Distribution:
WM File: 3109.9
WMHL r/f
NMSS r/f
REBrowning
MJBell
DJFehringer
PMORnstein & r/f
HJMiller
JOBunting
PSJustus
JTGreeves
PSB C Seeley
PDR

3109.9/PMO/83/09/14/0

SEP 23 1983

MEMORANDUM FOR: Harold S. Bassett, Director
Division of Data Automation
and Management Information

THRU: Program Support Claudia Seeley

FROM: Michael J. Bell, Chief
High-Level Waste Licensing
Management Branch
Division of Waste Manangement

SUBJECT: REQUEST FOR IMPLEMENTATION OF THE TOUGH COMPUTER PROGRAM ON THE BROOKHAVEN SYSTEM

This is to request your assistance to input into the NRC - Brookhaven Computer System, the TOUGH computer program acquired from Lawrence Berkeley Laboratory. This code will be used in the assessment of High-Level waste repositories. The enclosed tape contains the TOUGH computer program, several pre-processor programs, and several sample input sets for TOUGH. Input documentation is provided as an enclosure.

We would appreciate having this program implemented by October 21, 1983.

Michael J. Bell, Chief
High-Level Waste Licensing
Management Branch
Division of Waste Management

Enclosure
As Stated

cc: James Shields

WM Record File 109.9
WM Project 1
Docket No.
PDR ✓
LPDR
Distribution:
(Return to WM, 623-SS) 15

*SEE PREVIOUS CONCURRENCE

OFC	WMHL *	WMHL	PSB				
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DATE	9/ /83	9/23/83	9/ /83				

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PDR WASTE
WM-1 PDR

3109.9/PMO/83/09/14/0

MEMORANDUM FOR: Harold S. Bassett, Director
Division of Data Automation
and Management Information
Office of Resource Management

FROM: Michael J. Bell, Chief
High-Level Waste Licensing
Management Branch
Division of Waste Manangement

THROUGH: Program Support Branch

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OFC	WMHL	WMHL					
NAME	PMOrnstein:lem	MJBell					
DATE	9/16/83	9/ /83					

3. THE INPUT STRUCTURE

3.1 Data Blocks

The types of data needed to characterize a system are summarized in Table 8. The input of TOUGH is organized into "blocks", each of which corresponds to one of the data groups given in Table 8. In addition, there is a data block with computational parameters. There is no special data block for boundary conditions; these have to be specified through appropriately chosen elements, interfaces, initial conditions, and sinks/sources. An overview of the most general input structure is given in Table 9.

The first data card must be the TITLE-card. The last data card must be the ENDCY-card, with ENDCY punched in columns 1-5. The data blocks between TITLE and ENDCY can be provided in arbitrary order, except that block ELEME must precede block CONNE. The blocks ELEME and CONNE must either be both provided through data cards, or both through a disk file called MESH. The block GENER will be omitted if there are no sinks or sources in the problem. If block START is present, consisting of one data card with START punched in columns 1-5, the block INCON can be incomplete, with elements in arbitrary order, or it can be absent altogether. Elements for which no initial conditions are specified in INCON will then be assigned default initial conditions as given in block PARAM, and default porosities as given in block ROCKS. If START is not present, INCON must contain information for all elements, in exactly the same order as the elements are listed in block ELEME. However, element names which have not been defined in ELEME may appear in CONNE, GENER, and INCON. Such items will be ignored and a diagnostic will be printed.

The format for data blocks ELEME, CONNE, GENER, and INCON is the same when these data are provided as disk files as when they are provided as part of the input deck. A sequence of identical items can be specified on a single data card. Also, the indices needed for cross-referencing elements, interfaces, and sources

