the preprocessor, are described in Reilly and Harbaugh (1993a). The preprocessor generates a data set that is to be used with the General Finite-Difference Package (Harbaugh, 1992) of the U.S. Geological Survey modular finite-difference ground-water flow model.

Past applications:

New.

Availability:

Report (which contains the program on diskette) is available from either the USGS ESIC--Open-File Report Section or NWIS.

Related program:

Goode, D.J., and Appel, C.A., 1992, Finite-difference interblock transmissivity for unconfined aquifers and for aquifers having smoothly varying transmissivity: U.S. Geological Survey Water-Resources Investigations Report 92-4124, 79 p.

Most significant change to original program:

The interblock transmissivity calculated by the modular finite-difference model of McDonald and Harbaugh (1988) is a weighted harmonic mean. This report described changes to that model to incorporate alternative interblock transmissivity functions for the cases of linear spatial variation of transmissivity in a confined aquifer and either uniform hydraulic conductivity or hydraulic conductivity that varies linearly with distance in an unconfined aquifer.

Past applications:

New.

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Related program:

Hsieh, P. A., and Freckleton, J. R., 1993, Documentation of a computer program to simulate horizontal-flow barriers using the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 92-477, 32 p.

Most significant changes to original program:

The horizontal-flow-barrier (HFB) package simulates thin, vertical, low-permeability geologic features that impede the horizontal flow of ground water. These geologic features are approximated as a series of HFB's conceptually situated on the boundaries between pairs of adjacent cells in a finite-difference grid. Two key assumptions underlie the HFB package—the width of the barrier is negligibly small in comparison to the horizontal dimensions of the cells in the grid and the barrier has zero storage capacity.

Past applications:

New program.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Related program:

McDonald, M.G., Harbaugh, A.W., Orr, B.R., and Ackerman, D.J., 1992, A method of converting no-flow cells to variable-head cells for the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 91-536, 99 p.

Most significant changes to original program:

The original model, MODFLOW, could simulate the desaturation of variable-head model cells, which resulted in their conversion to no-flow cells, but could not simulate the resaturation of cells. This report described an option that was added to MODFLOW to allow cells to convert from no-flow to variable head; this process is called "wetting" a cell. Examples of situations for which the wetting capability is useful are the recovery of water levels when pumping wells are turned off, and the mounding that can occur in response to irrigation applied to the land surface above an aquifer. This wetting capability also is very useful in situations where cells incorrectly go dry (convert to no

flow) as part of the iterative solution process. During the iterative solution process, heads in some cells may decrease to less than their final values, which may cause such cells to go dry. The new wetting capability allows such cells to convert back to wet.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Related program:

Leake, S.A., Leahy, P., and Navoy, A.S., in press, Documentation of a computer program to simulate transient leakage from confining units using the modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 94-59.

Most significant changes to original program:

The computer package TLK1 represents a new method of simulating transient leakage from confining beds. The method incorporated into the TLK1 package is a solution of integrodifferential equations that describe flow at the upper and lower boundaries of confining units. The package is applicable to confining units in which flow is nearly vertical, confining unit properties do not vary vertically, the specific storage of the confining unit does not vary with head, and the confining unit is bounded below by an aquifer and above by an aquifer or a specified-head boundary. The TLK1 package can not simulate transient leakage in a confining unit bounded on top or bottom by an impermeable boundary.

The TLK1 package allows simulation of transient leakage without use of additional model layers to simulate flow in the confining units. Use of this package for some problems is more accurate and less computationally intensive than use of model layers to simulate confining units.

Past applications:

New program.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Two-Dimensional--Parameter Estimation

Program Documentation:

Cooley, R.L., and Naff, R.L., 1990, Regression modeling of ground-water flow: Techniques of Water-Resources Investigations of the U.S. Geological Survey, book 3, chap. B4, 232 p., diskette in pocket.

Description:

Regression procedures are used to solve for one or more of the following parameters: transmissivity, vertical hydraulic conductance (hydraulic conductivity divided by thickness) of sediments that underlie a stream or of an aquitard that overlies or underlies the aquifer, areally distributed recharge or discharge values, specific discharges normal to segments of the model boundary, and hydraulic heads at segments of the model boundary. This regression is based on steady-state observed heads, prior estimates of the regression parameters and their reliability, and known fluxes into or out of the aquifer.

Numerical features:

A rectangular grid is formed by two sets of mutually parallel and variably spaced lines. In this report, the intersections of the grid lines are called nodes, and the intragrid areas bounded by four adjacent nodes are called cells. The flow parameters, such as transmissivity, vertical hydraulic conductance, and distributed recharge and discharge, are assumed to be constant within a cell. Aquifer properties are characterized by zones, which are made up of a collection of cells. An integrated finite-difference method is used to develop a discrete form of solution of the flow equation. Various statistics associated with the regression analysis are computed.

Past applications:

Several.

Remarks:

An application of a preliminary version of the program, with modifications, was described in Garabedian (1986). Cooley (1993) described changes to the computer code that allow any model parameters to be transformed to natural logarithms and that improve the procedure for computing the parameter that is used to damp changes in the values of model parameters for each iteration of the solution method. In addition, instructions are given on how to input prior information on parameters separately from the set of initial parameter values.

Availability:

Report is available from the USGS Map Distribution. The computer program is contained on a diskette that comes with the report.

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Coupled Ground-Water and Surface-Water Flow Model

Program Documentation:

Swain, E.D., and Wexler, E.J., 1993, A coupled surface-water and ground-water flow model for simulation of stream-aquifer interaction: U.S. Geological Survey Open-File Report 92-138, 162 p.

Description:

The program couples the ground-water flow model MODFLOW with the surface-water flow model BRANCH to form a package called MODBRANCH. MODFLOW is a modular three-dimensional finite-difference ground-water model (McDonald and Harbaugh, 1988, see description under "three-dimensional finite-difference"), and BRANCH (Schaffranek, Baltzer, and Goldberg, 1981) is a one-dimensional finite-difference model used to simulate the unsteady flow in a single open network of reaches composed on interconnected channels. The "linkage" between the aquifer and the surface-water models is a term that corresponds to the flow (commonly referred to as the "leakage") across the streambed between the stream and the aquifer in response to a difference in heads in the two places. BRANCH is based on a comprehensive set of unsteady flow equations and, within the limitations inherent in a one-dimensional formulation of streamflow, can accommodate a variety of open-channel flow problems.

Numerical features:

The BRANCH code was modified (to form BRANCH') to allow it to be called from MODFLOW. The surface-water time-step size selected in using BRANCH' must be such that the ground-water time step is an integral multiple of the surface-water time step. The leakage flow rates between the stream and the aquifer calculated by using BRANCH' are averaged over an entire ground-water time step and used in MODFLOW as the leakage for the time step. The aquifer head used at each BRANCH' time step is linearly interpolated from heads calculated by using MODFLOW at the beginning and end of its time step. This approach necessitates multiple interactions between BRANCH' and MODFLOW for each MODFLOW time step. The authors reported that while this approach may not be as numerically stable at high leakage rates as the implicit calculation of leakage in MODFLOW, it is needed to maintain mass balance between the two models.

Past applications:

New program.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

Related program:

Swain, E. D., 1993, Documentation of a computer program (Streamlink) to represent direct-flow connections in a coupled ground-water and surface-water model: U.S. Geological Survey Water-Resources Investigations Report 93-4011, 62 p.

Most significant change to original program:

The program Streamlink allows direct-flow connections to be simulated among the MODFLOW ground-water model, the channel stage RIVER package (see McDonald and Harbaugh, 1988), the flow-routing stream package (see Prudic, 1989) and the unsteady open-channel model BRANCH by using the MODBRANCH coupling program. Two of the new connections are useful in modeling direct inlet/outlet between channels and the lakes or wetlands when the lakes or wetlands are represented by a high-conductivity aquifer block. Four other connections allow the three channel packages to connect to each other, thus modeling different sections of a channel network with various methods. The appeal of this flexibility in channel representation is that for some field problems, computation time can be reduced significantly by using the simpler packages for some of the channel sections without incurring a loss in accuracy.

Past applications:

New program.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Soil Moisture Accounting Program Coupled to a Two-Dimensional Unconfined/Confined Aquifer System

Program Documentation:

Reed, J.E., Bedinger, M.S., and Terry, J.E., 1976, Simulation procedure for modeling transient water-table and artesian stress and response: U.S. Geological Survey Open-File Report 76-792, 173 p.

Description:

The program (called SUPERMOCK) was designed to simulate transient stress and response of an aquifer system that consists of a confined aquifer overlain by a water-table aquitard; climatic conditions and soil and vegetative properties, as well as the hydraulic properties of the aquifer system, must be taken into consideration. This aquifer system can be in various degrees of hydraulic connection with streams and lakes. The model has three components—a soil-moisture accounting component that

computes changes in soil-moisture storage and recharge and discharge from the zone of aeration to the water table; a vertical-flow component that computes the altitude of the water table in the fine-grained water-table aquitard that overlies the confined aquifer; and a horizontal flow component that computes accretion to the confined aquifer and its nonsteady heads. Simulated stresses on the confined aquifer include changes in stream stage, withdrawal by wells and infiltration or evapotranspiration or both, through the fine-grained zone above the confined aquifer.

Numerical features:

The grid is a rectangular array of nodes, which are at the intersection of two sets of mutually perpendicular lines (rows and columns). The spacing of nodes can differ in either direction. Data on properties of the aquifer and boundary conditions are specified at each node. Finite-difference numerical approximations are used. The resulting matrix problem is solved by using the ADIP (alternating-direction implicit procedure).

