

# 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

## **T**ransport **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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- 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 TOUGH2 T2VOC	geothermal, nuclear waste general purpose environmental	aqueous, gas (water, air) aqueous, gas (water, NCGs) aqueous, gas, NAPL (water, air, VOC)	released 1987 released 1991 released 1995
ITOUGH2	inverse modeling: sensitivity analysis, uncertainty propagation	multi (multi)	released 1999
TOUGH2 V 2.0 TMVOC	general purpose environmental	multi (multi) aqueous, gas, NAPL (water, air, multiple VOCs and NCGs)	released 1999 released 2002
TOUGHREACT	reactive chemistry	aqueous, gas, solid (multi)	release 2004 (expected)
TOUGH-FLAC	geomechanics	aqueous, gas (water, CO <sub>2</sub> )	research code

† NAPL, nonaqueous phase liquid; NCG, noncondensable 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.

LBNL-43134

## 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-condensable 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 (Phillip, 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 transition; 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 (Doughly and Pruess, 1991, 1992)	Pruess (1991); Doughly and Pruess (1992)
4	coupled heat and mass transport	1-D, linear	non-isothermal convection, diffusion	code verification (Avidomin, 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 (Avidomin, 1964, Ross, 1982)	#3 in Moridis and Pruess (1992)
6	Thesis problem (flow toward a well)	1-D, radial	single-phase, isothermal, viscous forces	validation against analytical solution (Thesis, 1935)	#2 in Moridis and Pruess (1995) #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 (1992)
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

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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	Lasverier heat transfer solution	2-D, cartesian	conductive and convective heat transfer in porous media	code verification against analytical solution (Lasverier, 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 (Papadopoulos, 1965)	this paper
16	single-phase transient flow with irregular grid	2-D, cartesian	transient flow in horizontal, isotropic, isothermal aquifer	verification of irregular grid capability using This 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 Carslaw 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 Odeh 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 Hasan (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.

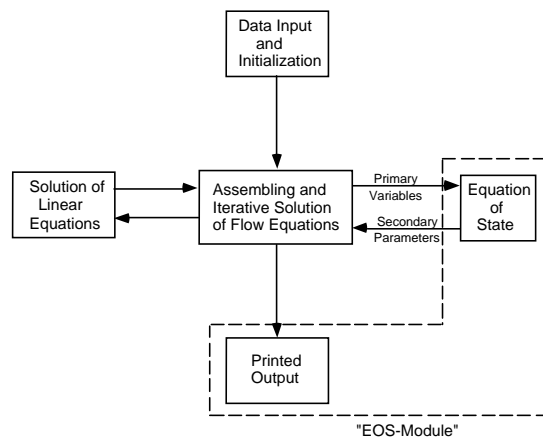
The only differences for different fluid systems, such as *water-air*, *water-dissolved salts*, *brine-CO<sub>2</sub>*, or *water-gas-oil*, are in the material properties: densities, viscosities, partitioning of fluid components among phases, etc. ...

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

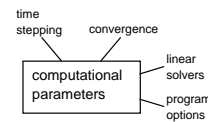
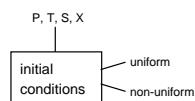
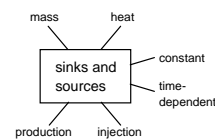
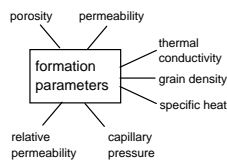
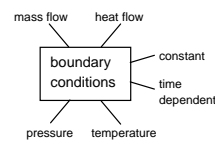
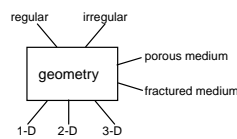
\* optional constant-temperature capability

2005: ECO2N\* – water, NaCl, CO<sub>2</sub>

## 1999-Additions

Module	Capabilities
EOS7 *	water, brine, air
EOS7R *	water, brine, air, parent daughter radionuclides
EOS8 *	water, "dead" oil, condensible gas non -
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, Version 2.0: Bugs and Fixes**

**April 27, 2007**  
**module eos.f**  
**Bug:** In eos.f, two parameters used for internal generation of gravity-capillary equilibrium initial conditions were not initialized when no REFVCO specifications were used.

