PACKAGE ID - 001205MLTPL00 STOMP

KWIC TITLE - Subsurface Transport Over Multiple Phases

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LIMITATION CODE -COPY **AUDIENCE CODE -** LIM

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DESCRIPTION - STOMP is a computer model designed to be a general purpose tool for simulating subsurface flow and transport, that complements other analytical capabilities developed by Pacific Northwest National Laboratory's Hydrology Group. The simulator was specifically designed to provide scientists and engineers from various disciplines with multidimensional analysis capabilities for modeling subsurface flow and transport phenomena. STOMP's target capabilities were guided by proposed or applied remediation activities at sites contaminated with volatile organic compounds and/or radioactive material. Developed with the support of the U.S. Department of Energy, Office of Environmental Restoration and Waste Management, the simulator's modeling capabilities address a variety of subsurface environments, including nonisothermal conditions, fractured media, multiple-phase systems, non-wetting fluid entrapment, soil freezing conditions, nonaqueous phase liquids, first-order chemical reactions, radioactive decay, solute transport, dense brines, nonequilibrium dissolution, and surfactant enhanced dissolution and mobilization of organics.

PACKAGE CONTENTS - Media Directory; Software Abstract; PNNL-11216; PNNL11218; PNNL-11217; Media Includes Source Code, Sample Problem Input and Output;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - The STOMP simulator solves the partial-differential equations that describe the conservation of mass or energy quantities by employing integrated-volume finite-difference discretization to the physical domain and backward Euler discretization to the time domain. The resulting equations are nonlinear coupled algebraic equations, which are solved using Newton-Raphson iteration. The simulator has been written with a variably source code that allows the user to choose the solved governing equations (e.g., water mass, air mass, dissolved-oil mass, oil mass, salt mass, thermal energy). Depending

PACKAGE ID - 001205MLTPL00 STOMP

METHOD OF SOLUTION -(CONT) on the chosen operational mode the governing transport equations will be written over one to four phases (e.g., aqueous phase, gas phase, NAPL phase, ice phase, solid phase) Solute transport, radioactive decay, and first-order chemical reactions are solved using a direct solution technique (e.g., Patankar's power-law formulation, TVD scheme) following the solution of the coupled flow equations. Input is directed through semi-formatted text files and output is available through a variety of user directed formats. The simulator recognizes a number of boundary condition types and allows their specification both internally and externally to the computational domain.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - Machine dependent

PROGRAMMING LANGUAGES - ANSI FORTRAN 77

SOFTWARE LIMITATIONS - The STOMP simulator solves multiple-phase subsurface flow and transport problems for variably saturated geologic media systems. The fundamental premise of the numerical theory for the simulator is that flow of liquids through geologic media is described by Darcy's Law. This assumption eliminates the need to solve a separate momentum equation, which makes the simulator unsuitable for solving problems involving flow of liquids through pipes, channels, river beds, canals, etc. From a more general perspective, the simulator attempts to model subsurface flow and transport phenomena through mathematical descriptions of a finite number of physical processes, according to a set of governing equations. The formulation of these mathematical descriptions and the selection of the governing flow and transport equations has required a number of assumptions be taken. A description of these assumptions and specifics about the governing equations and associated constitutive theories is documented in the STOMP Theory Guide (White and Oostrom 1996).

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - In effect the STOMP simulator is a collection of subsurface flow and transport codes that are distingushed by the solved governing equations. This operational mode approach allows the simulation to be customized to the problem of interest, thus eliminating the additional work associated with solving extraneous governing equations. The STOMP simulator has a diverse number of operational modes: Water, Water-Air, Water-Air-Energy, Water-Salt, Water-Air-Salt-Energy, Water-Oil, Water-Oil-Air, Water-Dissolved Oil-Oil, Water-Dissolved Oil-Dissolved Surfactant-Oil, and Water-Dissolved Oil-Oil-Air. In addition to the operational mode features, the STOMP simulator is unique in its capabilities related to the relative permeability-saturation-capillary pressure (k-s-P) functions.

PACKAGE ID - 001205MLTPL00 STOMP

UNIQUE FEATURES -(CONT)
RELATED SOFTWARE - The STOMP simulator generates several output files according to user directives: screen, output, plot.n, restart.n, surface; where .n refers to an integer number related to the simulation time step. These output files contain user directed simulation results of field variables, surface variables, and fluxes. Several utility type programs have been written in FORTRAN 77 that translate or extract the data in these files into forms used by other plotting or visualization packages. In the scalar version (FORTRAN 77) of the STOMP simulator all output files contain data in ASCII text format, which can be read by text editors. Input files can be generated through a text editor following the formatting guidelines described in the STOMP User's Guide or a Macintosh based graphical user interface called sTeP can be employed.

HARDWARE REQS - Hardware requirements for the STOMP simulator are entirely dependent on the dimensions of the computational domain and the number of solved equations. failure to successfully execute a particular simulation can occur through insufficient memory or execution speed. Although the simulator will execute on personal computers the computational spatial and temporal domains will be severely limited. The simulator was principally designed for use on workstation, mainframe, and supercomputer level computer platforms, executing the UNIX operating system.

TIME REQUIREMENTS - As with most computational fluid dynamics type simulators, problem size (i.e., number of unknowns, grid cells, and dimensions) and execution speed are limited by the executing computer's available memory and compute cycle speed. Execution time requirements depend on the size and dimensionality of the computational domain, the number of solved equations, the degree of nonlinearity in the constitutive equations, and the number of time steps executed. Executin speeds for a single iteration are roughly proportional to the number of unknowns in the linear system to the 2.5 power. The number of iterations per time step depends on the degree of nonlinearity associated with the constitutive equations. Execution times can range from seconds for one-dimensional column simulations involving the flow of the aqueous phase to weeks for three-dimensional problems of transient heat transfer through multiple-phase systems.

REFERENCES - W.E. Nichols, N.J. Aimo, M. Oostrom, and M.D. White, STOMP Subsurface Transport Over Multiple Phases, Application Guide, PNNL-11216, October 1997; M.D. White and M. Oostrom, STOMP Subsurface Transport Over Multiple Phases, User's Guide, PNNL-11218, October 1997; M.D. White and M. Oostrom, STOMP Subsurface Transport Over Multiple Phases, Theory Guide, PNNL 11217, October 1997.

ABSTRACT STATUS - Released AS-IS 3/18/98

SUBJECT CLASS CODE - H

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SPONSOR - DOE/EM

PACKAGE TYPE - AS - IS