TOUGH2

- General overview: code development, capabilities, methods, architecture
- Simulation of flow systems: approach, data needs
- TOUGH2 user interface and preparation of input data

Developed at Lawrence Berkeley National Laboratory
http://www-esd.lbl.gov/TOUGH2/

TOUGH2

Transport **O**f **U**nsaturated **G**roundwater and **H**eat

- *Geothermal reservoir engineering*
- *Nuclear waste disposal*
- *Vadose zone hydrology*
- *Environmental remediation*
- *Oil and gas*
- *Carbon storage (sequestration)*

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Energy Science and Technology Software Center	phone	(865) 576-2606
P.O. Box 1020	fax	(865) 576-6436
Oak Ridge, Tennessee 37831	email	estsc@adonis.osti.gov
U.S.A.	http://www.osti.gov/estsc/	

- Nuclear Energy Agency (NEA) data bank: http://www.nea.fr/
- Thunderhead Engineering (PetraSim): http://www.thunderheadeng.com/petrasim/index.html

TOUGH Family of Codes

Table 1. Development of the TOUGH codes.*

Simulator	Application	Phases (components)†	Comments
MULKOM	geothermal, nuclear waste, oil and gas	multi (multi)	research code, operational 1981, no public release
TOUGH	geothermal, nuclear waste	aqueous, gas (water, air)	released 1987
TOUGH2	general purpose	aqueous, gas (water, NCGs)	released 1991
T2VOC	environmental	aqueous, gas, NAPL (water, air, VOC)	released 1995
iTOUGH2	inverse modeling: sensitivity analysis, uncertainty propagation	multi (multi)	released 1999
TOUGH2 V 2.0	general purpose	multi (multi)	released 1999
TMVOC	environmental	aqueous, gas, NAPL (water, air, multiple VOCs and NCGs)	released 2002
TOUGHREACT	reactive chemistry	aqueous, gas, solid (multi)	release 2004 (expected)
TOUGH-FLAC	geomechanics	aqueous, gas (water, CO_2)	research code

† NAPL, nonaqueous phase liquid; NCG, noncondensible gas; VOC, volatile organic compound.

* Pruess, K. The TOUGH Codes—A Family of Simulation Tools for Multiphase Flow and Transport Processes in Permeable Media, *Vadose Zone J.*, Vol. 3, pp. 738 - 746, 2004

Development of the TOUGH/MULKOM Family of Codes

- Problem-driven: geothermal, nuclear waste, oil and gas, environmental, hydrogeology, greenhouse gases
- Flexibility: modular structure
- Robustness: fully implicit, residual-based formulation
- Openness: source code, internal and external documentation
- Referenceability: version control
- Technology transfer: code distribution (ESTSC), user support, collaborations

The TOUGH codes are currently in use in over 300 organizations in more than 30 countries.

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TOUGH2 USER'S GUIDE, VERSION 2.0

Karsten Pruess
Curt Oldenburg
George Moridis

Earth Sciences Division, Lawrence Berkeley National Laboratory
University of California, Berkeley, California 94720

November 1999

TOUGH2 - Capabilities

- single-phase flow of water, water with tracer
- two-phase flow of water, vapor, and non-condensible gas
- multiphase flows of multicomponent fluids
- non-isothermal flows with phase change (boiling and condensation)
- dissolution and precipitation of salt (NaCl)
- heat conduction, gas diffusion
- vapor pressure lowering
- 1-D, 2-D, 3-D; heterogeneous media
- double-porosity, dual-permeability, and multiple interacting continua (MINC) methods for fractured media
- T2VOC, TMVOC: contamination problems with non-aqueous phase liquids (NAPLs)
- inverse model iTOUGH2
- **TOUGHREACT: reactive chemistry**
- TOUGH-FLAC: geomechanics

Pruess, K., A. Simmons, Y.S. Wu and G. Moridis. TOUGH2 Software Qualification. Lawrence Berkeley National Laboratory Report LBL-38383, February 1996.