**Fix:** In the DO 11 N=1 NM loop near the top of subroutine EOS, add two lines of coding to initialize parameters ZREF and SRP, as follows:  
 DO 11 N=1 NM  
 iformat(= REFCO) then  
 ...  
 ZREF=0  
 SRP=0  
 endif

**March 9, 2006**  
**CO2TAB fluid property table for module geo2.f, routine eo2tab.f for generating CO2 property tables**  
**Bug:** For low temperatures (c. 25 deg.C), the density, viscosity, and specific enthalpy data in the CO2TAB fluid property table supplied with the ECO2N module had lower accuracy at the very highest pressure point (1000 bar). Errors reached 1.5 % for density, almost 30 % for viscosity, and 1.5 % for specific enthalpy.  
 The eo2tab.f routine that was supplied with the ECO2N package for generating fluid property tables has deteriorating accuracy at low temperatures, when pressures approach or exceed 100 bar.

**Fix:** The deterioration in accuracy arose from a flaw in the search interval for the iteration used in eo2tab.f to find the real gas compressibility factor Z. Click here for downloading an improved routine eo2tab.f for generating CO2TAB, in which the search interval was revised to avoid this problem. The revised eo2tab.f follows the iterative function process for determining Z with a Newtonian iteration.  
 Click here to download the updated CO2TAB file generated with the revised eo2tab.f. Please let us know of any problems by e-mail to [K.Francis@sl.gov](mailto:K.Francis@sl.gov).  
 Note that the updated CO2TAB has small differences from the previous version throughout, even for the table points at lower pressures that had satisfactory accuracy. The differences arise because the iteration process for Z is now slightly different. This will have small effects on simulation results, but it may lead to some changes in the behavior of a simulation run, when occasionally convergence now is achieved in a different number of iterations, so that subsequently the accurate time step control may lead to a different choice of delta t. Once that happens, time truncation errors will of course be different. For testing proper simulations of ECO2N by comparing results for sample problems with those given in the user's guide, we recommend using the original CO2TAB.

**March 8, 2006**  
**Fix:** The problem occurs because of a conditional switching of relative permeabilities at interfaces in which a nodal distance is zero, as is the case for fracture nodal distances generated by the MNC method. It is recommended to simply comment out (or delete outright) the following two lines in subroutine MULTI, module G.U.F.  
 IF(DI.EQ.0 .AND. REL.20.NE.0) REL.1=REL.2  
 IF(DI.EQ.0 .AND. REL.10.NE.0) REL.2=REL.1  
 (These two lines occur a few lines after the following line)  
 C-----PERFORM APPROPRIATE UPSTREAM WEIGHTING FOR MOBILITIES.  
 Note that Drel triggers other switches as well that should not be changed. These other switches are "static," depending only on input parameters, not on parameters such as relative permeabilities that may change during a simulation.

**March 8, 2006**  
**module 12.f**  
**Bug:** Occasionally severe convergence problems are encountered when using the MNC method to simulate multiphase flow problems in fractured reservoirs.

**July 8, 2004 Fluid injection at time-dependent rates.**  
**Bug:** When specifying injection of a fluid component at time-dependent rates (ITABs) in GENER, only giving tabular data for times and rates but not for specific enthalpies (ITAB in record GENER, I) enthalpy data will be read. Note that when a fluid component is injected at "small" rates (traces), specific enthalpies may for convenience be specified as zero.

**Fix:** When using time-dependent injection, it is mandatory that tabular data for specific enthalpy of injected fluid be provided as well as only giving tabular data for times and rates but not for specific enthalpies (ITAB in record GENER, I) enthalpy data will be read. Note that when a fluid component is injected at "small" rates (traces), specific enthalpies may for convenience be specified as zero.

