

Volume I:
User's Guide

for

UTCHEM-9.0

A Three-Dimensional
Chemical Flood Simulator

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1.0 INTRODUCTION



UTCHEM is a three-dimensional chemical flooding simulator. The solution scheme is **analogous** to IMPES, where pressure is solved for implicitly, but concentrations rather than saturations are then solved for explicitly. Phase saturations and concentrations are then solved in a flash routine. An energy balance equation is solved explicitly for reservoir temperature. The energy balance equation includes heat flow between the reservoir and the over- and under-burden rocks.

The major physical phenomena modeled in the simulator are:

- dispersion
- diffusion
- dilution effects
- adsorption for oil, surfactant and polymer
- interfacial tension
- relative permeability
- capillary pressure
- **hysteresis** in relative permeability and capillary pressure
- capillary trapping
- cation exchange
- phase density
- compositional phase viscosity
- phase behavior (pseudoquaternary)
- aqueous reactions
- **partitioning of chemical species between oil and water**
- dissolution/precipitation
- cation exchange reactions involving more than two cations
- in-situ generation of surfactant from acidic crude oil
- pH dependent surfactant adsorption
- organic biodegradation capability
- multiple organic species
- equilibrium and nonequilibrium organic dissolution in aqueous phase
- dual porosity option for simple phase tracer flow
- polymer properties: shear thinning viscosity, inaccessible pore volume, permeability reduction, adsorption
- gel properties: viscosity, permeability reduction, adsorption
- tracer properties: partitioning, adsorption, radioactive decay, reaction (ester hydrolyzation), dead-end pore (capacitance)
- temperature dependent properties: viscosity, tracer reaction, gel reactions, Surfactant phase behavior
- gas mobility reduction due to foam
- mixed-wet oil/water capillary pressure and relative permeability

See Section 2 of the UTCHEM Technical Documentation for the general formulation of the simulator.

User notes:

2.0 OPERATION OF THE SIMULATOR

The UTCHEM simulator is run on a CRAY SV1 at the Texas Advanced Computing Center affiliated with The University of Texas at Austin (UNICOS operating system), a DEC Alpha system (DEC/Compaq XP1000) at the Center for Petroleum and Geosystems Engineering (OSF/1 operating system), and several WINDOWS-based PC workstations (Windows operating system, running at 450 MHz with 256MB RAM; depending on the size of the problem, the code will also run on slower PCs with less RAM).

2.1 Input and Output Files

UTCHEM requires two input files (HEAD and INPUT) for non-restart runs. For restart runs, a binary restart file (INPUT2) is required in addition to the original input data files used for the previous run. The HEAD input file gives UTCHEM information regarding the name and size of the problem to be run; it is described in Section 2.2. A detailed description of the data in the second input file is given in Section 3.0 and the data in the restart data file is documented in Appendix A.3. A number of UTCHEM input example files demonstrating a variety of petroleum oil-field and groundwater applications are available to UTCHEM users. The oil-field applications include water, single-well tracer, interwell tracer, polymer, profile control using gel, surfactant/polymer, and high pH alkaline/surfactant/polymer flooding. The groundwater applications include contaminant infiltration, water flushing, partitioning interwell tracer, surfactant enhanced aquifer remediation, and bioremediation.

We provide all users with two sample input files for testing purposes (see the distribution package for copies of the files). The first sample input file (EX01) is for a 3D surfactant/polymer flood. In that file, the surfactant properties are for petroleum sulfonate and the polymer properties are based on the typical data for xanthan gum. CPU usage for the EX01 example run is about 55 seconds on the DEC/Compaq XP1000 and about 286 seconds on the 450MHz Windows PC. The second sample input file (EX21) is for a 2-D contamination event in the saturated zone of an aquifer. CPU usage for the EX21 example run is about 14 seconds on the DEC/Compaq XP1000 and about 90 seconds on the 450MHz Windows PC. If

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you would like to receive additional sample input files, please contact Joanna L. Castillo (joanna@mail.utexas.edu or 512-471-3229) for details.

The input files are summarized in the following table.

