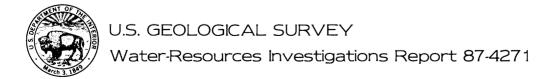# Selected Reports that Include Computer Programs Produced by the U.S. Geological Survey for Simulation of Ground-Water Flow and Quality

By Charles A. Appel and Thomas E. Reilly

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SELECTED REPORTS THAT INCLUDE COMPUTER PROGRAMS PRODUCED BY THE U.S. GEOLOGICAL SURVEY FOR SIMULATION OF GROUND-WATER FLOW AND QUALITY

By

Charles A. Appel and Thomas E. Reilly

ABSTRACT

A summary list of reports that document numerical models that simulate ground-water flow and quality is presented. The list documents the reference by giving a description of each model program, its numerical features, a qualitative expression of the number of past applications and where to obtain a copy. All reports included in the list have been published or developed by the U.S. Geological Survey and most contain listings of the computer programs.

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INTRODUCTION

Numerical models provide a powerful aid in understanding and assessing ground-water systems. The U.S. Geological Survey has contributed significantly to the development and use of models for the analysis of ground-water problems. The status of ground-water modeling in the Geological Survey before 1975 was documented in U.S. Geological Survey Circular 737 (Appel and Bredehoeft, 1976). Developments in the field have taken place since that time and many useful computer codes have been published. This report gives information on selected computer programs published or developed by the Geological Survey or by the Geological Survey 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, and where to request copies of the report and, in some cases, the computer code.

Depending on the nature of the problem, there may be more than one computer program or one category of programs that can be applied. 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 relatively thick zone separating strictly fresh water from strictly salt water, 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.

Although all reports 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.

The format used here is to first list the report by category describing the general program followed by selected reports that describe modifications to that program. Information on each report is separated by one solid horizontal line. Three solid lines mark the end of the list of those reports based on that basic computer program. However, in a few cases, a program listed under one category was derived from a program in another category. For example, some of the reports listed under "freshwater-saltwater" describe programs that are modifications to ground-water flow programs described under the category "flow-saturated". Also, some reports could be included under other categories. For example, the reports by Grove and Stollenwerk (1984) and Lewis, Voss, and Rubin (1986) describe models for the transport of fluids that are affected both by physical and chemical processes. Both of those reports could have been included under "chemical equilibrium" instead of the category of "solute transport" in which they are contained in this report.

Purpose and Scope

The purpose of this report is to make available a relatively comprehensive list of computer programs that have been produced by the U.S. Geological Survey for simulation of ground-water problems. The main criteria used in compiling the list is that the report must be published and include 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
WATSTORE Program Office
437 National Center
Reston, Virginia 22092
(703) 648-5695

Books and Open-File Reports Section
U.S. Geological Survey
Federal Center, Box 25425
Denver, Colorado 80225
(303) 236-7476

NTIS, U.S. Department of Commerce
5825 Port Royal Road
Springfield, Virginia 22161

SELECTED REPORTS

Summary List of Computer Programs

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Individual Descriptions

FLOW-SATURATED

Two-Dimensional Finite Difference

Reference: 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: Simulates steady and non-steady ground-water flow in an irregularly shaped aquifer that can be a confined or unconfined aquifer, or both. The aquifer's transmissive properties 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 using 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: Many field problems.

Remarks: Up to a few years ago, one of the most used flow models for two-dimensional problems.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE.

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 is presented assuming the D4 (alternating diagonal) node ordering scheme. For moderate size grids this solver can be computationally more efficient than iterative matrix methods.

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Past applications: Many

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE.

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 presented for the two-dimensional ground-water flow problem. Application to a field problem of this method as compared to the Iterative Alternating Direction Implicit Procedure (IADIP) and the Strongly Implicit Procedure (SIP) methods showed the conjugate gradient method to compare favorably with IADIP and 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: Very few

Availability: Report from Books and Open-File Reports Section.

Related program: Ozbilgin, Melih M., and Dickerman, David C., 1984, 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 assumes that the water level in streams in hydraulic connection with an aquifer are not appreciably affected by the flow between those streams and the aquifer. The Ozbilgin and Dickerman (1984) report describes a method that, because it relates stream discharge to the depth of water in the stream at that place (using the Manning formula), accounts for changes in stream-water level associated with changes in stream discharge resulting from flows between the aquifer and the stream.

