U.S NUCLEAR REGULATORY COMMISSION
DIVISION OF WASTE MANAGEMENT

TRIP REPORT

MODELING OF FLUID FLOW
AND CONTAMINANT TRANSPORT
IN FRACTURED OR GRANULAR POROUS MEDIA

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TECHNICAL ASSISTANCE IN HYDROGEOLOGY
PROJECT B - ANALYSIS
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M E M O R A N D U M

TO: Mark Logsdon
FROM: Catherine Kraeger-Rovey CKR
DATE: August 3, 1987
SUBJECT: Trip Report - Attendance at Holcomb Research Institute Short Course, July 27 - 31, 1987.

On Sunday, July 26, 1987, I flew to Indianapolis to attend a five-day short course at Holcomb Research Institute (Butler University) entitled "Modeling of Fluid Flow and Contaminant Transport in Fractured or Granular Porous Media". This memorandum summarizes the content of the course and my impressions of the applicability of course material to analysis of flow and transport problems at BWIP.

ANALYTIC TECHNIQUES

The first one and one-half days of the course were taught by Dr. Edward O. Sudicky, Research Assistant Professor at the Institute for Groundwater Research, Department of Earth Sciences, University of Waterloo, Ontario. Dr. Sudicky lectured on flow and transport in fractured rock, the concept of dual porosity, and analytic techniques for solving flow and transport problems in dual porosity media, given conceptual models having relatively simple geometry. As part of the course material, we were provided copies of several papers authored or co-authored by Sudicky; these papers contained the detailed derivations of the analytic techniques on which Sudicky lectured.

The course also included a set of five IBM-compatible micro-computer disks containing the "CRACK" package of computer programs, which utilizes some of the analytic techniques presented in the lectures to solve flow and transport problems for the following geometries:

- Transport in a single fracture with matrix diffusion but no dispersion along the fracture axis

- Transport in a single fracture with matrix diffusion and with dispersion along the fracture axis

- Transport in a system of parallel fractures with matrix diffusion but no dispersion along the fracture axis.

- Transport in a single fracture with matrix diffusion but no dispersionn along fracture axis; flow field is radial diverging.

The five disks contain the ASCII source codes (disk 1), and executable versions of several of the codes, with variations available for fixed or variable time steps (disk 2 = fixed; disk 3 = variable) The codes are written in Microsoft BASIC. Disks 2 and 3 also include a plot routine for graphically displaying the results produced by the models. Disk 5 contains both FORTRAN source and executable codes for interactive and non-interactive versions of the parallel fracture model, utilizing Laplace transforms to obtain solutions. Disk 5 also contains a demonstration data file for use with the interactive version of this model. Disk 4 was blank when we received it, and formatted for use in storing data files we generated in two hands-on sessions. I was able to generate my own demonstration files for several of the models. Demonstration data sets were also given in the documentation for some of the models.

The documentation for the CRACK package is fairly sketchy, but since we have the lecture notes and published papers for the theoretical background, plus the source code that can be listed, detailed documentation in the form of a "user's manual" is not really necessary. The programs are fairly user-friendy. Though the conceptual models these programs simulate have fairly simple, one-dimensional geometry, they appear to be quite applicable to many problems, provided the user understands the physical system, and the assumptions and limitations of the model, and operates intelligently within those constraints.

FINITE ELEMENT THEORY, DUAL POROSITY, AND THE "TRAFRAP" MODEL

The remaining three and one-half days of the five-day course were taught by Dr. Peter S. Huyakorn, formerly with GeoTrans, Inc. and presently Executive Vice President of the Technology Department for HydroGeoLogic, Inc., Herndon, Virginia. Dr. Huyakorn began by presenting several lectures on finite element theory and the concept of dual proposity in subsurface flow and contaminant transport. With this material as background, he spent several lectures describing the TRAFRAP finite element code and its applications. Although Dr. Huyakorn's lecturing pace was uncomfortably rapid, his subject material was excellent. This is one of the best presentations I've seen of finite element theory and dual porosity flow and transport. For me, this was a very worthwhile refresher course.