Table 8: DATA GROUPS FOR A SIMULATION PROBLEM

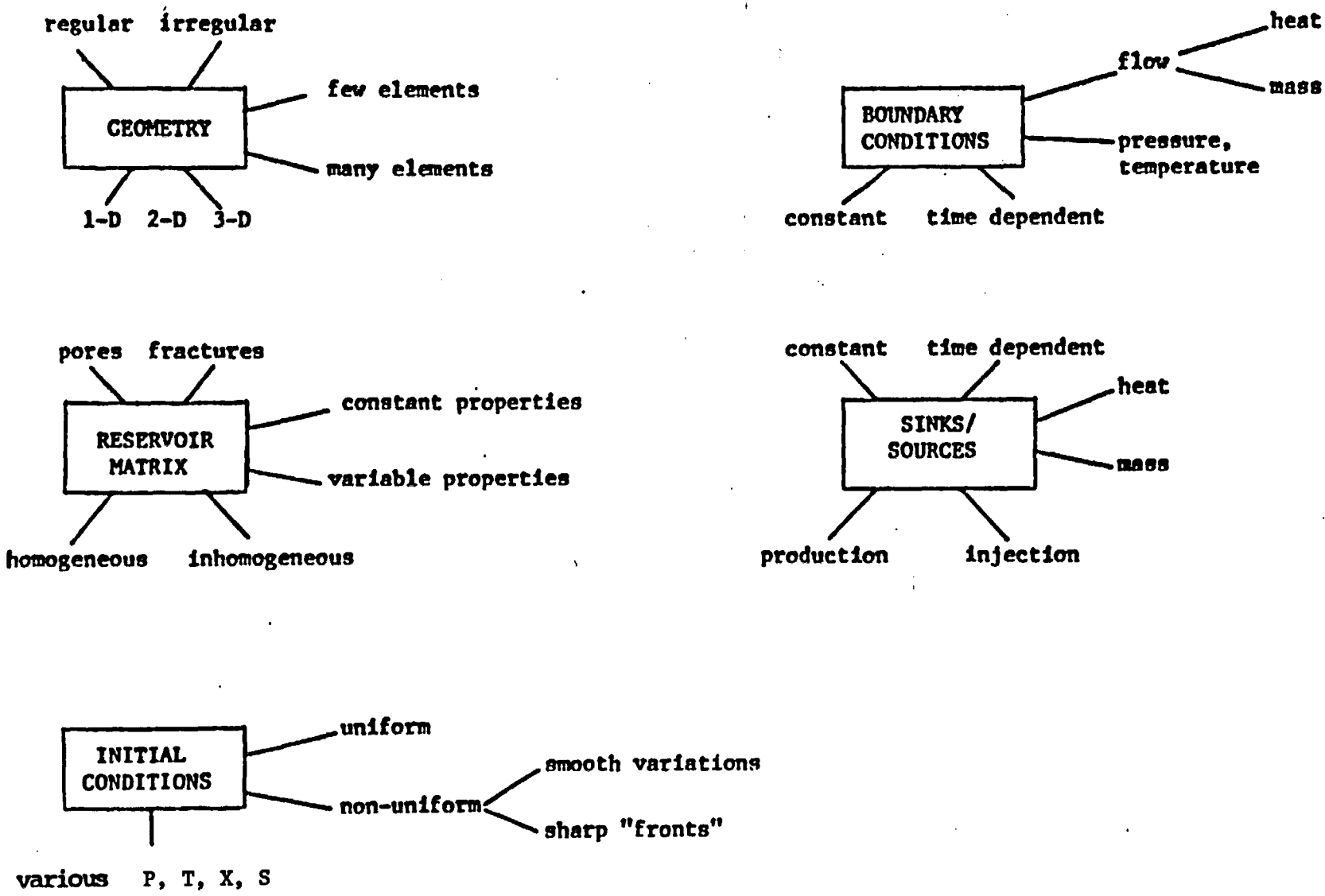

Table 9: INPUT DATA BLOCKS[1]

Block	Description
TITLE (first card)	One data card containing a header that will be printed on every page of output.
ROCKS	Material parameters for the various reservoir domains.
PARAM	Computational parameters (time stepping information, program options).
RPCAP	Parameters for relative permeability and capillary pressure functions.
TIMES (optional)	List of (physical) times at which printout is to be generated.
*ELEME	List of grid elements. } MESH - information
*CONNE	List of interfaces (connections). } MESH - information
*GENER (optional)	List of mass or heat sinks/sources.
*INCON (optional)	List of initial conditions and (optional) restart information.
START (optional)	One data card allowing a more flexible initialization.
ENDCY (last card)	One card closing the TOUGH input deck.