Past applications: Very few.

Availability: Report from Books and Open-File Reports 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 assumes that model grid boundaries are places where either the head is specified or the fluxes across the boundary are specified. This report describes a head-controlled flux condition for the model grid boundary that allows both head and flux to change. The assumptions made are 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 boundary and the constant-head boundary. The storage properties of the aquifer and the confining bed in the strip are neglected.

Past applications: Limited

Availability: Report from Books and Open-File Reports Section.

Two-Dimensional Finite Element Galerkin

Reference: 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-
168 contain documentation of program developed by J. V. Tracy).

Description: Model simulates steady and non-steady two-dimensional
ground-water flow in an irregularly shaped confined or unconfined
aquifer. The aquifer's transmissive and storage properties 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 using an input stage-discharge relationship 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 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. By a "regular" grid, it is meant that the region is
subdivided by a given number of columns, each of which has an equal
number of elements, where the columns need not be parallel or of
the same lengths. The effect is of a deformed rectangular grid.
Applying the Galerkin method results in an associated matrix problem
which is solved using a direct method. Mass balances are computed
for each time step and the cumulative volumes.

Past applications: Several field problems.

Availability: Report from Book and Open-File Reports Section. Computer
program and report from WATSTORE.

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

References: 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 was designed to simulate transient stress
and response of an aquifer system that consists of a confined
aquifer overlain by a water-table aquitard taking into consideration
climatic conditions and soil and vegetative properties as well as
the hydraulic properties of the aquifer system. 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 computes changes in soil-moisture storage, and
recharge and discharge from the zone of aeration to the water
table; a vertical-flow component computes the altitude of the water
table in the fine-grained water-table aquitard overlying the confined
aquifer; and a horizontal-flow component computes accretion to the
confined aquifer and its non-steady heads. Simulated stresses on
the confined aquifer simulated 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, where
the nodes 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 using the ADIP (alternating-direction implicit procedure).

Past applications: A few field applications.

Availability: Report from Books and Open-File Reports Section.

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Cylindrical Coordinates

Reference: Reilly, Thomas 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, such as at a pumping well, recharge basin, or injection well. It is capable of simulating anisotropic, inhomogenous, confined, or pseudo-unconfined - 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 from the Books and Open-File Reports Section. Computer program and report from WATSTORE.

Two-Aquifer System

References: Mallory, Michael 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 is from the report: Durbin, Timothy J., 1978, Calibration of a mathematical model of the Antelope Valley ground-water basin, California: U.S. Geological Survey Water-Supply Paper 2046, 51 p. The model was developed by T. Durbin. It simulates steady and non-steady ground-water flow in an irregularly shaped two-aquifer system. The areal extent of the two aquifers do not have to be coincident. The aquifers' transmissive and storage properties 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 using the point iterative successive over-relation method (PSOR).

Past applications: A few field applications.

Availability: Report from NTIS (PB #80140932).

Quasi-Three Dimensional Aquifer System

Reference: Weeks, John 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 non-steady ground-water flow in an irregularly shaped flow system consisting of aquifer layers and confining layers. Changes in storage in the confining layers are assumed 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 subdivided 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 which is solved 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 John D. Bredehoeft in 1969. That generic program was used widely before about 1980. The methodology is described in Bredehoeft and Pinder (1970).

Availability: Report from NTIS (PB #284-341).

Three-Dimensional

References: Trescott, Peter 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, Documentation of finite-difference model for simulation of three-dimensional ground-water flow, supplement to Open-File Report 75-438: U.S. Geological Survey Open-File Report 76-591, 21 p.

Description: Simulates steady and non-steady flow 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 characterized by alternating layers of "high" and "low" hydraulic conductivities, a modified 3-D 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 at significantly lower computational effort.

Numerical features: The flow region is considered to be subdivided 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 subdividing 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 using the SIP iterative (the Strongly Implicit Procedure) 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: Up to very recently, one of the most used models for three-dimensional flow problems.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE.