Table 9. Summary of Validation Problems

#	PROBLEM TITLE	DIMENSIONS	FEATURES	ISSUES	REFERENCES
1	infiltration	1-D, linear horizontal	isothermal	code verification against known semi-analytical solution (Philip, 1955; Ross et al., 1982)	#2 in Pruess (1987); also #1 in Moridis and Pruess (1992)
2	flow to a geothermal well	1-D, radial	water and steam only, no air; sensible and latent heat effects; coupled fluid and heat flow	phase transitions; propagating boiling front; code verification against known semi-analytical and numerical solutions (Garg, 1978, 1980)	#4 in Pruess, (1987), also #4 in Moridis and Pruess (1992)
3	transient heat pipe	1-D, linear	coupled fluid and heat flow with air; liquid-gas counter-flow with very strong binary diffusion; sensible and latent heat effects	code verification against similarity solution (Doughty and Pruess, 1991, 1992)	Pruess (1991); Doughty and Pruess (1992)
4	coupled heat and mass transport	1-D, linear	non-isothermal convection, diffusion	code verification (Avdonin, 1964, Ross, 1982)	# 2 in Moridis and Pruess (1992)
5	heat transport	1-D, radial	single phase non-isothermal, convection, diffusion, sensible and latent heat effects	code verification (Avdonin, 1964, Ross, 1982)	#3 in Moridis and Pruess (1992) #2 in Moridis and Pruess (1995)
6	Theis problem (flow toward a well)	1-D, radial	single-phase, isothermal, viscous forces	validation against analytical solution (Theis, 1935)	#1 in Moridis and Pruess (1995)
7	Coupled fluid and heat flow in fracture	1-D, radial	heat conduction, MINC, fracture-matrix flow, single-phase, non-isothermal	verification	Pruess and Wu (1993)
8	infiltration	2-D, cartesian	isothermal, two-phase heterogeneous medium, seepage face mixed boundary condition, interference between liquid and gas, gravity effects	validation against experimental data (Vauclin et al., 1979)	#6 in Moridis and Pruess (1995)

TOUGH2 SOFTWARE QUALIFICATION - FEBRUARY 1996 32

Pruess, K., A. Simmons, Y.S. Wu and G. Moridis. TOUGH2 Software Qualification. Lawrence Berkeley National Laboratory Report LBL-38383, February 1996.

Table 9 (cont). Summary of Validation Problems

#	PROBLEM TITLE	DIMENSIONS	FEATURES	ISSUES	REFERENCES
9	convection cell	2-D, cylindrical	single phase, non-isothermal, heterogeneous soil, no mass flow boundary, flow channeling, sensible and latent heat effects	validation against lab experiment (Reda, 1984)	#7 in Moridis and Pruess (1992) 3 in Moridis and Pruess (1995)
10	two-phase flow	2-D, cylindrical	simultaneous heat and mass flow, phase change, time-variant pressure boundary, interference between liquid and gas phase	validation against lab experiment (Kruger and Ramey, 1974; Faust and Mercer, 1979)	#8 in Moridis and Pruess, 1992
11	Warren-Root Solution	1-D, radial	transient flow, double-porosity medium	code verification against analytical solution (Warren and Root, 1963)	this paper
12	Lauwerier heat transfer solution	2-D, cartesian	conductive and convective heat transfer in porous media	code verification against analytical solution (Lauwerier, 1955)	this paper
13	handling of thermophysical properties	NA	water, water vapor, air	TOUGH2 calculated properties compared to steam tables (CRC, 1993)	this paper
14	vapor pressure lowering	NA	coupling between capillary and vapor adsorption effects, and vapor pressure	comparison with predictions from Kelvin's equation	this paper
15a	heterogeneous	1-D	single-phase slightly compressible liquid	code verification against analytical solution of Moridis (1995)	this paper
15b	flow to single well with anisotropic formation	2-D	single-phase, slightly compressible fluid, infinite anisotropic aquifer	code verification against analytical solution (Papadapoulos, 1965)	this paper
16	single-phase transient flow with irregular gird	2-D, cartesian	transient flow in horizontal, isotropic, isothermal aquifer	verification of irregular grid capability using Theis solution	this paper

Pruess, K., A. Simmons, Y.S. Wu and G. Moridis. TOUGH2 Software Qualification. Lawrence Berkeley National Laboratory Report LBL-38383, February 1996.