[1]Blocks labeled with a star * can be provided as disk files, in which case they would be omitted from the input deck.

will be generated by TOUGH rather than having them provided by the user. Usually these features are useful when a new simulation problem is initiated.

During initialization, TOUGH writes the following disk files from information provided through input data blocks:

- a file MESH, consisting of blocks ELEME and CONNE;
- a file GENER, consisting of the block GENER;
- a file INCON, consisting of the block INCON.

At the completion of a run, the results needed for a subsequent continuation of the problem are written onto a file SAVE. This file is compatible with INCON, and can be provided for a subsequent run either as a disk file, or as part of the data deck.

We expect the user to initiate a problem with ELEME, CONNE, GENER, and INCON as part of the input deck, using the START-option for flexibility and convenience. Typically, the user will want to run only a few time steps initially, examine the results and then restart the problem with time steps chosen to give an optimum compromise between accuracy and efficiency. The file SAVE of a completed run must be provided as file INCON for a continuation run. Apart from initial conditions, file SAVE also transmits information on times and time steps for a restart.

3.2 TOUGH = Input Formats

The input data to be provided for a TOUGH simulation is summarized in Figure 2. The blocks ROCKS, ELEME, CONNE, GENER, and INCON can have a variable number of cards, depending upon how many items the user wishes to specify. The end of these variable-length blocks is indicated with a blank card. (For CONNE, GENER, and INCON it is possible to have, instead of the blank card, a card with "+++" punched in columns 1-3, followed by some element and source cross-referencing information in the case of CONNE and GENER, and followed by restart-information in the case of INCON; see below.)

We shall now explain the cards and variables in detail. Clarifying examples will be given in Section 5.

All input and output of TOUGH is in standard metric units.

TITLE is the first card of the deck, containing a header of up to 80 characters, to be printed on every page of output. This can be used to identify a problem. If no header is desired, leave this card blank.

ROCKS introduces material parameters for up to 27 different reservoir domains.

Card ROCKS.1

Format (A5, I5, 7E10.4)
MAT, NAD, DM, POR, (PER (I), I = 1,3), CM, CH

MAT material name (rock type).

NAD if zero or negative, porosity will remain constant (i.e. compressibility = 0, expansivity = 0);
> 1: will read another data card with compressibility and expansivity;
> 2: will read two additional cards with parameters for relative permeability and capillary pressure functions.

DM rock density (kg/m^3).

POR default porosity (void fraction) for all elements belonging to domain "MAT" for which no other porosity has been specified in block INCON.

PER(I), I = 1,3 absolute permeabilities along the three principle axes, as specified by ISOT in block CONNE.

CM rock heat conductivity (W/m°C).

CH rock specific heat (J/kg°C). Domains with CH > 10^4 J/kg° will not be included in material balances. Flows entering or leaving domains with CH > 10^4 J/kg°C will always be 100% upstream weighted. This provision is useful for boundary nodes, which are given very large volumes so that their thermodynamic state remains constant.

Card ROCKS.1.1 (optional, NAD > 1 only)

Format (2E10.4)
COM, EXPAN

COM compressibility (m^2/N), $\frac{1}{\phi}\left(\frac{\partial\phi}{\partial P}\right)_T$

EXPAN expansivity (1/°C), $\frac{1}{\phi}\left(\frac{\partial\phi}{\partial T}\right)_P$

Card ROCKS.1.2 (optional, NAD > 2 only)

Format (I5, 5X7E10.4)
IRP, (RP(I), I = 1,7)

IRP integer parameter to choose type of relative permeability function.

RP(I), I = 1, ..., 7 parameters for relative permeability function.

Card ROCKS.1.3 (optional, NAD > 2 only)

Format (I5, 5X7E10.4)
ICP, (CP(I), I = 1,7)

ICP integer parameter to choose type of capillary pressure function.

CP (I), I = 1, ..., 7 parameters for capillary pressure function.

Repeat cards 1, 1.1, 1.2, and 1.3 for up to 27 reservoir domains.

Card ROCKS.2 A blank card closes the ROCKS data block.

