

Summary review of available models for groundwater flow and contaminant migration

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Technical Documents in Hydrology



International
Hydrological Programme
United Nations Educational,
Scientific and Cultural Organization

UNESCO
Paris, 1993



INTERNATIONAL HYDROLOGICAL PROGRAMME



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*PROCEEDINGS of the
Workshop on Hydrological Impact
of Nuclear Power Plant Systems
(Paris, 23-25 September 1992)*

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(P. Giuliani, ENEA/ANTAR)

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HYDROGEOLOGICAL FACTORS IN NUCLEAR POWER PLANT SITING

1. General considerations

The purpose of siting investigations and studies for nuclear power plants -NPP- is to ensure that people and environment are not affected by the potential radioactive releases from the NPP, both in normal operating conditions and in accident conditions.

Thus, in siting, three main areas are studied:

- the actions of the plant on the environment (potential radioactive releases),
- the actions of the environment on the plant (earthquakes, floods, extreme meteorological phenomena, man-made phenomena, etc.),
- characteristics of the site area influencing the impact of the NPP, such as population density and distribution, meteorological diffusion characteristics, hydrological and hydrogeological setting of the site, land and water uses in the site region, etc..

Among the components of the environment, groundwater is one of the most sensitive. It occurs in a very wide spectrum of geological settings: groundwater exists within fractures and fissures of any dimension in hard rocks, like granite or basalt, or within small or large pores in sedimentary rocks or soils.

The velocity of groundwater may be as low as centimeters per year or as high as several tens of meters per year.

All these factors combine in making the prediction of groundwater movement extremely difficult.

The groundwater system is therefore a very fragile one, because contaminants introduced in the system remain there for extremely long periods and move slowly towards outlets like wells or springs. A contaminant may well spend many years in a groundwater system and its movement may in some cases be very difficult to detect or predict.

The siting of NPP takes into careful account hydrogeology. Accidental releases of radioactive materials into the ground may result in the direct contamination of groundwater. Also releases in the atmosphere or in surface waters may reach the groundwater system through deposition on the ground and subsequent leaching into groundwater or through penetration of surface waters into the ground. Contaminants can then move in the groundwater system and eventually reach water extraction points for use by the public.

In summary, radioactive releases to the groundwater can be:

- direct into the groundwater system,
- onto the ground surface and then slowly leached into the groundwater by infiltration of precipitation,
- into the atmosphere and thus widely dispersed at varying distances from the site, then deposited and leached into the ground.

Sites for nuclear installations are carefully analyzed from the hydrogeological point of view. There are no precise and quantitative criteria for site acceptability from this point of view. While in extreme cases it may be clear if a site is acceptable or not, intermediate cases are usually not easy and have to be assessed carefully.

The purpose of siting from the hydrogeological point of view is to select a site where the possibility of interaction with major aquifers is reduced to the minimum and where it is possible to predict with a high degree of confidence the path and the time of transit to potential users of the groundwater.

Among the aspects to be considered:

- mechanism, geometry and other characteristics of the release (source term),
- location of the nearest groundwater use,
- main groundwater discharge points to surface waters,
- depth to local and regional water tables,

- groundwater flow direction and gradients to determine pathways and travel times to accessible environments,
- distance from the site to the main regional aquifers and their recharge areas,
- groundwater-related human activities that could affect the site.

Many site characteristics related to hydrogeology can be influenced by the construction of the plant; the possible consequences of such changes should be evaluated.

There are several stages in a siting investigation. In the first, more general stage, a large region in which a number of possible sites can be selected, is surveyed. In the site survey stage the investigations are usually based on information or data already published or available easily; this process can produce areas which are either very clearly not acceptable or which may be worth of a more detailed and accurate investigation.

The following stage is much more detailed and much local specific investigation is performed. Ad hoc studies are performed, drilling for a better knowledge of aquifers, studies on water uses etc. At the end of this stage a certain number of possible site areas is usually available.

In the third and last stage a final comparison of the few potential sites is done, with extensive local investigations and detailed analysis of data. This stage is concluded with the qualification of the selected site from the hydrological point of view.

It is important to remember that a siting investigation for a NPP is an extremely complex and difficult process, which may take several years. Not only one has to study a large number of natural and man-made events which may influence the safety of a site, but also the possible interactions of the different phenomena among themselves.

In the following some details of the hydrogeological analysis of a site will be given as well as a discussion of the role played by the use of mathematical models in this analysis.

2. Hydrogeological investigations

At this stage the information collected is usually obtained from published documents and maps. It includes:

- data on existing and projected major water uses
- identification of major discharge and extraction points
- indication of groundwater flow
- location, extent and interrelationship of the main hydrogeologic units in the region
- average flow rates and prevailing flow directions of groundwater in the major hydrogeologic units
- charge and discharge information on the main hydrogeologic units
- information on the local and regional water tables, including their seasonal fluctuations

In general not all of the information mentioned is available at this very preliminary stage of siting. However, information of this nature, even if not complete, will help in a first screening of potential site areas.

More detailed information is collected for the comparison of the site areas which may be taken into further consideration; it includes:

- characteristics of the major hydrogeologic units and their interconnections.
- type and stratigraphy of the geological formations at each site, including their geological setting. This data are obtained from existing maps and from the exploratory drilling performed at the site areas.
- seasonal and quantitative data on recharge and depletion of relevant hydrogeologic units; their relationship with surface waters.

- water uses in the region, both actual and predicted.
- climatological data, especially precipitation
- geochemical properties of subsurface material

On the basis of data and information such as that listed above a comparison of potential sites can be performed.

After a site has been finally selected, very detailed local and site area investigations are started. The purpose of the study at the site evaluation level is to understand the hydrogeological situation to the extent of being able to assess the concentration of the released radioactive material in the groundwater and the transport path with its related time of travel to the points of possible water use.

At this final stage a large amount of data and information is needed, and a good detail is necessary in order to perform the assessments.

Much exploratory work is performed at and near the site, samples are collected, monitoring of the groundwater systems is begun- and monitoring of many parameters will continue during the entire lifetime of the plant-; some of this work is performed in parallel with other siting investigations, such as geology, soil mechanics, surface hydrology.

It must be stressed that the study of groundwater flow is very difficult and the prediction of groundwater transport of contaminants of any nature is further complicated by the various physico-chemical processes occurring between the contaminants and the water-bearing rocks and soils. Only in very simple cases it is possible to predict with confidence the paths of contaminants and the travel times.

Among the most difficult situations to analyse are the cases of very ample variations of water table levels in which it is sometimes possible to define a large number of groundwater regimes, each one with its own velocities and directions of transport, the presence of salt water wedges intruding in the groundwater system in estuarine locations. In cases like these the use of physical models in the laboratory may help in

understanding the actual behaviour of groundwater.

3. Models

To predict the behaviour of a contaminant in the groundwater and to evaluate potential exposures to the population, many computer models are nowadays commonly available. It is important to recognize that computer models allow us to analyze data collected from surface and subsurface explorations. The results of computer analyses will, however, strongly depend on the completeness and accuracy with which the system has been defined.

In many instances, the computer model averages characteristics over large areas and the results may not be sufficiently detailed to address a concern at a specific location.

Therefore, it is important that models to be used be frequently updated and/or adapted to incorporate changes in the data base occurring during the construction and operation of the facility, such as those caused by excavation works for foundations. Furthermore, existing and potential water users should clearly be identified and added to the model as well as water quality and changes in direction and travel time.