Related program: Torak, Lynn 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: Make corrections and
     extend the application of the Trescott 3-D program to simulations
     involving leaky rivers, evaportranspiration as a linear function of
     depth to water, and discharge to drains and springs.

Past applications: Many.

Availablity: Report from Books and Open-File Reports Section. Computer
     program and report from WATSTORE.

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Related program: Helgesen, John O., Larson, Steven P., and Razem,
     Allan C., 1982, Model modifications for simulation of flow through
     stratified nodes in eastern Ohio: U.S. Geological Survey Water-
     Resources Investigations Report 82-4019, 109p.

Most significant changes to original program: (1) The calculation for
     vertical leakage between adjacent aquifer layers allows for the case
     where a lower aquifer converts from confined to unconfined conditions;
     (2) 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; (3) recharge from
     precipitation to any layer can be simulated; (4) water-budget
     calculations are made for each layer; and (5) spring flow from the
     top aquifer can recharge the next lower aquifer.

Past applications: Few.

Availability: Report from Books and Open-File Reports Section.

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Related program: 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 No. 27, 87 p.

Most significant change to original program: (1) Transient-leakage
     effects in confining layers were simulated, and (2) a program was
     added to quantify the effect of making selected changes in

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aquifer parameter values on computed heads. That 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.

Past applications: Few.

Availability: Report from:

> Louisiana Department of Transportation and Development
> Office of Public Works
> Baton Rouge, Louisiana

Related program: Leahy, P. Patrick, 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.

Most significant changes to original program: Modifications are
presented that (1) permit the simulation of confining-bed and
aquifer pinchouts without the use of artificial hydraulic
parameters, (2) reduce the computer-memory requirements for
aquifer systems having complex external boundary shapes,
(3) include the capability to approximate transient leakage from
confining layers.

Past applications: Few.

Availability: Report from Books and Open-File Reports Section.

Related program: Meyer, Walter R., and Carr, Jerry 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.
(plus 107 p. appendix)

Most significant change to original program: Land subsidence induced
by ground-water extraction is 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 from:

　　　　Texas Natural Resources Information System
　　　　P.O. Box 13087
　　　　Austin, Texas 78711

Three-Dimensional

Reference: 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: The same basic capabilities as the computer program of
Trescott (1975, U.S. Geological Survey Open-File Report 75-438)
except that (1) this program uses "cube" input commands which allow
the modeler to change aquifer parameters by zones that are believed
to have uniform values and reinitialize the model with relatively
few input records; (2) a data-swapping procedure between the central
memory and peripheral storage devices exploits the nature of the
SIP 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 which involve more blocks than can be handled by the
approach of having all of 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: Same as Trescott (1975, U.S. Geological Survey
Open-File Report 75-438) except that an analytical-numerical
approximation is included for transient leakage from the confinng
beds.

Past applications: Few.

Availability: Report from Books and Open-File Reports Section.

Related program: Hearne, Glenn 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
reported on in Open-File Report 80-421 (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 more implicit the calculation of flow at
such boundaries, and to allow the program to execute on a CRAY-1
computer.

Past applications: Few.

Report from Books and Open-File Reports Section.

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Three-Dimensional Finite-Difference Method

Reference: McDonald, Michael G., and Harbaugh, Arlen W., 1984, A
modular three-dimensional finite-difference ground-water flow model:
U.S. Geological Survey Open-File Report 83-875, 528 p.

Description: The model simulates steady and non-steady flow in an
irregularly shaped flow system in which aquifer layers can be
confined, unconfined, or a combination of confined and unconfined.
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 direction alined 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 model's outer boundary 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 subdivided
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
using either the SIP (strongly implicit procedure) or 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: Currently the most used numerical model in the U.S. Geological
Survey for ground-water flow problems.

Availability: Report from Books and Open-File Reports Section. Computer
program from WATSTORE Program Office. To be released in the series
Techniques of Water-Resources Investigations of the United States
Geological Survey.

Related program: Kuiper, Logan 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 interation termination.

Past applications: Just published.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE.

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Two-Dimensional--Parameter Estimation

Reference: Cooley, Richard L., and Naff, Richard L., 1985, Regression
modeling of ground-water flow: U.S. Geological Survey Open-File
Report 85-180, 450 p.