Past applications:

A few field applications.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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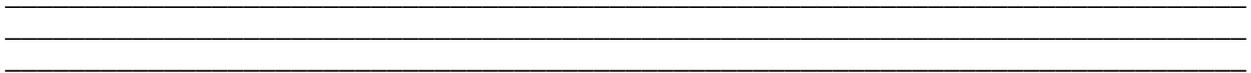
FLOW-VARIABLY SATURATED

Two-Dimensional

Program Documentation:

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

Description:

Simulates isothermal, two-dimensional movement of liquid water in variably saturated porous media. The mathematical model of this physical process is developed by combining the law of conservation of fluid mass with a nonlinear form of Darcy's law. The resultant mathematical model, or flow equation, is written with total hydraulic potential as the dependent variable. This allows straightforward treatment of saturated and unsaturated conditions. In addition, the model can simulate "difficult" nonlinear problems, such as those caused by infiltration into dry soils and by discontinuities in permeabilities and porosities.

Numerical features:

The model can analyze problems in one and two dimensions with planar or cylindrical geometries. The spatial derivatives in the flow equation are approximated by central differences written about grid-block boundaries. Time derivatives are approximated by a fully implicit backward scheme. Nonlinear storage terms are linearized by an implicit Newton-Raphson method. Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighting, the arithmetic mean, or the geometric mean of values from adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance-weighted harmonic means. The linearized matrix equations are solved by using SIP (the strongly implicit procedure).

Past applications:

Several.

Remarks:

Some additional modifications to the computer program VS2D are described in Healy (1990), which is listed in the section "Solute Transport--Variably Saturated."

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Related program:

Healy, R.W., 1987, Simulation of trickle irrigation, an extension to the U.S. Geological Survey's computer program VS2D: U.S. Geological Survey Water-Resources Investigations Report 87-4086, 61 p.

Most significant changes to original program:

A method for use with VS2D is presented for simulating water movement through unsaturated porous media in response to a constant rate of application from a surface source. Because the rate at which water can be absorbed by soil is limited, the water will pond; therefore, the actual surface area over which the water is applied may change with time and, in general, will not be known beforehand. An iterative method is used to determine the size of this ponded area at any time. This method will be most useful for simulating trickle irrigation and may be of value for simulating movement of water in soils as a result of an accidental spill.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Two-Dimensional Diffusion

Program Documentation:

Ishii, A.L., Healy, R.W., and Striegl, R.G., 1989, A numerical solution for the diffusion equation in hydrogeologic systems: U.S. Geological Survey Water-Resources Investigations Report 89-4027, 86 p.

Description:

This program provides a numerical solution of the linear diffusion equation in one or two dimensions in cartesian or cylindrical coordinates. Applications of the program include molecular diffusion, heat conduction, and fluid flow in confined ground-water systems. The flow media may be anisotropic and heterogenous.

Numerical features:

The model uses a block-centered finite-difference method. The resulting matrix equation is solved by the method of preconditioned conjugate gradients. The model allows the specification of various boundary conditions for any number of stress periods.

Past applications:

Very few.

Remarks:

The report describes application of the model to a hypothetical two-dimensional field situation that involves gas (methane in this case) diffusion in the unsaturated zone.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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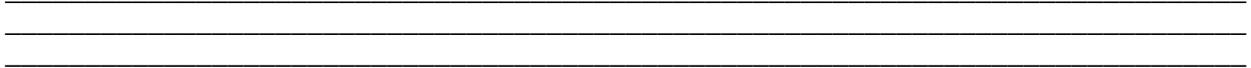
SOLUTE TRANSPORT--SATURATED

One-Dimensional Finite-Difference Method

Program Documentation:

Grove, D.B., and Stollenwerk, K.G., 1984, Computer model of one-dimensional equilibrium-controlled sorption processes: U.S. Geological Survey Water-Resources Investigations Report 84-4059, 58 p.

Description:

A numerical solution to the one-dimensional solute-transport equation with equilibrium-controlled sorption and a first-order irreversible-rate reaction is presented. Sorption reactions include Langmuir, Freundlich, and ion-exchange, with or without equal valence.

Numerical features:

General equations that describe transport and reaction processes are solved by finite-difference methods; nonlinearities are accounted for by iteration.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Two-Dimensional Method of Characteristics

Program Documentation:

Konikow, L.F., and Bredehoeft, J.D., 1978, Computer model of two-dimensional solute transport and dispersion in ground water: Techniques of Water-Resources Investigations of the United States Geological Survey, book 7, chap. C2, 90 p.

Goode, D.J., and Konikow, L.F., 1989, Modification of a method-of-characteristics solute-transport model to incorporate decay and equilibrium-controlled sorption or ion exchange: U.S. Geological Survey Water-Resources Investigations Report 89-4030, 65 p.

Description:

This model simulates solute transport in flowing ground water. It is applicable to one- or two-dimensional problems that involve steady-state or transient flow. The model computes changes in concentration over time caused by the processes of advective transport, hydrodynamic dispersion, mixing or dilution from fluid sources, and the following types of chemical reactions: first-order irreversible-rate reaction, such as radioactive decay; reversible equilibrium-controlled sorption with linear, Freundlich, or Langmuir isotherms; and reversible equilibrium-controlled ion exchange for monovalent or divalent ions. The first type of reaction is accounted for by an exponential decay term applied directly to the particle concentration. The second and third types of reactions are incorporated through a retardation factor, which is a function of concentration for nonlinear cases. Gradients of fluid density, viscosity, and temperature are assumed not to affect the velocity distribution. However, the aquifer may be heterogeneous and anisotropic.

The model has been evolving since its first release in the report by Konikow and Bredehoeft (1978). The updated model is reflected in the Goode and Konikow (1989) report, and both reports are required for a complete documentation.

Numerical features:

The model couples the ground-water flow equation with the solute-transport equation. The digital computer program uses the IADIP (iterative alternating-direction implicit procedure) to solve a finite-difference approximation to the ground-water flow equation and the method of characteristics to solve the solute-transport equation. The model uses a particle-tracking procedure to represent convective transport and a two-step explicit procedure to solve a finite-difference equation that describes the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity. This explicit procedure has several stability criteria, but the consequent time-step limitations are automatically determined by the program.

Past applications:

Widely used.

Remarks:

This is one of the most-used models for solute-transport problems. Complete documentation of the current version of this model requires the Konikow and Bredehoeft (1978) report and the report by Goode and Konikow (1989).

Availability:

The Konikow and Bredehoeft (1978) report is available from the USGS Map Distribution. The Goode and Konikow (1989) report is available from the USGS ESIC Open-File Report Section. Computer program and both reports (including updates to the program) are available from NWIS program office.

Related program:

Garabedian, S.P., and Konikow, L.F., 1983, Front-tracking model for convective transport in flowing ground water: U.S. Geological Survey Water-Resources Investigations Report 83-4034, 55 p.

Most significant change to original program:

Unlike the original program this program does not represent dispersion and dilution. The model tracks representative water or tracer particles, initially located along specified lines, as they move in response to the ground-water velocity field.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Related program:

Sanford, W.E., and Konikow, L.F., 1985, A two-constituent solute-transport model for ground water having variable density: U.S. Geological Survey Water-Resources Investigations Report 85-4279, 88 p.

Most significant change to original program:

This model was developed to simulate advective solute transport and dispersion of either one or two constituents in ground water in a cross-sectional plane where the density and viscosity of one constituent is a function of concentration.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Two-Dimensional Finite-Element Galerkin Method

Program Documentation:

Lewis, F.M., Voss, C.I., and Rubin, Jacob, 1986, Numerical simulation of advective-dispersive multisolute transport with sorption, ion exchange and equilibrium chemistry: U.S. Geological Survey Water-Resources Investigations Report 86-4022, 165 p.

Description:

This model simulates fully saturated two-dimensional transient, or steady-state, areal or cross-sectional, constant-density ground-water flow and multisolute transport. The options for transport under the condition of local equilibrium are linear sorption and up to two aqueous complexations and binary ion exchange and a single complexation reaction that involves one of the exchanging species.

Numerical features:

This model, SATRA-CHEM, is a modified version of the computer program SUTRA (Voss, 1984a). A finite-element Galerkin method is used for spatial approximations of the dependent variable and backwards finite-difference method for its time derivative. Hydraulic conductivities of each element can be anisotropic and variable in direction and magnitude. Boundary conditions and source/sink terms can vary with time.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Dual-Porosity Flow and Transport

Program Documentation:

Glover, K. C., 1987, A dual-porosity model for simulating solute transport in oil shale: U.S. Geological Survey Water Resources Investigations Report 86-4047, 88 p.

Description:

This model simulates three-dimensional flow and advective transport and hydrodynamic dispersion in an aquifer that has parallel fractures separated by nonfractured rock with significant porosity and negligible hydraulic conductivity. The flow and transport are assumed to take place primarily in the fractures with the potential for the exchange of solute between fluid in the fracture and the nonfractured rock by

molecular diffusion. Such diffusion is simulated by including a source-sink term developed from the analytical solution for the problem of mass transfer from two parallel, constant-concentration boundaries into the intervening material.

Numerical features:

By using the finite element Galerkin procedure, the differential equations that describe flow and mass transport are approximated by a system of linear equations. The system of equations are solved by selected forms of Gauss elimination.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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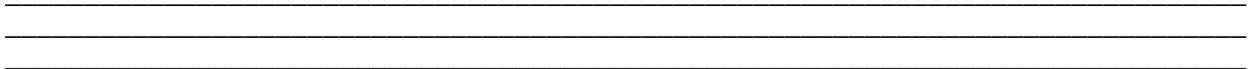
SOLUTE TRANSPORT--VARIABLY SATURATED

Two-Dimensional Finite-Difference Method

Program 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, 125 p.