Some of the models are very simple in nature and are based on a once-through or constant release rate approach assuming homogeneous and isotropic conditions in a water-bearing formation.

More complex models take into account heterogeneity and anisotropy of the overall geological setting, dispersion characteristics and sorption phenomena.

Processes and factors

The processes and factors that govern the movement of radionuclides in the hydrogeological environment must be identified and evaluated. The final use for such information on the site and its environs is:

(a) to calculate the length of time for the contaminant to reach the accessible

environment and (b) to predict the concentration levels resulting from severe

releases from a nuclear facility into a water-bearing formation. This is usually achieved by modelling the radionuclide transport from the site specific release point to potential outlets to the human environment.

Among the many natural processes that affect the movement of radionuclides and their concentration distribution in the aquifer the physical and chemical ones play the major role. Since their importance can vary with varying source and site characteristics, they should be properly evaluated and monitored to establish a realistic and current input to the models.

The principal transport routes to be considered are:

- (a) the movement of radionuclides through the unsaturated zone and their interaction with the soil or rock.
- (b) the transport, dilution, dispersion and sorption of radionuclides in the saturated zone.

Deterministic modelling

Since system analysis theory gives only partial insight into the physical mechanisms that may influence the radionuclide transport, a deterministic modelling approach is appropriate, where such a model is needed and where some prior information on geological structure and aquifer parameter values is available.

In the past, the deterministic modelling has concentrated on lumped and one-dimensional models while the more recent solute and water transport models deal with distributed and 2-3 dimensional systems.

Mathematical models representing groundwater flow range from a simple expression of Darcy's Law to a detailed representation of the transient flow, using complex numerical methods. By use of appropriate boundary conditions and aquifer parameters, the groundwater velocity can be determined. The reduction in radionuclide concentration at the point of interest can be determined by solving the equations for hydrodynamic dispersion and sorption.

Numerical models (finite element and finite difference models) in combination with multicompartmental models seem to be a promising way to get a better insight into the actual water flow. This deterministic approach suffers from the problem of how to treat variations in the hydraulic conductivity due to inhomogeneous aquifer structure. Such inhomogeneity influences the dispersion phenomenon. Inhomogeneities of the confining beds can also cause spatial variations of the hydraulic communication between the various groundwater bodies. Stochastic treatment of these inhomogeneities seems to be an appropriate procedure, although the practical experience in this field is limited. The validity of these models should be checked by sensitivity tests of the applied model to variances of the individual input parameters.

To the extent limited by the accuracy of the model and the input data, the selected model should comply with the following main objectives:

- (a) It should be capable of computing the rate of contaminant movement i.e. travel time and the rate of movement to the accessible environment.
- (b) It should be capable of portraying the direction of flow within each of the aquifer units of concern.
- (c) It should be capable of computing the distribution of the concentration of radionuclides migrating through the geologic material.
- (d) It should be capable of assessing the effective capacity of the geologic media to contain the released contaminant and, of determining the amounts of radionuclides reaching the outlets of the system in near as well as far future periods of time.
- (e) It should be capable of analysing:
 - the potential effects of the postulated releases.
 - the significance of changes that can occur in the groundwater system during normal as well as abnormal operational conditions of the given nuclear facility.
 - the effectiveness of a preventive and/or mitigative system or systems in controlling and containing/removing contaminated groundwater.

To achieve these goals, the information relevant to the overall groundwater system, both on regional and local bases, should be available.

The extent and quality of required data will largely depend on:

- The source term under consideration, i.e. the type of nuclear facility and its operational conditions, effectiveness of safety measures.
- the complexity of the hydrogeological system.
- the environmental characteristics of the site, in relation to the important groundwater resources in the region and the land use.

References used in the preparation of this text:

- IAEA - Safety Guide no. 50-SG-S7

"Nuclear Power Plant Siting: Hydrogeologic aspects", 1984

- IAEA - TECDOC - 482

"Prevention and mitigation of groundwater contamination from radioactive releases", 1988.

SUMMARY REVIEW OF AVAILABLE MODELS IN GROUNDWATER FLOW AND CONTAMINANT MIGRATION

1. Sources of documentation

Several directories and reviews have been published quite recently describing features and capabilities of groundwater and contaminant transport models.

The most comprehensive review is the 1985 American Geophysical Union (AGU) monograph from Van der Heijde et al "Groundwater Management: The Use of Numerical Models". This study includes, besides flow and transport models, also heat transport, deformation and multipurpose codes.

Other references are available from the International Ground Water Modeling Center (IGWMC) Newsletters, their 1992 Software Catalog and Model Annotated Retrieval System (MARS) database. A Summary of Subsurface Hydrological and Hydrochemical Models has been prepared by Mangold and Tsang in 1992 including geochemical, solute transport and hydrochemical models.

More specific model studies and reviews related to radionuclide migration in the geosphere have been developed within international programs for radioactive waste disposal assessment methodologies.

These models are summarized in a directory prepared under a EC Research Program (1984). This directory actually reviews several kinds of codes: nuclide inventory, leaching, geochemistry, heat transfer codes and coupled processes codes. Total system analysis programs are also included. Another source of radionuclide migration programs is the 1991 catalog of the NEA (OECD) Data Bank that describes the codes tested and available at the Bank itself.

A list of selected reports that document numerical models produced by the U.S.G.S. has been prepared by Appel and Reilly.

It should be stressed that most radionuclide migration codes have been implemented for waste disposal applications and that little efforts have been dedicated in the past to modeling hydrogeologic processes for nuclear power plant siting aspects or for risk assessment of radionuclide release in groundwater from power plant accidents.

However, it is generally true that contaminant transport codes may be applied independently of the nature and origin of the source; rather it is important that the code may simulate all relevant processes and account for all critical site features.

2. Model classification and features

The surveyed models belong to the category of "prediction models" which simulate the behaviour of the groundwater system and its response to stresses in terms of spatial and temporal changes in the movement of water and contaminant distribution.

The processes described by these models include fluid flow, mass transport by convection and dispersion and some geochemical processes.

A common feature of all models surveyed is that their predictions are deterministic (one value) rather than probabilistic (a range of values of varying probabilities).

Representation in the spatial domain is always by distributed parameters. Almost all flow models are based on Darcy's law, valid for porous media. Few of them treat fracture flow.

In the hydrogeological domain groundwater models are distinguished in saturated and unsaturated, hydraulic (if Dupuit approximation holds) or hydrodynamic, single phase or multiphase (water + air, water + sea water), confined, semiconfined, or phreatic. Numerical models generally handle nonhomogeneous and anisotropic parameters.

Spatial dimensions, in numerical models, are 2D or 3D. Some codes allow for a better simulation of seepage problems, near-field, or unsaturated flow problems by 2D vertical profile representation of the domain. For more general migration and environmental impact assessment studies, 2D areal perspectives are adopted.

