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August 1987

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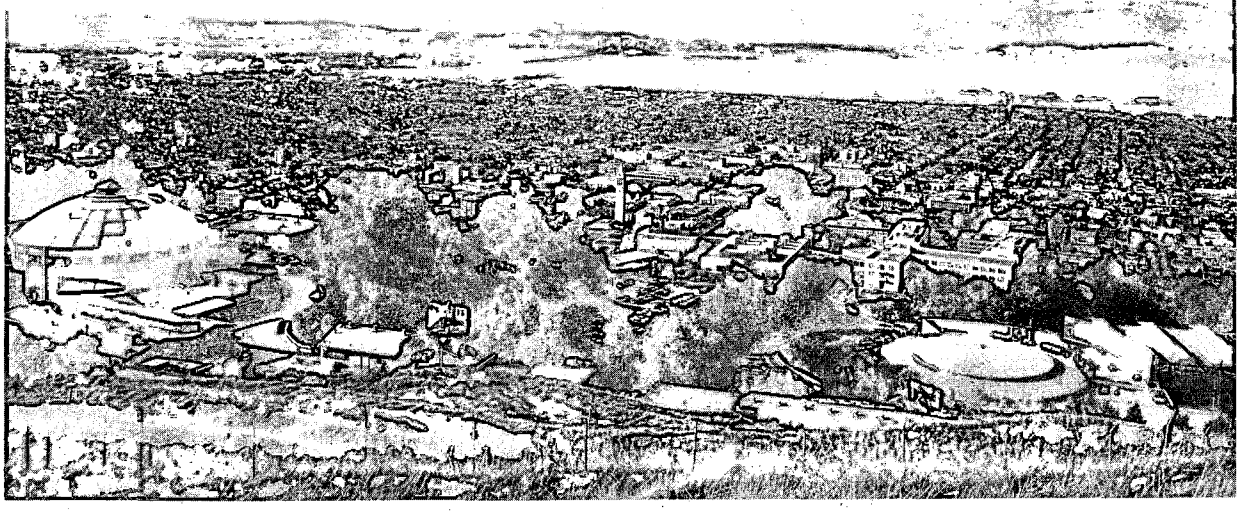

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SUMMARY OF HYDROLOGIC AND HYDROCHEMICAL MODELS WITH POTENTIAL APPLICATION TO DEEP UNDERGROUND INJECTION PERFORMANCE

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General Introduction: Hydrologic, Geochemical and Hydrochemical Models

The numerical simulation of hydrological systems has become an established method in hydrologic studies. Numerical models have been successfully applied to a variety of practical hydrologic field problems. This indicates their potential usefulness in investigating deep underground injection performance. Some of them cover aspects of mass transport such as flow of conservative solutes in three-dimensional porous media in strata of different permeability and storativity, flow in anisotropic porous media, non-isothermal (coupled fluid and heat) flow, and to a limited extent, flow in unsaturated and fractured media. Many of these models are capable of calculating transient as well as steady flows. Both initial conditions and boundary conditions to the system may be specified in a detailed way, and even boundary conditions changing with time may be included.

Similarly, the modeling of equilbrium aqueous chemistry has become well established. Speciation models can calculate the ions and complexes that will be formed, their thermodynamic activities, and the saturation state of the water with respect to different species and minerals. A variety of different chemical reactions can be modeled, including dissolution/precipitation, sorption, redox, acid-base, complexation, mineral alteration and gas-solution equilibria. Several kinds of models have been successfully employed to study a variety of different phenomena in ground water chemistry.

The joining of hydrologic solute transport models and the aqueous chemical models is an active area of research by a number of research groups. Some of the efforts along this line have combined these two kinds of models, but they very often are restricted to a constant velocity flow field in one dimension. Generally, a coupled hydrochemical model would incorporate a full three-dimensional flow field with capabilities to simulate heterogeneities and different hydrologic strata with complex boundary

conditions dynamically. It would also incorporate a large number of chemical reactions including kinetics. Such a model would represent a most powerful tool at the state of the art of numerical simulation of hydrochemical systems. The limitation would be the availability of large computers and of experienced code users. For this reason sometimes simpler models and codes are preferred.

Input Parameters Needed

The hydrochemical models need certain parameters and other information to be specified as input to the calculations. These are the geometry of the subsurface system (conceptual model), the hydrologic properties and the chemical properties. The geometrical input includes a spatial discretization of the underground domain into sufficiently small volumes so that the spatial variations in hydrologic, thermodynamic and chemical parameters can be adequately resolved. The connections between volume elements must also be specified so that the flow field may be modeled. The hydrologic characteristics of different rocks in the domain of interest must also be given, such as the permeability, porosity, compressibility and density. For nonisothermal flow, the thermal characteristics such as thermal conductivity and heat capacity need to be included. The water properties of density, viscosity, expansivity and compressibility, all of which are a function of temperature and some a function of salinity as well, must be incorporated. The chemical data needed include elemental concentrations, chemical and mineralogical analyses of the rocks, the pH and redox potential Eh of the water, and a thermodynamic data base for all the species under consideration. All these data are obtained with various degrees of confidence from field measurements at the site of interest or from laboratory measurements (especially chemical properties). Some of the data may be already tabulated in existing reference works (especially properties of water and certain kinds of thermodynamic data).

Compilation of the Codes

The following summaries of codes useful for investigating contaminant transport associated with underground injection disposal were produced mainly from secondary references that summarize and evaluate these codes. In only a few cases was the documentation for the code or the code developer available to consult. Whenever possible, references have been compared with one another to ensure accuracy. The information contained in these summaries should be treated as a compilation that may be useful to guide readers to make an initial selection of appropriate codes and to study source materials. For any code of interest, it is best to consult the details given in the references or to contact the authors directly to ascertain all the needed details, and to be informed of the most recent developments.

Explanation of the Tables

The seven tables in this report summarize some essential features of current computer codes that may be useful for various aspects of contaminant transport and reactions. The 57 codes that have been selected are arranged into three broad classes which correspond to their general area of application: geochemical models, solute transport models for both saturated and unsaturated media, and hydrochemical models that combine the chemical and transport models. Among these classes, the models for transport were sufficiently numerous that separate tables were made according to whether they incorporated three dimensions or fewer than three dimensions, and flow path network models were made a separate table.