Description:

This report documents VS2DT, which simulates two-dimensional solute transport in
porous media under variably saturated conditions. The program is an extension of the
U.S. Geological Survey's computer program VS2D (Lappala, Healy, and Weeks,
1987), which simulates water movement through variably saturated porous media. The
extension consists of four new subroutines and slight modifications to existing routines.
VS2DT may be a useful tool in studies of water quality, ground-water contamination,
waste disposal, or ground-water recharge.

Numerical features:

VS2DT uses a finite-difference approximation to the advection/dispersion equation, as
well as the nonlinear water-flow equation (based on total hydraulic head). It can
simulate problems in one, two (vertical cross section), or three dimensions (axially
symmetric). The porous media may be heterogeneous and anisotropic, but principal
directions must coincide with the coordinate axes. Boundary conditions for flow can
take the form of fixed pressure heads, infiltration with ponding, evaporation from the
soil surface, plant transpiration, or seepage faces. An extension to Healy's (1987)
program also allows simulation of infiltration from trickle irrigation. Boundary
conditions for solute transport include fixed solute concentration and fixed mass flux.
Solute source/sink terms include first-order decay, equilibrium partitioning to the solid
phase (as described by Langmuir or Freundlich isotherms), and ion exchange. The
design of the program is modular, so that programmers can easily modify subroutines
and functions to apply the model to particular field, laboratory, or hypothetical
problems.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer
program and report are available from NWIS.

SOLUTE AND HEAT TRANSPORT--SATURATED

Three-Dimensional Finite-Difference Method

Program Documentation:

INTERCOMP Resource Development and Engineering, Inc., 1976, A model for calculating effects of liquid waste disposal in deep saline aquifers: U.S. Geological Survey Water-Resources Investigations Report 76-61, 263 p.

Description:

A transient, three-dimensional model was developed to solve the three coupled governing equations for pressure, mass and heat transport. Although this program was initially developed to simulate certain aspects of waste injection into confined saline aquifers, it also is suitable for other applications that involve significant spatial variation in temperature and solute mass.

Numerical features:

The model is a finite-difference solution to the pressure, energy, and mass-transport equations. Equation parameters, such as viscosity and density, are allowed to be functions of the dependent variables of the equations. Multiple-user options allow the choice of three dimensional cartesian or r and z radial coordinates; various finite-difference methods; iterative and direct matrix solution techniques; restart options; and various provisions for output display.

Past applications:

Limited.

Remarks:

See Kipp (1987) for a current model of similar capabilities.

Availability:

Report is available from NTIS (PB–256 903/AS).

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Related program:

INTERA Environmental Consultants, Inc., 1979, Revision of the documentation for a model calculating effects of liquid waste disposal in deep saline aquifers: U.S. Geological Survey Water-Resources Investigations Report 79-96, 79 p.

Most significant changes to original program:

The additions and modifications in this revision include a free water surface, vertical recharge, equilibrium-controlled linear adsorption, and a first-order irreversible rate reaction. These, plus additional modifications, make this model more adaptable to general hydrologic problems and those that involve waste disposal with simple chemical reactions.

Past applications:

Several.

Remarks:

See Kipp (1987) for a current model of similar capabilities.

Availability:

Report is available from NTIS (PB–80 122 542). Computer program and report are available from NWIS.

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Three-Dimensional Finite-Difference Method

Program Documentation:

Kipp, K.L., Jr., l987, HST3D—A computer code for simulation of heat and solute transport in three-dimensional ground-water flow systems: U.S. Geological Survey Water-Resources Investigations Report 86-4095, 5l7 p.

Description:

The Heat- and Solute-Transport Program (HST3D) simulates ground-water flow and associated heat and solute transport in three dimensions. This program is a descendant of the computer codes developed by INTERCOMP Resource Development and Engineering Inc. (1976) and revised by INTERA Environmental Consultants, Inc. (1979). HST3D may be used for analysis of such problems as those related to subsurface-waste injection, landfill leaching, saltwater intrusion, freshwater recharge and recovery, radioactive-waste disposal, hot-water geothermal systems, and subsurface-energy storage. The three governing equations are coupled through the interstitial pore velocity; the dependence of the fluid density on pressure, temperature, and solute-mass fraction; and the dependence of the fluid viscosity on temperature and solute-mass fraction. The solute-transport equation is for only a single solute species with possible linear-equilibrium sorption and linear decay.

Numerical features:

Finite-difference techniques are used to discretize the governing equations by using a point-distributed grid. The flow-, heat- and solute-transport equations are solved, in turn, after a partial Gauss-reduction scheme is used to modify them. The modified equations are more tightly coupled and have better stability for the numerical solutions. Two techniques are available for solution of the finite-difference matrix equations. One technique is a direct-elimination solver, in which equations are reordered by alternating diagonal planes. The other technique is an iterative solver, in which two-line successive overrelaxation is used.

Past applications:

Several.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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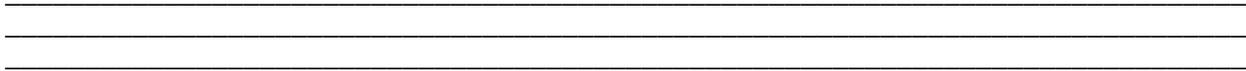
FLOW-SATURATED FRESHWATER/SALTWATER

Two-Dimensional Areal

Program Documentation:

Mercer, J.W., Larson, S.P., and Faust, C.R., 1980, Finite-difference model to simulate the areal flow of saltwater and freshwater separated by an interface: U.S. Geological Survey Open-File Report 80-407, 88 p.

Description:

The model is capable of simulating ground-water flow of saltwater and freshwater separated by an interface. The partial differential equations are integrated over the thicknesses of freshwater and saltwater, which results in two equations that describe the flow characteristics in the areal domain. The program is designed to simulate such time-dependent problems as those associated with the development of coastal aquifers and can treat water-table or confined conditions with steady-state leakage of fresh water. The program generally will be most applicable to the analysis of regional aquifer problems in which the zone between saltwater and freshwater can be considered to be a surface (sharp interface).

Numerical features:

The equations are approximated by using finite-difference techniques. The resulting algebraic equations are solved for the dependent variables, freshwater and saltwater heads using an iterative solution method.

Past applications:

Few field problems.

Remarks:

See Essaid (1990) for an updated three-dimensional model (SHARP) with similar capabilities.

Availability:

Report is available from the USGS ESIC--Open-File Reports Section. Computer program and report are available from NWIS.

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Two-Dimensional Areal

Program Documentation:

Voss, C.I., 1984b, AQUIFEM-SALT—A finite-element model for aquifers containing a seawater interface: U.S. Geological Survey Water-Resources Investigations Report 84-4263, 37 p.

Description:

This is an areal ground-water model that simulates head changes in and movement of only the freshwater in an aquifer. The freshwater and saltwater are assumed not to mix because they are separated by an effectively sharp interface. Vertical hydrostatic equilibrium in the freshwater and saltwater is assumed, and the model ignores any time lag that may result from transient horizontal saltwater flow as the interface attempts to readjust to a new hydrostatic equilibrium elevation. Parts of the freshwater lens may be confined above and below by less permeable units.

Numerical features:

A Galerkin finite-element formulation is used.

Past applications:

Few field problems.

Remarks:

This model is a modification to AQUIFEM, which is described by Pinder and Voss (1979). The computer code was prepared by George Pinder, Emil Frind, Peter Trescott, and Clifford Voss. Copies of that report may be obtained from:

AQUIFEM-SALT
U.S. Geological Survey
431 National Center
Reston, VA 22092

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Three-Dimensional (Sharp interface)

Program Documentation:

Guswa, J.H., and LeBlanc, D.R., 1985, Digital models of ground-water flow in the Cape Cod aquifer system, Massachusetts: U.S. Geological Survey Water-Supply Paper 2209, 112 p.

Description:

This model is a modification of the three-dimensional ground-water flow model described in Trescott (1975) and Trescott and Larson (1976). The modifications are based on the assumptions that the zone between fresh and saline ground water can be treated as an interface, that the saline-water zone is static, and that the flow system is in a state of dynamic equilibrium. Because the pressure in such a flow field must be continuous across the assumed interface, a relation can be written between the freshwater head and the elevation that must be satisfied at each point of the interface, which depends on the equivalent freshwater head along the seabed and the density difference between the freshwater and saline water. The computational scheme used requires that the starting head values be sufficiently large to define an interface position that is seaward of and deeper than the real interface position. During an iteration sequence, the calculated interface moves landward and upward until it is in balance with the freshwater flow system. The transmissivity of those zones that are calculated to be below the interface are assumed to be zero for computational purposes because the saline water is assumed to be static.

Past applications:

Few.

Availability:

Report is available from the USGS Map Distribution.

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Three-Dimensional (Sharp Interface)

Program Documentation:

Sapik, D.B., 1988, Documentation of a steady-state saltwater-intrusion model for three-dimensional ground-water flow, and user's guide: U.S. Geological Survey Open-File Report 87-526, 174 p.

Description:

This report describes changes made to Trescott's (1975) three-dimensional finite-difference ground-water flow program so that a steady-state sharp interface between freshwater and saltwater can be simulated. The model simulates flow only in the freshwater region and incorporates a Ghyben-Herzberg type approximation to locate the freshwater/saltwater interface.

Past applications:

Very few.

Availability:

Report is available from the USGS ESIC--Open-File Reports Section.

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Three-Dimensional (Sharp Interface)

Program Documentation:

Essaid, H.I., 1990, SHARP—A quasi-three-dimensional finite-difference simulation model for freshwater and saltwater flow in layered coastal aquifer systems: U.S. Geological Survey Water-Resources Investigations Report 90-4130, 181 p.

