TOUGHREACT V3.32 QUICK REFERENCE GUIDE

FLOW.INP

REACT Reactive transport flags (**MOPR - M**ethods **O**r **P**arameters **R**eactive Transport): Format 20**I1**
12345678901234567890

MOPR(1) = 0 Reactive transport (flow, transport, reaction).
= 1 Flow, no reactive transport, chemical input files read.
= 2 Flow, no reactive transport, no chemical input files read. Equivalent to running TOUGH2.
= 3 Flow and transport without chemical reactions.
= 4 Transport and chemical reactions using velocity field from first time step.
= 5 Transport (no chemical reactions) using velocity field from first time step.

MOPR(2) > 0 Writes transport coefficient matrix, Darcy velocities, porosities, and other data in *runlog.out*. *Very large output!*

MOPR(3) > 0 Writes source terms, aqueous concentrations, permeability, porosity, and capillary pressure correction factor, and other parameters in *runlog.out*. *Very large output!*

MOPR(4) ≥ 2 Force at least one flow iteration (MOPR(4) =2 is normally suggested).
= 1 Do not force at least one fluid flow iteration. Must be set to 1 for chemical quasi-stationary-state (QSS) option.

MOPR(5) = 1 Reduced output in file *flow.out* (no printout at every time step).
= 2 In addition to (1), porosities and permeabilities are not written to the SAVE file.

MOPR(6) > 0 Leverett scaling of capillary pressure owing to permeability/porosity differences.
= 1 Capillaries assumed to be tubes having a circular cross-section.
= 2 Capillaries assumed to be channels (e.g., planar fractures).
= 3 Leverett scaling assuming porosity-weighted capillary (Φ=0.0) and channel flow (Φ=1.0).

MOPR(7) ≥ 0 Specification of output precision in tecplot-format output files (up to 8 decimal digits). Zero or blank gives the default of 4 digits.

MOPR(8) ≥ 1 Outputs mineral saturation indices, for each grid block, in file *min_SI.dat*.
≥ 2 Outputs mineral reaction rates (mol/kg H_2O/s) in file *rctn_rate.out*.
≥ 3 Outputs reactive surface areas (m^2/kg H_2O) and related parameters in file *rct_sfarea.out*.
≥ 4 Outputs mass balance information in file *mbalance.out*.
≥ 5 Outputs mineral and rock thermal conductivities and heat capacities (Cp) and calculated rock Cp coefficients in file *thermalparam.out*.
= 6 Outputs system and mineral heats of reaction in file *heatreaction.out*.

MOPR(9) = 1 Temperature-dependent mineral and rock heat capacities calculated from coefficients in thermodynamic database.
= 2 Temperature-dependent mineral and rock thermal conductivities calculated from coefficients in thermodynamic database.
= 3 Temperature-dependent mineral and rock heat capacities *and* thermal conductivities calculated from coefficients in thermodynamic database.

MOPR(10) ≥ 1 Time step length not reduced as a result of increased chemical iterations.

MOPR(11) = 1 Enables sedimentation/compaction by forward explicit advection of solids and aqueous species. Sedimentation velocities must be added as extra zone columns in file *solute.inp.*

MOPR(12) = 1 Includes heats of reaction calculated from log(K) values in thermodynamic database and writes heats of reaction and source terms in file *heatreaction.out*.

MOPR(13) = 1 Temperature-dependent mineral and rock densities based on thermal expansion coefficients from thermodynamic database (input working, calculations not implemented yet).

MOPR(14) ≥ 0 Exponent for output of *SAVE* and *savechem* files. Files are written out according to NTSAVE*(10**MOPR(14)), where NTSAVE is dimensioned in file *flowpar.inc* (default = 100).

MOPR(15) = 1 Permeability multiplier (see TOUGH2 V2.1 manual).

MOPR(15) = 2 Permeability calculated from porosity (see TOUGH2 V2.1 manual).

MOPR(16) = 1 Reads heterogeneous mineral volume fractions from input file *min_volf.inp*.

MOPR(17) Not used. Can be left blank or set to zero

MOPR(18) = 1 Reads Arrhenius parameters from thermodynamic database for species and temperature-dependent aqueous diffusion coefficient calculations (total transported concentrations).

MOPR(19)- MOPR(20) Not used. Can be left blank or set to zero.

PARAM Fluid and heat flow flags, time stepping, convergence, and other calculation options.

PARAM.1

Format (2I2, 3I4, 24I1, 10X, 2E10.4) NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), TEXP, BE

NOITE Maximum number of Newtonian iterations per time step (default is 8).

KDATA = 0,1 Prints a selection of the most important variables.

KDATA = 2 Prints mass and heat fluxes and flow velocities.

KDATA = 3 Prints primary variables and their changes. If KDATA is increased by 10, printout will occur after each Newton-Raphson iteration (not just after convergence).

KDATA = 4 Writes flow output to VisIT-compatible Tecplot-format file "flowdata.tec" instead of flow.out. Mass and heat fluxes, velocities and vector components are in file "flowvector.tec" .

MCYC Maximum number of time steps (9999 runs until maximum time MSEC is reached).

MSEC Maximum duration, in CPU seconds, of the simulation (default is infinite).

MCYPR Printout at every multiple of MCYPR steps (9999 only writes times listed in TIMES block).

MOP(1) > 0 Short printout for non-convergent iterations will be generated.

MOP(2) > 0 Printout of CYCIT messages.