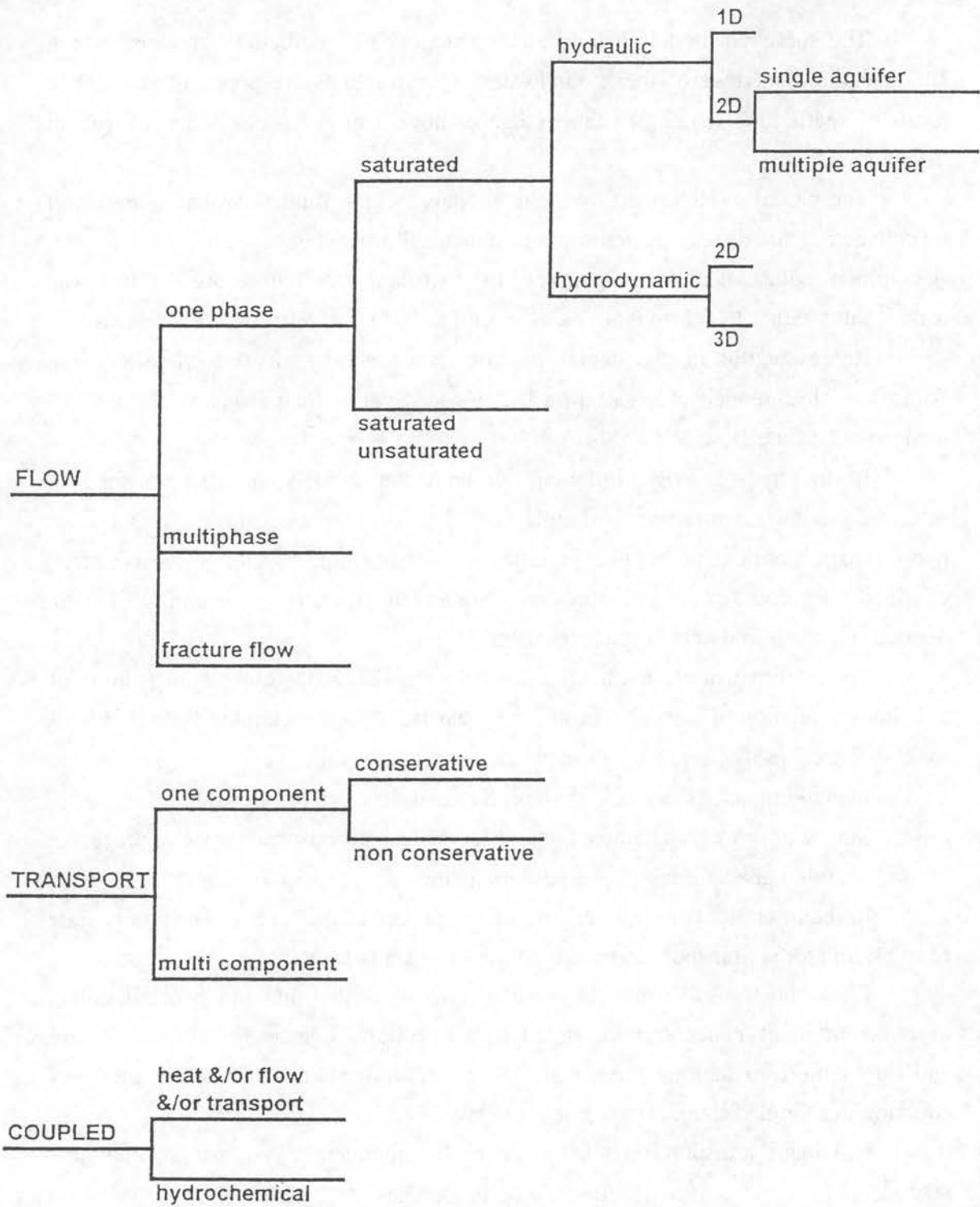
Mass transport is generally non-conservative and adsorption/decay processes (as well as other geochemical processes) are included.

In the time domain flow and transport processes may be either steady-state or transient (some transport codes are limited to steady flow).

Flow and transport models are generally sequential and independent unless high contaminant concentration, or high temperature, affect groundwater density and flow pattern to such an extent that flow equation needs to be joined to transport equation in a single "coupled processes" model.

Few mass transport models handle multicomponent systems and chemical reactions. In these cases reactions among species or with soil, described by geochemical models, may be coupled to transport processes in hydrochemical models.

This tentative classification is represented in the following scheme (from Van der Heijde, modified).



Classification of groundwater flow and contaminant transport prediction models

3. Mathematical methods

Almost all models reviewed use numerical methods to solve the partial differential equations of flow and transport. They are adopted when analytical solutions are too restrictive and are not able to represent, to the required accuracy, the behaviour and features of the system. Analytical methods are generally adopted in a preliminary assessment phase when not enough data are available to run a numerical code.

For all numerical methods the general approach is to discretize the spatial and temporal domain and to transform the field equations into a set of algebraic equations with one equation required for each node or cell and/or time step.

The requirements of numerical methods are that the solution should be convergent and stable: this means that the numerical solution should converge to the true solution as the grid of discrete points is refined and that errors introduced at each step of calculations should not produce unacceptable oscillations in the results.

These qualities are sometimes tested through verification of the numerical method against analytical solutions.

The most common numerical methods employed are the finite difference (FDM) or finite element methods (FEM). For transport models the method of characteristic (MOC) and random walk methods are sometimes employed.

The FDM uses a rectangular grid discretization and can follow different approximation schemes such as the forward or backward (implicit) difference or the central difference Crank Nicholson scheme. Solution methods for the linear algebraic equations may be direct (Gaussian Elimination and Cholesky Factorization) or iterative (Gauss Seidel, Successive Over Relaxation, Conjugate Gradient Method).

In general direct methods carry out a sequence of operations once and provide an exact solution, ignoring computer round-off errors; for large problems such methods may require vast amounts of computer storage. Iterative methods may fail to converge for some problems, for example for steady state problems which are poorly conditioned. Iterative methods require little computer storage and are generally fast. Conjugate Gradient Method is becoming popular for solving groundwater problems.

The FEM provides a much better approximation of the system geometry since the finite elements may have an arbitrary shape: in 2D they may be linear triangles, distorted rectangles or shapes with curved boundaries. In the FEM an integral approach is used to form the linear algebraic equations. The method used

to define the equations is the Weighted Residuals and in particular Galerkin's method which is widely used in hydrogeological models. Solution is then sought by iterative or direct procedures.

For multi-dimensional problems the domain boundaries and internal regions of changes in aquifer characteristics are better discretized by the FEM which allows also a more efficient representation of anisotropies and stress areas. FEM is more indicated for unsaturated flow problems as it is easier to incorporate the high nonlinearity of hydraulic properties above the water table; phreatic aquifer problems, where the saturated thickness varies with time, are also easily modelled by FEM letting the mesh expand or contract with the water table.

FDM is generally preferred for approximating the time derivative; so it may happen that a mixed FEM-FDM solution is adopted.

In a similar way FDM and FEM are applied to solve the advection-dispersion equation for solute transport; but it is generally recognized that these methods may introduce numerical dispersion and instability problems to the result. Some modification to the traditional methods as, for example, the upstream weighting function for the Galerkin FEM, may guarantee a more stable solution.

The Method of Characteristics (or Particle in Cell) has been developed to overcome dispersion introduced by FDM and FEM calculation processes. This method starts from a discretized velocity field (generated for example by FDM) where a number of particles, representing a certain solute concentration, are inserted within each cell. Then each particle is advected (moved) by its cell velocity and the new particle concentration is computed in each cell. The dispersion is taken into account and concentrations are updated by this factor. This procedure is repeated for each time step. This method is useful for highly advective transport where a finite element mesh should be very finely discretized. On the other hand the method suffers from the need of an accurate recording of a large number of particles that may increase in number as they move downstream dispersion. Numerical dispersion and oscillations may be introduced, but to a less extent also by this method.