Description:

This model is a quasi-three-dimensional, numerical, finite-difference model that simulates freshwater and saltwater flow separated by a sharp interface in layered coastal aquifer/confining unit systems. SHARP facilitates regional simulation of coastal ground-water conditions in layered systems and includes the effects of saltwater dynamics on the freshwater flow system.

Numerical features:

The model accommodates multiple layered aquifers separated by confining units. Each aquifer is handled as a single layer with hydraulic properties that can vary spatially. The leakance (the ratio of vertical hydraulic conductivity to bed thickness) of confining layers also can vary spatially. The uppermost aquifer of the system may be confined, unconfined, or semiconfined with an areally distributed recharge. Temporal variations in recharge and pumping are accounted for by multiple pumping periods. The boundary conditions that may be simulated in the model are prescribed flux boundaries, constant freshwater and (or) constant saltwater-head boundaries, and leaky head-dependent boundaries in the uppermost aquifer. The program is written in FORTRAN 77.

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Three-Dimensional (Variable Density)

Program Documentation:

Weiss, Emanuel, 1982, A model for the simulation of flow of variable-density ground water in three dimensions under steady-state conditions: U.S. Geological Survey Open-File Report 82-352, 59 p.

Description:

The computer program associated with this model is a preprocessor for the constant density three-dimensional ground-water flow model by Trescott (1975). This preprocessor enables simulation of variable density flow fields, where the density is known throughout the three-dimensional flow field and is assumed to be constant in time (the density distribution does not change as a result of the movement of the fluid). Information on the density distribution and elevation of the layers is processed by the preprocessor, and the output from the preprocessor is calculated sources and sinks that when entered into the Trescott code will simulate the variable density flow field. Included in the report is a computer program for calculating ground-water density from aquifer depth, temperature, and dissolved solids concentration.

Numerical features:

The information required for the program's operation is aquifer elevation, thickness, and ground-water density. The report contains two FORTRAN programs that are used to generate the necessary flow-model input. The model is based on the same three-dimensional finite-difference scheme as the Trescott (1975) model.

Past applications:

Very few field problems.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Three-Dimensional (Variable Density)

Program Documentation:

Kuiper, L.K., 1985, Documentation of a numerical code for the simulation of variable density ground-water flow in three dimensions: U.S. Geological Survey Water Resources Investigations Report 84-4302, 80 p.

Description:

This is a numerical program for the simulation of variable density time-dependant ground-water flow in three dimensions. The ground-water density, although variable in space, is assumed to be approximately constant in time and known. The integrated finite difference grid elements in the program are rectangular when viewed from the vertical direction, but their top and bottom surfaces follow the curvature of the geologic strata in the modeled area.

Numerical features:

The program uses the integrated finite difference method. The SIP (strongly implicit procedure), SOR (successive overrelaxation), and eight different PCG (preconditioned conjugate gradient) methods are used to solve the approximating matrix equations.

Past applications:

Very few field applications.

Remarks:

The theoretical development, on which the numerical code is based, is described in Kuiper (1983).

Availability:

Report is available from the USGS ESIC--Open-File Reports Section. Computer program and report are available from NWIS.

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Three-Dimensional (Variable Density and Multiaquifer wells)

Program Documentation:

Kontis, A.L., and Mandle, R.J., 1988, Modification of a three-dimensional ground-water flow model to account for variable water density and effects of multiaquifer wells: U.S. Geological Survey Water Resources Investigations Report 87-4265, 78 p.

Description:

   This report described changes made to the constant density three-dimensional ground-
   water flow model of Trescott (1975) that allow it to be used for variable density flow
   fields in which the spatial distribution of the fluid density is assumed not to change with
   time. The report also described changes made to simulate wells open to more than a
   single aquifer.

Numerical features:

   In addition to describing the variable-density and multiple-well modifications to the
   Trescott model, two new computer programs were described. Those programs compute
   ground water and pure water density and dynamic viscosity and the horizontal and
   vertical hydraulic conductances and variable density input data for the Trescott model.
   A SSOR (slice-successive-over-relaxation) matrix solver is described.

Past applications:

   Limited.

Availability:

   Report is available from the USGS ESIC--Open-File Report Section.

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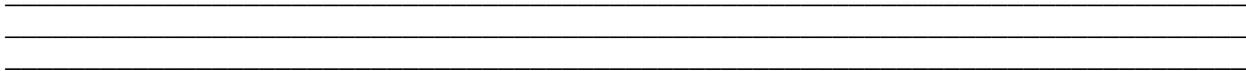
HEAT TRANSPORT

Two-Dimensional Single- and Two-Phase

Program Documentation:

Faust, C.R., and Mercer, J.W., 1977, Version I—A finite-difference model of two-dimensional, single- and two-phase heat transport in a porous medium: U.S. Geological Survey Open-File Report 77-234, 84 p.

Description:

The model can simulate two-dimensional (areal) flow of compressed water, two-phase mixtures, and super-heated steam over a temperature range of 10 to 300 ^{o}C. The model can handle the conversion from single-phase to two-phase flow. The dependent variables solved for are pressure and enthalpy. The aquifer is assumed to be underlain and overlain by impermeable layers that allow only conduction of heat. The aquifer permeability, porosity, and thickness can vary spatially. The permeability can be anisotropic in each block, but the principal directions must be aligned with the coordinate axes.

Numerical features:

The modeled area is divided into rectangular grid blocks (with nodes at the block centers) in which the fluid and aquifer properties are assumed to be uniform.

Past applications:

Limited.

Remarks:

It was recognized that the model would require some sophisticated changes and additions before a complicated field problem could be simulated; consequently, the model was considered to be a research tool only.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.
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Two-Dimensional Single-Phase

Program Documentation:

Mercer, J.W., and Pinder, G.F., 1975, A finite-element model of a two-dimensional, single-phase heat transport in a porous medium: U.S. Geological Survey Open-File Report 75-574, 115 p.

Description:

This program simulates the two-dimensional areal equations of ground-water flow and heat transport. The program solves for aquifer pressures and temperatures and allows vertical flow of heat and liquid through an overlying confining bed. An areally distributed heat function may be used to approximate a heat source below the aquifer.

Numerical features:

The Galerkin finite-element method is used. The basic shape of the elements are quadrilaterals, but the sides may be curved, depending on the degree of polynomial used to describe the side. Linear, quadratic, and cubic basis functions are available. The elements are designed to allow the basis functions on different sides of the same element to be polynomials of different degrees. Backward or central differences are used for time derivative.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Three-Dimensional

Program Documentation:

Reed, J.E., 1985, Digital model for simulating steady-state ground-water and heat flow: U.S. Geological Survey Water-Resources Investigations Report 85-4248, 134 p.

Description:

This model simulates the three-dimensional equation of ground-water and single-phase heat flow by convective flow and conduction. The thermal conductivity of the saturated rock materials and the volumetric specific heat for the fluid are assumed constants. The heat flows accounted for are geothermal heat flow, conduction to the land surface, convection from recharge from precipitation, and convection to or from fixed-head boundaries. Because the model assumes that fluid density is constant, buoyancy effects caused by fluid-density variations that result from temperature differences are not considered.

Numerical features:

The program is based on separate finite-difference approximations of the ground-water flow equation and of the convective-dispersive heat-flow equation. The ground-water

flow and heat flow models are interdependent because hydraulic conductivity in the ground-water flow model is a function of temperature and convective flow in the heat-flow model is a function of ground-water flow. The ground-water flow and heat-flow models use block-centered, finite-difference approximations. The hydraulic conductivity and porosity can vary from block to block. The program uses an iterative procedure that alternately solves the ground-water flow and heat-flow equations improving the estimate of convective flux after solution of the ground-water flow equation and improving the estimate of hydraulic conductivity after solution of the heat-flow equation. Time of travel is determined by particle tracking through the modeled region.

Past applications:

Limited.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Three-Dimensional

Program Documentation:

Hayba, D.O., and Ingebritsen, S.E., in press, The computer model HYDROTHERM, A three-dimensional finite-difference model to simulate ground-water flow and heat transport in the temperature range of 0 to 1,200 $^{\circ}$C: U.S. Geological Survey Water-Resources Investigations Report 94-4045.

Description:

The HYDROTHERM model simulates the flow of pure water and heat in a porous medium. The model allows for spatial and temporal variations of permeability, porosity, and thermal conductivity. HYDROTHERM incorporates pure-water equations of state that cover the temperature range of 0 to 1,200 $^{\circ}$C and pressures from 0.5 bars to 10 kbars. The governing equations are expressions of mass and energy conservation that are posed in terms of pressure and enthalpy. The advantage of pressure and enthalpy as the dependent variables is that they uniquely specify the thermodynamic state of the fluid under both single- and two-phase conditions. Major assumptions are that the rock matrix can be treated as a porous medium; that the water and rock are in thermal equilibrium; and that capillary pressure is negligible. The intrinsic permeability can be anisotropic in each block, but the principal directions are assumed to be aligned with the coordinate axes. Rock density and specific heat are assumed to be constants.

Numerical features:

The modeled region can be represented using cartesian or radial coordinate systems.The governing equations for the model require values for fluid densities, viscosities, and temperature. HYDROTHERM uses a bicubic interpolation routine to derive, for any given pressure-enthalpy pair, values of density, viscosity, and temperature, as well as the local gradients of those values with respect to pressure and enthalpy. For a fully three-dimensional model, the numerical solution technique used is slice-successive overrelaxation embedded in a Newton-Raphson iteration. The report describes five example problems solved using HYDROTHERM to demonstrate the thermodynamic range and multi-dimensional performance of the model.