MOP(3) > 0 Printout of MULTI (flow and accumulation terms).

MOP(4) > 0 Printout of QU (sinks/sources).

MOP(5) > 0 Printout of EOS (equation of state) messages.

MOP(6) > 0 Printout of LINEQ (linear equations).

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

MOP(8) Interface area reduction for relative permeability (fixed) or via active fracture model.

MOP(8) = 1 Fixed interface area reduction factor to relative permeability from RP(6).

MOP(8) = 2 Active Fracture Model interface area reduction factor to relative permeability times RP(7).

MOP(9) Determines the composition of produced fluid with the MASS option (see GENER).

= 0 According to relative mobilities in the source element.

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

MOP(10) Interpolation formula for heat conductivity as a function of liquid saturation (Sl).

= 0 C(Sl) = CDRY + SQRT(Sl)* [CWET - CDRY]

= 1 C(Sl) = CDRY + Sl * (CWET - CDRY)

MOP(11) Evaluation of mobility and permeability at interfaces.

= 0 Mobilities upstream weighted with WUP (PARAM.3), permeability is upstream weighted.

= 1 Mobilities averaged between adjacent elements, permeability is upstream weighted.

= 2 Mobilities upstream weighted, permeability is harmonic weighted.

= 3 Mobilities averaged between adjacent elements, permeability is harmonic weighted.

= 4 Mobility and permeability are both harmonic weighted.

MOP(12) Interpolation procedure for time dependent sink/source data (flow rates and enthalpies).

= 0 Triple linear interpolation; tabular data are used to obtain interpolated rates and enthalpies for the beginning and end of the time step; the average of these values is then used.

= 1 Step function; rates and enthalpies are taken as averages of the table values corresponding to the beginning and end of the time step.

= 2 Rigorous step rate capability for time dependent generation data. Times and generation rates are interpreted to mean that sink/source rates and enthalpies are piecewise constant.

MOP(13) Not used.

MOP(14) = 0 Fixed rock thermal conductivities and heat capacities from ROCKS as in TOUGH2 V2.1.

= 1 Temperature-dependent grain heat capacities (ROCKS, line 4; 4 coefficients (E14.6))

= 2 Temperature-dependent rock thermal conductivity (ROCKS, line 3; 3 coefficients (E10.4)).

= 3 Temperature-dependent rock thermal conductivity *and* heat capacity as described above.

MOP(15) Determines conductive heat exchange with impermeable confining layers (see section 7.4).

= 0 Heat exchange is off.

= 1 Heat exchange is on for grid blocks that have a non-zero heat transfer area in block ELEME.

MOP(16) ≥ 2 Automatic time step control. Time step size doubled if convergence occurs within MOP(16) Newton-Raphson iterations. MOP(16) should typically be set in the range of 2 – 6, unless the wellbore simulator option (MOP(17) is invoked and then it usually must be set from 8 - 9.

MOP(17) ≥ 1 Invokes single-phase wellbore simulator for turbulence and friction effects on pressure. Initial wellbore permeability is assumed to be in permeability direction '3', and is used to

calculate the wellbore diameter assuming Poiseulle flow. Only grid block connections designated as 'ISO=5' in CONNE will be subject to wellbore flow calculations.

= 1 Wellbore permeability calculated from average value of current turbulence/friction calculation and the value from previous iteration (more stable).

= 2 Wellbore permeability from geometric mean of current and previous iteration (less stable).

MOP(18) = 0 Perform upstream weighting for interface density.

> 0 Average interface density between the two grid blocks, unless one of the two phase saturations is zero, upstream weighting will be performed.

MOP(19) Switch used by EOS modules for conversion of primary variables (section 6).

MOP(20) Switch for vapor pressure lowering in EOS4; see Table 10.

MOP(21) Selects the linear equation solver (see section 7.6).

= 0,1 Defaults to DSLUCS.

= 2 DSLUBC, bi-conjugate gradient solver.

= 3 DSLUCS (default).

= 4 DSLUGM, generalized minimum residual preconditioned conjugate gradient solver.

= 5 DLUSTB, stabilized bi-conjugate gradient solver.

= 6 LUBAND, banded direct solver.

MOP(22) Not used.

MOP(23) Not used.

MOP(24) Determines handling of multiphase diffusive fluxes at interfaces.

= 0 Harmonic weighting of fully coupled effective multiphase diffusivity.

= 1 Separate harmonic weighting of gas and liquid phase diffusivities.

TEXP: Parameter for temperature dependence of gas phase diffusion coefficient (see Eq. D.8).

BE: Parameter for effective strength of enhanced vapor diffusion; if set to a non-zero value, will replace the parameter group for vapor diffusion (see Eq. D.3 and section D.4).

PARAM.2

Format (4E10.4, A5, 5X, 3E10.4) TSTART, TIMAX, DELTEN, DELTMX, ELST, GF, REDLT, SCALE

TSTART: Starting time of simulation in seconds (default is 0).

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 records with time step information. Note that -NDLT must be provided as a floating point number, with decimal point.

DELTMX: Upper limit for time step size in seconds (default is infinite).

ELST: Set equal to the name of one element to obtain a short printout after each time step. If set to "wdata" the file "GASOBS.DAT" will be created with printout at each time step of gas and liquid phase saturations, relative humidity, and gas pressure for elements listed below PARAM.2.

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

REDLT: Factor to reduce time step in case of convergence failure or other problems (default is 4).

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