Also in the Random Walk Method the transport equation is solved by representing the mass of contaminant with a large a number of particles. Each particle is moved independently at each time step according to a step equation which is statistically equivalent to the advection/dispersion equation. Concentration at each time step in each cell is calculated by computing the number of particles in that area. This method does not introduce numerical dispersion. A large number of particles may be required for some problems and boundary conditions may be difficult to prescribe. Nevertheless this method is becoming very popular in groundwater solute transport models.

4. Model selection criteria

Factors that have been considered in selecting a number of groundwater flow and solute transport models refer mainly to their capability to simulate processes relevant to the problem of NPP siting and to represent different site configurations and hydrogeological characteristics.

Another criteria refers to the "popularity" of the model i.e. to the number of users, tests and real cases where the model has been successfully applied and to the validation and verification exercises which the model has gone through.

Model documentation, availability and references generally come along with their popularity.

This selection approach is probably quite different from that followed when a site or scenario specific assessment has to be carried out and a code must be chosen. In that case, selection of the code depends very much on the complexity and features of the groundwater system conceptual model and on the interfaces of the groundwater system model with source term and biosphere models.

In some cases the choice may reflect the user familiarity with the particular mathematical (numerical) approach adopted in the program. However for solving a particular problem, code selection is strongly "site specific".

The present review aims only at a presentation of a number of deterministic groundwater flow and transport codes, collected also outside the "nuclear domain", representative of the state of the art.

5. Description of selected codes

Selected codes are briefly described in the form of summary reports according to a number of identification items that should help in characterizing codes capabilities .

The items 'Name of Program' and 'Author', refer to one version of the code. Other versions may exist with slightly different names, contributions from other authors and slightly different or additional features.

Contents of items 'Applications to date', 'Method of solution', 'Program operation', 'Availability' and 'References' are taken from the Sources of Documentation cited (see above Par.1 and Bibliography). Only in a few cases direct informations or program manuals were available.

Programs are listed in alphabetical order. A synoptic table, assembling all key-features of selected codes, is shown at the end of this Paragraph.

Name of program

AQUA

Author

Vatnaskil Consulting Engineers, Reykjavik, Iceland

Program functions

AQUA solves confined/unconfined groundwater flow, contaminant (or heat) transport 2D problems in nonhomogeneous and anisotropic media at steady state and transient conditions. Decay, adsorption and dispersion are included. The program allows for a large number of pumping and injection wells with time varying rates and areal variation of leakage and infiltration. Several flow and concentration boundary conditions are permitted. AQUA solves problems on regional and local scale (horizontal and vertical perspectives) as well as seepage problems.

Applications to date

Prediction of groundwater contamination from geothermal power plants in Iceland. Surface pond disposal of geothermal wastewater.

Method of solution

Galerkin finite element method is used to solve groundwater flow and transport equations.

Program operation

AQUA is written in Fortran 77.

Input is prepared by keyboard entry or with a mouse or digitizer supported by several efficient graphical preprocessors. The finite element mesh is automatically generated and condensed. Input and output files format knowledge is not necessary. The package includes also graphical postprocessors.

AQUA Extended Memory version runs on a 386/486 PC with 4Mb RAM.

Availability

AQUA is a commercial code distributed in Europe by Natural System Software and in the US by Scientific Software Group.

References

- Holm, S.L., Kjaran, S.P., Ingolfsson, A. : Computational Hydraulics and Hydrology in Iceland. Proceedings of the Nordic Hydrological Conference in Reykjavik, 1988.
- Kjaran, S.P., Sigurdsson, S. : Treatment of time derivative and calculation of flow when solving groundwater problems by Galerkin finite element methods. Advances in Water Resources, Vol.4, March 1981.

Name of program

ASM

Author

W. Kinzelbach, University of Kassel
R. Rausch, University of Stuttgart, Germany

Program functions

ASM simulates groundwater flow and solute transport in a 2D space. The program handles both steady state and transient flow conditions, confined, phreatic and leaky-confined aquifers. Media can be heterogeneous and anisotropic. Time varying pumping and injection rates, recharge and permanent or instantaneous solute injection may be modeled. It includes transport processes such as dispersion, molecular diffusion, decay and adsorption.

Applications to date

Used for first estimates in assessing field problems. Widely used as educational tool.

Method of solution

ASM uses a 2D node centered finite difference scheme. The algebraic equations are solved either by the alternating direction implicit method or the conjugate gradient method. Pathlines and isochrones are computed by Prickett or Pollock interpolation schemes.

Solute transport is simulated by the random-walk method.

Program operation

ASM is written in Microsoft QuickBasic.

The program is menu driven and fully interactive. All input is prepared via input menus in a machine user dialogue. Areal data are inserted by moving the cursor on the model grid and entering numerical values. Output is graphically displayed in terms of contour lines, flow vectors, pathlines, time series at observation wells and mass balance.

ASM runs on PCs with 640Kb RAM.

Availability

The code is available directly from the author or from IGWMC together with its manual and technical support.

References

Kinzelbach W., 1986. Groundwater modeling - An Introduction with Sample program in Basic. Development in Water Science, 25, Elsevier. Amsterdam.

Name of program

AT123D

Author

G.T. Yeh, Oak Ridge National Laboratory, (presently at Pennsylvania State University) , USA

Program functions

The program is based on an analytical solution for transient 1-2 or 3D transport in homogeneous anisotropic aquifers. The program allows for simulation of advection, diffusion, dispersion, retardation and first order decay. Simulation of various source configurations and boundary conditions is possible, as well as horizontal and vertical transverse dispersion that can be input independently. The model calculates concentration distribution in space and time. Flow field is only stationary.

Applications to date

The code has been checked against head calculations and laboratory experiments. It has been applied to radioactive waste and hazardous chemical transport in aquifer systems.

Method of solution

Analytical solution are expressed by Green's function representation.

Program operation

The program is written in Fortran IV.

AT123D input is read from a file which must be prepared by line editor or word processor. Results are also output to a file. The version included in the RISKPRO package is supported by pre and post processors.

The code runs on PCs with 384K RAM.

Availability

The code has been published and is available from IGWMC together with source code, example data sets and documentation by G.T. Yeh. The RISKPRO package is distributed by General Science Corporation.

References

G.T. Yeh, 1981, AT123D: Analytical Transient One-, Two- and Three-Dimensional Simulation of Waste Transport in the Aquifer System. ORNL-5602, Environmental Sciences Division, Oak Ridge National Laboratory.

Name of program

CFEST

Author

Gupta S.K.,C.R. Cole, C.T. Kincaid and A.M. Monti, Office of Nuclear Waste Isolation, Battelle Memorial Institute and Pacific Northwest Laboratory, USA.

Program functions

CFEST is an updated and extended version of the code FE3DGW which is a 3D groundwater flow program.

CFEST is a coupled fluid, energy and solute transport code for analyzing anisotropic, isothermal and non-isothermal events in confined, unconfined, semiconfined, multiaquifer systems.

Multidimensional, density dependent flow, steady state and transient conditions may be modeled. Improvements of the code include stochastic parameters and boundary conditions.