Past applications:

New.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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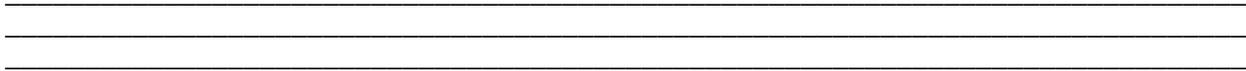
SOLUTE OR HEAT TRANSPORT--SATURATED AND UNSATURATED

Two-Dimensional Finite-Element Galerkin Method

Program Documentation:

Voss, C.I., 1984a, A finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport: U.S. Geological Survey Water-Resources Investigations Report 84-4369, 409 p.

Description:

The model may be employed for areal and cross-sectional modeling of saturated ground-water flow systems and for cross-sectional modeling of unsaturated zone flow. Solute-transport simulation that uses SUTRA may be employed to model natural or man-induced chemical species transport, which includes processes of solute sorption, production, and decay, and may be applied to analysis of ground-water contaminant transport problems and aquifer restoration designs. In addition, solute-transport simulation with SUTRA may be used for modeling of variable density leachate movement and for cross-sectional modeling of saltwater intrusion in aquifers, with either dispersed or relatively sharp transition zones between freshwater and saltwater. SUTRA energy-transport simulation may be employed to model thermal regimes in aquifers, subsurface heat conduction, aquifer thermal energy storage systems, geothermal reservoirs, thermal pollution of aquifers, and natural hydrogeologic convection systems.

Numerical features:

The model employs a two-dimensional hybrid finite-element and integrated-finite-difference method to approximate the governing equations that describe the following simulated interdependent processes: fluid density-dependent saturated or unsaturated ground-water flow and either transport of a solute in the ground water, in which the solute may be subject to equilibrium adsorption on the porous matrix, and both first- and zero-order production or decay, or transport of thermal energy in the ground water and solid matrix of the aquifer.

Past applications:

Many.

Remarks:

A graphical postprocessor developed by Souza (1987) is available for use with the computer code. This postprocessor facilitates interpretation of the simulation results.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report (including an update to the program) are available from NWIS.

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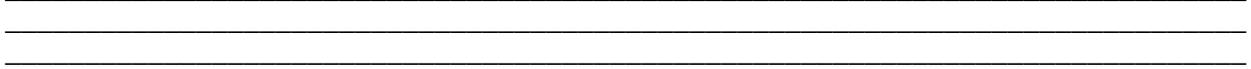
AQUIFER MANAGEMENT

Two-Dimensional Saturated Flow

Program Documentation:

Lefkoff, L.J., and Gorelick, S.M., 1987, AQMAN—Linear and quadratic programming matrix generator using two-dimensional ground-water flow simulation for aquifer management modeling: U.S. Geological Survey Water-Resources Investigations Report 87-4061, 164 p.

Description:

AQMAN provides a link between a modified version of the two-dimensional ground-water flow model of Trescott, Pinder, and Larson (1976) and any optimization program that expects an input file written in MPS (Mathematical Programming System) format. AQMAN uses the modified Trescott ground-water flow model to solve the basic ground-water flow equation to determine aquifer responses to the stresses that cannot be controlled because of physical limitations or either legal or socioeconomic demands (the unmanaged stresses) and that can be controlled (the managed stresses). A management problem is to determine the distribution of pumping and (or) recharge that minimizes or maximizes some user-specified objective function while satisfying user-specified constraints on the ground-water hydraulic conditions. AQMAN creates a data file written in MPS format that contains all the hydrologic information and management objectives needed by an optimization program to solve the management problem. MPS format is required by most standard linear and quadratic programming optimization packages.

Numerical features:

The spatial discretization of the aquifer is that used by the Trescott, Pinder, and Larson (1976) program. AQMAN requires that the management time periods, during which a particular decision variable is constant or a particular set of constraints apply, are equal in duration. AQMAN is written to handle either a linear or quadratic objective function. Various types of constraints can be defined for pumping and (or) recharge rates and on ground-water heads, gradients, and velocities. AQMAN assumes that the relation between aquifer stress and water-level response is essentially linear, that is, that linear superposition of solutions to the transient ground-water flow equation is appropriate.

Past applications:

Few.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Three-Dimensional Saturated Flow

Program Documentation:

Puig, J.C., and Rolon-Collazo, L.I., in press, User's manual for AQMAN3D—A mathematical programming system dataset generator for aquifer management using the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 92-481.

Description:

The computer code AQMAN3D provides a link between the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model, MODFLOW (see McDonald and Harbaugh, 1988), and any standard optimization program that uses MPS (Mathematical Programming System) input format. The program creates the input fields that will be used by the optimization program. The relation between AQMAN3D and MODFLOW is comparable to the relation between AQMAN (see Lefkoff and Gorelick, 1987) and the two-dimensional ground-water flow model of Trescott, Pinder, and Larson (1976), except that AQMAN3D permits applications to three-dimensional problems as opposed to the two-dimensional problem limitation of AQMAN.

Numerical features:

The user of AQMAN3D must be familiar with the MODFLOW code (see McDonald and Harbaugh, 1988) and documentation and should be familiar with the AQMAN documentation (see Lefkoff and Gorelick, 1987) to understand the basic concepts of aquifer-management modeling and problem formulation for linear and quadratic programming. One of the main differences between AQMAN3D and the AQMAN code is that AQMAN3D has three-dimensional capability.

Past applications:

This is a new code.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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CHEMICAL MASS BALANCE

Mass Balance and Electron Conservation

Program Documentation:

Parkhurst, D.L., Plummer, L. N., and Thorstenson, D. C., 1982, BALANCE—A computer program for calculating mass transfer for geochemical reactions in ground water: U.S. Geological Survey Water-Resources Investigations Report 82-14, 29 p.

Description:

BALANCE is a FORTRAN computer program designed to help define and quantify chemical reactions between ground water and soluble mineral assemblages. Given the chemical concentrations of various elements in water samples from two points along a flow path, together with the chemical compositions of a set of minerals, organic substances, or gases that are presumed to be the only, or at least dominant, potential reactive phases in the system, this program calculates the mass transfer (amounts of selected phases that dissolve or precipitate) necessary to account for the observed changes in element concentrations between the two water samples. Additional constraints can be included in the problem formulation to account for mixing two end-member waters with or without mineral-water interaction, redox reactions, and in a simplified form, isotopic composition.

Numerical features:

The number of potential reactive or product phases must equal the number of elements, except for mixing problems, in which case the number of reactive or product phases must be equal to the number of elements minus one. If oxidation reduction is considered, then an additional phase may be added. BALANCE solves a set of simultaneous linear equations that mathematically represent the conservation of mass for selected elements, conservation of electrons, and conservation of isotopic species.

Past applications:

Many.

Remarks:

The purpose of BALANCE is to derive balanced reactions of the form:

Initial Water + Reactant Phases → Final Water + Product Phases
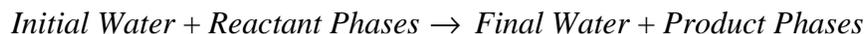
A "reaction model" is defined by the user-selected phases and the calculated amount of each phase necessary to satisfy this equation. Because the BALANCE models are not constrained by any thermodynamic criteria, the output may imply reactions that are not thermodynamically possible. Plummer, Parkhurst, and Thorstenson (1983) discussed methods for identifying reaction models that can be eliminated from consideration because they do not satisfy available thermodynamic, petrographic, mineralogic, or isotopic information.

Availability:

Report is available from NTIS (PB-82 255 902). Computer program and report are available from NWIS.

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Characterization of Natural Waters

Program Documentation:

Bodine, M.W., Jr., and Jones, B.F., 1986, THE SALT NORM—A quantitative chemical-mineralogical characterization of natural waters: U.S. Geological Survey Water-Resources Investigations Report 86-4086, 130 p.

Description:

The SALT NORM is the quantitative ideal equilibrium assemblage that would crystallize if the water evaporated to dryness at 25 $^{\circ}$C and 1 bar pressure under atmospheric partial pressure of CO_2. This assemblage is called ideal, in part, because certain liberties are necessarily inherent in the selection of the particular normative salts; for example, because the standard chemical potentials of many compound salts that are not found as minerals are unknown, those were excluded as possible normative salts. The SALT NORM is a computer program written in FORTRAN IV that quantitatively distributes 18 selected solutes (Mg, Ca, Na, K, Li, NH_4, Sr, Ba, Cl, SO_4, HCO_3, CO_3, F, Br, I, NO_3, B, PO_4) reported from an analysis into normative salts that are assigned from 63 selected possible normative salts to allow only stable associations on the basis of the Gibbs phase rule, available free energy values, and observed low-temperature mineral association.

Examination of over 500 salt norms calculated from water analyses that represent a wide range of concentrations and hydrochemical settings has suggested that certain key phases or assemblages are characteristic of solute origin.

Past applications:

Few.

Remarks:

Normative analysis of ground waters was used as an aid in the interpretation of the origin and evolution of waters in the Rustler Formation in southeastern New Mexico by Bodine and Jones (1990) and the Madrid Basin in Spain by Jones and Llamas (1989).

Report is available from the USGS ESIC--Open-File Report Section. Computer program and report are available from NWIS.

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Mass Balance Reaction Models That Satisfy Specified Constraints

Program Documentation:

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

Description:

NETPATH is an interactive FORTRAN 77 computer program used to interpret net geochemical mass balance reactions between an initial and final water along a hydrologic flow path. Given the chemical and isotopic data for two points on a flow path, NETPATH determines every possible geochemical mass balance reaction model that indicates the masses of plausible minerals and gases that must enter or leave the initial water along the flow path to define exactly a set of selected elemental, electron transfer, and isotopic constraints observed in a final (evolutionary) water. The calculations are of use in interpreting geochemical reactions, mixing proportions, evaporation and (or) dilution of waters, and mineral mass transfer in the chemical and isotopic evolution of natural environmental waters. If sufficient isotopic data are available, then Rayleigh distillation calculations are applied to each mass balance model that satisfies the constraints to predict carbon, sulfur, and strontium isotope compositions at the end point and an adjusted ^{14}C content that is useful for radiocarbon dating.