Table 9 (cont). Summary of Validation Problems

#	PROBLEM TITLE	DIMENSIONS	FEATURES	ISSUES	REFERENCES
17a	heat conduction	1-D, linear	semi-infinite rock column, step change in T; ignores flow effects	code verification against analytical solution of Carslaw and Jaeger (1959)	this paper
17b	binary vapor diffusion	1-D	vapor and air diffusion in gas phase, semi-infinite rock column; ignores vapor adsorption	code verification against analytical solution of Carlsaw and Jaeger (1959)	this paper
17c	gas flow with Klinkenberg effects	1-D	steady single-phase gas flow across linear rock column, isothermal	code verification of gas permeability enhancement at low pressures (Klinkenberg, 1941)	this paper
18	horizontal well with compressible liquid	3-D	anisotropic reservoir	code verification against analytical solution of Goode and Thambynayagam (1987)	this paper
19	single-phase gas flow	1-D, radial	flow to single vertical well at center of bounded cylindrical formation	code verification against analytical solution of Kabir and Hasen (1986)	this paper
20	water absorption into porous matrix	1-D, radial	fracture-matrix interaction in two-phase flow	code verification against semi-analytical solution	Zimmerman et al, (1990)

TOUGH2 - Methods

- set up general mass-and-energy balance equations
- space discretization by integral finite differences (IFD)
- applicable to 1-D, 2-D, 3-D regular or irregular grid geometries; single porosity or multi-continua (fractured media)
- fully implicit time weighting
- simultaneous, iterative solution of all mass- and energy-balances
- phase (dis-)appearance handled by switching primary variables
- preconditioned conjugate gradients, direct solvers
- different fluid property modules for different applications

TOUGH2 - Architecture

The equations describing multiphase, multicomponent fluid and heat flow have the same mathematical form, regardless of the number and nature of fluid components and phases present.

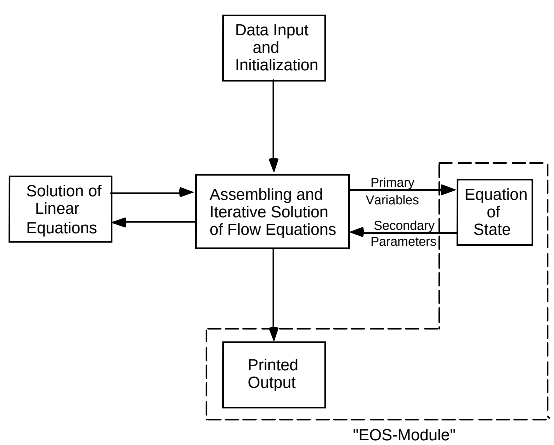
The only differences for different fluid systems, such as *water-air*, *water-dissolved salts*, *brine-CO_2*, or *water-gas-oil*, are in the material properties:
densities, viscosities, partitioning of fluid components among phases, etc. ...

This suggests to set up a "modular" simulator architecture, consisting of

- a core module for assembling and solving the flow and transport equations,
- fluid property or "equation-of-state" (EOS) modules, that supply thermophysical and transport property data for the fluid system(s) at hand,
- modules for inputting and outputting data.

The modular architecture just described is known as "MULKOM," and is implemented in the TOUGH family of codes. It offers great flexibility in applications to different kinds of flow problems.

Modular Architecture for TOUGH2



TOUGH2 Fluid Property Modules

1991-Release

Module	Capabilities
EOS1 *	water, water with tracer
EOS2	water, CO2
EOS3 *	water, air
EOS4	water, air, with vapor pressure lowering
EOS5 *	water, hydrogen

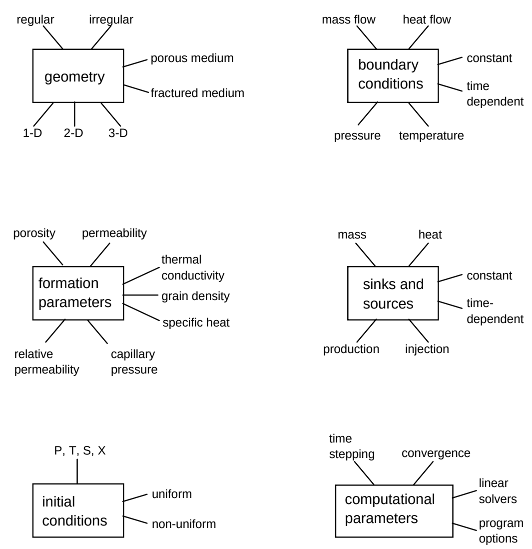
* optional constant-temperature capability