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
underlying a stream or of an aquitard overlying or underlying 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.

Availability: Report from Books and Open-File Reports Section. Computer
program and report from WATSTORE.

Related program: Garabedian, S. P., 1986, Application of a parameter-
estimation technique to modeling the regional aquifer underlying
the eastern Snake River Plain, Idaho: U.S. Geological Survey Water-
Supply Paper 2278, 60 p.

Most significant changes to original program: The original program assumes
that observed heads are in wells that coincide with node points. The
program listed in this report includes a modification to account for
observation heads at places other than node points.

Past applications: Limited.

Availability: Report from the Books and Open-File Reports Section.

Two-Dimensional

Reference: 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 both 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 using the strongly implicit procedure.

Past applications: Just published.

Remarks: A modification to the computer program VS2D allows simulation of water movement through unsaturated media in response to a constant rate of application of water at the land surface (Healy, 1987). Because the rate at which water can be absorbed by soil is limited, the water will pond and the 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.

Availability: Report from Books and Open-File Reports Section. Computer program and report available from WATSTORE.

SOLUTE TRANSPORT--SATURATED

One Dimensional Finite-Difference Method

Reference: Grove, David B., and Stollenwerk, Kenneth 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 describing transport and reaction
processes are solved by finite-difference methods, with non-linearities
accounted for by iteration.

Past applications: Limited.

Availability: Report from Books and Open-File Reports Section.
Computer program and report from WATSTORE.

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Two-Dimensional Method of Characteristics

Reference: 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, Chapter C2, 90 p.

Description: This model simulates solute transport in flowing ground water. It is applicable to one- or two-dimensional problems involving steady-state or transient flow. The model computes changes in concentration over time caused by the processes of convective transport, hydrodynamic dispersion, and mixing or dilution from fluid sources. The original model assumes that the solute is nonreactive, but a subsequent update includes modifications to the program that will allow the model to simulate a first-order irreversible-rate reaction or equilibrium-controlled sorption-desorption for a linear isotherm. Gradients of fluid density, viscosity, and temperature are assumed not to affect the velocity distribution. However, the aquifer may be heterogeneous and anisotropic.

Numerical features: The model couples the ground-water flow equation with the solute-transport equation. The digital computer program uses an alternating-direction implicit procedure to solve a finite-difference approximation to the ground-water flow equation, and it uses the method of characteristics to solve the solute-transport equation. The latter 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: One of the most used models for solute-transport problems.

Availability: Report from Books and Open-File Reports Section. Computer program and report (including updates to the program) from WATSTORE program office.

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Related program: Garabedian, Stephen P., and Konikow, Leonard 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: 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 from Books and Open-File Reports Section.

Related program: Sanford, Ward E., and Konikow, Leonard 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 where there is a two-dimensional-
density-dependent flow.

Past applications: Limited.

Availability: Report from Books and Open-File Reports Section. Computer
program and report from WATSTORE program office.

Two-Dimensional Finite-Element Galerkin Method

Reference: Lewis, Frank M., Voss, Clifford 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: 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: (a) linear sorption and up to two aqueous complexations, and (b) binary ion exchange and a single complexation reaction involving one of the exchanging species.

Numerical features: This model, SATRA-CHEM, is a modified version of the computer code SATRA, which itself is a simplified version of the flow and solute-transport model SUTRA. 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 from Books and Open-File Reports Section.

Dual Porosity Flow and Transport

Reference: Glover, Kent 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: Simulates three-dimensional flow and advective transport and hydrodynamic dispersion in an aquifer having parallel fractures separated by a matrix (blocks) of materials that have significant porosity and negligible hydraulic conductivity. It is assumed that the flow and transport take place primarily in the fractures with the potential for the exchange of solute between fluid in the fracture and the adjacent matrix (blocks) 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: Using the finite element Galerkin procedure the differential equations describing flow and mass transport are approximated by a system of linear equations which are solved by selected forms of Gauss elimination.

Past applications: Just published.

Availability: Report from Books and Open-File Reports Section.