Numerical features:

The number of potential reactive or product phases must be at least as great as the constraints (except for the case of mixing). Constraints can be chemical elements, expression of electron conservation, or conservation of a particular isotope of an element.

If there are many more phases than constraints, then the total number of reaction models can be very large. Long computation times may be required to find all possible models. The total number of reaction models can be reduced by either deleting unnecessary phases or designating them for dissolution or precipitation only and then including appropriate forcing conditions for phases. For a phase to be "forced" means that every reaction model considered must contain that phase.

Past applications:

Many.

Remarks:

NETPATH combines information on mineral saturation indices with mass balance modeling to identify and quantify mineral reactions in the system. This interactive program allows the user to build a file that contains chemical and isotopic data for each water; runs the water analyses through a modified version of the speciation model, WATEQF (Plummer, Jones, and Truesdell, 1976); and uses output from the speciation step and the user's selection of two (or three) water analyses, chemical and isotopic mass balance constraints, and a set of plausible reactions to construct a set of possible chemical evolution models.

Availability:

Report (including diskette) is available from the USGS ESIC--Open-File Report Section and NWIS. The diskette contains source and executable code.

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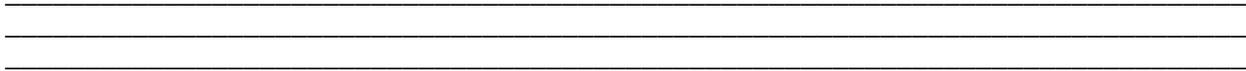
AQUEOUS SPECIATION

Speciation of Major and Some Minor Elements in 0 to 100 °C Temperature Range

Program Documentation:

Truesdell, A.H., and Jones, B.F., 1973, WATEQ—A computer program for calculating chemical equilibrium of natural waters: National Technical Information Service PB-220 464, 77 p.

Description:

This model calculates the distribution of inorganic aqueous species (that is, free ions and complexes) of major and important minor elements in low temperature natural waters. The thermodynamic data base included in the program contains equilibrium constants for about 150 reactions. Input to the program includes the chemical analysis results for 20 selected solutes (Ca, Mg, Na, K, Cl, SO_4, HCO_3, Fe, H_2S, CO_3, SiO_2, NH_4, B, PO_4, Al, F, NO_3, Li, Sr, and Ba), and field measurements of the water temperature and pH. Measurements of Eh and dissolved oxygen, as well as some other trace element analyses, may be included.

A mass balance equation can be written for each analyzed constituent that relates the sum of the concentrations of the free ions and complexes to the total concentration measured for that constituent. By means of experimentally developed equilibrium constants, the law of mass action relates the chemical activities of the various ion pairs to the activities of the complexes that involve that constituent. Taken together, the mass balance and the equilibrium relations form a set of nonlinear equations that involve the unknown concentrations of free ions and complexes. These are nonlinear because the activities are equal to the product of the concentration and an activity coefficient, where the activity coefficient depends on the ionic strength, which is a measure of the total concentration of charged ions in solution. Aqueous activity coefficients are calculated by using a novel extended form of the "extended Debye-Hückel equation," which contains two ion-specific parameters instead of one. The inclusion of the second parameter allows a more accurate calculation of activity coefficients beyond the 0.1 ionic strength limit usually considered by the traditional extended Debye-Hückel equation.

The program output is typical of a speciation code. It includes concentrations and thermodynamic activities of aqueous species, major ion activity ratios that can be used to help determine the water-rock reactions that may be controlling water compositions, and mineral-saturation indices that express the state of disequilibrium of the water with respect to various mineral phases.

A method of successive approximation called the continued fraction method is used with the activity coefficients calculated from ionic strengths updated at each iteration. When the mass balance for the anions is within 0.5 percent of the analytical values, the iteration is stopped. The program was written in PL/1 for IBM 360 computers. WATEQ was one of the first-generation programs developed for general use that uses the method of successive approximation to solve equilibrium problems in aqueous geochemistry (Nordstrom and others, 1979).

Past applications:

Many.

Remarks:

The methodology (everything but the computer listing) also was published in: Truesdell and Jones (1974).

A series of computer programs have been developed based on this original WATEQ model that have added to, or otherwise modified, the thermodynamic data base and chemical species considered or changed the mathematics used to approximate the solution to the set of nonlinear equations. However, the Truesdell and Jones (1974) paper remains important because of its description of the basic methodology. See Ball and Nordstrom (1991) for a newer code that uses the same general methodology but has an expanded and improved thermodynamic data base.

Availability:

Report that includes computer program listing is available from NTIS (PB-220 464). Truesdell and Jones (1974) is available from NWIS.

Related program:

Plummer, L.N., Jones, B.F., and Truesdell, A.H., 1976, WATEQF-A FORTRAN IV version of WATEQ—A computer program for calculating chemical equilibrium of natural waters: U.S. Geological Survey Water-Resources Investigations Report 76-13, 70 p. (Revised 1984).

Most significant changes to original program:

WATEQ, which was originally written in the PL/1 language, is reprogrammed in FORTRAN IV. With a few exceptions, the thermochemical data, speciation, activity coefficients, and general calculation procedure for this version of the program is equivalent to the original version. WATEQF includes 14 species of manganese and computes saturation data for 21 manganese minerals. A value for pE can now be set by the dissolved oxygen relation of Sato (1960) and by $SO_4^=/S^=$. In addition to the Debye-Hückel equation, the Davies equation can be used to calculate the activity coefficients.

The carbon-bearing species are computed from titration alkalinity, carbonate alkalinity, or total carbon in solution. The computational method of convergence on mass balance for anions has been improved.

Past applications:

Many.

Remarks:

This is a widely used program. The Ball and Nordstrom (1991) code refined and supplemented the thermodynamic data base and has improved capabilities. Either Truesdell and Jones (1973) or (1974) are needed to understand the basic methodology. A modified version of WATEQF is included in the NETPATH program (Plummer, Prestemon, and Parkhurst, 1991).

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Original report (PB–261 027) and magnetic tape of original computer program (PB–261 026) are available from NTIS.

Related program:

Ball, J.W., Nordstrom, D.K., and Jenne, E.A., 1980, Additional and revised thermochemical data and computer code for WATEQ2--A computerized chemical model for trace and major element speciation and mineral equilibria of natural waters: U.S. Geological Survey Water-Resources Investigations Report 78-116, 109 p. (Second printing, 1981.)

Most significant changes to original program:

This program expands and revises WATEQ to include consideration of ion association and solubility equilibria for 10 selected elements (Ag, As, Cd, Cs, Cu, Mn, Ni, Pb, Rb, and Zn). Certain polysulfides and additional complexes of Br, I, and bisulfides have been added, as have various metastable solids, sparingly soluble salts, and several complexes of major ions. The complete program is in the PL/1 language and is a corrected and revised extension of the original WATEQ program (Truesdell and Jones, 1973, 1974).

Past applications:

Many.

Remarks:

Ball, Jenne, and Nordstrom (1979) should be read to understand this program because it describes the functions of various parts of the computer program and the changes in

logic made to the WATEQ chemical model. The report by Nordstrom and others (1984) refined and supplemented the thermodynamic data base. See also Nordstrom and others (1990).

The report by Ball, Nordstrom, and Zachmann (1987) described WATEQ4F, which is a FORTRAN 77 version of WATEQ2 that has been adapted for operation on a personal microcomputer with math coprocessor and professional FORTRAN compiler. Limited data-base revisions are made that include the addition of several ion pairs. An updated version of WATEQ4F is described in Ball and Nordstrom (1991).

Availability:

Report is available from NTIS (PB-80 224 140).

Related program:

Ball, J.W., Jenne, E.A., and Cantrell, M.W., 1981, WATEQ3—A geochemical model with uranium added: U.S. Geological Survey Open-File Report 81-1183, 81 p.

Most significant changes to original program:

Procedures for the calculation of the speciation of uranium solutes and the activity products of uranium solid phases have been added to the WATEQ2 chemical model, and an error in the WATEQ2 program has been corrected, as well as a few problems with the previous text.

Past applications:

Few.

Remarks:

The program WATEQ4F, which was described by Ball and Nordstrom (1991), includes the capabilities of the WATEQ3 model.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

Related program:

Ball, J.W., and Nordstrom, D.K., 1991, User's manual for WATEQ4F, 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, 189 p., and diskette in pocket.

Most significant changes to original program:

The report states that it replaces Ball, Nordstrom, and Jenne (1980), Ball, Jenne, and Cantrell (1981), and Ball, Nordstrom, and Zachmann (1987), as the primary reference and user's manual for WATEQ4F. The entire library of reactions and thermodynamic data used in WATEQ4F is included in this report. Previously, Ball, Nordstrom, and Zachmann (1987) was the principal documentation for a FORTRAN 77 version of WATEQ2 that was designed to run on a personal microcomputer. This report supersedes that report and reflects the following primary changes in the model: the addition of Se, U, five Fe, Mn, and Ba carbonate reactions and the $FeCl^+$ and $SrSO_4^0$ complexes to the model calculations; revision of the user options for the control of redox calculations; significant revision of the thermodynamic data base, from Nordstrom and others (1990); and inclusion of the entire WATEQ4F data base in the report.