START (optional)

A card with START punched in columns 1-5, allows a more flexible assignment of initial conditions.

PARAM introduces computation parameters.

Card PARAM.1

Format (2I2, 3I4, 19I1).
NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 19).

NOITE specifies the maximum number of iterations per time step (default value is 8)

KDATA specifies amount of printout (default = 1).

0 or 1: print a selection of the most important variables.

2: print fluxes.

3: print primary variables and their changes.

If the above values for KDATA are increased by 10, printout will occur after each iteration (not just after convergence).

MCYC maximum number of time steps to be calculated.

MSEC maximum duration, in machine seconds, of the simulation (default is infinite).

MCYPR printout will occur for every multiple of MCYPR steps (default is 1).

MOP(I), I = 1,19 allows choice of various options.

MOP(1) if unequal 0, short printout for non-convergent iterations will be suppressed.

MOP(2) through MOP(6) generate additional printout in various subroutines, if set ≠ 0. The amount of printout increases with MOP(I).

MOP(2) CYCIT (main subroutine).

MOP(3) MULTI (flow- and accumulation-terms).

MOP(4) QU (sinks/sources).

MOP(5) EOS (equation of state).

MOP(6) LINEQ (linear equations).

MOP(7) if unequal 0, a printout of input data will be provided.

Calculational choices are as follows:

MOP(9) determines the composition of produced fluid. The relative amounts of phases are determined:

0: according to relative mobilities in the source element.

1: source fluid has the same phase composition as the producing element.

MOP(11) determines evaluation of mobilities at interfaces.

0: mobilities are upstream weighted with WUP (default is WUP = 1).

1: mobilities are spatially interpolated between adjacent elements.

MOP(12) determines interpolation procedure for time-dependent generation data.

0: step function option.

1: triple linear interpolation.

MOP(13) if unequal zero, perform new matrix decomposition only when the number of pivot failures is a multiple of MOP(13). This option is available only with MOP(14) = 2.

MOP(14) determines handling of pivot failures in matrix decomposition.

0: perform new decomposition.

1: reduce time step, stay with old decomposition.

2: ignore pivot failure and proceed (MOP(13)) = 0, or number of pivot failures not a multiple of (MOP(13)).

MOP(16) provides automatic time step control. Time step size will be doubled, if convergence occurs within ITER < MOP(16) iterations.

Card PARAM.2

Format (4E10.4, A5, 5X3E10.4)
TSTART, TIMAX, DELTEN, SCALE, ELST, GF, REDLT, DIFF.

TSTART starting time of simulation in seconds.

TIMAX time in seconds at which simulation should stop (default is infinite).

DELTEN length of time steps in seconds. If DELTEN is a negative integer, DELTEN = -NDLT, the program will proceed to read NDLT cards with time step information.

SCALE scale factor to change the size of the mesh (default = 1.0).

ELST set equal to the name of one element to obtain a short printout after each time step.

GF magnitude (m/sec^2) of the gravitational acceleration vector. Blank or zero gives "no gravity" calculation.

REDLT factor by which time step is reduced in case of failure (default is 5.).

DIFF strength parameter for diffusive vapor flux (for free gas, DIFF = 2.12×10^{-5} m^2/s).

Card PARAM.2.1, 2.2, etc.

Format (8E10.4)
(DLT(I), I = 1, 100)

DLT(I) length (in seconds) of time step I.

This set of cards is optional for DELTEN = -NDLT, a negative integer: Up to 13 cards can be read, each containing 8 time step sizes. If the number of simulated time steps exceeds the number of DLT(I), the simulation will continue with time steps equal to the last non-zero DLT(I) encountered.

Card PARAM.3

Format (8E10.4)
RE1, RE2, FOR, WUP, WNR, DFAC, SING, U

RE1 convergence criterion for relative error (default = 1.E-5).

RE2 convergence criterion for absolute error (default = 1.E-2).

FOR weighting factor for time differencing (it is strongly recommended to use only default value = 1., i.e., fully implicit). Generally, 0. < FOR < 1.

WUP upstream weighting factor for mobilities and enthalpies at interfaces (default = 1.0). 0 < WUP < 1.