Input File Name	Contents
HEAD	Run number and array dimensioning information
INPUT	Input data; described in detail in Section 3.0
INPUT2	Restart run data (binary input file RESTAR created by an earlier run)

The number of output files generated by UTCHEM varies depending upon several control flags set by the user in the input file. See Section 3.0 for more information on how to set those flags. **Output file names are created by appending a suffix to the run number specified in the HEAD input file.** For example, if the run number is TEST01, the echo print output file generated by UTCHEM would be TEST01.ECHO. All output files are **ASCII files** which can be edited with a standard text editor unless otherwise specified. The output files are summarized in the following table.

Output file extension	Contents
ALKP	Alkaline option related profile plotting data, created if IREACT>1 and IPALK=1
BIOD	Biodegradation option plotting data, created if IPBIO=1 and IBIO=1
CAPP	Capacitance property profile plotting data, created if IPCAP=1 and ICAP=1
COMP_AQ	Aqueous phase composition plotting data, created if ICKL=1
COMP_ME	Microemulsion phase composition plotting data, created if surfactant is present and ICKL=1
COMP_OIL	Oleic phase composition plotting data, created if ICKL=1
CONCP	Component concentration profile plotting data, created if IPCTOT=1
SALT	Effective salinity plotting data, created if surfactant is present and ICSE=1
DISS	Mass transfer option plotting data, created if INONEQ=1 and IMASS=2 and ICOR>0
ECHO	Echo print of the input file information
FOAM	Foam option plotting data, created if IGAS=2 and IFOAMP=2
FRAC	Dual porosity plotting data, created if IPCAP=1 and ICAP=2
GFILEP	Gel property profile plotting data, created if IREACT=1 or 4 and IPGEL=1

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HIST01	Well history plotting data for well #1; described in Appendix A
HIST02	Well history plotting data for well #2
...	...
HIST _{xx}	Well history plotting data for last well
HYST	Hysteresis option plotting data, created if (IHYST=1 or IPERM=3) and IHYSTP=1
MESH	Number of gridblocks and distances to center of gridblocks in each direction
OVERAL	History of overall properties; described in Appendix A
PERM	Permeability and porosity data
PRESP	Phase pressure profile plotting data, created if IPPRES=1
PROF	Formatted profile data; described in Appendix A
RESTAR	Stored restart run data; described in Appendix A (binary file)
RPERM	Phase relative permeability plotting data, creating if IPER=1
SATP	Phase saturation profile plotting data, created if IPSAT=1
TEMP	Temperature profile, created if IENG=1 and IPTTEMP=1
TRAC01	Aqueous (or gas) phase tracer concentration for the 1st tracer at observation points, created if IPOBS>0; described in Appendix A
TRAC02	Aqueous (or gas) phase tracer concentration for 2nd tracer at observation points
...	...
TRAC _{xx}	Aqueous (or gas) phase tracer concentration for the last tracer at observation points
TRAP	Interfacial tension and phase trapping plotting data, created if ICNM=1 and ITRAP>0
TTABLE	Table of time steps and Courant numbers
VISC	Phase viscosity plotting data, created if IVIS=1
WARN	Warning messages

2.2 Description of HEAD file

The variables listed in the table below give UTCHEM information regarding the name and size of the problem to be run. All values should be equal to those specified in the main input file (INPUT). The values can be larger than those specified in the main input file but it is recommended they not be in order to maintain as small an executable file as possible. Note that **the values must not be smaller than those in the main input file or the program will not execute properly.**

Example HEAD file:

```

utex21
NX  NY  NZ  N  NWELL
49  1   24  8   3
NTW  NTA
0    0
NO   NPHASE
0    4
NSUB MSUB
0    0

```

The first line of the HEAD file contains the run number which is a 6-character string used as a **prefix** for output file names generated by UTCHEM (as described in Section 2.1). We strongly recommend this be **the same as RUNNO in the main input file** so as to avoid confusion. The following table contains definitions of the variables used in the HEAD file.