SOLUTE AND HEAT TRANSPORT--SATURATED

Three-Dimensional Finite-Difference Method

Reference: INTERCOMP Resource Development and Engineering, Inc., 1976, A model for calculating effects of liquid waste disposal in deep saline aquifer: U.S. Geological Survey Water-Resources Investigations Report 76-61, 253 p.

Description: A transient, three-dimensional model developed to solve the three coupled governing equations for pressure, mass-transport and heat-transport. Although this program was initially developed to simulate certain aspects of waste injection into saline aquifers, it also is suitable for many other applications.

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 equations' dependent variables. Multiple user options allow the choice of x, y, and z 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.

Availability: Report from NTIS (PB #256903/AS).

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 involving waste disposal with simple chemical reactions.

Past applications: Several.

Availability: Report from NTIS (PB #80122542). Computer program and report from WATSTORE program office.

Three-Dimensional Finite-Difference Method

Reference: Kipp, Kenneth L., Jr., 1987, 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, 517 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). The HST3D program may be used for analysis of problems such 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 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, using equations reordered by alternating diagonal planes. The other technique is an iterative solver, using two-line successive overrelaxation.

Past applications: Just published.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE program office.

FLOW-SATURATED FRESHWATER-SALTWATER

Two-Dimensional Areal

Reference: Mercer, J. W., Larson, S. P., and Faust, C. R., 1980, Finite-difference model to simulate the areal flow of salt water and fresh water 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 salt water and fresh water separated by an interface. The partial differential equations are integrated over the thicknesses of fresh water and salt water resulting in two equations describing the flow characteristics in the areal domain. The program is designed to simulate time-dependent problems such as those associated with the development of coastal aquifers, and can treat water-table conditions or confined conditions with steady-state leakage of fresh water. The program will generally be most applicable to the analysis of regional aquifer problems in which the zone between salt water and fresh water can be considered a surface (sharp interface).

Numerical features: The equations are approximated using finite-difference techniques and the resulting algebraic equations are solved for the dependent variables, fresh-water head and salt-water heads using an iterative solution method.

Past applications: A very few field problems.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE program office.

Two-Dimensional Areal

Reference: Voss, Clifford I., 1984, 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 and are separated
by an effectively sharp interface. Vertical hydrostatic equilibrium
in both the freshwater and saltwater is assumed and the model
ignores any time lag resulting 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, a model which is
described by Pinder and Voss (1979). Copies of that report may
be obtained from:

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

Availability: Report from Books and Open-File Reports Section.

Three-Dimensional (Sharp interface)

Reference: Guswa, John H., and LeBlanc, Denis 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, and the saline-water zone is static and 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 relationship can be written between the freshwater head and the elevation that must be satisfied at each point of the interface that 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 which 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 taken to be zero for computational purposes because of the assumption that the saline water is static.

Past applications: Few.

Availability: Report from Books and Open-File Reports Section.

Three-Dimensional (Variable Density)

Reference: 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 constant in time
(the density distribution does not change due to 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: Information required for the program's operation is:
aquifer elevation, thickness, and ground-water density. The report
contains two FORTRAN programs 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 from Books and Open-File Reports Section.

Three-Dimensional (Variable Density)

Reference: 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 code 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 code 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 code uses the integrated finite difference method.
The strongly implicit procedure (SIP), successive over-relaxation (SOR),
and eight different preconditioned conjugate gradient (PCG) 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 from Books and Open-File Reports Section.
Computer program and report from WATSTORE.

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Three-Dimensional (Variable Density and Multiaquifer wells)

Reference: 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 (in press).

Description: This report describes 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 it is reasonable to assume that the spatial distribution of the fluid density does not change with time and that contains wells open to more than a single aquifer.

Numerical features: Beside describing the variable-density and multiple-well modifications to the Trescott model, two new computer programs are described. Those programs compute (1) ground-water density, pure water density, and dynamic viscosity, and (2) the horizontal and vertical hydraulic conductances and variable density input data for the Trescott model. A slice-successive-over-relaxation (SSOR) matrix solver is described.

Past applications: Limited.

Availability: Report from Books and Open-File Reports Section.