Predicted variables are head, temperature and concentration.

Applications to date

FE3DGW and CFEST have been used in research and field applications. Verification has been performed by comparison with PATH analytical code and by participation in the international Hydrocoin Program.

Field applications refer to modeling of:

- . Sutter Basin, California;
- . Long Island Ground Water System, New York;
- . Nuclear waste repository assessment in salt and basalt formations.

Specific applications are regional hydrologic characterization and simulation of coupled transport of fluid, heat and salinity.

Method of solution

Galerkin finite element method is used to solve differential equations for pressure, temperature and concentration coupled with fluid density and viscosity. The code employs bilinear quadrilateral elements in all two-dimensional analysis and three-linear quadrilateral elements in 3D simulations.

Program operation

The code is written in Fortran IV.

Input data are in the form of well log data describing stratification, hydraulic properties of each geological layer, fault zones, surface water boundaries, withdrawal and injection wells.

Pre and post processing programs for graphic display of input and output data and variables are available.

The code is designed to use the virtual memory capability of main frame computers. It has been developed for the DEC VAX 11/780 under VAX/VMS although other mainframe or minicomputer implementations are known.

Availability

The program is available through the code custodian of ONWI at Battelle or at the NEA (OECD) Data Bank together with its manual and supportive documentation. The report is also available from NTIS-US Department of Commerce.

References

Gupta S.K., C.R. Cole, C.T. Kincaid and A.M. Monti (1987). Coupled Fluid, Energy and Solute Transport (CFEST) Model. Formulation and User's Manual. BMI/ONWI 660. Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio.

Name of program

CHEMTRN

Author

C.W. Miller and L.V. Benson, Lawrence Berkeley Laboratory, Berkeley, California, USA.

Program functions

CHEMTRN allows for a comprehensive geochemical simulation of the 1D transport of solutes in a porous medium. The model includes the effects of advection, dispersion, aqueous complexation, sorption, reversible precipitation/dissolution and the dissociation of water. Sorption is modelled by ion exchange and surface complexation. Irreversible dissolution may also be modelled. Extension to 2D or 3D is possible by solving the chemical equations along predetermined streamlines although this approach does not allow for dispersion normal to the flow.

Applications to date

The code has been verified by comparing it with two analytical solutions and a field experiment. It has been applied to nuclear waste isolation and chemical contaminant transport.

Method of solution

The transport equations are discretized to yield a set of finite difference equations. These are solved simultaneously with the chemical equations by the Newton-Raphson method.

Program operation

The code is written in Fortran IV.

It has been used on CDC 7600 and VAX 11/780. No pre/post processors or graphic output are known.

Availability

The code is public and available through the US National Energy Software Center. User manual with theory and example problems is provided.

References

Miller, C.W., Toward a comprehensive model of chemical transport in porous media. Scientific basis for Nuclear Waste Management VI, Mater. Res. Soc. Symp. Proc., 15,1983.

Miller, C.W. and L.V. Benson. Simulation of solute transport in a chemically reactive heterogeneous system: Model development and application. Water Resou. Res., 19,1983.

Name of program

FASTCHEM

Author

C.J. Hostetler and R.L. Erikson, Battelle PNL/EPRI,USA

Program functions

FASTCHEM consists of six codes that combine 2D flow field calculation, geochemistry and coupled transport. Saturated/unsaturated flow is modelled by the EFLOW module. The geochemistry module ECHEM is based on the geochemical code MINTEQA2. The geochemical submodel simulates aqueous complexation reactions, solubility reactions, adsorption, ion-exchange, oxidation/reduction. ETUBE is the water-parcel tracking code that transforms the 2D flow field in 1D path lines. The module EICM couples transport equations with chemical relations. The transport processes of advection, hydrodynamic dispersion and molecular diffusion are included in EICM.

Applications to date

The transport and reactive transport processes simulations have been verified against six analytical solutions.

The code has been applied (and developed) for studying waste disposal from electric utility fossil fuel plants.

Method of solution

Flow equation is solved by the finite element method. In the transport analysis a two-step algorithm is used.

Program operation

The package is divided into input/output intensive codes for PC 640K and calculation intensive codes for mainframe computers. A communication link is provided to connect the workstation with the mainframe computer. The workstation codes perform the interactive preprocessing (ECPR) and postprocessing (EGRF) functions of the package. The mainframe codes are not interactive but can be run independently to examine individual aspects of the geohydrochemical problem.

Availability

The code is proprietary.

References

Hostetler C.J., and R.L. Erikson, FASTCHEM package, vol.5, User's guide to the EICM coupled geohydrochemical transport code, Rep. EA-5870-CCM, EPRI, Palo Alto, Calif.,1989.

Name of program

FEMWATER\LEWASTE

Author

G.T. Yeh, Oak Ridge National Laboratory (presently at Pennsylvania State University), USA

Program functions

FEMWATER\LEWASTE is a 2D finite element code for modeling saturated, unsaturated flow and transport. Steady state and transient problems may be applied to heterogeneous and anisotropic porous media. Decay, dispersion and sorption are included. Input relative permeability functions is required. Predicted variables are head distribution, velocity vectors, moisture content, concentration distribution.

A 3D version of both programs is available .

Method of solution

The code uses the finite element Galerkin formulation. Finite differences method is used to approximate the time derivative. LEWASTE is an improvement of the former FEMWASTE code that uses the Eulerian-Lagrangian approach.

Applications to date

The program has been used for solid waste disposal and shallow trench burial problems, seepage pond leakage and similar groundwater contamination studies. It has been compared with several analytical solutions and other programs. FEMWATER is one of the HYDROCOIN codes. FEMWATER\FEMWASTE is also in the list of NRC repository siting codes. The program is widely used in the US and in Europe by private companies, universities and government agencies.

Program operation

The code is written in Fortran IV.

The program has been used on IBM 360, CDC and UNIVAC mainframes. 2D and 3D PC versions have also been developed. The program does not include pre or post processors but a PC version with supporting graphics for input and output display is known to exist.

Availability

The code is of public domain. It is available from NEA Data Bank with user's manual, source code and documentation.

References

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

Yeh, G.T., FEMWASTE: A finite element model of waste transport through saturated-unsaturated porous media: First revision, Rep. ORNL5601/R1, Oak Ridge Natl. Lab., 1989.

Name of program

FTRANS

Author

Huyakorn, P.S., Geotrans Inc. / ONWI

Golis, M.J., Battelle Project, Columbus, Ohio, USA

Program functions

FTRANS is a 2D code designed to simulate groundwater flow and transport of radionuclides in a fractured porous medium. The model takes into account fluid interactions between the fracture and porous matrix blocks, advective-dispersive transport in the fractures and diffusion in the porous matrix, and chain reactions of radionuclides.

The program uses a dual porosity or a discrete fracture modeling approach or a combination of the two. Aquifer may be confined/semiconfined, anisotropic and heterogeneous. A FTRANS-2 version exists that models multiaquifer, quasi-3D systems. A version that accounts for coupled thermal fluid capability and density dependent flow and solute transport also exists.

Applications to date

The code has been applied to the transport of ^{237}Np from a waste repository in a uniform flow field.

It has been tested within the international INTRACOIN program of transport codes intercomparison.

Method of solution

The finite element method is adopted with the upstream weighting scheme to simulate flow in the fractures.