WNR weighting factor for increments in Newton/Raphson - iteration (default = 1.0). 0 < WNR < 1.

DFAC increment factor for computing derivatives (default = 1.E-8).

SING correction for matrix elements which are numerically zero (default = 0.).

U pivoting parameter (default = 0.1). 0 < U < 1; increased value for U will make criterion for pivot selection more stringent, resulting in better numerical stability at the expense of more storage for matrix decomposition. — MA28

Card PARAM.4

Format (3E20.14)
DEP(I), I = 1,3

This card holds a set of primary variables which are used as default initial conditions for all elements for which no other value is specified in block "INCON" (with option "START" only).

DEP(1) pressure (Pa)

DEP(2) > 1.5: temperature (°C) (single-phase points).
< 1.5: gas saturation (two-phase points).

DEP(3) > 1.5: temperature (°C) (two-phase points).
< 1.5: air mass fraction (single phase points).

RPCAP introduces information on relative permeability and capillary pressure functions, which will be applied for all flow domains for which no data were specified in cards ROCKS.1.2 and ROCKS.1.3.

Card RPCAP.1

```
Format (I5,5X7E10.4)
IRP, (RP(I),I = 1,7)
```

IRP integer parameter to choose type of relative permeability function.

RP(I), I = 1, ..., 7 parameters for relative permeability function.

Card RPCAP.2

```
Format (I5,5X7E10.4)
ICP, (CP(I), I = 1,7)
```

ICP integer parameter to choose type of capillary pressure function.

CP(I), I = 1, ..., 7 parameters for capillary pressure function.

TIMES permits the user to obtain printout at specified times (optional). This printout will occur in addition to printout specified in card PARAM.1.

Card TIMES.1

Format (2I5,2E10.4)
ITI, ITE, DELAF, TINTER

ITI number of times provided (ITI < 100).

ITE total number of times desired (ITE < 100).

DELAF maximum time step size after any of the prescribed times have been reached. default = ∞

TINTER time increment for times with index ITI, ITI+1, ..., ITE.

Card TIMES.2, TIMES.3, etc.

Format (8E10.4)
(TIS(I), I = 1, ITI)

TIS(I) list of times (in ascending order) at which printout is desired.

ELEME introduces element information.

Card ELEME.1

Format (A3, I2, 2I5, A3, A2, E10.4)
EL, NE, NSEQ, NADD, MA1, MA2, VOLX

EL, NE 5-character code name of an element. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ number of additional elements having the same volume and belonging to the same reservoir domain.

NADD increment between the code numbers of two successive elements. (Note: the maximum permissible code number NE + NSEQ * NADD is < 99.).

MA1, MA2 a five character material identifier corresponding to one of the reservoir domains as specified in block ROCKS. If the first three characters are blanks, the last two characters must be numbers in which case they would indicate the sequence number of the domain as entered in ROCKS.

VOLX element volume (m^3).

Repeat card ELEME.1 for the number of elements desired.

Card ELEME.2 A blank card closes the ELEME data block.

CONNE introduces information for the connections (interfaces) between elements.

Card CONNE.1

Format (A3, I2, A3, I2, 4I5, 4E10.4)
EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX

EL1, NE1 code name of the first element.

EL2, NE2 code name of the second element.

NSEQ number of additional connections in the sequence.

NAD1 increment of the code number of the first element between two successive connections.

NAD2 increment of the code number of the second element between two successive connections.

ISOT set equal to 1, 2, or 3; specifies absolute permeability to be PER(ISOT) for the materials in elements (EL1, NE1) and (EL2, NE2), where PER is read in block ROCKS. This allows assignment of different permeabilities, e.g., in the horizontal and vertical direction.

D1
D2 distance (m) from center of first and second element, respectively, to their common interface.

AREAX interface area (m^2).

BETAX cosine of the angle between the gravitational acceleration vector and the line between the two elements. GF x BETAX > 0 (<0) corresponds to first element being above (below) the second element.

Repeat card CONNE.1 for the number of connections desired.

Card CONNE.2 A blank card closes the CONNE data block. (For an alternative, see note at the end of Chapter 3).