Two-Dimensional Single- and Two-Phase

Reference: Faust, Charles R., and Mercer, James W., 1977, Finite-
difference model of two-dimensional, single- and two-phase heat
transport in a porous medium-version I: 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° C. The model can handle the
conversion from single-phase flow to two-phase flow. The dependent
variables solved for are pressure and enthalpy. The aquifer is
assumed 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 anistropic in
each block but the principal directions must be alined with the
coordinate axes.

Numerical features: The modeled area is subdivided into rectangular
grid blocks (with nodes at the block centers) in which the fluid
and aquifer properties are assumed uniform.

Past applications: Limited.

Remarks: When developed, the model was considered to be a research
tool because it was recognized that some sophisticated changes and
additions would need to be made before a complicated field problem
could be simulated.

Availability: Report from Books and Open-File Reports Section.

Two-Dimensional Single-Phase

Reference: Mercer, James W., and Pinder, George 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: Simulates 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 used for time derivative.

Past applications: Limited.

Availability: Report from Books and Open-File Reports Section.

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Three-Dimensional

Reference: 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: Simulates three-dimensional equation of ground-water
flow 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 fluid density is constant, buoyancy effects caused by fluid-
density variations resulting from temperature differences are not
considered.

Numerical features: The ground-water flow and heat-flow models are
block-centered, finite-difference approximations with interblock
transmissivity calculated as the harmonic mean of the two adjacent
blocks. Block lengths can vary in each of the three coordinate
directions. 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, updating convective flux
after solution of the ground-water flow equation, and updating
hydraulic conductivity after solution of the heat-flow equation.
Direct solution is used for each equation.

Time of travel is determined by particle tracking through the modeled
region.

Past applications: Limited.

Availability: Report from Books and Open-File Reports Section.

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SOLUTE OR HEAT TRANSPORT--SATURATED AND UNSATURATED

Two-Dimensional Finite-Element Galerkin Method

Reference: Voss, Clifford I., 1984, 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 (SUTRA) 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 using SUTRA may be employed to model natural or man-induced chemical species transport including processes of solute sorption, production and decay, and may be applied to analyze 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 salt-water intrusion in aquifers in near-well or regional scales, with either dispersed or relatively sharp transition zones between fresh water and salt water. 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 two interdependent processes that are simulated: (1) fluid density-dependent saturated or unsaturated ground-water flow, and either (2a) 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-order and zero-order production or decay, or, (2b) transport of thermal energy in the ground water and solid matrix of the aquifer.

Past applications: A few field problems.

Remarks: A graphical post-processor developed by Souza (1987) is available for use with the computer code. This post-processor facilitates interpretation of the simulation results.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE program office.

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AQUIFER MANAGEMENT

Two-Dimensional Saturated Flow

Reference: Lefkoff, L. Jeff, and Gorelick, Steven 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: The computer program AQMAN provides a link between
    a modified version of the two-dimensional ground-water flow model
    of Trescott, Pinder, and Larson (1976) and any standard Mathematical
    Programming System input format. AQMAN uses the modified Trescott
    model to solve the basic ground-water flow equation to determine
    aquifer responses to both the stresses that cannot be controlled
    because of physical limitations or legal, or socio-economic demands
    (the unmanaged stresses) and to the stresses that can be controlled
    (the managed stresses). A management problem is to use that aquifer
    response information together with an optimization program to deter-
    mine 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.
    The program, AQMAN, creates the input files to be used by an
    optimization program. These input files contain all the hydrologic
    information and management objectives needed by an optimization
    program to solve the management problem.

Numerical features: The spatial discretization of the aquifer is that
    used by the Trescott, Pinder, and Larson (1976) program. AQMAN
    requires that the time periods during which a particular decision
    variable is constant on a particular set of constraints applies
    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 relationship between aquifer stress and water-
    level response is essentially linear (i.e., that linear superposition
    of solutions to the transient ground-water flow equation is appropriate).

Past applications: Just published.

Availability: Report from Books and Open-File Reports Section and the
    computer program and report from the WATSTORE program office.

CHEMICAL EQUILIBRIUM

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

Reference: Truesdell, Alfred H., and Jones, Blair F., 1973, WATEQ, A computer program for calculating chemical equilibrium of natural waters: NTIS PB-220 464, 77 p.