Program operation

The program is written in Fortran IV.

It was designed to operate on a CDC Cyber 740. It can be used on its own or in conjunction with other flow codes, such as NETFLO and STFLO which perform a preliminary simplistic steady state flow calculation.

Availability

The code is proprietary but a tested version is available from NEA Data Bank. Code custodian is at ONWI, Battelle Project Management Division.

References

Huyakorn, P.S., B.H. Lester and J.W. Mercer. An efficient finite element technique for modeling transport in fractured porous media, 1, Single species transport, Water Resour. Res., 19(3), 1983a.

Name of program

HST3D

Author

K.L. Kipp, United States Geological Survey

Program functions

HST3D simulates saturated groundwater flow and associated heat and solute transport in three dimensions. 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 fluid viscosity on temperature and solute mass-fraction.

Confined, semiconfined and phreatic aquifers with heterogeneous and/or anisotropic media are modelled. Advection, dispersion, molecular diffusion and linear decay are included together with linear equilibrium adsorption.

Applications to date

HST3D has been verified against eight analytical solutions and also compared to the finite element transport code SUTRA.

Applications include subsurface waste injection, landfill leaching, saltwater intrusion, freshwater recharge and recovery, radioactive waste disposal, geothermal systems.

Method of solution

HST3D uses the finite difference method to solve groundwater flow and heat/solute transport equations. Two solution techniques are available, one is a direct elimination solver, using equations reordered by diagonal planes, the other is an iterative solver, using two-line successive overrelaxation.

Program operation

HST3D is written in Fortran 77.

The code runs on main frame PRIME, VAX and CRAY computers. A PC version and an extended memory version that runs on 386/486 PCs with 4Mb RAM exist.

The EM version includes pre and postprocessors which allow easy entry and editing of the input and an output format suitable for the SURFER graphics package.

Availability

HST3D is public and available from USGS and IGWMC.

References

Kipp K.L., 1987, HST3D: A computer code for simulation of heat and solute transport in three-dimensional groundwater flow systems. USGS Water-Resources Investigations Report 86-4095.

Name of program

MMT

Author

W. Ahlstrom, J.F. Washburn, J. Golis, PNL and Battelle Project Management Division, USA

Program functions

MMT solves the 1D equation for transport of solutes in groundwater systems, with uniform velocity and transport properties.

MMT treats convective transport, sorption/desorption effects and hydrodynamic dispersion only along flow direction.

MMT may take into account transport of several contaminants at the same time, simulates decay processes and transport of daughter nuclides.

2D and 3D versions of the code exist that may simulate saturated/unsaturated flow, confined, semiconfined, phreatic aquifers, precipitation\dissolution reactions and ion exchange. Transport of decay products is only one-dimensional.

Applications to date

MMT is used to simulate radionuclide transport from waste disposal sites or, more generally, transport of groundwater solutes.

The code has been verified against analytical results for a variety of one-dimensional problems, and was applied to one two-dimensional field study. It has participated in the INTRACOIN benchmark exercises and is listed in the catalog of NRC repository siting codes. It has been tested also at the NEA Data Bank.

Method of solution

The Discrete -Parcel Random Walk method (DPRW) is used to model mass transport coupled equations.

Program operation

MMT is written in Fortran 77.

MMT is supported by several post processors that filter and smooth the output to reduce statistical fluctuations.

The program runs on a CDC Cyber 740.

Availability

The code is public and available from NEA Data Bank together with source code and example cases. The 3D version MMT-DPRW is available at Battelle PNL.

References

Washburn J.F., F.E. Kaszeta, C.S. Simmons and C.R. Cole (1980). Multicomponent mass transport model: a model for simulating migration of radionuclides in groundwater. PNL-3179, Pacific Northwest Laboratory.

Name of program

MOC and MOC DENSE

Author

L.F. Konikow and J.D. Bredehoeft (MOC)

L.F. Konikow and W.E. Sanford (MOC DENSE), United States Geological Survey

Program functions

MOC is a 2D method for simulation of non-conservative solute transport in saturated groundwater systems. It computes changes in the spatial concentration distribution over time caused by convective transport, hydrodynamic dispersion, mixing or dilution from recharge, radioactive decay, reversible equilibrium-controlled sorption with linear, Freundlich or Langmuir isotherms and reversible equilibrium -controlled ion- exchange for monovalent or divalent ions. MOC may model heterogeneous and anisotropic aquifers. Flow equation is solved before simulating transport problems. MOC DENSE is a version that can simulate solute transport and dispersion of either one or two constituents where there is a 2D density dependent flow.

Applications to date

MOC in its original USGS version, or enhancements provided by software houses, is a very widely used solute transport code (possibly the most used at present) for a variety of different applications in the US and in Europe.

Method of solution

MOC uses the Alternating Direction Implicit (ADI) scheme or the Strongly Implicit Procedure (SIP) to solve the finite difference approximation of the groundwater flow equation.

MOC 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.

Program operation

MOC is written in Fortran IV.

A pre-processor is included to facilitate input preparation. Output processors or graphic routines are not included in the package but several products have been developed for MOC by software houses.

MOC runs on a 640K RAM PC. An extended memory version is also available that requires a 386/486 PC with 2Mb RAM.

Availability

The code is public and available from USGS and IGWMC together with source code and user's manual. Training courses are organized in the US and in Europe.

References

Konikow, L.F. and Bredehoeft J.D., 1978, Computer model for two dimensional solute transport and dispersion in groundwater. Techniques of Water Resources Investigations of the USGS, Book 7, Chapt. C2.

Goode, D. J. and L.F. Konikow, Modification of a method of characteristics solute transport model to incorporate decay and equilibrium-controlled sorption or ion exchange. Water-Resources Investigations Rep. 89-4030, USGS, 1989.

Name of program

MODFLOW

Author

M.G. McDonald and A.W. Harbaugh, United States Geological Survey.

Program functions

The model simulates steady and transient flow in a 2D irregularly shaped flow systems in which aquifer layers may be confined, unconfined or a combination of confined and unconfined. Quasi or fully three-dimensional flow through layered aquifer systems can also be simulated. The model allows for analysis of external influences such as wells, areal recharge, drains, evapotranspiration and streams.

Applications to date

The program is very widely used (possibly the most used at present) for modelling groundwater flow. Training courses are held in the US and in Europe.

Method of solution

The code uses two different techniques for the solution of the finite difference equations: the Strongly Implicit Procedure and the Slice-Successive Overrelaxation Procedure (SSOR).

Program operation

MODFLOW is written in Fortran 77.

The program has a modular structure that consists of a series of highly independent subroutines called 'modules'. The modules are grouped into 'packages'; each package deals with a specific feature of the hydrologic system which is to be simulated. Pre and postprocessors are included to facilitate input preparation and to reformat part of the output for use in graphic display. Various implementations and enhancements of the code are available from software houses.

The code runs on a 640K RAM PC.

The extended memory version, that includes the Stream Routing package and the Preconditioned Conjugate-Gradient2 solution package, requires 2M RAM.

A mainframe version based on the extended memory version, is available.

Availability

MODFLOW is available from USGS and from IGWMC with Fortran source code and manual.

References

- McDonald, M.G. and Harbaugh A.W., 1984, A modular three-dimensional finite-difference groundwater flow model. USGS Open-file Rep. 83-875.

