

PACKAGE ID - 000219MLTPL03 ITOUGH2(PC)

KWIC TITLE - Inverse Modeling for TOUGH2 Family of
Multiphase Flow Simulators

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

COMPLETION DATE - 01/19/1999 **PUBLICATION DATE** - 03/01/1999

DESCRIPTION - ITOUGH2 assumes the user either has, or is intimately familiar with the use of TOUGH2 and its documentation as it is needed for proper use of ITOUGH2. ITOUGH2 provides inverse modeling capabilities for the TOUGH2 family of numerical simulators for non-isothermal multiphase flows in fractured-porous media. The ITOUGH2 can be used for estimating parameters by automatic modeling calibration, for sensitivity analyses, and for uncertainty propagation analyses (linear and Monte Carlo simulations). Any input parameter to the TOUGH2 simulator can be estimated based on any type of observation for which a corresponding TOUGH2 output is calculated. ITOUGH2 solves a non-linear least-squares problem using direct or gradient-based minimization algorithms. A detailed residual and error analysis is performed, which includes the evaluation of model identification criteria. ITOUGH2 can also be run in forward mode, solving subsurface flow problems related to nuclear waste isolation, oil, gas, and geothermal reservoir engineering, and vadose zone hydrology.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Includes User Guides: LBNL-40040 REV. 1, LBNL-40041 REV. 1, LBNL-40042 REV. 1, Source Code, Auxiliary Material, Compilation Instructions, Linking Instructions, Sample Problem Input Data, Installation Instructions; TOUGH2 or TOUGH2PC documents as required;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 CD Rom

METHOD OF SOLUTION - Integral Finite Differences, Newton-Raphson, direct and iterative equation solvers, Minimization algorithms: Levenberg-Marquardt, Simplex, Simulated Annealing.

COMPUTER - MLT-PLTFM

OPERATING SYSTEMS - Lahey Compiler

PROGRAMMING LANGUAGES - FORTRAN 77, Unix Bourne Shell Script

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SOFTWARE LIMITATIONS - Use of the forward program TOUGH2 is a prerequisite for the use of ITOUGH2, and should be ordered with ITOUGH2 if the user does not already have TOUGH2. Adjustable problem size.

SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - Sophisticated forward model (TOUGH2), extensive error and uncertainty analysis.

RELATED SOFTWARE - TOUGH2 and T2-VOC.

OTHER PROG/OPER SYS INFO - Machine-dependent system calls (provided for all platforms)

HARDWARE REQS - Greater than 32MB RAM recommended.

TIME REQUIREMENTS - 1 minute to several days.

REFERENCES - S. Finsterle, iTOUGH2 Sample Problems, LBNL-40042-Rev.1, March 1999; S. Finsterle, iTOUGH2 User's Guide, LBNL-40040-Rev.1, March 1999; S. Finsterle, iTOUGH2 Command Reference, LBNL-40041-Rev.1.

ABSTRACT STATUS - Released AS-IS 7/12/1999.

SUBJECT CLASS CODE - HR

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
I CODES
MULTIPHASE FLOW
HEAT FLOW
POROUS MATERIALS
RADIOACTIVE WASTE DISPOSAL
GEOTHERMAL FLUIDS
HYDROLOGY

EDB SUBJECT CATEGORIES -

990200 052002 152001

SPONSOR - DOE/DP

PACKAGE TYPE - AS - IS