Description: Calculates the distribution of inorganic aqueous species (i.e, 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 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, Ba, and field measurements of the water temperature and pH. If available, 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. Also, the law of mass action relates, by an experimentally developed equilibrium constant, 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 non-linear equations involving the unknown concentrations of free ions and complexes. These are non-linear because the activities are equal to the product of the concentration and an activity coefficient, where the activity coefficient depends on the ionic strength, a measure of the total concentration of charged ions in solution. But, the concentration of those ions are some of the unknowns being sought. The activity coefficients are calculated for the major ions using an extended form of the Debye-Huckel equation containing two parameters that vary in a known way with the ions.

The program output includes the ratio of the activity product to the solubility equilibrium constant for various mineral phases which show the degree of saturation of the water with each mineral considered.

Numerical features: A method of successive approximation is used with the activity coefficients calculated from an updated ionic strength each iteration. When the mass balance for the anions agree with the analytical values within 0.5 percent, the iteration is stopped. The program was written in PL/1 for IBM 360 computers.

Past applications: Many.

Remarks: The methodology (everything but the computer listing) was
published also in:

> Truesdell, Alfred H., and Jones, Blair F., 1974, WATEQ, A
> computer program for calculating chemical equilibrium of
> natural waters: Journal of Research, U.S. Geological Survey,
> V. 2, No. 2, p. 233-248.

While other computer programs have evolved that may 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 rate of non-linear equations, many of them refer to this paper
for a description of the basic methodology and the thermodynamic data.

Availability: Report that includes computer program listing from NTIS
(PB-220 464). Truesdell and Jones (1974) paper from WATSTORE.

Related program: Plummer, L. Niel, Jones, Blair F., and Truesdell,
Alfred H., 1976 (Revised edition January 1984), WATEQF-A FORTRAN IV
version of WATEQ, A computer program for calculating chemical equili-
brium of natural waters: U.S. Geological Survey Water-Resources
Investigations Report 76-13, 70 p.

Most significant changes to original program: The WATEQ computer program
that originally was written in the PL/1 language is reprogrammed in
FORTRAN IV. With but 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 the $SO_4^=/S^=$ ratio.
In addition to the Debye-Huckel equation, the Davies equation can
be used to calculate the activity coefficients. The carbon-bearing
species are computed from either 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 report by Nordstrom et al
(1984) refines and supplements the thermodynamic data base. Either
the report Truesdell and Jones (1974) or (1973) are needed because
this report is a supplement to the earlier report.

Related program: Ball, James W., Nordstrom, D. Kirk, and Jenne,
    Everett 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 September 1981).

Most significant changes to original program: Expands and revises the
    model, WATEQ, to include consideration of ion association and solubi-
    lity equilibria for the 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.

Past applications: Many.

Remarks: An adjunct paper that 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 is
    Ball, Jenne, and Nordstrom (1979). The report by Nordstrom et al
    (1984) refines and supplements the thermodynamic data base.

    The report by Ball, Nordstrom, and Zachmann (1987) describes 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.

Availability: Report from NTIS (PB-80 224 140).

Related program: Ball, James W., Jenne, Everett A., and Cantrell,
    Mark 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 is corrected as are a few
problems with the previous text describing WATEQ2.

Past applications: Few.

Availability: Report from Books and Open-File Reports Section.

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Speciation of Major and Many Minor Elements in 0-350°C Temperature Range

Reference: Kharaka, Yousif K., and Barnes, Ivan, 1973, SOLMNEQ: Solution-mineral equilibrium computations: U.S. Geological Survey Computer Contribution, NTIS Report PB-215 899, 81 p.

Description: SOLMNEQ is a computer program written in PL/1 for the IBM 360 computers. SOLMNEQ computes the equilibrium distribution of 162 inorganic aqueous species generally present in natural waters over a temperature range of 0° to 350°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 developed in part from the programs WATCHEM (Barnes and Clark, 1969) and WATEQ (Truesdell and Jones, 1973, 1974).

