DCS

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: Workshop on Modeling Reactive Multispecies-Multicomponent Transport Through Subsurface Media
20-5704-072

DATE/PLACE: November 17-20, 1992; Penn State University, State College, PA

AUTHOR: David R. Turner

DISTRIBUTION:

CNWRA	NRC	SwRI
J. Latz	M. Knapp	S. Rowe
W. Patrick	S. Fortuna	
Directors	B. Stiltenpole	
Element Managers	B. Morris	
GS Element Staff	F. Costanzi	
PA Element Staff	M. Silberberg	
	J. Randall	
	G. Birchard	
	V. Colten-Bradley	
	H. Astwood	
	J. Bradbury	

150023

9301150154 921218
PDR WASTE
WM-11 PDR

426.1
WM-11
NH05

delete all distribution except: CF, PDR & NUDOCS full text.

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: Workshop on Modeling Reactive Multispecies-Multicomponent Transport Through Subsurface Media

DATE/PLACE: November 17-20, 1992; Penn State University, State College, PA

AUTHOR: David R. Turner

PERSONS PRESENT:

CNWRA	NRC
David Turner	V. Colten-Bradley
	H. Astwood

BACKGROUND: Contaminant transport through subsurface media is affected in a complex manner by both chemical and hydrological processes. Reactive transport models commonly rely on simplifications to lump these processes into one or two empirical parameters. To handle solute transport in a more realistic manner, computer codes should couple hydrologic transport with geochemical reactions. This can either be accomplished by direct substitution of chemical reactions into the transport equations to produce a set of non-linear partial differential equations, or by two-step coupling of transport and chemistry in a sequential manner. The coupled reactive transport code HYDROGEOCHEM relies on the second method, using the total analytical concentration of components as the primary dependent variable. HYDROGEOCHEM uses two separate modules, EQMOD which performs the equilibrium geochemical calculations, and HYDROFLOW, a finite element model of hydrologic flow through saturated-unsaturated media. HYDROGEOCHEM is a fairly new code, and this was the first workshop conducted in its application to field problems. Thirty-six professionals from the U.S., Europe, and Canada attended (See Attachment A).

WORKSHOP ACTIVITIES:

The workshop lasted four days and was basically arranged so that one day each was spent on geochemistry and transport. The final two days involved description of EQMOD, HYDROFLOW, and HYDROGEOCHEM, with time allotted for hands-on experience (See Attachment B).

The geochemistry lecture was conducted by Dr. Brian Dempsey of the Penn State University Department of Civil & Environmental Engineering. The talk covered the fundamentals of equilibrium chemistry, including mass action, mass balance, charge balance, precipitation/dissolution, Reduction-Oxidation, ion exchange, and sorption. Particular attention was paid to modeling chemical equilibrium in terms of constructing matrices to handle the linear and nonlinear algebraic equations involved in mass balance and mass action. There was also some discussion of data sources, and the construction of the EQMOD program.

The second day of the workshop was conducted by Dr. George Yeh, also of Penn State and the principal author of the HYDROGEOCHEM code. Dr. Yeh began by discussing flow modeling with the HYDROFLOW model, introducing the governing equations and describing the types of boundary and initial conditions that can be imposed on a given system. The structure of HYDROFLOW was discussed, and the roles of the different subroutines. A fair bit of time was also spent on constructing input files, defining the different variables and describing the formatting requirements for input using a sample problem. Initial values and parameter properties must be specified at each node in the finite element mesh, and input rapidly becomes very complex. Input is unformatted, but there is no preprocessing currently available for constructing the input files, although there is some shorthand notation available for initializing large portions of the finite element mesh that have common properties.

Dr. Yeh also discussed the structure of EQMOD and the construction of the equilibrium geochemical model. This module can also be executed as a stand-alone code, and is similar in structure to MINTEQA2. A set of base components are related by a set of geochemical reactions and mass action expressions. Aqueous complexation, adsorption/desorption, ion exchange, acid/base, reduction/oxidation, and precipitation/dissolution reactions are all handled using equilibrium mass action/mass balance constraints. There are some plans to incorporate reaction kinetics into the code as well. EQMOD does not come with an attached database, and all thermodynamic data relevant to the geochemical system must be entered as part of the input file. Similar to HYDROFLOW, preprocessing is not currently available for the construction of input files, and input can get rather complex. However, the freedom to use different thermodynamic data sets makes it possible to evaluate the effects of aqueous speciation on transport. Ionic strength effects are corrected using either the Davies or the Debye-Hückel equations. Temperature/pressure effects are handled if there is log K data available for input, but are not handled automatically by the code. If EQMOD is being used as part of a coupled transport and geochemistry simulation, initial component concentrations must be specified for each element in the finite element mesh.