The attached abstract from the model documentation describes the capabilities of the TRAFRAP model. Like SWIFT, the TRAFRAP model handles both flow and contaminant transport in a system comprised of both fractured and porous media. The present version of the code is two-dimensional. TRAFRAP does NOT have the capability, as do SWIFT and PORFLO, of modeling any temperature effects. This appears to be its major limitation at the present time. The major advantages of the TRAFRAP code are its reasonable length (about 3700 lines), and its complete accessibility to users (I brought back a listing with me, and tapes or diskettes of the code are available, so that the model can be run on a variety of computer systems, possibly including IBM-compatible micros).

Relative to SWIFT, TRAFRAP is very user-friendly. I have developed and worked with a number of FORTRAN codes of this size and similar function, and am confident that I can fully comprehend the workings of this one, so that I will have some confidence in applying the model and correctly interpreting the results it generates.

Part of Dr. Huyakorn's lecture time was spent discussing the details of preparing input data for various test cases for use with the TRAFRAP model. Though time was limited, we did have two opportunities to access the model on HRI's VAX computer, and run some test problems. My lab partner and I succeeded in generating a dataset that was not provided, and made a run of the model with it. I brought back printouts of results from several model runs for a variety of flow and transport cases.

A printout of the TRAFRAP code was provided to us as part of the course material. The code was not provided on disk or tape as part of the course, but is available to participants for an additional $95.00. The following tape formats are available:

Format A: VAX/VMS; ANSI-Labeled

Format B: ASCII; 1600 BPI; Record size 80; Block size 80; no labels

Format C: EBCDIC; 1600 BPI; Record size 80; Block size 80; no lables

Obviously, a main-frame computer is needed in order to use any of these formats. Holcomb Research Institute will provide technical support, principally in the form of telephone consultation, for use of these code formats.

In addition, HRI will provide the FORTRAN source code plus test data files on IBM-PC, 5.25-inch, double-sided, double-density, diskettes. HRI does not represent this version as "executable"; we are on our own with this version to make it work with whatever computer we choose. HRI will provide technical support, but they will not guarantee that the code will ever actually run.

I am fairly confidant that we can work with either tape or diskette format of the code. Some considerations that may enter into the decision whether to obtain a diskette version of the code are:

- The overall size of the code is similar to the size of the USGS MODFLO code, for which a PC version is available, and widely used (with some limitations - there are some problems using very many of the options of MODFLO at one time, or using the SIP matrix solver on a PC).

- Double precision is used for some of the arrays, but can be replaced with single precision; the result is a model that is less precise, but no less correct, given the same input data, time steps, etc.

- The code is modularized into a number of subroutines, so that it may be possible to drop unused subroutines from the code for various applications, to achieve a program that can be run on one of NWC's micro-computers.

- As a last resort, if we can't make the code work on a micro, we could probably read the source code off the diskette onto a hard disk, then transmit it to a main-frame computer.

Whether we purchase the code, and if so in what format, depends on the NRC's authorization for us to use it or have it ready for use, and NWC's preference for what format we can best work with. I will wait for your go-ahead before I proceed to order a copy of the TRAFRAP code. To my knowledge, there is no time limit; the code should be available to short-course participants at the $95.00 price indefinitely.

ABSTRACT

TRAFRAP-WT (TRAnsport in FRActured Porous media with Water Table boundary conditions) is a two-dimensional finite element code designed to simulate groundwater and solute transport in fractured or granular aquifers. This code was developed under a joint cooperation between HydroGeoLogic, Inc. and the International Ground Water Modeling Center of Holcomb Research Institute. TRAFRAP-WT is a new enhanced version of the TRAFRAP code documented by Huyakorn et al. (1986). It is capable of treating both confined and water table fractured aquifers. Fractured porous media are represented using both discrete-fracture and dual porosity approaches. The flow and transport equations are solved using improved finite element algorithms with special features designed to handle aquifer-aquitard systems and options to account for water table boundary conditions and fracture skin effects. This report describes mathematical equations of the physical system being modeled, the numerical techniques employed, and the code organization and utility.

The TRAFRAP-WT code takes into account: (a) fluid interactions between the fractures and porous matrix blocks; (b) advective-dispersive transport in the fractures and diffusion in the porous matrix blocks and fracture skin; and (c) chain reactions of radionuclide components. Major advantages of TRAFRAP-WT are: (a) capability to model the fractured system using either the dual-porosity or the discrete-fracture modeling approach or a combination of both; and (b) capability to simulate both flow and transport in the same code.