Name of program

MT3D

Author

Z. Zheng, Papadopoulos & Ass., Inc., USA

Program functions

MT3D simulates convection and dispersion of contaminants in a 2D or 3D space. Adsorption with linear or Freundlich isotherms, first order decay and biodegradation are included. Steady state flow fields from confined/unconfined aquifers may be considered. Nonhomogeneous and anisotropic media are modelled.

Applications to date**Method of solution**

The code is implemented with three mixed Eulerian-Lagrangian options: the method of characteristics, the modified method of characteristics and a hybrid of this two methods. This approach combines the strength of MOC for eliminating numerical dispersion and the computational efficiency of MMC. MT3D can also be used in standard finite difference formulation.

Program operation

MT3D is intended to be used in conjunction with USGS MODFLOW: in fact MT3D supports its hydrogeologic features and discretization options and uses MODFLOW groundwater head calculation. The program has a modular architecture similar to that of MODFLOW.

Utility and post-processing programs are available to transform concentration matrices into files directly legible by commercial graphic packages.

The source code is written in Fortran 77. The executable programs are compiled to run on 386/486 based PCs and 68020/30/40 based Mcintosh.

Availability

The code is available from the authors together with source code and user's manual.

References

Name of program

NAMMU

Author

R. Atkinson et al., AERE, Harwell, UK

Program functions

NAMMU solves density dependent, steady-state or transient, saturated/unsaturated flow, coupled flow and heat transport, solute transport and steady-state brine transport. One, two and three dimensions problems may be solved. Multilayered aquifers with heterogeneous and/or anisotropic parameters are modeled. Fracture elements may be included and different physical equations may be applied in different sub-regions of the domain.

Transport processes simulated are advection, dispersion, diffusion, decay and chemical adsorption.

Applications to date

Nammu is a general purpose code but it has been mostly applied to radionuclide transport problems (repository design). Comparison with analytical solution has been performed. The program has been tested in the international intercomparison Hydrocoin project and verified in several other international projects.

Method of solution

The finite element method is adopted. Transients are solved by Gear's method or Crank-Nicholson; non-linear problems are linearised by Newton-Raphson or quasi Newton-Raphson; parameter stepping for hard non-linear problems is provided; equations are solved by a very fast direct frontal solver.

Program operation

NAMMU is written in Fortran 77.

Several graphic options for input and output data are provided. Standard interfaces for addition of user routines for non-standard input, solvers or output are included. Standard defaults for ease of use by new and inexperienced users is provided.

The code runs on mainframe IBM, CRAY and SUN.

Availability

The code is available under license from AERE.

References

Atkinson R., A.W. Herbert, C.P. Jackson, P.C. Robinson and M.G. Williams:
NAMMU User Guide (release 4), AERE Harwell, Theoretical Physics Division,
1984.

Name of program

PATHS

Author

R.W. Nelson, Battelle Pacific Northwest Laboratories, USA

Program functions

The program evaluates contamination problems in unsteady 2D isotropic and homogeneous confined aquifers using analytical solutions. Advection, adsorption, ion exchange and decay processes are modelled. The code gives the flow path network. Dispersion is not included.

The code has been designed to make a quick and inexpensive preliminary evaluation of contamination problems.

Applications to date

Its applications have included release of radioactive wastes from storage or reprocessing facilities and release of contaminants from sewage pond and copper tailings reservoir. It has been verified against results of two other codes. PATHS has been used in research, field and education.

Method of solution

Analytical solutions are used for the flow equation and the modified fourth order Runge-Kutta method for the pathline equation.

Program operation

Interactive code.

Availability

The code is available from the author together with user's instructions.

References

Nelson R.W. and J.A. Schur. PATHS - Groundwater hydrologic model (assessment of effectiveness of geologic isolation systems) Rep. PNL-3162, Battelle, 1980.

Name of program

RANDOM WALK

Author

T.A. Prickett, T.G. Naymik, C.G. Lonquist, Illinois State Water Survey, USA.

Program functions

RANDOM WALK is a 1D or 2D code for simulation of groundwater flow and solute transport.

It solves steady/transient problems in heterogeneous aquifers under water table and/or artesian or leaky artesian conditions. Effects of wells, recharge, evapotranspiration and springs may be modelled as well as conversion of storage coefficients from artesian to water table conditions.

Convection, diffusion, sorption, reduction/oxidation reactions and first order decay solute processes are included.

Applications to date

The code has been applied to hazardous waste sites analysis, research, educational purposes and more general field applications. The code is widely used in the US by several organizations.

Method of solution

Solutions for groundwater flow include a finite difference formulation. The solute transport portion of the code is based on a particle-in-a-cell technique for the convective mechanism and a random-walk technique for the dispersion effects.

Program operation

RANDOM WALK is written in Fortran.

Both a mainframe and a PC version exist. The PC version runs on 640K RAM PC.

Availability

The code is public and available from IGWMC with source code, documentation and example data sets.

References

Prickett T.A., T.G. Naymik and G.C. Lonquist, A 'Random Walk' solute transport model for selected groundwater quality evaluations, Bull.65, Illinois State Water Survey, 1981.

Name of program

SUTRA

Author

C.I. Voss, United States Geological Survey.

Program operation

The program simulates fluid movement and the transport of either energy or dissolved substances in a 2D porous medium. The processes simulated are: fluid density-dependent saturated or unsaturated flow; transport of solutes in groundwater by convection, dispersion, adsorption, decay; transport of thermal energy in the groundwater and in the solid matrix of the aquifer.

Flow models may be areal or cross-sectional for saturated flow and cross-sectional for unsaturated flow.

Boundary conditions, source and sinks may be time dependent.

The IGWMC modified version includes three options for moisture characteristic curve for unsaturated flow simulation.

Applications to date

Prediction of hazardous waste migration from land disposal sites; assessment of well pumping tests; analysis of aquifer restoration, waste confinement, hydraulic barriers, liners and water quality protection systems, geothermal reservoirs, saltwater intrusion. The code has been verified by comparison to four analytical solutions, several other codes and field experiments.

Method of solution

SUTRA employs a 2D hybrid finite element and integrated finite difference method to approximate the governing equations.

Program operation

SUTRA is written in Fortran 77.

The program includes a post-processor SUTRA-PLOT that can draw the input mesh and the output predicted variables in the form of contour plots.

The program exists in mainframe and 640K PC version.

An extended memory version also is available that needs 4M RAM. Several versions of the program and processors are available from software companies.

Availability

The code is available from IGWMC and from USGS together with user's manual.

References

Voss C.I., Saturated-unsaturated transport (SUTRA), USGS Water Resour. Invest., 84-4369, 1984.

Name of program

SWIFT

Author

R.M Cranwell, Sandia National Laboratories
M. Reeves, INTERA environmental consultants
D.S.Ward, Geotrans, Inc.

Program functions

SWIFT solves the coupled or individual equations governing saturated fluid flow, heat transport, brine displacement in geologic porous and fractured media. Fluid flow may be transient and steady-state, aquifers may be confined, semiconfined or phreatic. One, two and three dimensions are available. Mass transport and thermal dispersion processes are included. Both dual porosity and discrete-fracture conceptualization may be considered for the fractured zone. Migration within the rock matrix is characterized as a one-dimensional process. Ion-exchange and reduction/oxidation reactions may be simulated.