GENER introduces sinks and/or sources.

Card GENER.1

Format (A3, I2, A3, I2, 4I5, 5X,A4, A1,3E10.4)
EL, NE, SL, NS, NSEQ, NADD, NADS, LTAB, TYPE, ITAB, GX, EX, HG

EL, NE code name of the element containing the sink/source.

SL, NS code name of the sink/source. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ number of additional sinks/sources with the same injection/production rate.

NADD increment between the code numbers of two successive elements with identical sink/source.

NADS increment between the code numbers of two successive sinks/sources.

LTAB number of points in table of generation rate versus time. Set 0 or 1 for constant generation rate. For wells on deliverability, LTAB denotes the number of open layers, to be specified only for the bottommost layer.

TYPE HEAT - heat sink/source.
COM1 - component 1 (water). } injection only
COM2 - component 2 (air)
MASS - mass production rate specified.
VOL - volumetric production rate specified.
DELV - well on deliverability, i.e. production occurs against specified wellbore pressure. If well is completed in more than one layer, bottommost layer must be specified first, with number of layers given in LTAB. Subsequent layers must be given sequentially for a total number of LTAB layers.

− = prod.
+ = inj.

ITAB if set unequal to blank, table of specific enthalpies will be read (LTAB > 1 only).

GX constant generation rate; positive for injection, negative for production; GX is mass (kg/sec) for a MASS sink/source, volume (m^3/sec) for a volumetric sink/source, and energy (J/kg) for a HEAT sink/source. For wells on deliverability, GX is productivity index PI (m^3).

EX fixed specific enthalpy (J/kg) of the fluid for mass injection (GX>0). For wells on deliverability, EX is bottomhole pressure PWB (Pa), for the topmost producing layer in which the well is open.

HG thickness of layer (m); wells on deliverability only; or, density (kg/m^3) of injected fluid (GX positive).

Card GENER.1.1 (optional, LTAB>1 only)

Format (4E14.7)
F1(L), L=1, LTAB

F1 generation times.

Card GENER.1.2 (optional, LTAB>1 only)

Format (4E14.7)
F2(L), L=1, LTAB

F2 generation rates. WATTS

Card GENER. 1.3 (optional, LTAB>1 and ITAB ≠ 1Hb only)

Format (4E14.7)
F3(L), L=1, LTAB

F3 specific enthalpy of produced or injected fluid.

Repeat cards GENER.1, 1.1, 1.2, and 1.3 for up to 20 sinks/sources.

Card GENER.2 A blank card closes the GENER data block. (For an alternative, see note at the end of Chapter 3.)

INCON introduces initial conditions.

Card INCON.1

Format (A3, I2, 2I5, E15.9)
EL, NE, NSEQ, NADD, PORX

EL, NE code name of element.

NSEQ number of additional elements with same initial conditions.

NADD increment between the code numbers of two successive elements with identical initial conditions.

PORX porosity (void fraction); if zero or blank, porosity will be taken as specified in block ROCKS if option START is used.

Card INCON.2

Format (3E20.14)
X1, X2, X3

Set of primary variables for the element specified in card INCON.1.

X1 pressure (Pa)

X2 > 1.5: temperature (°C) (single-phase points).
< 1.5: gas saturation (two-phase points).

X3 > 1.5: temperature (°C) (two-phase points).
< 1.5: air mass fraction (single phase points).

Card INCON.3 A blank card closes the INCON data block. (For an alternative, see note below).

ENDCY closes the TOUGH data deck and initiates the simulation.

Note on closure of blocks CONNE, GENER, and INCON

The "ordinary" way to indicate the end of any of the above data blocks is by means of a blank card. There is an alternative available if the user makes up an input deck from the files MESH, GENER, or SAVE, which have been generated by a previous TOUGH run. These files are written exactly according to the specifications of data blocks ELEME and CONNE (file MESH), GENER (file GENER), and INCON (file SAVE), except that the blocks CONNE, GENER, and INCON terminate with a card with "+++" in columns 1-3 followed by some cross-referencing and restart information. TOUGH will accept this type of input, and in this case there is no blank card at the end of the indicated data blocks.