

PACKAGE ID - 000219MLTPL05 TOUGH2V2.0

KWIC TITLE - Unsaturated Groundwater and Heat Transport
Model

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LIMITATION CODE -COPY **AUDIENCE CODE** - UNL

COMPLETION DATE - 12/01/1999 **PUBLICATION DATE** - 12/01/1999

DESCRIPTION - TOUGH2V2.0 is a new and improved version of TOUGH2 for simulating fluid flow and heat transfer in porous media. It is upwardly compatible with and includes all of the capabilities of the earlier version, including the flexibility to handle different fluid mixtures (water, water with tracer; water, CO₂; water, air; water, air, with vapor pressure lowering; and water, hydrogen), facilities for processing of geometric data (computational grids), and an internal version control system to ensure referenceability of code applications. Improvements in TOUGH2V2.0 include (1) several new EOS modules for different fluid mixtures, including brines and water-soluble and volatile tracers, (2) enhanced capabilities for previously released fluid property modules, (3) description of diffusion and dispersion in multiphase systems, (4) strongly coupled flow and transport processes, (5) coupling between flow in geothermal reservoirs and wellbores in two-phase conditions, (6) tracer transport with sorption and radioactive decay, (7) flow in media with strong heterogeneity, and (8) a new package of preconditioned conjugate gradient routines for more robust solution of numerically difficult problems. In addition, numerous enhancements were made to facilitate applications to more diverse and demanding flow problems. The T2VOC code for three phase flow of water, air, and a non-aqueous phase liquid (NAPL) has been fully integrated into and is now part of the TOUGH2V2.0 program package. TOUGH2V2.0 comes with a new self-contained users guide that includes technical specifications, a complete reference of input data formats and a collection of sample problems. TOUGH2V2.0 is a multi-dimensional numerical model for simulating the coupled transport of water, vapor, air, and other fluids, and heat in porous and fractured media. The program provides options for specifying injection or withdrawal of heat and fluids. (more in OTHER PROG/OPER SYS INFO)

PACKAGE CONTENTS - Media Directory; Software Abstract; NOTE ON DOCUMENTATION; READ.ME XDDB File; Overview of Code Revisions; Media Includes User Guide (LBNL-43134), Source Code, Auxiliary

PACKAGE ID - 000219MLTPL05 TOUGH2V2.0

PACKAGE CONTENTS - (CONT) Materials, Compilation Instructions, Linking Instructions, Sample Problem Input Data, Installation Instructions;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD ROM

METHOD OF SOLUTION - TOUGH2V2.0 performs a fully-coupled, simultaneous solution of mass and energy balance for multi-component, multi-phase fluids in permeable media coupled with a multiphase extension of Darcy's Law, and Fickian diffusion and dispersion. The governing equations are discretized using integral finite difference for space and fully-implicit first-order finite differences in time. The resulting non-linear algebraic equations are solved by Newton-Raphson iteration. Iteration is continued until all residuals are reduced below user-specified convergence tolerances. The linear equations arising at each iteration step can be solved with a variety of techniques, including direct matrix methods, and iterative approaches using preconditioned conjugate gradients.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - Operating System-Independent (Requires 64 bit compiler to provide double precision arithmetic)

PROGRAMMING LANGUAGES - FORTRAN 77

SOFTWARE LIMITATIONS - Storage requirements increase with number of grid blocks (mesh size). Maximum problem dimensions can be specified through PARAMETER statements in the main program, or through an INCLUDE file.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - TOUGH2V2.0 has a flexible modular structure that allows modeling of different fluid mixtures. The integral finite difference method used is equivalent to conventional finite differences for regular grid systems, but offers additional flexibility by allowing irregular grids to represent geologic or geometric features. One, two, and three-dimensional systems and single or multiple continuum media are all treated on the same footing. There is an extensive record of code verifications and worked problems.

RELATED SOFTWARE - TOUGH2V2.0 supersedes the previous versions of TOUGH2, which in turn superseded the TOUGH Code. Utility programs to facilitate TOUGH2 applications, such as preprocessing of calculational grids, specification of initial and boundary conditions, and interfacing with graphics programs, are freely available for downloading from the TOUGH2 homepage on the web at

PACKAGE ID - 000219MLTPL05 TOUGH2V2.0

RELATED SOFTWARE - (CONT) <http://www-esd.lbl.gov/TOUGH2/>

OTHER PROG/OPER SYS INFO - (DESCRIPTION CONT.) Although primarily designed for geothermal reservoir studies, and isolation of high level nuclear waste in partially saturated geological media, TOUGH2V2.0 should also be useful for a wider range of problems in heat and moisture transfer, and in the drying of porous materials. The simulator was primarily developed for problems involving strongly heat driven flow. To describe these phenomena a multiphase approach to fluid and heat flow is used, which fully accounts for the movement of gaseous and liquid phases, their transport of latent and sensible heat, and phase transitions between liquid and vapor. TOUGH2V2.0 takes account of fluid flow in both liquid and gaseous phases occurring under pressure, viscous, gravity forces according to Darcy's Law. Interference between the phases is represented by means of relative permeability functions. The code handles multiphase diffusion effects coupled with phase partitioning, and represents capillary and phase adsorption effects for the liquid phase. Heat transport occurs by convection and diffusion, accounting for sensible and latent heat, and by conduction with thermal conductivity dependent on water saturation. TOUGH2V2.0 can also efficiently model isothermal flow problems, such as unsaturated flow described by Richard's equation, or water and tracer transport in groundwater aquifers. TOUGH2V2.0 includes the proprietary software package MA28 from the Harwell Subroutine Library.

HARDWARE REQS - A flow problem with up to 800 grid blocks, 2400 connections (interfaces) between them, and 3 equations per grid block requires approximately 4 Megabytes of RAM. More detailed information is available in the user's guide.

TIME REQUIREMENTS - Highly variable depending on problem size and simulation time. Many simple flow problems with a few hundred grid blocks can be run in a matter of minutes on workstations. Large, complex 3-D problems with 50,000 - 100,000 grid blocks in heterogenous media may run for days.

REFERENCES - K. Pruess, C. Oldenburg, and G. Moridis, TOUGH2 User's Guide Veriosn 2.0, LBNL-43134, November 1999.

ABSTRACT STATUS - Released AS-IS 12/14/1999.

SUBJECT CLASS CODE - HR

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
T CODES
GEOTHERMAL ENERGY
RADIOACTIVE WASTE DISPOSAL
RESERVOIR ENGINEERING

PACKAGE ID - 000219MLTPL05 TOUGH2V2.0

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EDB SUBJECT CATEGORIES -
990200

SPONSOR - DOE/DP

PACKAGE TYPE - AS - IS