Variable	Definition
NX	Number of gridblocks in X-direction
NY	Number of gridblocks in Y-direction
NZ	Number of gridblocks in Z-direction
N	Number of components (cannot be less than 8)
NWELL	Number of wells
NTW	Number of water tracers
NTA	Number of air tracers
NO	Number of organic components
NPHASE	Number of phases (<u>set to 3 when there is no gas phase or 4 if gas is present</u>)
NSUB	Number of subgrids in lateral direction (check for ICAP=2)
MSUB	Number of subgrids in vertical direction (check for ICAP=2)

2.3 Compilation and Execution on Workstations



The UTCHEM distribution package for workstations contains the FORTRAN-90 source files (all ending with a ".f" file extension), two files used for compiling the code (Commodule and Makev9), input files for the ex01 sample run (ex01.data and ex01.head), and input files for the ex21 sample run (ex21.data and ex21.head). Make sure you place all files in the same directory on your workstation. Then, follow these steps in order to compile and execute the code:

1. Issue the command:

```
Commodule
```

This will compile the modules before building the executable file.

2. To build an executable file called utchem9.exe, issue the command:

```
make -f Makev9 FC=f90
```

Note that the example makefile assumes the use of the ~~f90 FORTRAN compiler~~.

3. Run UTCHEM in the background using a command file (in the example below, the file is called work.job). Note that the work.job file needs to be executable. Use any text editor to create your job file and then issue the command:

```
chmod +x work.job
```

at the UNIX prompt to make sure the work.job file is executable. Then, submit the job file by issuing the following command:

```
work.job &
```

at the UNIX prompt.

Example work.job file:

```
rm -r ex01.dir
mkdir ex01.dir
cd EX01.dir
ln -s ../ex01.head HEAD
ln -s ../ex01.data INPUT
time ../utchem9.exe
gzip *
```

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The `work.job` file needs to be modified to reflect the directory structure you create for running UTCHEM jobs. See the table on the following page for a description of the contents of the `work.job` file.

Command line	Description
<code>rm -r ex01.dir</code>	Removes the <code>ex01.dir</code> directory if it already exists. Make sure you've copied files from previous runs (if you want to save them) to another location before executing the <code>work.job</code> file because all files in the <code>ex01.dir</code> directory will be deleted when the directory is deleted.
<code>mkdir ex01.dir</code>	Create a subdirectory in which to place the new simulation results.
<code>cd ex01.dir</code>	Make <code>ex01.dir</code> the current working directory.
<code>ln -s ../ex01.head HEAD</code> <code>ln -s ../ex01.data INPUT</code>	Create symbolic links to the <code>ex01.head</code> and <code>ex01.data</code> input files (which are located up one level in the directory structure). When the program looks for the files <code>HEAD</code> and <code>INPUT</code> , it will automatically be pointed to the <code>ex01.head</code> and <code>ex01.data</code> files, respectively.
<code>time ../utchem9.exe</code>	Run the program (which is located up one level in the directory structure).
<code>gzip *</code>	Add this line to the <code>work.job</code> file to compress all files in order to save space (if necessary).

2.4 **Compilation and Execution on a WINDOWS-based PC**

The UTCHEM distribution package for PCs contains the FORTRAN-90 source files (all ending with a ".f" file extension), input files for the ex01 sample run (ex01.data and ex01.head), and input files for the ex21 sample run (ex21.data and ex21.head). At The University of Texas at Austin, we compile UTCHEM on PCs using the Digital FOFTRAN compiler. UTCHEM will probably compile successfully using other compilers with little or no modification if those compilers have been updated within the last year and contain FORTRAN-90 features. Copy the source files (all files ending with the ".f" file extension in the distribution package) to a directory on your hard disk and then follow the steps below to compile UTCHEM using the Digital FORTRAN compiler:


1. Launch Visual Studio.
2. Select "New" from the File menu. In the dialog box that appears, click on the "Projects" tab and select Win32 Console Application, provide a project name ("utchem9" for this example), and select the location on your hard disk in which you'd like the executable code to be placed. Click on OK.
3. Select "Add to Project..." and then "File..." from the Project menu. Navigate to the location of the source files. Select "All files (*.*)" so all the files can be seen. Control-click on the three module source files (module1.f, module11.f, and module12.f). Click on OK.
4. Select "Build utchem9.exe" from the Build menu. This will generate a couple of error messages regarding the Library module file and error executing df.exe. Disregard these message.
5. Select "Add to Project..." and then "File..." from the Project menu. Navigate to the location of the source files. Select "All files (*.*)" so all the files can be seen. Select all the source files. Click on OK.
6. Select "Build utchem9.exe" from the Build menu. You will get a warning that the module files have already been compiled. Click on OK.
7. Wait patiently while the code compiles. Upon completion, exit Visual Studio. An executable version of the code called utchem9.exe will be placed in the Debug folder within the utchem9 project folder.


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8. Copy the input and head files to the directory containing `utchem9.exe` and name them `INPUT` and `HEAD`. Make sure the files have no file extensions (like `".txt"` or `".dat"`).
9. Double click on `utchem9.exe`. A screen will appear and will remain visible until execution of the job has completed. Periodically, the simulation time, the number of time steps, time step in days, and Courant number will be written to the screen. Your output files will appear in the same directory from which you launched `utchem9.exe`.

UTCHEM
INPUT DATA DESCRIPTION

3.0 INPUT DATA DESCRIPTION

 The main UTCHEM input file (called INPUT) consists of comment lines and data lines. All comment lines are ignored by the UTCHEM simulator. It is important to note, however, that the number of comment lines between data lines is fixed. The first twenty-two lines of the input file are reserved for comment lines used to briefly describe the input file. Each data line is preceded by three comment lines (except for the input described in Section 3.5). The input file is basically divided into seven sections and each of those input sections (except Section 3.5) is preceded by an additional seven comment lines. The user should update the comment lines as the input file is modified in order to make using the simulator easier.

 All non-character data is free-formatted. This means that for each read statement, it is only necessary to leave a blank space between data elements. Note that the first data element for a given read statement must be on a new line in the input file. Subsequent data elements for that read statement can span as many lines as necessary. Implicit type matching is used; that is, all ~~REAL variables begin with the letters A-H or O-Z and all integer variables begin with the letters I-N.~~

 The following is a list of variables as they are read by UTCHEM. The variable names appear in all-caps on a single line in the order they are read by the program (variables that are new to the latest version of UTCHEM are printed in ***italicized boldface*** as well). Every list of variables is followed by a description of each variable and corresponding units or possible values if applicable. All of the variables listed in the input description will be read by the program unless otherwise noted; therefore, a dummy value will be read by the program for variables not pertinent to the problem being run.

User notes:

3.1. Title and Reservoir Description Data

The first input section consists of the title and reservoir description data.

Please remember that there are 22 comment lines at the beginning of this section and that each data line is preceded by three comment lines.

3.1.1 RUNNO

RUNNO - Run number.

Note: The run number can consist of any combination of six non-blank alphanumeric characters. This information will be printed as the first line of every output file and used as a prefix for file names of output files. We strongly recommend that this be identical to the first line of the HEAD file so as to avoid confusion. If you are using the UTCHEM-GUI program, this will be done automatically.

3.1.2 TITLE

TITLE - Title and run description.

Note: The title can consist of any combination of alphanumeric characters spanning three lines in the input file (not to exceed 80 characters per line). The title must span three lines and any of those lines can be blank.

3.1.3 IMODE, IMES, IDISPC, ICWM, ICAP, IREACT, IBIO, ICOORD, ITREAC, ITC, IGAS, IENG

IMODE - Flag indicating if the problem to be run is a first run or a restart simulation.

Possible Values:

- 1 - First simulation run
- 2 - Restart simulation

Note: See Appendix A for more details on how to run restart simulations.

IMES - Flag indicating if a constant or automatic time-step is to be used.

Possible Values:

- 1 - Constant time-step size is used
- 2 - Automatic time-step size selector based on method of relative changes for the first three components is used
- 3 - Automatic time-step size selector based on method of relative changes for all the components is used
- 4 - Automatic time-step size selector based on changes in dimensionless concentration for all the components is used

Note: The automatic time-step selector is recommended. See input lines 3.7.9 through 3.7.13 and Appendix E for more details on the above options.