Code Summaries in the Tables

There are three formats of code summaries in the tables corresponding to the three classes of models. In each table, the codes are listed in alphabetical order by code name except for the hydrochemical models, where they are ordered by date because in

many cases there is no formal name given in the literature for the code. For the geochemical models, wherever possible the number of elements, species, gases, etc. are listed from the available information. Also, the relationship between these codes and earlier and related codes is mentioned. In all the tables, an explanation of the abbreviations employed in the body of the table is provided below. For the transport codes, a different format was chosen in order to show clearly the features for both the flow processes and transport processes included in the model. The flow processes have a considerable variety of features, so no attempt was made to give them general categories. With the transport processes, however, there are specific processes which may be considered by the user to be important for a particular application, so they are listed for each code to make clear its capabilities and to facilitate comparison among the different codes. Information for the hydrochemical models is generally more limited because they are the most recently developed kind of model. Beneath each part of the table is a short note concerning the incorporation of kinetic calculations in the models.

Applications and Field Validations

Examples of applications of these codes and their validation by field experiments (whenever available) are given in the Appendix. An attempt has been made to find the examples most relevant to deep underground injection. We hope that this summary will guide the readers in their choosing of a code most appropriate for their problem.

A Discussion of Procedures to Apply Mathematical Models to Underground Injection Evaluation

Applications are site-specific, but the following procedures may provide some guidance in attempting to model a particular system of interest. They are based on an idealized approach to modeling subsurface flow processes. Before embarking on a modeling exercise, we need to determine:

(1) what are the observables of interest,

(2) what is the the accuracy required for the prediction of these observables,

(3) the range of conditions for which the model is valid.

For example, the observables of interest could be point tracer concentration at a given time, or the integrated tracer output concentration over a spatial region and a time period of a few thousand years. The former depends on fine details of the heterogeneity of the geologic medium; we suspect no currently available model is able to give the correct predictions except under very special conditions. For the latter, however, methods may perhaps be developed to calculate the integrated quantities.

It is important to establish the range of applicability of selected models. We do not believe that a model can be developed that is appropriate for all situations. Defining the applicability ranges can perhaps help to avoid applications of the models to conditions for which they are not suitable.

In mathematical modeling of geologic systems, it is useful to differentiate between processes and model structures. Model structures can also be referred to as geometric structures. Processes are physical and chemical phenomena, such as buoyancy flow, colloidal transport, and dissolution and precipitation. Model structures represent geologic and geometric characteristics of the medium, such as faults, layering and heterogeneity. Processes can probably be studied in the laboratory and described by mathematical equations, whereas model structures are site- and scale-dependent and are part of the

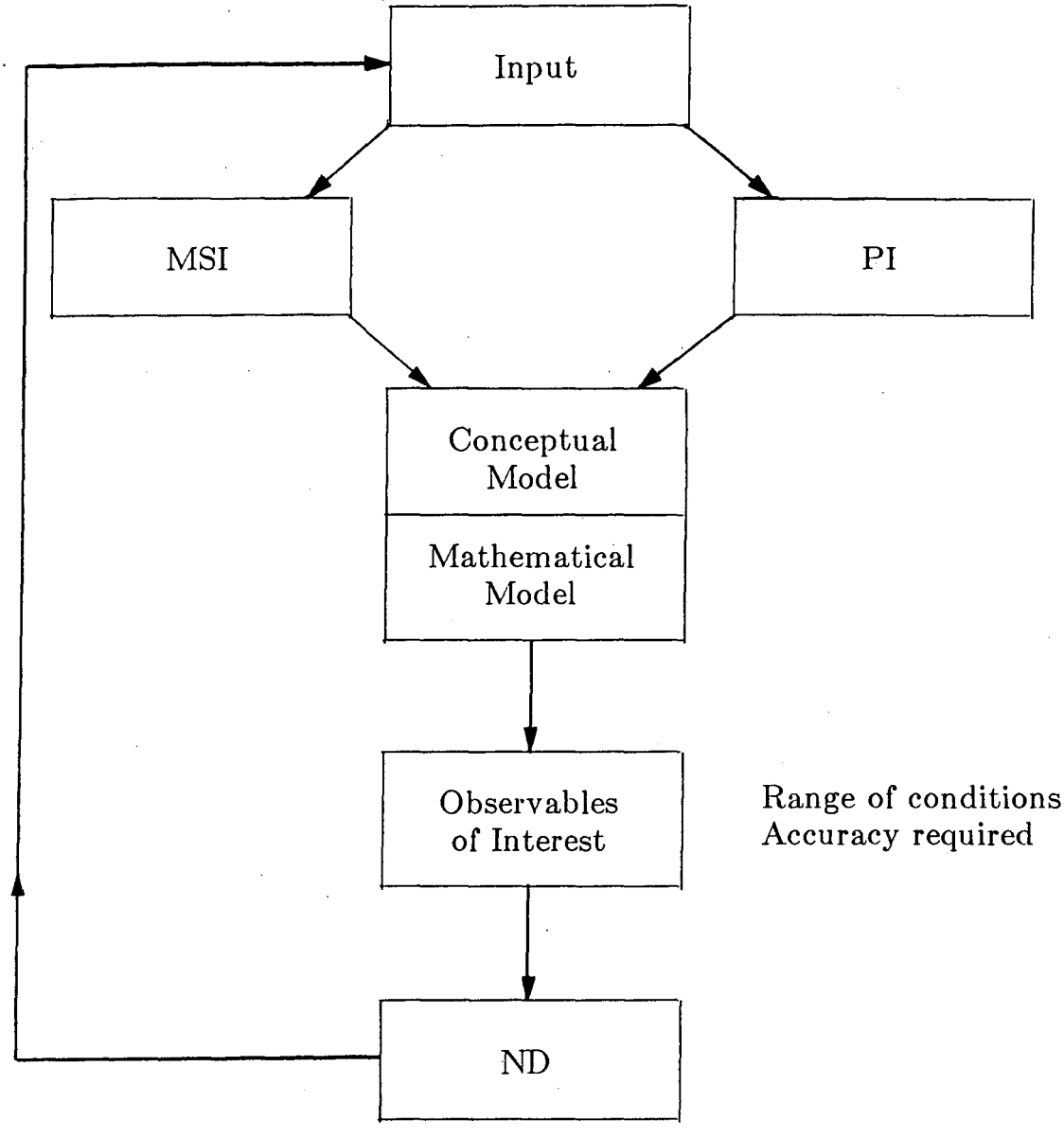
input data to the model. For a successful modeling study, one needs both the proper process identification (PI) and the proper model structure identification (MSI). Failure of matching modeling results with the field data could be due to errors in PI and/or MSI. Processes and model structure are approached quite differently. For example, models of processes can be studied generically, but models of geometric structure are site-specific. In practice, there are often cases where processes and model structure are intimately correlated.