2005: ECO2N* – water, NaCl, CO_2

1999-Additions

Module	Capabilities
EOS7 *	water, brine, air
EOS7R *	water, brine, air, parent - daughter radionuclides
EOS8 *	water, "dead" oil, non - condensible gas
EOS9	variably-saturated isothermal flow according to Richards' equation
EWASG*	water, salt (NaCl), non - condensible gas (includes precipitation and dissolution, with porosity and permeability change; optional treatment of vapor pressure lowering effects)
T2VOC	water, air, NAPL (implementation of T2VOC within TOUGH2)

Data Groups for a Flow Simulation



Model Calibration (History Matching)

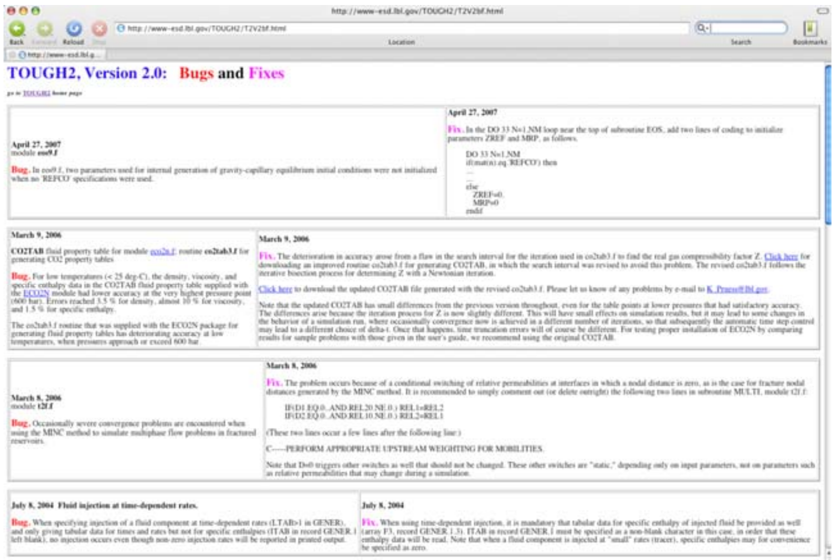
- make guesses for poorly constrained parameters
- run simulation
- compare the outcome with field observations
- revise parameters to try and reduce discrepancies

trial-and-error process, or "inverse modeling”
(iTOUGH2 - automatic history match)

Got Bugs?

- We know of no methodology that would allow to systematically find and correct all bugs in a big complex code.
- Users have to assume that codes may have bugs - it is the user’s responsibility to check and verify their code applications.
- What to do?
  - be very careful in writing/changing codes and developing applications
  - keep unbroken chain of test applications and sample problems
  - compare with semi-analytical solutions, other codes
  - compare with data (lab, field)
  - maintain records (internal version control)
  - wide dissemination: the more a code gets used, the greater the likelihood that bugs will be found and fixed
  - user community: win-win
  - we maintain web site with bugs and fixes
    (http://www-esd.lbl.gov/TOUGH2/T2V2bf.html)

Got Fixes!



TOUGH2 Input Data Blocks

Keyword	Function
TITLE (first record)	one data record (single line) with a title for the simulation problem
MESHM	optional; parameters for internal grid generation through MESHMaker
ROCKS	hydrogeologic parameters for various reservoir domains
MULTI	optional; specifies number of fluid components and balance equations per grid block; applicable only for certain fluid property (EOS) modules
SELEC	used with certain EOS-modules to supply thermophysical property data
START	optional; one data record for more flexible initialization
PARAM	computational parameters; time stepping and convergence parameters; program options
DIFFU	diffusivities of mass components
FOFT	optional; specifies grid blocks for which time series data are desired
COFT	optional; specifies connections for which time series data are desired
GOFT	optional; specifies sinks/sources for which time series data are desired