IDISPC - Flag indicating which type of numerical dispersion control is used.

Possible Values:

- 0 - Single point upstream method is used
- 2 - Two point upstream method is used
- 3 - Improved total variation diminishing third order method is used

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Note: These methods are applied to both **concentration** and **relative permeability**.

ICWM - Flag indicating if the concentration well model is used or not.

Possible Values:

- 0 - Concentration well model is not used
- 1 - Concentration well model is used

Note: **The concentration well model (ICWM=1) can only be used with vertical wells (IDIR(M)=3).**

ICAP - Flag indicating if the capacitance model is used or not.

Possible Values:

- 0 - Capacitance model or dual porosity option is not used
- 1 - Capacitance model is used
- 2 - Dual porosity option is used for single phase tracer flow

Note: **The dual porosity option (ICAP=2) is available only if IMODE=1, IUNIT=0, and ICOORD=1.**

IREACT - Flag indicating if gel reactions or alkaline options are used or not.

Possible Values:

- 0 - Gel reactions are not used
- 1 - Gel reactions are used
- 2 - Geochemistry option with no acidic crude is used
- 3 - Geochemistry option with acidic crude is used
- 4 - IREACT=2 and gel reactions are used

IBIO - Flag indicating whether or not biodegradation reactions occur

Possible Values:

- 0 - No biodegradation reactions
- 1 - Biodegradation reactions occur

ICOORD - Flag indicating which coordinate system is used.

Possible Values:

- 1 - Cartesian coordinate system is used
- 2 - Radial coordinate system is used
- 3 - Cartesian coordinate system with variable-width gridblock is used (2-D cross section only)
- 4 - Curvilinear grid definition of the X-Z cross section is used (2-D or 3-D)

Note: **For ICOORD=4, the 3-D grid consists of the 2-D cross sectional grid repeated at specified intervals (uniform or non-uniform) in the Y direction, according to the definition of DY1. The curvilinear grid option is not available with the temperature equation option.**

ITREAC - Flag indicating if a tracer reaction is used or not.

Possible Values:

- 0 - Tracer reactions are not used
- 1 - Tracer reactions are used

ITC - Flag indicating if second-order time approximation is used or not.

Possible Values:

- 0 - Second-order time approximation is not used
- 1 - Second-order time approximation is used

Note: We recommend that second-order time approximation (ITC=1) only be used with higher-order dispersion methods (IDISPC>1).

IGAS - Flag indicating if gas phase is considered or not.

Possible Values:

- 0 - Gas is not present
- 1 - Gas is present
- 2 - Gas is present and foam option is used

IENG - Flag indicating if temperature variation is considered or not.

Possible Values:

- 0 - Isothermal simulation
- 1 - Temperature equation is solved

3.1.4 NX, NY, NZ, IDXYZ, IUNIT

NX - Number of gridblocks along X-axis (ICOORD=1, 3, or 4) or number of gridblocks in radial direction (ICOORD=2).

Note: This value should be equal to or smaller than the NNX parameter in UTCHEM.

NY - Number of gridblocks along Y-axis.

Note: This value should be equal to or smaller than the NNY parameter in UTCHEM. It should be set equal to 1 if the user is running a 1-D problem or a 2-D cross sectional problem. If ICOORD=2, this value is automatically set equal to 1.

NZ - Number of gridblocks along Z-axis.

Note: This value should be equal to or smaller than the NNZ parameter in UTCHEM. It should be set equal to 1 if the user is running a 1-D problem or a 2-D areal problem.

IDXYZ - Flag indicating constant or variable grid size.

Possible Values:

- 0 - Constant grid size
- 1 - Variable grid size on a regional basis
- 2 - Variable grid size

Note: IDXYZ must be set equal to 2 if ICOORD=3.

IUNIT - Flag indicating English or Metric units.