Past applications:

Many.

Remarks:

As of 1993, this version of the WATEQ-generated ion-association models has the most complete and current library of reactions and thermodynamic data.

Availability:

Report is available from the USGS ESIC--Open-File Report Section. Report and computer program (on diskette) are available from NWIS.

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CHEMICAL MASS TRANSFER

System CaO-MgO-Na_2O-K_2O-CO_2-H_2SO_4-HCl-H_2O

Program Documentation:

Plummer, L.N., Parkhurst, D.L., and Kosiur, D.R., 1976, MIX2—A computer program for modeling chemical reactions in natural waters: U.S. Geological Survey Water-Resources Investigations Report 75-61, NTIS Report PB 251 668, 73 p.

Description:

MIX2 utilizes an aqueous model akin to WATEQ and constraints of mass and electrical balances to compute the pH and equilibrium distribution of inorganic species in solution as a result of net reaction in the system—CaO-MgO-Na_2O-K_2O-CO_2-H_2SO_4-HCl-H_2O. The system is assumed to be closed in the sense that the mixing calculations do not reflect changes in mass of the constituent or constituents in mixtures because of the exchange or interaction with adjacent systems. In addition, MIX2 allows for mineral precipitation along the reaction path in maintaining a fixed ion activity product in solution for a given mineral.

Numerical features:

MIX2 is written in FORTRAN IV. A successive approximation method is used to calculate the distribution of the aqueous species that is similar to that used in WATEQ (Truesdell and Jones, 1974), except that MIX2 uses cation and anion mass balances to determine convergence.

An iterative approach is used in finding the pH of a solution that, through convergence on mass balance in the aqueous model, will result in perfect electrical neutrality. In estimating the number of moles of a specified mineral to be dissolved or precipitated to bring the solution to equilibrium with a specified mineral and accompanying mass and charge balance, an iterative cyclic approach also is used.

Past applications:

Many.

Remarks:

The program, PHREEQE, which is described in Parkhurst, Thorstenson, and Plummer (1980), is considered to be a replacement for MIX2.

Availability:

Report is available from NTIS (PB-251 668/AS). Computer program and report also are available from NWIS.

Mineral and Water/Gas Interactions at Low Temperatures

Program Documentation:

Parkhurst, D.L., Thorstenson, D.C., and Plummer, L.N., 1980 PHREEQE—A
computer program for geochemical calculations: U.S. Geological Survey Water-
Resources Investigations Report 80-96, 195 p. (Revised 1990.)

Description:

PHREEQE is a FORTRAN 77 computer program that models geochemical reactions.
The program calculates the following quantities during a reaction simulation: hydrogen
ion activity (pH), relative electron activity, total concentration of elements, the
amounts of minerals (or other phases) transferred into or out of the aqueous phase, the
distribution of aqueous species, and the relative saturation of the aqueous phase with
respect to specified mineral phases. PHREEQE can simulate several types of reactions,
which include addition of reactants to a solution, mixing of two waters, and titrating one
solution with another. In each of these cases, PHREEQE can simultaneously maintain
the reacting solution at equilibrium with multiple specified mineral phases.

With step-by-step manipulation by the user, PHREEQE can be used to analyze the
progress of a reaction in a geochemical system in which an irreversible reaction is
occurring. Reaction progress is measured by locating the intersection of the reaction
path with mineral phase boundaries (specified by the user as the plausible phases
present) and in defining the reaction paths across the mineral stability fields between
the mineral phase boundaries. The revised 1990 report includes a new thermodynamic
data base that is consistent with the data published by Nordstrom and others (1990).
The data base includes data on 19 elements, 133 aqueous species, and 43 minerals.

Numerical features:

Because of the nonlinear nature of the problem of determining a distribution of species
that simultaneously satisfies electron neutrality, conservation of electrons, mass
balance for each element, mineral equilibrium, and the mass action equation, numerical
convergence to a solution is not assured, although most problems attempted have been
solved. Problems that involve oxidation/reduction processes are more likely to cause
such convergence difficulties because the equilibrium concentrations of some species
can vary dramatically from a fully/oxidizing to a fully/reducing environment.

PHREEQE uses a continued fraction scheme to calculate species distribution and a
modified Newton-Raphson iterative technique for pH, pE, and mass transfer estimates.

Past applications:

Many.

Remarks:

The geochemical reaction model PHREEQE has been used with ground-water flow and solute-transport models to simulate a variety of problems that involve the combined effects of complex chemical processes and the physical processes of advection and dispersion. Sanford and Konikow (1989) used PHREEQE in conjunction with a two-constituent solute-transport model (MOCDENSE) that allows for variable density fluids to study calcite dissolution and related porosity changes in coastal freshwater/saltwater mixing zones in carbonate aquifers. Engesgaard and Kipp (1992) described a one-dimensional multiple species geochemical reaction transport model, MST1D. MST1D iterates sequentially between solving the transport equations by means of an implicit finite-difference method and solving a set of nonlinear algebraic equations that describe chemical mass transfer and aqueous speciation by using PHREEQE. Glynn, Engesgaard, and Kipp (1991) discussed a geochemical reaction mass-transport model PHREEQM. PHREEQM decouples geochemical reaction transport into three steps—advection, application of PHREEQE to calculate chemical equilibration, and simulation of the dispersion process by mixing the contents of each cell with that of its adjacent cells by using mixing factors calculated as a function of aquifer dispersivity and molecular diffusion.

Availability:

Original PHREEQE report is available from NTIS (PB–81 167 801). Revised (1990) computer program and revised report are available from NWIS. The report and computer program for PHRQINPT (Fleming and Plummer, 1983) are provided by NWIS as companions to the report and program for PHREEQE.

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Related program:

Fleming, G.W., and Plummer, L.N., 1983, PHRQINPT—An interactive computer program for constructing input data sets to the geochemical simulation program PHREEQE: U.S. Geological Survey Water-Resources Investigations Report 83-4236, 108 p.

Most significant changes to original program:

PHRQINPT facilitates formulation of the input data file to PHREEQE. It interactively asks the user for values of variables required by PHREEQE, explains the meaning and significance of each variable when required, and internally checks to make sure that values entered are valid.

Past applications:

Many.

Report is available from the USGS ESIC--Open-File Reports Section. The report and computer program are provided by NWIS as companions to the report and computer program for PHREEQE.

Related program:

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 p., two diskettes in pocket.

Most significant changes to original program:

This report described PHRQPITZ, which makes geochemical calculations in brines and other electrolyte solutions of high concentrations by using the Pitzer virial-coefficient approach for activity-coefficient corrections. Reaction/modeling capabilities include calculation of aqueous speciation and mineral-saturation index, mineral solubility, mixing and titration of aqueous solutions, irreversible reactions and mineral-water mass transfer, and reaction path. The program has been adopted from PHREEQE. (Parkhurst, Thorstenson, and Plummer, 1980). The report described how PHRQPITZ can be used to simulate the reaction path that corresponds to the evaporation of seawater.

Past applications:

Few.

Remarks:

The diskettes included with the report contain a machine-readable copy of the PHRQPITZ source code and of the source code to the interactive input program PITZINPT.

Availability:

Report (including diskette) is available from the USGS ESIC--Open-File Report Section and NWIS.

Speciation of Major and Many Minor Elements With Mineral and Water Interactions
in the 0 to 350 $^{\circ}$C temperature range

Program Documentation:

Kharaka, Y.K., and Barnes, Ivan, 1973, SOLMNEQ—Solution-mineral equilibrium
computations: U.S. Geological Survey Computer Contribution, National Technical
Information Service PB-215 899, 81 p.

Description:

SOLMNEQ is a computer program written in PL/1 for the IBM 360 computers. It
computes the equilibrium distribution of 162 inorganic aqueous species generally
present in natural waters over a temperature range from 0 to 350 $^{\circ}$C from the reported
concentrations of Ca, Mg, Na, K, Ag, Al, Ba, Cu, Fe, Hg, Li, Mn, Pb, Sr, Zn, Cl, SO_4,
HCO_3, SiO_2, $As(OH)_4$, PO_4, F, H_3BO_3, NH_3, CO_3, NO_3, and pH; Eh is optional. The
state of reaction of the aqueous solution with respect to 158 minerals also are computed
by means of saturation indices.

Numerical factors:

A method of successive approximations is used in which convergence is based on the
mass balance for the anions.

Past applications:

Many.

Remarks:

Because the temperature range of the SOLMNEQ data base goes considerably higher
than the other speciation programs of the Water Resources Division, it is the most
suitable choice for "hot" waters. Logic of the program was developed in part from
WATEQ (Truesdell and Jones, 1973, 1974) and WATCHEM (Barnes and Clark, 1969).

See Kharaka and others (1988) for an updated and improved version of this model.

Availability:

Report is available from NTIS (PB-215 899).

Related program:

Kharaka, Y., Gunter, W.D., Aggarwal, P.K., Perkins, E.H., and DeBraal, J.D., 1988,
SOLMINEQ.88—A computer program for geochemical modeling of water-rock
interactions: U.S. Geological Survey Water-Resources Investigations Report 88-4227,
420 p.

Most significant changes to original program:

This report updates the computer model SOLMNEQ. This version, which was renamed SOLMINEQ.88 (SOLution MINeral EQuilibrium, 1988), is written in FORTRAN 77 and has an improved algorithm for faster execution. This version has a revised thermodynamic data base, more inorganic (260) and organic (80) aqueous species and minerals (220), and computed pH and mineral solubilities at subsurface temperatures and pressures. New modeling options have been added to SOLMINEQ.88 that can be used to study the effects of boiling, mixing of solutions, and partitioning of gases between water, oil and gas phases. SOLMINEQ.88 has mass-transfer capabilities that can be used to study the effects of ion exchange, adsorption/desorption, and dissolution/precipitation of solid phases.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Related Program:

DeBraal, J.D., and Kharaka, Y.K., 1989, SOLINPUT—A computer code to create and modify input for the geochemical program SOLMINEQ.88: U.S. Geological Survey Open-File Report 89-616, 140 p.