Figure 1 illustrates the above discussion. Ideally there should be an element in the model that can be used to suggest what further measurements are needed to improve the confidence level of the predictions. These further measurements are shown in the figure as network design (ND), which is the design of a network of measurement points with specified time schedules to improve the model inputs. The procedure can be repeated or iterated (line connecting ND to Input in the figure) until one of the following two outcomes are reached:

(1) the prediction converges so that additional measurements do not result in a change in prediction, or

(2) the prediction does not converge and additional measurements are so expensive and time-consuming so that further work is not practical. In this case, we arrive at the "acceptable" result that the model predictions are not useful.

The above discussion leads to some implications in regard to application of performance prediction models. There are two aspects associated with system performance, i.e., the appropriate processes and the geometric structure, as discussed above. By the latter, we also include the boundary and initial conditions. However, we should emphasize that there are also two stages to arrive at proper performance predictions. The first stage involves system comprehension or a basic understanding of the main



MSI = Model or Geometrical Structure Identification

PI = Process Identification

ND = Network Design for further measurements

Figure 1. Diagram of idealized procedure to apply mathematical models to underground injection evaluation.

features of the system. This includes the identification of appropriate processes and geometric structures as well as generic studies and research of their effects. Once a basic understanding is obtained, the second stage involving a few sequential steps may be carried out. Firstly, the performance measures are selected. These are the "bottomline" quantities which have to be predicted in order to determine whether the performance is satisfactory or acceptable. Based on these an idealization or simplification of the in-situ geometric structures is carried out, and relevant and significant processes are identified and represented by appropriate mathematical formulation. To be able to do this implies that the first stage concerning system comprehension has already been achieved. This step of idealization is probably always necessary because it is impossible to obtain data on all details of the system, and even if we had all the data, it would be impractical to perform calculations on all these details.

After simplification and idealization are done, then sample calculations for the particular site or bounding calculations can be carried out. One may remark here that the bounding calculations follow the step of idealization or simplification which in turn depends on system comprehension or a basic understanding of the system. Thus, meaningful bounding calculations cannot be done without a basic knowledge of the geometric structure and processes present. Here the importance of the first stage in performance assessment is again emphasized. Following the bounding calculations in the second stage, sensitivity studies should be made and ranges of applicability determined. None of the bounding calculation results can be accepted without qualification. An awareness of the ranges of applicability is of great value.

In general, the use of mathematical models requires a certain amount of experience. Use of numerical methods often involves decisions regarding time steps, spatial grid design, upstream weighting factors, or implicit-explicit parameters, as well as the best ways to avoid truncation errors and numerical oscillations. If these decisions are

made incorrectly, extraordinary computer effort may be required for a given calculation or wrong answers may be obtained.

Therefore, the application of complicated numerical models requires substantial experience and knowledge of the computer codes. Consultation with model developers and experienced model users is essential. Numerical models are only tools, after all; no special dispensation from conceptual errors automatically accompanies their use.

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TABLES OF CODE SUMMARIES

Table 1 GEOCHEMICAL MODELS (Parts 1 - 2)

Table 2 SOLUTE TRANSPORT MODELS--SATURATED MEDIA, 2-D (Parts 1 - 3)

Table 3 SOLUTE TRANSPORT MODELS--SATURATED MEDIA, 3-D

Table 4 FLOW PATH NETWORK MODELS

Table 5 SOLUTE TRANSPORT MODELS--UNSATURATED MEDIA, 2-D

Table 6 SOLUTE TRANSPORT MODELS--UNSATURATED MEDIA, 3-D

Table 7 HYDROCHEMICAL MODELS (Parts 1 - 3)

TABLE 1. GEOCHEMICAL MODELS (Part 1)

Model	EQUILIB	EQ3/6	GEOCHEM	MINTEQ
Authors	J.R. Morrey D.W. Shannon	T.J. Wolery	G. Sposito S.V. Mattigod	A.R. Felmy et al.
Date	1981	1979	1980	1983
Ref.	1.1	1.2	1.3	1.4
Inst.	EPRI-PNL	LLNL	UCR	EPA-PNL
Type	spec.	EQ3: spec. EQ6: path	spec.	spec.
Solution Methods	ligand projection	N-R	N-R	N-R, ligand projection
Elements	26	>40	45	31
Aqueous Species	200	~650	1853	373
Organics	no	no	889	no
Gases	7	15	3	3
Redox Elements	9	>16	7	8
Activity Coeff.	D-H	D-H & Pitzer	Davies	Davies & D-H
Sorption	no	no	SC	6 models
Precip./ Dissol. Minerals	186	~650	250	328
Temp. (°C)	0 - 300	0 - 300	25	25
Pressure (bars)	1	1 & saturation pressure above 100 °C	1	1
Earlier & Related Models	PATHI	PATHI	REDEQL	REDEQL, MINEQL, & WATEQ

Note: All models employ chemical equilibrium calculations.

Explanation of abbreviations in the table:

Category	Explanation
Type	path = reaction path, spec. = speciation
Solution Methods	N-R = Newton-Raphson
Activity Coeff.	D-H = extended Debye-Huckel equation
Sorption	SC = surface complexation model

TABLE 1. GEOCHEMICAL MODELS (Part 2)

Model	PHREEQE	TRANSCHEM	WATEQ3
Authors	D.L. Parkhurst et al.	M. Rafal S.J. Sanders	J.W. Ball et al.
Date	1980	1986	1981
Ref.	1.5	1.6	1.7
Inst.	USGS	OLI Systems	USGS
Type	reaction path	speciation	speciation
Solution Methods	N-R, continued fraction	N-R	N-R
Elements	19	100	30
Aqueous Species	120	300	227
Organics	yes	50	12
Gases	3	50	yes
Redox Elements	3	10	yes
Activity Coeff.	Davies & D-H	Bromley-Zemaitis, Pitzer	D-H
Sorption	IE	IE	no
Precip./ Dissol. Minerals	21	50	309
Temp. (°C)	0 - 100	-25 - 200	0 - 100
Pressure (bars)	1	1 - 200	1
Earlier & Related Models	MIX	ECES	WATEQ series, new: WATEQ4

Note: All models employ chemical equilibrium calculations.