The final day of the workshop was devoted to the structure of HYDROGEOCHEM and its application to site specific problems. The hydrologic transport equations and geochemical equilibrium reaction equations were reintroduced and the strategy used by the program in solving iteratively the two subsystems of equations was outlined. Input was described through the analysis of sample input files. Input is very complex, and requires a large number of values to be specified for each element in the mesh. Dr. Yeh discussed some strategies that may be used to improve the likelihood of convergence for a given problem, and stressed that "embarrassingly simple" problems should be attempted first. The function of different subroutines was discussed, and the different variables (30 program control variables in addition to all of the necessary boundary and initial conditions) were defined in the context of the sample problems.

IMPRESSIONS/CONCLUSIONS: HYDROGEOCHEM is clearly an elaborate code that is designed to consider a wide range of hydrologic and chemical processes. The input for the code is very complex and data intensive. The real challenge in applying the code to a given problem may be in providing reasonable values for all of the parameters required in the initial input files. It is largely up to the modeler to define realistic problems that are simple enough to be amenable to sensitivity analysis.

The workshop included copies of the source code (FORTRAN 77) for EQMOD, HYDROFLOW, and HYDROGEOCHEM, but it is up to the user to compile these into executable elements. Since the code is quite involved, perhaps more time should have been spent on describing hardware/software requirements for successful compilation and execution of the program. Some hands-on experience with the different programs was provided, but there was so much information to digest that it was difficult to do more than run the sample problems supplied with the source code. The information provided with the short course was extensive, and the user's manuals provided with the different programs were comprehensively documented, although some errors were corrected in class. Although some of the lecture notes were provided during the workshop, they need to be presented in a more organized fashion and provided at the outset so that participants can get more out of the material presented. This is particularly important given some of the complications introduced by language difficulties.

PENDING ACTION(S): Investigate installation and compilation of EQMOD, HYDROFLOW, and HYDROGEOCHEM on CNWRA computer facilities.

RECOMMENDATIONS: One point that was not discussed (and has apparently not been done yet) was the comparison of model results to field or laboratory results. Given the interesting results from some of the test problems and the complexities of the code, this is an important next step in evaluating the "reasonableness" of the output. To this end, the code needs to be compiled and compared against "real" data; migration studies for radionuclides with relatively simple chemistry, such as Cs and Sr may be suitable.

PROBLEMS ENCOUNTERED: None.

REFERENCES: None. See attachments for listing of participants and short course agenda.

SIGNATURE:

David R. Turner

12/18/92
Date

CONCURRENCE:

Budhi Sagar
Technical Director

12/18/92
Date

ATTACHMENT A

WORKSHOP PARTICIPANTS

11/17/1992 to 11/20/1992

The Pennsylvania State University
University Park, Pennsylvania

FINAL REGISTRATION LIST

Abrams, Robert H.	Stanford University Dept. of Geology Stanford, CA 94305-2115
Afifi, Sameh M.	Colorado State University 1600 W. Plum #20C Ft. Collins, CO 80521
Ahsan, Muhammad A.	U.S. Bureau of Reclamation P.O. Box 25007 D-5711, DFC, Bldg. 67 Denver, CO 80225-0007
Astwood, Heather M.	Nuclear Regulatory Commission Mail Stop OWFN 4-H-3 Washington, DC 20555
Baehr, Arthur L.	U.S. Geological Survey 810 Bear Tavern Road West Trenton, NJ 08628
Barden, Michael J.	Wisconsin Dept. of Natural Resources P.O. Box 7921 Madison, WI 53707
Bennett, David G.	WS Atkins Science & Technology Woodcote Grove Ashley Road Epsom, Surrey, Kt185BW United Kingdom
Burau, Richard G.	University of California LAWR Davis, CA 95616
Choi, Inn G.	Westinghouse Savannah River Co. Savannah River Tech. Center Aiken, SC 29808

11/17/1992 to 11/20/1992

The Pennsylvania State University
University Park, Pennsylvania

FINAL REGISTRATION LIST

Colten-Bradley, Virginia A.	Nuclear Regulatory Commission Mail Stop One White Flint North 4-H-3 Washington, DC 20555
Doerr, G. Brett	CH2M Hill P.O. Box 4400 Reston, VA 22090-1483
Evans, Tracy M.	Woodward-Clyde Consultants 900 Fourth Avenue, Suite 3440 Seattle, WA 98164
Farley, Kevin J.	Clemson University Environmental Systems Engineering Clemson, SC 29634-0919
Feng, Husheng	Bechtel Corporation 50 Beale Street P.O. Box 193965 San Francisco, CA 94119
Fox, Fred L.	GEONICS P.O. Box 5356 Clinton, NJ 08809
Germain, Diane	INRS - Georessources C.P. 7500 Ste-foy, Quebec G1V 4C7 Canada
Glynn, Pierre D.	U.S. Geological Survey 432 National Center Reston, VA 22052
Guo, Lei	Triegel and Assoc., Inc. 1235 Westlakes Drive Suite 320 Berwyn, PA 19312