Most significant changes to original program:

This report documented SOLINPUT, which is an interactive computer program designed to create and modify input files for the geochemical code SOLMINEQ.88.

Past applications:

Many.

Availability:

Report is available from the USGS ESIC--Open-File Report Section.

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Non-ideal Solid-Solution Aqueous-Solution Reactions

Program Documentation:

Glynn, P.D., 1991a, MBSSAS—A code for the computation of Margules parameters and equilibrium relations in binary solid-solution aqueous-solution systems: Computers and Geoscience, v. 17, no. 7, p. 907-966.

Description:

MBSSAS (Margules parameters and equilibrium relations in Binary Solid-Solution Aqueous-Solution systems) is a FORTRAN program that can be used in calculating thermodynamic equilibrium, stoichiometric saturation, and pure-phase saturation states in binary solid-solution aqueous-solution systems. "Binary" is used here to mean two-cation single-anion solid solutions. The results of these calculations can be used to construct phase diagrams and to model mineral-water reactions in natural and contaminated systems.

Past applications:

New.

Remarks:

Geochemical mass-transfer and mass-transport codes commonly ignore mineral impurities and defects and assume the minerals behave as constant-composition solids. MBASSAS can be useful in estimating the effects of mineral impurities on mineral solubility calculations made by programs like PHREEQE and to estimate the equilibrium partitioning between isotopically pure minerals and common minerals (Glynn, 1991b).

Availability:

Computer program is available from NWIS.

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SUMMARY AND CLOSING REMARKS

The computer programs listed in this report have been published or developed by the U.S. Geological Survey and solve problems that concern the physics and chemistry of ground water. Some programs are included for either historical purposes or documentation of a specific method. Thus, not all programs are being widely used. Some programs have been released so recently that the statements on past applications cannot indicate the potential usefulness of these programs. A few programs have been or are being used in many studies and have been so noted.

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Appendix 1. List of acronyms used to identify selected computer programs, and the report to which they refer.

Acronym	Full Name	Reference
AQMAN	Linear and quadratic programming matrix generator using two-dimensional ground-water flow simulation for aquifer management modeling	Lefkoff, L. J., and Gorelick, S. M., 1987
AQMAN3D	A mathematical programming system dataset generator for aquifer management using the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model	Puig, J. C., and Rolon-Collazo, L. I., in press
AQUIFEM-SALT	A finite-element model for aquifers containing a seawater interface	Voss, C. I., 1984b
AX	An axisymmetric finite-difference flow model to simulate drawdown in and around a pumped well.	Rutledge, A. T., 1991
BALANCE	A computer program for calculating mass transfer for geochemical reactions in ground water	Parkhurst, D. L., Plummer, L. N., and Thorstenson, D. C., 1982
HOTWTR	Three-dimensional finite-difference model for ground-water flow and single phase (liquid) heat transport	Reed, J.E., 1985
HST3D	A computer code for simulation of heat and solute transport in three-dimensional ground-water flow systems	Kipp, K. L., 1987
HYDROTHERM	A three-dimensional finite-difference model for ground-water flow and multiphase heat transport in the temperature range of 0 to 1,200°C	Hayba, D.O., and Ingebritsen, S.E., in press
INTERCOMP	A model for calculating effects of liquid waste disposal in deep saline aquifer	INTERCOMP, 1976; INTERA, 1979
MBSSAS	Margules parameters and equilibrium relations in Binary Solid-Solution Aqueous-Solution systems	Glynn, P. D., 1991a

Acronym	Full Name	Reference
MMSP	A statistical processor for analyzing simulations made using the modular finite-difference ground-water flow model	Scott, J. C., 1990
MODBRANCH	A coupled surface-water and ground-water flow model for simulation of stream-aquifer interaction	Swain, E. D., and Wexler, E. J., 1993
MOC	Computer model of two-dimensional solute transport and dispersion in ground water	Konikow, L. F., and Bredehoeft, J. D., 1978; Goode, D. J., and Konikow, L. F., 1989
MOCDENSE	A two-constituent solute-transport model for ground water having variable density	Sanford, W. E., and Konikow, L. F., 1985
MODFE	A MODular Finite-Element model (MODFE) for areal and axisymmetric ground-water-flow problems	Torak, L. J., 1993a, b and Cooley, R. L., 1992
MODFLOW	A modular three-dimensional finite-difference ground-water flow model	McDonald, M. G., and Harbaugh, A. W., 1988
MODFLOWARC	Modifications of the U.S. Geological Survey Modular, finite-difference, ground-water flow model to read and write geographical information system file	Orzol, L. L., and McGrath, T. S., 1992
MODFLOWP	A computer program for estimating parameters of a transient, three-dimensional, ground-water flow model using nonlinear regression	Hill, M. C., 1992
MODPATH	Computer programs to compute and display pathlines using results from the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model	Pollock, D. W., 1989, 1990
NETPATH	An interactive code for modeling net geochemical reactions along a flow path	Plummer, L. N., Prestemon, E. C., and Parkhurst, D. L., 1991

Acronym	Full Name	Reference
PHREEQE	PHREEQE-A computer program for geochemical calculations	Parkhurst, D. L., Thorstenson, D. C., and Plummer, L. N., 1980 (Revised edition - August 1990)
PHRQINPT	An interactive computer program for constructing input data sets to the geochemical simulation program PHREEQE	Fleming, G. W., and Plummer, L. N., 1983
PHRQPITZ	A computer program incorporating Pitzer's equations for calculation of geochemical reactions in brines	Plummer, L. N., Parkhurst, D. L., Fleming, G. W., and Dunkle, S. A., 1988
RADFLOW	A Galerkin finite-element flow model to predict the transient response of a radially symmetric aquifer	Reilly, T. E., 1984
RADMOD	Computer program for the simulation of cylindrical flow to a well using the U.S. Geological Survey Modular Finite-Difference Ground-Water Flow Model	Reilly, T. E., and Harbaugh, A. W., 1993b
SALT NORM	A quantitative chemical-mineralogical characterization of natural waters	Bodine, M. W., Jr., and Jones, B. F., 1986
SATRA-CHEM	Numerical simulation of advective-dispersive multisolute transport with sorption, ion exchange and equilibrium chemistry	Lewis, F. M., Voss, C. I., and Rubin, Jacob, 1986
SHARP	A quasi-three-dimensional finite-difference simulation model for freshwater and saltwater flow in layered coastal aquifer systems	Essaid, H. I., 1990
SOLINPUT	A computer code to create and modify input for the geochemical program SOLMINEQ.88	DeBraal, J. D., and Kharaka, Y. K., 1989
SOLMINEQ	Solution-mineral equilibrium computations	Kharaka, Y. K., and Barnes, Ivan, 1973
SOLMINEQ.88	A computer program for geochemical modeling of water-rock interactions	Kharaka, Y., Gunter, W. D., Aggarwal, Pradeep K., Perkins, E. H., and DeBraal, J. D., 1988

Acronym	Full Name	Reference
SUPERMOCK	Simulation procedure for modeling transient water-table and artesian stress and response	Reed, J. E., Bedinger, M. S., and Terry, J. E., 1976
SUTRA	A finite-element simulation model for saturated-unsaturated, fluid-density-dependent ground-water flow with energy transport or chemically-reactive single-species solute transport	Voss, C. I., 1984a
SUTRAPLOT	A graphical display program for SUTRA Finite-Element Simulation Model	Souza, W. R., 1987
Trescott-2D	Finite-difference model for aquifer simulation in two dimensions	Trescott, P. C., Pinder, G. F., and Larson, S. P., 1976
Trescott-3D	Finite-difference model for simulation of three-dimensional ground-water flow	Trescott, P. C., 1975; Trescott, P. C., and Larson, S. P., 1976; Torak, L. J., 1982
TRIAG	A finite-element model for flow in a two-aquifer system	Mallory, M. I., 1979
VS2D	Computer program VS2D to solve the equations of fluid flow in variably saturated porous media	Lappala, E. G., Healy, R. W., and Weeks, E. P., 1987
VS2DT	Simulation of solute transport in variably saturated porous media	Healy, R. W., 1990
WATCHEM	Chemical properties of ground water	Barnes and Clark, 1969
WATEQ	A computer program for calculating chemical equilibrium of natural waters	Truesdell, A. H., and Jones, B. F., 1973; Truesdell, A. H., and Jones, B. F., 1974
WATEQF	A FORTRAN IV version of WATEQ, A computer program for calculating chemical equilibrium of natural waters	Plummer, L. N., Jones, B. F., and Truesdell, A. H., 1976 (Revised edition January 1984)
WATEQ2	Additional and revised thermochemical data and computer code for WATEQ2--A computerized chemical model for trace and major element speciation and mineral equilibria of natural waters	Ball, J. W., Nordstrom, D. K., and Jenne, E.A., 1980

Acronym	Full Name	Reference
WATEQ3	A geochemical model with uranium added	Ball, J. W., Jenne, E. A., and Cantrell, M. W., 1981
WATEQ4F	Revised thermodynamic data base and test cases for calculating speciation of major, trace, and redox elements in natural waters	Ball, J. W., and Nordstrom, D. K., 1991
ZONEBUDGET	A computer program for calculating subregional water budgets using results from the U.S. Geological Survey modular three-dimensional finite-difference ground-water flow model	Harbaugh, A. W., 1990