Explanation of abbreviations in the table:

Category	Explanation
Solution Methods	N-R = Newton-Raphson
Activity Coeff.	D-H = extended Debye-Huckel equation
Sorption	IE = ion exchange

TABLE 2. SOLUTE TRANSPORT MODELS--SATURATED MEDIA, 2-D (Part 1)

Model	FTRANS	GROUNDWATER PACKAGE	GROVE/ GALERKIN	GWTHERM
Authors	P.S. Huyakorn et al.	J. Marlon-Lambert I. Miller	D.B. Grove	A. Runchal et al.
Date	1983	1978	1977	1979
Ref.	2.1	2.2	2.3	2.4
Inst.	GeoTrans	Golder Assoc.	USGS	Dames & Moore
Solution Methods	FEM, UW for fractures	Galerkin FEM, L-U decomposition (Doolittle method), UW for transport	Galerkin FEM, SOR iterative, cubic basis functions, FDM for flow	IFDM, ADI
System	anisotropic, heterogeneous, conf. or semi-conf. aq.	anisotropic, heterogeneous, layered & conf. or unconf. aq.	anisotropic, heterogeneous	anisotropic, heterogeneous, unconf. aq.
Flow Processes	transient, 2-D flow & transport in fractures, 1-D in matrix	transient	transient	transient, nonisothermal, particle-tracking option
Transport Processes				
Advection	yes	yes	yes	yes
Dispersion	yes	yes	yes	yes
Diffusion	yes	yes	no	yes
Sorption	yes	yes	no	yes
Decay	yes	yes	yes	yes
Other		ion exchange	ion exchange, multiple species	

Explanation of Abbreviations in the Table:

Category	Explanation
Solution Methods	ADI = alternating direction implicit finite difference method FDM = finite difference method, FEM = finite element method IFDM = integrated finite difference method L-U = lower-upper triangular matrix form SOR = successive overrelaxation method, UW = upstream weighting
System	conf./semi-conf./unconf. aq. = confined/semi-confined/unconfined aquifer

TABLE 2. SOLUTE TRANSPORT MODELS--SATURATED MEDIA, 2-D (Part 2)

Model	KONBRED	MAGNUM2D-CHAINT	PTC	RESTOR
Authors	L.E. Konikow J.D. Bredehoeft	R.G. Baca et al.	C.H. Lai G.S. Bodvarsson	J.W. Warner
Date	1978	1981	1986	1981
Ref.	2.5	2.6	2.7	2.8
Inst.	USGS	Rockwell (Hanford)	LBL	Colorado State U.
Solution Methods	FDM, ADI for flow, method of characteristics for transport	2-D FEM for matrix, 1-D FEM for fractures, Galerkin	FDM, 2nd order Godunov method	Gauss-Seidel or point SOR, leap frog solution
System	anisotropic, heterogeneous, conf. or semi-conf. or unconf. aq.	anisotropic, heterogeneous, double porosity	anisotropic, heterogeneous	anisotropic, heterogeneous, conf. or semi-conf. aq.
Flow Processes	transient	transient, nonisothermal, transport in fractures only	transient, nonisothermal	transient
Transport Processes				
Advection	yes	yes	yes	yes
Dispersion	yes	yes	yes	yes
Diffusion	no	yes	no	yes
Sorption	yes	yes	no	no
Decay	yes	yes	no	no
Other		multiple species	precipitation/ dissolution	2 species, reactions with binary cation exchange

Explanation of Abbreviations in the Table:

Category	Explanation
Solution Methods	ADI = alternating direction implicit finite difference method FDM = finite difference method, FEM = finite element method SOR = successive overrelaxation method
System	conf./semi-conf./unconf. aq. = confined/semi-confined/unconfined aquifer

TABLE 2. SOLUTE TRANSPORT MODELS--SATURATED MEDIA, 2-D (Part 3)

Model	SALTRP	SHALT	VCHFLD
Authors	L. Picking	J.F. Pickens G.E. Grisak	Intera Env. Consultants
Date	1980	1979	1981
Ref.	2.9	2.10	2.11
Inst.	Stone and Webster Eng.	Environment Canada	Intera Env. Consultants
Solution Methods	Galerkin FEM	Galerkin FEM, triangular elements, sequential solution	Galerkin FEM, Gaussian elim. or SOR, bilinear basis functions
System	confined aquifer	anisotropic, heterogeneous, confined or unconfined aquifer	anisotropic, heterogeneous, confined aquifer
Flow Processes	transient	transient, nonisothermal	
Transport Processes			
Advection	yes	yes	yes
Dispersion	yes	yes	yes
Diffusion	yes	yes	yes
Sorption	no	yes	yes
Decay	no	yes	no
Other	salt transport & dissolution	ion exchange	5 species transport & reactions

Explanation of Abbreviations in the Table:

Category	Explanation
Solution Methods	elim. = elimination, FEM = finite element method SOR = successive overrelaxation method

TABLE 3. SOLUTE TRANSPORT MODELS--SATURATED MEDIA, 3-D

Model	AT123D	CFEST	PORFLOW	SWENT	SWIFT
Authors	G.T. Yeh et al.	S.K. Gupta	A.K. Runchal et al.	S.B Pahwa	R.T. Dillon et al.
Date	1981	1982	1985	1983	1978
Ref.	3.1	3.2	3.3	3.4	3.5
Inst.	ORNL	PNL	Analytic & Comput. Res.	Intera Env. Consultants	SNL, GeoTrans
Solution Methods	analytical using Grn. fn.	Galerkin FEM, linear elements, sequential soln.	IFDM, ADI	two line SOR iter. or direct ordered, Gaussian elim.	two line SOR iter. or direct ordered, Gaussian elim.
System	isotr., homog., conf. aq.	anisotr., heterog., conf. or semi-conf. or unconf. aq.	anisotr., heterog., conf. or semi-conf. aq.	anisotr., heterog., conf. aq.	anisotr., heterog., fractures, conf. or semi-conf. or unconf. aq.
Flow Processes	trans., only steady uniform flow	trans., nonisoth.	trans., nonisoth., density is fn. of conc.	trans., well-bore, nonisoth., density is fn. of conc.	trans., well-bore, nonisoth., density is fn. of conc.
Transport Processes					
Advection	yes	yes	yes	yes	yes
Dispersion	yes	yes	yes	yes	yes
Diffusion	yes	yes	yes	yes	yes
Sorption	yes	no	yes	yes	yes
Decay	yes	no	yes	yes	yes
Other			multiphase, dissolution	salt dissolution, leaching	salt dissolution, leaching

Explanation of Abbreviations in the Table:

Category	Explanation
Solution Methods	ADI = alternating direction implicit finite difference method elim. = elimination, FEM = finite element method, Grn. fn. = Green's function IFDM = integrated finite difference method, iter. = iteration soln. = solution, SOR = successive overrelaxation method
System	anisotr. = anisotropic conf./semi-conf./unconf. aq. = confined/semi-confined/unconfined aquifer heterog. = heterogeneous, homog. = homogeneous, isotr. = isotropic
Flow Processes	conc. = concentration, fn. = function, nonisoth. = nonisothermal, trans. = transient