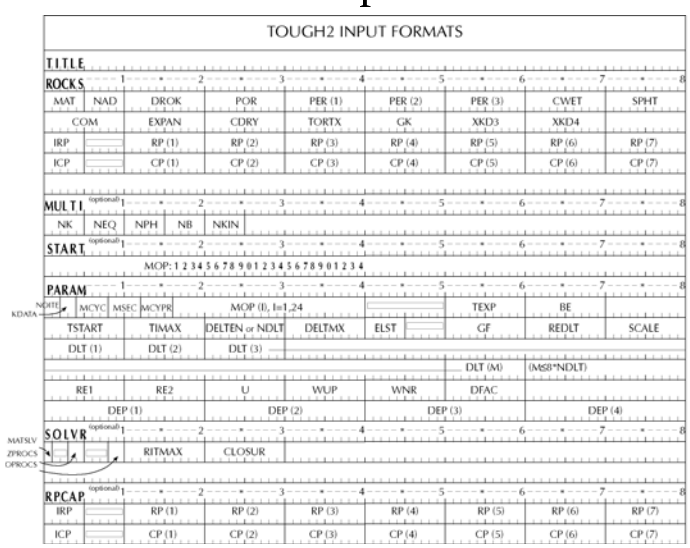
RPCAP	optional; parameters for relative permeability and capillary pressure functions
TIMES	optional; specification of times for generating printout
*ELEME	list of grid blocks (volume elements)
*CONNE	list of flow connections between grid blocks
*GENER	optional; list of mass or heat sinks and sources
INDOM	optional; list of initial conditions for specific reservoir domains
*INCON	optional; list of initial conditions for specific grid blocks
NOVER (optional)	optional; if present, suppresses printout of version numbers and dates of the program units executed in a TOUGH2 run
ENDCY (last record)	one record to close the TOUGH2 input file and initiate the simulation
ENDFI	alternative to “ENDCY” for closing a TOUGH2 input file; will cause flow simulation to be skipped; useful if only mesh generation is desired

Blocks labeled with a star * can be provided as separate disk files, in which case they would be omitted from the INPUT file.