Applications to date

The code has been verified against several analytical solutions for flow, heat and transport, laboratory results and a radioactive decay code. SWIFT has been compared to several field studies in heat storage and groundwater contamination. It has been applied in studies of high level nuclear waste isolation and underground deep injection. It has been tested in the international intercomparison Hydrocoin and Intracoin projects. It belongs to the list of NRC repository siting codes. The code is widely used by research institutions and companies both in the US and in Europe. The code has been tested also at NEA Data Bank.

Method of solution

The program uses the finite difference method. Centered or backward space and time differencing are allowed. The matrix equation may be solved iteratively or directly.

Program operation

The code was originally written for a CDC 7600 in Fortran IV. Several PC versions and extended memory versions exist that need a 386/486 and 2Mb or 4 Mb RAM. These versions are generally supported by processors and graphics.

Availability

The code is public, available from NRC, together with user's manual and self teaching guide. Enhanced PC versions are distributed by software houses.

References

Reeves, M., D.S. Ward, N.D. Johns and R.M. Cranwell, 1986a. Theory and implementation for SWIFTII, the Sandia waste isolation flow and transport model for fractured media, release 4.84, NUREG7CR-3328, SAND83-1159, Sandia National Laboratories.

Name of program

USGS-2D-FLOW / USGS-3D-FLOW

Author

P.C. Trescott et al., United States Geological Survey

Program functions

Models for simulation of 2D horizontal and vertical flow and quasi or fully 3D saturated flow in anisotropic, heterogeneous, confined, leaky-confined or water table aquifers or a combination of these. Stress terms may be well discharges, leakage from confining beds, constant recharge, evapotranspiration.

Applications to date

Both codes have been used to solve a variety of groundwater field problems. Up to few years ago they have been among the most used flow models in 2D and 3D simulations.

The programs belong to the list of NRC repository siting codes.

Method of solution

The finite difference method is used. The model has three numerical techniques available for solving simultaneous equations: the Strongly Implicit Procedure (SIP), the Alternate Direction Iterative procedure (ADI) and the Line Successive Overrelaxation method (LSOR).

Program operation

The programs are written in Fortran IV.

Main frame and 640K PC version (for USGS2D) are available.

Availability

The programs are public and available from USGS or from IGWMC together with source codes and documentation.

References

Trescott P.C., G.F. Pinder, S.P. Larson, Finite-difference model for aquifer simulation in two dimensions with results of numerical experiments. Techniques of Water-Resources Investigations of the USGS, Book 7, Chapt.C1, USGS, 1976.

Trescott P.C. (1975), Documentation of finite-difference model for simulation of three-dimensional ground-water flow. USGS Open-File Rep. 75-438.

Name of program

VERA

Author

C.J. Van Duyn, Delft Soil Mechanics Laboratory, The Netherlands

Program functions

VERA predicts head pressure and contaminant transport with dispersion in a 3D heterogeneous aquifer. It may simulate confined, semiconfined and/or water table aquifers as well as a multiaquifer system. Flow may be density-dependent, steady-state or transient. Two-phase flow is also modelled.

Solute transport processes are convection, dispersion, diffusion, adsorption, ion-exchange, radioactive decay and some chemical reactions. Heat transport may be simulated.

Applications to date

The code has been applied to low level radioactive waste migration and to problems involving sea-bed disposal. The original code HCTM from INTERA has been used for a number of contaminant transport problems and for mine dewatering applications.

Method of solution

The finite difference method is used either with direct Gaussian matrix inversion or line successive overrelaxation (LSOR). The method of characteristics is used for solute transport simulation.

Program operation

The code is written in Fortran IV.

Availability

The code is available only on a consultancy basis from DSML or by purchase.

References.

INTERA Environmental Consultants Inc. (1982): 'Hydrology Contaminant Transport Model'. INTERA, USA

ONWI (1981). 'Tabulation of Waste Isolation Computer Models'. Technical Report ONWI-78, 1981.

KEY FEATURES	MODELS																						
	RANDOM													RANDOM				RANDOM					
	AQ	AS	A2	CF	CH	CA	FE	ML	FW	HT	MS	MO	CO	DD	MT	NA	PA	WA	SU	SW	SG	US	VE
FLOW	X	X		X		X	X	X	X		X	X		X	X	X	X	X	X	X	X		X
TRANSPORT	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X				X
ID			X		X	X				X							X		X				
2D	X	X	X				X	X		X	X	X	X		X	X	X	X	X	X	X		
3D			X	X			X	X	X			X	X	X				X	X			X	X
F.E.M.	X			X		X	X	X							X			X					
F.D.M.		X			X				X		X	X	X				X	X	X	X	X		X
M.O.C.											X		X										X
R.W.		X								X							X						
ANALYTICAL			X													X							
SATURATED	X	X		X			X	X	X	X	X	X	X		X	X	X	X	X	X	X		X
NON-SATURATED							X			X									X				
ADVECTION	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X				X
DISPERSION	X	X	X	X	X	X	X	X	X	X	X		X	X		X	X	X	X				X
ADSORPTION	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X				X
ION EXCHANGE					X	X				X	X					X			X				X
DECAY	X	X		X		X	X	X	X	X	X		X	X	X	X	X	X	X	X			X
PRECIPIT/DISSOL					X	X				X													
FRACTURE FLOW								X							X				X				
MULTI SPECIES					X	X					*												
2 PHASE																							X
VARIABLE DENSITY				X					X		*			X				X	X				
COUPLED HFT				X					X					X				X	X				X
HYDROCHEMICAL					X	X																	

Bibliography

- Grant M.McD. and T.W. Broyd, Report on the revision of a directory of computer programs for assessment of radioactive waste disposal in geological formations. Atkins Research and Development/CEC Nuclear Science and Development, 1984.
- News from the Nea Data Bank No.13, November 1991, OECD/NEA Data Bank.
- IGWMC Software Catalog, February 1992, International Ground Water Modeling Center.
- Van der Heijde P. and M.S. Beljin, Available Solute Transport Models for Groundwater and Soil Water Quality Management, IGWMC,1986.
- Van der Heijde P., Y. Bachmat, J. Bredehoeft, B. Andrews, D. Holtz and S. Sebastian; Groundwater Management: the use of numerical models. AGU Water Resources Monograph Series, 1985.
- Javandel,I., C. Doughty, and C. F. Tsang; Groundwater transport: Handbook of Mathematical Models. AGU Water Resources Monograph Series, 1984.
- Mangold, D.C.,Tsang C.F., A summary of Subsurface Hydrological and Hydrochemical Models, Reviews of Geophysics, 29,1,1991.
- The International HYDROCOIN Project - Groundwater Hydrology Modelling strategies for Performance Assessment of Nuclear Waste Disposal - Level 1: Code Verification (1988), OECD/NEA and SKI, Swedish Nuclear Power Inspectorate.
- Appel C.A., T.E. Reilly; Selected Reports that include Computer Programs Produced by the U.S. Geological Survey for Simulation of Ground-Water Flow and Quality. USGS Water Resources Investigations Report 87-4271.
- IGWMC Ground Water Modeling Newsletters 1988 to 1991.
- Scientific Software Group 1991 Software catalog.
- Geraghty & Miller Software Newsletters 1991 and 1992.
- GeoTrans, Inc. Software listings, 1992.
- Hydraulic Research technical documents, HR Wallingford, 1991.
- MARS database summary reports, IGWMC 1992.