TABLE 4. FLOW PATH NETWORK MODELS

Model	DPCT	MMT	NUTRAN	NWFT/ DVM	PATHS	TRANS
Authors	F.W. Schwartz A. Crowe	S.W. Ahlstrom et al.	B. Ross et al.	J.E. Campbell et al.	R.W. Nelson J.A. Schur	T.A. Prickett et al.
Date	1980	1977	1979	1981	1980	1981
Ref.	4.1	4.2	4.3	4.4	4.5	4.6
Inst.	Univ. Alberta	PNL	Analytic Sciences	SNL	PNL	Ill. Water Survey
Dimensions	2	2	1	1	2	2
Solution Methods	random number for disper., FEM for flow	Monte Carlo for disper.	Grn. fn. for transp.	distr. vel. for disper. (Gaussian for contam.)	analytical flow potential	random-walk for disper.
System	aq. unconf.	isotropic, heterog., aq. conf. or semi-conf. or unconf.	anisotropic, heterog., aq. conf. or semi-conf.	isotropic, homog., aq. conf. or unconf.	isotropic, homog., aq. conf., cst. hd. pond	anisotropic heterog., aq. conf. or semi-conf. or unconf.
Flow Processes	s.s., water table	trans., sat. or unsat. flow	trans., withdrawl through wells	s.s., density is fn. of salt conc.	trans., line-source wells	trans.
Transport Processes						
Advection	yes	yes	yes	yes	yes	yes
Dispersion	yes	yes	yes	yes	no	yes
Diffusion	no	no	yes	no	no	yes
Sorption	yes	yes	yes	yes	yes	yes
Decay	yes	option (1-D)	yes	yes	no	yes
Other		precip./ dissol., ion exchange, mult. species	dissol., leaching	dissol., kinetic leaching	ion exchange	

Explanation of abbreviations in the table:

Category	Explanation
Solution Methods	contam. = contaminant, disper. = dispersion, distr. vel. = distributed velocity FEM = finite element method, Grn. fn. = Green's function, transp. = transport
System	aq. conf./semi-conf./unconf. = aquifer confined/semi-confined/unconfined cst. hd. = constant head, heterog. = heterogeneous, homog. = homogeneous
Flow Processes	conc. = concentration, fn. = function, sat./unsat. = saturated/unsaturated s.s. = steady state, trans. = transient
Transport Processes	dissol. = dissolution, mult. = multiple, precip. = precipitation

TABLE 5. SOLUTE TRANSPORT MODELS--UNSATURATED MEDIA, 2-D

Model	FEMWATER-FEMWASTE	FLOWS	SATURN	SUTRA	WAFE
Authors	G.T. Yeh D.S. Ward	J. Noorishad M. Mehran	P.S. Huyakorn et al.	C.I. Voss	B.J. Travis
Date	1980, 1981	1982	1983	1984	1986
Ref.	5.1	5.2	5.3	5.4	5.5
Inst.	ORNL	LBL	GeoTrans	USGS	LANL
Solution Methods	FEM, UW	Galerkin FEM, UW	Galerkin FEM & N-R for flow, FEM with infl. coeff. meth. & UW for transp.	FEM & IFDM	FDM, N-R, Gauss-Seidel
System	anisotr., heterog.	isotr., heterog.	anisotr., heterog.	anisotr., heterog.	anisotr., heterog.
Flow Processes	trans., density is fn. of moisture content	trans., discrete fractures	trans.	trans., nonisoth., variable density of solute	trans., nonisoth., fractures
Transport Processes					
Advection	yes	yes	yes	yes	yes
Dispersion	yes	yes	yes	yes	yes
Diffusion	yes	yes	yes	yes	yes
Sorption	yes	yes	yes	yes	yes
Decay	yes	yes	yes	yes	yes
Other			dissolution	3 sorption models	8 species, 4 sorption models, two-phase

Note: Model MMT of the Flow Path Network models (Table 4) also can calculate unsaturated flow.

Explanation of abbreviations in the table:

Category	Explanation
Solution Methods	FDM = finite difference method, FEM = finite element method IFDM = integrated finite difference method infl. coeff. meth. = influence coefficient method N-R = Newton-Raphson, transp. = transport, UW = upstream weighting
System	anisotr. = anisotropic, heterog. = heterogeneous, isotr. = isotropic
Flow Processes	fn. = function, nonisoth. = nonisothermal, trans. = transient

TABLE 6. SOLUTE TRANSPORT MODELS--UNSATURATED MEDIA, 3-D

Model	CHAMP	HCTM	SWANFLOW	TOUGH	TRACR3D	3D S/U T.M.
Authors	T.N. Narasimhan M. Alavi	Intera Env. Consultants	C. Faust J. Rumbaugh	K. Pruess	B.J. Travis	G. Segol E.O. Frind
Date	1986	1980	1985	1986	1984	1976
Ref.	6.1	6.2	6.3	6.4	6.5	6.6
Inst.	LBL	Intera Env. Consultants	GeoTrans	LBL	LANL	Univ. of Waterloo
Solution Methods	IFDM, iter., FEM for disper.	FDM, meth. of chars. for advection	FDM	IFDM	implicit FDM for flow, semi-implicit for transport	Galerkin FEM
System	anisotr., heterog., fractured & deformable porous media	anisotr., heterog., confined or unconfined aquifer	anisotr., heterog., confined or unconfined aquifer	anisotr., heterog., fractured-porous media	anisotr., heterog., deformable fractured-porous media	anisotr., heterog.
Flow Processes	trans.	trans.	trans.	trans., nonisoth.	trans.	trans., free surface
Transport Processes						
Advection	yes	yes	yes	yes	yes	yes
Dispersion	yes	yes	no	yes	yes	yes
Diffusion	yes	yes	no	yes	yes	yes
Sorption	yes	yes	no	no	yes	yes
Decay	yes	yes	no	no	yes	yes
Other			nonaqueous phase	dissolution, multiphase	multiple species, two-phase	

Explanation of abbreviations in the table:

Category	Explanation
Models	3D S/U T.M. = 3-D Saturated/Unsaturated Transport Model
Solution Methods	meth. of chars. = method of characteristics, disper. = dispersion FDM = finite difference method, FEM = finite element method IFDM = integrated finite difference method, iter. = iterative
System	anisotr. = anisotropic, heterog. = heterogeneous
Flow Processes	nonisoth. = nonisothermal, trans. = transient

TABLE 7. HYDROCHEMICAL MODELS (Part 1)

Model						CHEMTRN
Authors	J. Rubin R.V. James	D.A. Grove W.W. Wood	A.J. Valocchi et al.	A.A. Jennings et al.	M.P. Walsh et al.	C.W. Miller L.V. Benson
Date	1973	1979	1981	1982	1982	1983
Ref.	7.1	7.2	7.3	7.4	7.5	7.6
Inst.	USGS	USGS	Stanford	Notre Dame	Univ. of Texas	LBL
Dimensions	1	1	2	1	1	1
Coupling Relation	C-T	C-T	C-T	C-T	C-T	C-T
Coupling Method	direct	2-step	direct	direct	2-step	direct
Aqueous Speciation	no	yes	no	yes	yes	yes
Activity Coeff.	no	D-H	no	no	Davies	Davies
Sorption	IE	IE	IE	SC	L	IE, SC
Precip./ Dissol.	no	yes	no	no	yes	yes
Temp.	constant	constant	constant	constant	constant	constant

Note: All models employ chemical equilibrium calculations.