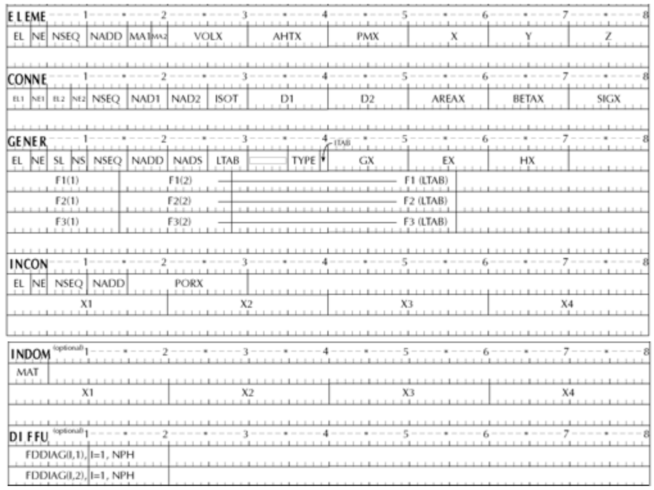
TOUGH2 Disk Files

File	Use
MESH (unit 4)	written in subroutine INPUT from ELEME and CONNE data, or in module MESHMAKER from mesh specification data; read in RFILE to initialize all geometry data arrays used to define the discretized flow problem
GENER (unit 3)	written in subroutine INPUT from GENER data; read in RFILE to define nature, strength, and time-dependence of sinks and sources
INCON (unit 1)	written in subroutine INPUT from INCON data; read in RFILE to provide a complete specification of thermodynamic conditions
SAVE (unit 7)	written in subroutine WRIFI to record thermodynamic conditions at the end of a TOUGH2 simulation run; compatible with formats of file or data block INCON for initializing a continuation run
MINC (unit 10)	written in module MESHMAKER with MESH-compatible specifications, to provide all geometry data for a fractured-porous medium mesh (double porosity, dual permeability, etc.); read (optionally) in subroutine RFILE to initialize geometry data for a fractured-porous system
LINEQ (unit 15)	written during linear equation solution, to provide informative messages on linear equation solution
TABLE (unit 8)	written in CYCIT to record coefficients of semi-analytical heat exchange at the end of a TOUGH2 simulation run; read (optionally) in subroutine QLOSS to initialize heat exchange coefficients in a continuation run
FOFT (unit 12)	written in FGTAB to provide time series data for elements for plotting
COFT (unit 14)	written in FGTAB to provide time series data for connections for plotting
GOFT (unit 13)	written in FGTAB to provide time series data for sinks/sources for plotting
VERS (unit 11)	written in all TOUGH2 program units with informational message on version number, date, and function; read in main program and printed to default OUTPUT at the conclusion of a TOUGH2 simulation run; printing of version information is suppressed when keyword NOVER is present in INPUT file

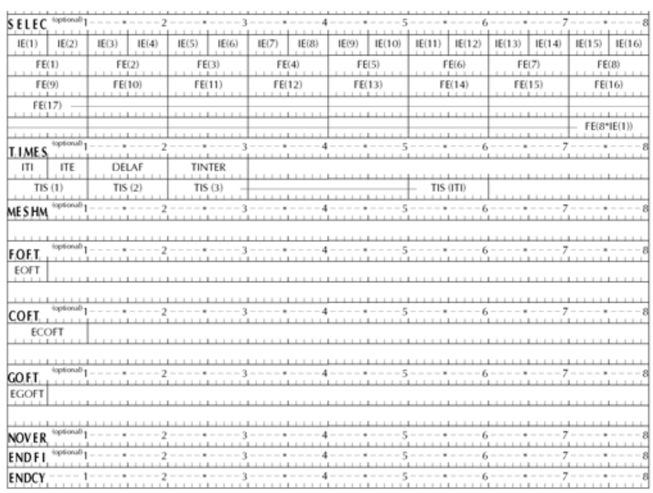
TOUGH2 Input Formats



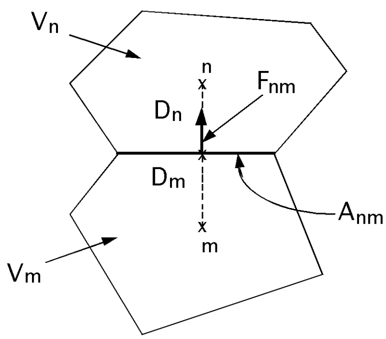
TOUGH2 Input Formats (cont'd)

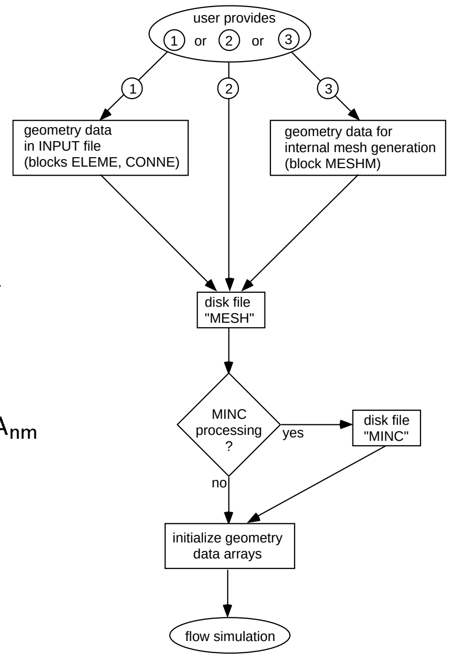


TOUGH2 Input Formats (cont'd)



User Options for Geometry Data





Linear Equation Solvers

MOP(21) = 1: direct solver MA28

MOP(21) = 2: DSLUBC, a bi-conjugate gradient solver

MOP(21) = 3: DSLUCS, a Lanczos-type bi-conjugate gradient solver

MOP(21) = 4: DSLUGM, a generalized minimum residual solver

MOP(21) = 5: DLUSTB, a stabilized bi-conjugate gradient solver

MOP(21) = 6: direct solver LUBAND