# 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 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
*ELEM	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 FG TAB to provide time series data for elements for plotting
COFT (unit 14)	written in FG TAB to provide time series data for connections for plotting
GOFT (unit 13)	written in FG TAB 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							
<b>TITLE</b>							
<b>ROCKS</b>							
MAT	NAD	DROK	POR	PER (1)	PER (2)	PER (3)	CWET SPHT
COM	EXPAN	CDRY	TORTX	GK	XXD3	XXD4	
IRP	RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)
ICP	CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)
<b>MULTI</b>							
NK	NEQ	NPH	NB	NKIN			
<b>START</b>							
MOP: 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4							
<b>PARAM</b>							
MCYC	MSEC	MCYPR	MOP (I), I=1,2,4		TEXP	BE	
TSTART	TMAX	DELTA or NDLT	DELTA	ELST	CF	REDT	SCALE
DLT (1)	DLT (2)	DLT (3)					
					DLT (M)	(MSB*NDLT)	
RE1	RE2	U	WUP	WNR	DFAC		
DEP (1)		DEP (2)		DEP (3)		DEP (4)	
<b>SOLVR</b>							
		RITMAX	CLOSUR				
<b>RPCAP</b>							
IRP	RP (1)	RP (2)	RP (3)	RP (4)	RP (5)	RP (6)	RP (7)
ICP	CP (1)	CP (2)	CP (3)	CP (4)	CP (5)	CP (6)	CP (7)

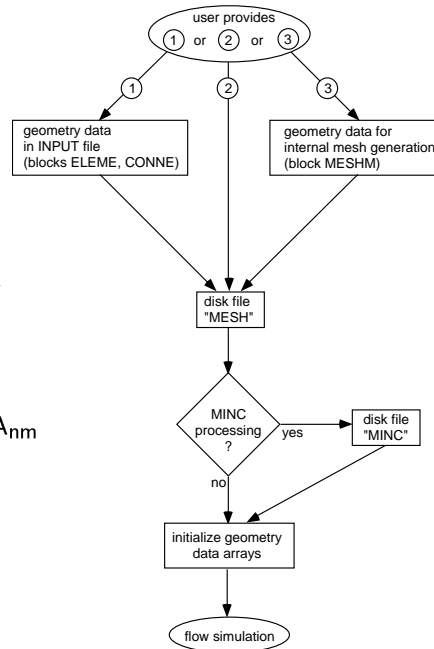
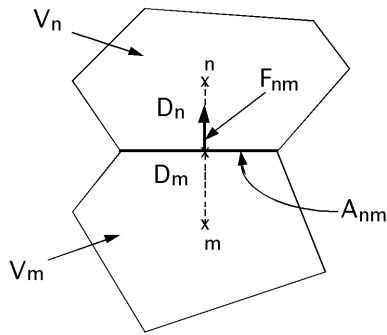
## TOUGH2 Input Formats (cont'd)

<b>E L E M E</b>											
EL	NE	NSEQ	NADD	MA1	MA2	VOLX	AHTX	PAX	X	Y	Z
<b>C O N N E</b>											
EL1	NE1	NE2	NSEQ	NAD1	NAD2	ISOT	D1	D2	AREAX	BETAX	SIGX
<b>G E N E R</b>											
EL	NE	SL	NS	NSEQ	NADD	NADS	LTAB	TYPE	GX	EX	HX
				F1(1)		F1(2)		F1 (LTAB)			
				F2(1)		F2(2)		F2 (LTAB)			
				F3(1)		F3(2)		F3 (LTAB)			
<b>I N C O N</b>											
EL	NE	NSEQ	NADD	PORX							
				X1		X2		X3		X4	
<b>I N D O M</b>											
MAT											
				X1		X2		X3		X4	
<b>D I F F U</b>											
FDDIAG(I), I=1, NPH											
FDDIAG(I), I=1, NPH											

## TOUGH2 Input Formats (cont'd)

<b>S E L E C</b>															
IE(1)	IE(2)	IE(3)	IE(4)	IE(5)	IE(6)	IE(7)	IE(8)	IE(9)	IE(10)	IE(11)	IE(12)	IE(13)	IE(14)	IE(15)	IE(16)
FE(1)		FE(2)		FE(3)		FE(4)		FE(5)		FE(6)		FE(7)		FE(8)	
FE(9)		FE(10)		FE(11)		FE(12)		FE(13)		FE(14)		FE(15)		FE(16)	
FE(17)		FE(18*IE(1))													
<b>T I M E S</b>															
ITI	ITE	DELAF		TINTER						TIS (IT)					
TIS (1)		TIS (2)		TIS (3)						TIS (IT)					
<b>M E S H M</b>															
<b>F O F T</b>															
EOFT															
<b>C O F T</b>															
ECOFT															
<b>G O F T</b>															
EGOFT															
<b>N O V E R</b>															
<b>E N D F I</b>															
<b>E N D C Y</b>															

## 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