Explanation of abbreviations in the table:

Category	Explanation
Coupling Relation	C-T = coupling between chemical relations and transport equations
Coupling Method	direct = chemical relations and transport equations solved simultaneously 2-step = chemical relations and transport equations solved sequentially
Activity Coeff.	D-H = extended Debye-Huckel equation
Sorption	IE = ion exchange, L = Langmuir adsorption SC = surface complexation model

TABLE 7. HYDROCHEMICAL MODELS (Part 2)

Model		CPT	MININR	FIESTA	CTM1D	
Authors	H.D. Schulz E.J. Reardon	D.C. Mangold C.F. Tsang	A.R. Felmy et al.	T.L. Theis et al.	J.R. Morrey C.J. Hostetler	P. Ortoleva
Date	1983	1983	1983	1983	1985	1985
Ref.	7.7	7.8	7.9	7.10	7.11	7.12
Inst.	Kiel Univ. Germany	LBL	PNL	Notre Dame	PNL	GeoChem Res. Assoc.
Dimensions	2	3	1	1	1	1
Coupling Relation	C-T	C-F	C-T	C-T	C-T	C-T
Coupling Method	2-step	2-step	2-step	2-step	2-step	direct
Aqueous Speciation	no	no	yes	yes	yes	no
Activity Coeff.	no	no	Davies & D-H	Davies	Davies & D-H	no
Sorption	IE	no	L	L	IE, TL	no
Precip./ Dissol.	yes	yes	yes	no	yes	yes
Temp.	constant	variable	constant	constant	constant	constant

Note: All models employ chemical equilibrium calculations, but the one by Ortoleva includes kinetics.

Explanation of abbreviations in the table:

Category	Explanation
Coupling Relation	C-F = coupling between chemical relations and fluid flow equation C-T = coupling between chemical relations and transport equations
Coupling Method	direct = chemical relations and transport equations solved simultaneously 2-step = chemical relations and transport equations solved sequentially
Activity Coeff.	D-H = extended Debye-Huckel equation
Sorption	IE = ion exchange, L = Langmuir adsorption, TL = triple layer model

TABLE 7. HYDROCHEMICAL MODELS (Part 3)

Model	CHMTRNS		DYNAMIX	TRANQL	THCC
Authors	J. Noorishad et al.	D.J. Kirkner et al.	T.N. Narasimhan et al.	G.A. Cederberg et al.	C.L. Carnahan
Date	1985	1985	1985	1985	1987
Ref.	7.13	7.14	7.15	7.16	7.17
Inst.	LBL	Notre Dame	LBL	Stanford	LBL
Dimensions	1	1	3	1	1
Coupling Relation	C-T	C-T	C-F	C-T	C-T
Coupling Method	2-step	direct	2-step	2-step	direct
Aqueous Speciation	yes	yes	yes	yes	yes
Activity Coeff.	Davies	no	Davies	no	Davies
Sorption	IE, SC	L	IE	SC	no
Precip./ Dissol.	yes	no	yes	no	yes
Temp.	constant	constant	constant	constant	variable

Note: The model by Noorishad et al. includes kinetics and carbon-13 fractionation in addition to equilibrium calculations.

The model by Kirkner et al. is only a kinetic model.

All the other models employ only chemical equilibrium calculations.

The models by Narasimhan and Carnahan include oxidation-reduction reactions.

Explanation of Abbreviations in the Table:

Category	Explanation
Coupling Relation	C-F = coupling between chemical relations and fluid flow equation C-T = coupling between chemical relations and transport equations
Coupling Method	direct = chemical relations and transport equations solved simultaneously 2-step = chemical relations and transport equations solved sequentially
Activity Coeff.	D-H = extended Debye-Huckel equation
Sorption	IE = ion exchange, L = Langmuir adsorption SC = surface complexation model

APPENDIX

APPLICATIONS AND FIELD VALIDATIONS

1.1 EQUILIB

This code has been verified and partially validated by comparing it to four other geochemical codes and to five laboratory experiments (Kincaid and Morrey, 1984) (general reference). It has been applied to studying mineral formation and corrosion in geothermal brines (Shannon et al., 1977; Morrey and Shannon, 1981).

1.2 EQ3/EQ6

This code is a sophisticated geochemical model that has capabilities ranging from simple solubility calculations to complicated kinetic simulations, is capable of modeling reaction paths, and it models both closed systems and flow-through open systems. A review of the development of the code, and some account of its verification and validation as well as its applications in various investigations in nuclear waste disposal has been given by Wolery et al. (1985) (see also Intera, 1983c; Delany and Wolery, 1984; Jackson and Wolery, 1985). It has been compared with similar reaction path codes (Nordstrom et al., 1979) (general reference), including PHREEQE (Intera, 1983d). The code was recently compared to leachate experiments and the code MINTEQ in Morrey et al. (1986) (general reference). One improvement mentioned by Wolery et al. (1985) permits the modeling of brines using Pitzer's equations. Some examples of applications are the modeling of mineral-ground water interactions (Kerrisk, 1984), the migration of ruthenium at the Nevada Test Site (Isherwood, 1984), the formation of deep ore deposits (Brimhall, 1980), and laboratory autoclave experiments (Knauss et al., 1985).

1.3 GEOCHEM

This code has been specifically constructed to model soil-aqueous chemistry. The thermodynamic data base includes several important organic ligands. All of the data are restricted to 25 °C and one atmosphere. For further information, see Sposito and Mattigod (1980).

1.4 MINTEQ

This code is a flexible geochemical model that calculates complex chemical equilibria with six models available for sorption. Its data base is restricted to 25 °C and one atmosphere. It has been partially validated by comparing it to leachate experiments (see below) and the validation of WATEQ3 with respect to uranium is expected to apply to MINTEQ, as it has been developed from WATEQ3's database.

The code has had a number of applications, including ground water analysis (Deutsch et al., 1982), restoration of an aquifer used for in situ uranium mining (Sherwood et al., 1984), reactions among uranium mill tailings, clay liners and natural sediments (Peterson et al., 1983), and uranium charge-form distributions determined by exchange resins (Jenne et al., 1984). A review of the development of the code with emphasis on its use for nuclear waste disposal has been given by Krupka and Morrey (1985). The code was recently compared to leachate experiments (including sorption) and the code EQ3/6 in Morrey et al. (1986) (general reference).