11/17/1992 to 11/20/1992

The Pennsylvania State University
University Park, Pennsylvania

FINAL REGISTRATION LIST

Liu, Chin-shu	NYS Dept. of Env. Conservation 50 Wolf Road Albany, NY 12233-3502
Maiwald, Ulrike	Freie Universitat Berlin Malteserstr, 74-100 Berlin 46, D-1000 Germany
Oston, Steven G.	TASC 55 Walkers Brook Drive Reading, MA 01867
Peterson, Stan R.	ICF Kaiser Engineers 11808 Northup Way Suite 104 Bellevue, WA 98005
Richer-LaFleche, Marc	INRS - Georessources C.P. 7500 Ste-Foy, Quebec Canada
Richey, Willis D.	5023 Bayard Street Pittsburgh, PA 15213
Runnells, Donald D.	University of Colorado Dept. of Geological Sciences Boulder, CO 80309-0250
Scharf, Richard L.	Iowa State University 2216 Agronomy Hall Ames, IA 50011
Seaman, John C.	University of Georgia Agronomy Dept. Miller Plant, Science Bldg. Athens, GA 30602

11/17/1992 to 11/20/1992

The Pennsylvania State University
University Park, Pennsylvania

FINAL REGISTRATION LIST

Shao, Chi	Unviersity of Georgia Geology Dept. Athens, GA 30602
Stone, Charles S.	M & E Pacific, Inc. 1001 Bishop Street Pauahi Tower, Suite 500 Honolulu, HI 96813
Sundberg, Kenneth R.	Phillips Petroleum Co. 252 Geoscience Bartlesville, OK 74004
Szecsody, Jim E.	Pacific Northwest Laboratories P.O. Box 999, M.S. K6-77 Richland, WA 99352
Timlin, Dennis J.	USDA:ARS Systems Res. Lab Bldg 007, Rm 008, Barc-West 10300 Baltimore Ave. Beltsville, MD 20705-2350
Turner, David R.	Ctr for Nuclear Waste Reg. Anly. 6220 Culebra Rd. San Antonio, TX 78288-0510
Winkler, Andreas H.	Freie Universitat Berlin Malteserstr 74-100 Berlin 46, D-1000 Germany
Wood, Dixon L.	Century Engineering, Inc. 32 West Road Towson, MD 21204
Yagecic, John R.	U.S. Army Corps of Engineers 111 North Canal Street Chicago, IL 60606-7206

ATTACHMENT B

WORKSHOP AGENDA

MODELING REACTIVE MULTISPECIES MULTICOMPONENTS TRANSPORT THROUGH SUBSURFACE MEDIA

November 17, 1992 - Geochemical Processes (Dempsey)

8:00 a.m.	Registration and Coffee
8:30	Opening Remarks
8:50	Aqueous complexation (Dempsey)
10:00	Coffee
10:30	Adsorption and Ion-Exchange (Dempsey)
	Precipitation-dissolution (Dempsey)
1:00 p.m.	Oxidation-reduction (Dempsey)
	Acid-base reactions (Dempsey)
2:30	Coffee
3:00	Geochemical equilibrium modeling (Dempsey)
	Geochemical kinetic modeling (Dempsey)

November 18, 1992 - Transport Processes (Yeh)

8:00 a.m.	Coffee
8:30	Saturated-unsaturated flow (Yeh)
10:00	Coffee
10:30	Multispecies-multicomponents transport (Yeh)
1:00 p.m.	Reactive chemical transport-practical consideration (Yeh)
2:30	Coffee
3:00	Numerical modeling of coupled hydrologic transport and geochemical equilibria (Yeh)

November 19, 1992 - Geochemical Equilibrium Model EQMOD

8:00 a.m.	Coffee
8:30	Program structure of EQMOD (Yeh)
10:00	Coffee
10:30	Direction for the use of EQMOD (Yeh)
1:00 p.m.	Example problems (Yeh)
2:30	Coffee
3:00	Computer lab with EQMOD (Yeh)

November 20, 1992 - Coupled Hydrological Transport and Geochemical Equilibria HYDROGEOCHEM

8:00 a.m.	Coffee
8:30	Program structure of HYDROGEOCHEM (Yeh)
10:00	Coffee
10:30	Direction for the use of HYDROGEOCHEM (Yeh)
1:00 p.m.	Example problems (Yeh)
2:30	Coffee
3:00	Computer lab with HYDROGEOCHEM (Yeh)