The paper by Aggarwal, Hull, Gunter, and Kharaka (1988, in press) describes the capabilities of a modified FORTRAN version of SOLMNEQ, called SOLMNEQF. SOLMNEQF calculates the equilibrium distribution of 236 aqueous species, including uranium, vanadium, and 18 organic species of acetate, oxylate, and succinate, and the saturation states of 196 minerals. SOLMNEQF can be used for simulating the effects on pH and solubility relationships resulting from (1) a change in temperature, (2) addition of gases (CO_2, H_2S, or NH_3) lost before pH measurement, (3) isothermal mixing of two solutions, (4) precipitation/dissolution of a given amount of a solid, and (5) the loss of steam by boiling.

Availability: Report from NTIS (PB-215 899).

CHEMICAL MASS TRANSFER

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

Reference: Plummer, L. Niel, Parkhurst, David L., and Kosiur, David R.,
1975, 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, 68 p.

Description: The computer program MIX2 utilizes an aqueous model akin
to WATEQ and constraints of mass balance and electrical balance 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 con-
stituent or constituents in mixtures owing to exchange or interaction
with adjacent systems. In addition, MIX2 allows for mineral preci-
pitation 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 both cation and anion mass
balances to determine convergence.

In finding the pH of a solution that, through convergence on mass
balance in the aqueous model, will result in perfect electrical
neutrality, an iterative cyclic approach is used. That approach
uses improved estimates of pH as input to the aqueous model for
convergence on mass balance which, in turn, results in new corres-
ponding values of charge balance. If electrical neutrality is not
acceptably well approximated, a new estimate of pH is computed and
the cycle starts over again.

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, described in a following section [Parkhurst,
Thorstenson and Plummer (1980)], is considered to be a replacement
for MIX2.

<u>Availability</u>: Report from NTIS (PB-251 668). Computer program and report also available from WATSTORE.

Balance Mass and Electrons

Reference: Parkhurst, David L., Plummer, L. Niel, and Thorstenson,
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 of two end-member waters with or without mineral-water inter-
action, 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,
an additional phase may be added. BALANCE solves a set of simultaneous
linear equations that represent mathematically 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 Solution + Reactant Phases = Final Solution + 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) discuss 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 from NTIS (PB-82 255 902). Computer program and
report also available from WATSTORE.

Balance Mass and Electrons

Reference: Parkhurst, David L., Thorstenson, Donald C., and Plummer,
L. Niel, 1980 (Revised edition - January 1985), PHREEQE-A computer
program for geochemical calculations: U.S. Geological Survey Water-
Resources Investigations Report 80-96, 193 p.

Description: PHREEQE is a FORTRAN 77 computer program that calculates
the following quantities during the reaction simulation: (1) hydrogen-
ion activity; (2) relative election activity; (3) total concentration
of elements; (4) the amounts of minerals (or other phases) transferred
into or out of the aqueous phase; (5) the distribution of aqueous
species; and (6) the relative saturation of the aqueous phase with
respect to specified mineral phases. PHREEQE can 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 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.

A preliminary thermodynamic data base is provided that includes 120
aqueous species of 19 elements and information for 24 minerals.

Numerical features: Because of the non-linear nature of the problem of
determining a distribution of species that satisfies simultaneously
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 involving oxidation-reduction
processes are more likely to cause such convergence difficulties
because the equilibrium concentrations of some species can vary drama-
tically from a fully-oxidizing to a fully-reducing environment.

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

Past applications: Many.

Remarks: To facilitate formulation of the input data file to the
computer program PHREEQE, the interactive computer program PHRQINPT
(Fleming and Plummer, 1983) was developed. The report describing
PHRQINPT is available from the Books and Open-File Reports Section.
The computer program PHRQINPT and the report describing its use also
are available from WATSTORE.

Reference: Bodine, M. W., Jr., and Jones, Blair 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°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 based on the Gibbs phase rule, available free energy values, and observed low-temperature mineral association.

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

Past applications: Just published.

Availability: Report from Books and Open-File Reports Section. Computer program and report from WATSTORE.

SUMMARY AND CLOSING REMARKS

The reports listed in this report have all been published or developed by the U.S. Geological Survey and contain listings of computer programs which solve problems concerning the physics and chemistry of ground water. Some reports are included for either historical purposes or for documentation of a specific method. Thus, not all programs are currently being widely used. Some programs have been released so recently that the statements on past applications cannot indicate the extent to which those programs probably will be used. A few programs have been or are being used on many studies. Those reports were so noted.

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