1.5 PHREEQE

This code is a very general geochemical model that can calculate both aqueous speciation and reaction paths in a wide variety of ground water environments (Parkhurst et al., 1980; Plummer et al., 1983; Intera, 1983a). It has been verified by comparing it

with EQ3/6 (Intera, 1983d). Applications include modeling of limestone ground waters of the northern Great Plains which constituted a partial field validation, and laboratory experiments of carbonate systems. A recent review of the development of the code and its potential applications in nuclear waste disposal has been given by Plummer and Parkhurst (1985).

1.6 TRANSCHEM

This code is proprietary. It has been verified and partially validated by comparing it to analytical solutions and laboratory experiments. The code has been used to model deep well injection of chemical wastes and aqueous electrolyte solutions generally (Scrivener et al., 1986).

1.7 WATEQ3

This code calculates complex geochemical aqueous speciation and solubility equilibria. The thermodynamic data base of the WATEQ versions, including WATEQ3, is probably the most thoroughly documented and evaluated of any available. The code has been verified by comparing it to similar equilibria programs by Nordstrom et al. (1979) (general reference), and extensively used in field ground water investigations of the USGS and others (Ball et al., 1981; Krupka and Jenne, 1982).

2.1 FTRANS

This code is proprietary. It has been applied to the transport of ^{237}Np from a waste repository in a uniform flow field (Huyakorn et al., 1983).

2.2 GROUNDWATER PACKAGE

This code is proprietary. Information is available in Marlon-Lambert (1978) and Javandel et al. (1984) (general reference).

2.3 GROVE/GALERKIN

This code has been compared to finite-difference codes and to analytical results. It can successfully simulate solute transport for an unreactive conservative solute, a solute with a first-order irreversible rate reaction, radioactive decay, and a solute with equilibrium-controlled ion exchange. It has been applied to a field problem involving an aquifer contaminated with chloride, tritium, and ^{90}Sr (Grove, 1977).

2.4 GWTHERM

This code is proprietary. It has been used in nuclear waste repository studies (Runchal et al., 1979).

2.5 KONBRED

This code has been verified by comparison with several analytical solutions (Konikow and Bredehoeft, 1978). It has been applied to a variety of field problems including chloride movement at the Rocky Mountain Arsenal (Konikow, 1977), chloride build-up in a stream-aquifer system (Konikow and Bredehoeft, 1974), and radionuclide transport at Idaho National Engineering Laboratory (INEL) (Robertson, 1974).

2.6 MAGNUM2D-CHAINT

MAGNUM2D has been verified by comparison with three analytical solutions. CHAINT was tested against an analytical solution based on the uranium decay series (Baca et al., 1981; King et al., 1981).

2.7 PTC

This code has been verified against seven analytical solutions (Bodvarsson, 1982) and validated by a series of field tests (Tsang and Doughty, 1985) for heat and mass flow. The solute transport portion has been verified by comparison with four analytical and numerical solutions (Lai et al., 1986).

2.8 RESTOR

This code has been applied to two-solute transport in calculating dual changes in concentration to two reacting solutes subject to binary cation-exchange in flowing ground water (Warner, 1981).

2.9 SALTRP

This code is proprietary. It has been tested against analytical solutions and against another numerical model (Science Applications, 1981) (general reference).

2.10 SHALT

This code has been verified against three analytical solutions and partially validated by a field pressure test (Pickens and Grisak, 1979; Davison, 1981; see also Thomas et al., 1982, general reference).

2.11 VCHFLD

This code is proprietary. Some information is available in Science Applications, Inc. (1981) (general reference).

3.1 AT123D

This code has been verified against hand calculations and laboratory experiments (Thomas et al., 1982) (general reference).

3.2 CFEST

This code has been verified against analytical and semianalytical solutions (Kincaid et al., 1984) (general reference). Its predecessor, FE3DGW, has been applied to a regional groundwater basin under Long Island, New York and a fault zone in Sutter Basin, California (Thomas et al., 1982; Kincaid and Morrey, 1984) (general references).

3.3 PORFLOW

This code is proprietary. The PORFLOW models have been extensively verified against a number of analytical solutions, experimental and field data, and other numerical models (Runchal and Sagar, 1985; Eyler and Budden, 1984; Fujioka and Runchal, 1982; Kline et al., 1975). Its applications have included chemical pollution of aquifers, ground water resource management, nuclear waste disposal, and geothermal storage (Runchal, 1987).

3.4 SWENT

This code is proprietary. This code has been verified against analytical solutions for eleven cases involving fluid flow, heat flow, inert component transport, and radionuclide transport. There are also three field applications where the predicted results are in reasonable agreement with the field observations in the code documentation (Intera, 1983b; Sykes et al., 1982a,b). The applications have included nuclear waste isolation, thermal energy storage in aquifers, and ground water contamination studies.

3.5 SWIFT

This code has been verified against eight analytical solutions for flow, heat and transport (Ward et al., 1984), laboratory results, and a radioactive decay code for radioactive decay (Reeves and Cranwell, 1981). It has been compared to three field studies in heat storage in aquifers and ground water contamination (Ward et al., 1984), and used to investigate a field site for ground water contamination (Ward et al., 1987a). It has also been applied in studies of nuclear waste isolation, and recently, underground deep injection (Ward et al., 1987b).

4.1 DPCT

This code has been applied to studying long-term effects of radioactive waste repositories (Schwartz and Crowe, 1980).

4.2 MMT

This code has been verified against analytical results for a variety of one-dimensional problems, and was applied to one two-dimensional field study (Ahlstrom et al., 1977; Washburn et al., 1980).

4.3 NUTRAN

This code is proprietary. It has been verified against a number of analytical solutions, and compared to two other codes for a one-dimensional problem. The code has been applied to transport of pollutants in ground water (Ross and Koplik, 1978) and transport of radioactive waste from a nuclear repository (Ross et al., 1981).

4.4 NWFT/DVM

This code has been verified against analytical results for several one-dimensional problems and compared to numerical results for radioactive decay chains (Campbell et al., 1981).

4.5 PATHS

This code has been verified against results of two other well-known codes. It was designed to permit a user to make a preliminary evaluation quickly and inexpensively. Its applications have included release of radioactive wastes from storage or reprocessing facilities, and release of contaminants from a sewage pond and a copper tailings reservoir (Nelson and Schur, 1980).

4.6 TRANS

This code has been compared with six analytical solutions and a field problem (Prickett et al., 1981), and also recently compared to several other codes and experimental data (Kincaid and Morrey, 1984; Morrey et al., 1986) (general references). It has been applied to ground water contamination problems (McDonald and Fleck, 1978).

5.1 FEMWATER-FEMWASTE

FEMWATER and FEMWASTE are closely affiliated codes for calculating flow and transport of solutes, respectively, that have been compared to three other codes for verification (Duguid and Reeves, 1976; Yeh and Ward, 1980, 1981; see also Kincaid and Morrey, 1984; Morrey et al., 1986, general references). They have been applied to seepage pond leakage and similar ground water contamination studies.

5.2 FLOWS

This code has been verified by comparing it with two other codes and an analytical solution (Heinze, 1984). It has been applied to flow in unsaturated fractured-porous media (Noorishad and Mehran, 1982).

5.3 SATURN

This code is proprietary. It has been verified by comparison with an analytical solution and another code (Huyakorn et al., 1983). This code has also been compared to several other codes and experimental data (Kincaid and Morrey, 1984; Morrey et al., 1986) (general references).

5.4 SUTRA

This code has been verified by comparisons to four analytical solutions, several other codes, and a field experiment (Voss, 1984). It can calculate fluid-density-dependent flow with heat or chemically-reactive single-species solute transport. It has applications to salt-water intrusion, thermal pollution of aquifers, and ground water contamination studies.

5.5 WAFE

This code has been verified by comparison with eight analytical solutions for flow of fluid and heat, and solute transport. The code has application to nuclear and chemical waste management, geothermal reservoir modeling, and hydrochemical transport modeling (Travis, 1986).

6.1 CHAMP

This code has been verified by comparison with two analytical solutions. It has application to chemical transport in waste disposal (Narasimhan and Alavi, 1986).

6.2 HCTM

This is a proprietary code which has been applied to ground water contamination from surface mining, tritium transport, in situ leaching and mine dewatering (Gardner et al., 1964; Price and Coats, 1973; Intera, 1980; see also Science Applications, Inc., 1981, general reference).

6.3 SWANFLOW

This code is proprietary. It has been verified by comparison with an analytical solution, three other numerical models, and a field experiment. The code has been applied to study transport of contaminants of different densities in the unsaturated and saturated zones (Faust, 1985).

6.4 TOUGH

This code has been verified by comparison with three analytical solutions (Pruess, 1986). It is based on a previous code MULKOM that has been extensively verified for heat and two-phase fluid flow (Pruess, 1983). This code is capable of modeling strongly heat-driven multi-phase flow. It has been applied to nuclear waste isolation in partially saturated fractured-porous media (Pruess and Wang, 1984; Pruess et al., 1985; Rulon, 1986).

6.5 TRACER3D

This code has been verified by comparison with eight analytical solutions for flow and transport and validated by comparison with three field experiments (Travis, 1984). It has been applied to study the hydrology and transport of colloids with radioactive materials (radiocolloids) at a low-level radioactive waste disposal site (Travis and Nuttall, 1987). It has application to tracer tests of aquifers, chemical waste management and hydrochemical transport in partially saturated or fully saturated fractured-porous media.

6.6 3D S/U T.M. (3-D Saturated/Unsaturated Transport Model)

This code has been applied to flow from ponds (Segol, 1976; see also Javandel et al., 1984, general reference).

7.1

This code was one of the first coupled hydrochemical models in the literature (Rubin and James, 1973). Its approach has formed the basis for many of the following codes, which have more extensive capabilities.

7.2

This code has been verified and partially validated by being compared to a laboratory experiment and a field experiment consisting of a case of artificial aquifer recharge at a field site. It has been used for water quality studies (Grove and Wood, 1979).

7.3

This code has been partially validated by comparison with several aspects of a field case of treated municipal effluent injected into a shallow aquifer (Valocchi et al., 1981).

7.4

This code has been verified by comparison to analytical solutions. It is capable of multicomponent transport. It has been used to model ground water contamination (Jennings et al., 1982).

7.5

This code has been verified and partially validated by comparison with a laboratory experiment and a field experiment. It has the capability of modeling different temperatures. It has been applied to acidizing formations in petroleum production (Walsh et al., 1982).

7.6 CHEMTRN

This code has been verified by comparing it with two analytical solutions and a and field experiment (Miller, 1983; Miller and Benson, 1983). It has been applied to nuclear waste isolation and chemical contaminant transport.

7.7

This code has been compared qualitatively to a field experiment (Schulz and Reardon, 1983).

7.8 CPT

This code is based on an earlier numerical model PT which has been verified against numerous analytical solutions (Bodvarsson, 1982) and validated by several field experiments (Tsang and Doughty, 1985) for fluid and heat flow (without chemical transport). It is one of the few codes listed that can model thermal effects in hydrochemical transport. It has been applied to tracer tests in geothermal (nonisothermal) reservoirs and changes in permeability due to temperature (Mangold and Tsang, 1983).

7.9

Information unavailable in general references used in this study, see Felmy et al., (1983).

7.10 FIESTA

This code has been compared with three analytical solutions (Theis, 1983; see also Morrey et al., 1986, general reference). It is based on two earlier codes, FEAP and MINEQL, that have been used for hydrological and chemical modeling, respectively.

7.11 CTM1D

This model uses MINTEQ as its parent geochemical code. It is used for coupled geochemical and solute transport (Morrey and Hostetler, 1985).

7.12

This code is proprietary. It has been compared to naturally occurring ore deposits and has application to flow with reactions including kinetics (Ortoleva, 1985; Moore, 1985).

7.13 CHMTRNS

This code has been verified against analytical solutions and another code, and the equilibrium part partially validated against a field experiment (Noorishad et al., 1985, 1987). It has been applied to nuclear waste isolation and radioactive carbon age-dating.

7.14

This code has been verified and partially validated by comparison with an analytical solution and a laboratory experiment. It includes the ability to model kinetic reactions. It is used to study migration of contaminants in ground water (Kirkner et al., 1985).

7.15 DYNAMIX

This code is a coupling of two well known codes, TRUMP (for transport) and PHREEQE (for equilibrium chemical reactions). The code has been partially validated by comparison to detailed field data (Narasimhan et al., 1985, 1986). It has been applied to leaching of uranium mill tailings and chemical transport.

7.16 TRANQL

This code has been verified and partially validated by being compared to several laboratory experiments and a field experiment. It has application to multicomponent reactive chemical transport (Cederberg et al., 1985).

7.17 THCC (Thermo-Hydro-Chemical Coupling)

This code has been verified by comparison with four analytical solutions. It is one of the few codes listed capable of modeling thermal effects of hydrochemical transport. It has application to nuclear waste isolation, hydrothermal ore formation, and

reactive migration of chemical waste (Carnahan, 1987).

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