Possible Values:

- 0 - English unit
- 1 - Metric unit

Note: These NX, NY, and NZ input values must be less than or equal to the NX, NY, and NZ values listed in the HEAD input file.

Simulation Gridblock Sizes (input lines 3.1.5-3.1.23)

3.1.5 XCORD(I), ZCORD(I), for I=1, (NX+1)×(NZ+1) (This line is read only if ICOORD=4)

Note: One line is required for each coordinate pair.

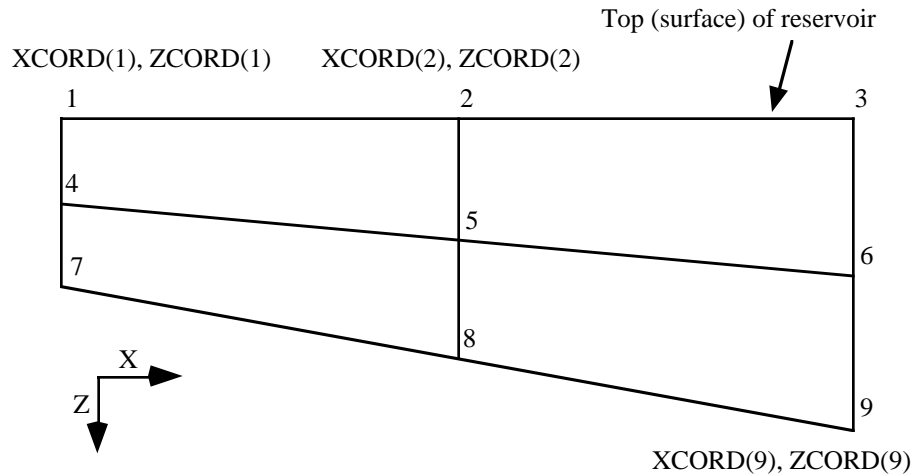
XCORD - Gridblock coordinate of Ith corner point in X-direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

ZCORD - Gridblock coordinate of Ith corner point in Z-direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: The coordinates of the corners (or vertices) of the 2-D X-Z cross section gridblocks are input in pairs as follows:

XCORD(1),	ZCORD(1)
⋮	⋮
⋮	⋮
XCORD(nodes),	ZCORD(nodes)

where nodes = (NX+1) × (NZ+1) and is the total number of corner points defining the X-Z cross section and Z is positive downward. The following figure illustrates the input order for an example X-Z cross section grid:



The number of gridblocks is equal to $NX \times NZ$ and the number of coordinate pairs (or nodes) is equal to $(NX+1) \times (NZ+1)$.

Cautionary warning: The X-Z cross section grid should be constructed by the user such that the curvilinear coordinate system is at least quasi-orthogonal. Departure from orthogonality will lead to numerical errors in the solution.

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Refer to the following table to help determine which input lines should be used to specify the gridblock size input values for different options:

ICOORD	IDXYZ	Input line(s)
1 (Cartesian coordinate system)	0 (constant grid size) 1 (regional variable grid) 2 (variable grid)	3.1.6 3.1.9–3.1.11 3.1.16, 3.1.17, 3.1.19
2 (Radial coordinate system)	0 (constant grid size) 1 (regional variable grid) 2 (variable grid)	3.1.7 3.1.12–3.1.14 3.1.20–3.1.22
3 (Cartesian coordinate system with variable-width gridblock)	0 (constant grid size) 1 (regional variable grid) 2 (variable grid)	(not applicable) (not applicable) 3.1.16, 3.1.18, 3.1.19
4 (Curvilinear grid)	0 (constant grid size) 1 (regional variable grid) 2 (variable grid)	3.1.8 3.1.15 3.1.17

3.1.6 DX1, DY1, DZ1 (This line is read **only if IDXYZ=0 and ICOORD=1**)

DX1 - Gridblock size in X direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.7 R(1), DX1, DZ1 (This line is read **only if IDXYZ=0 and ICOORD=2**)

R(1) - Wellbore radius.

Units: feet (IUNIT=0) or m (IUNIT=1)

DX1 - Distance between nodes in radial direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.8 DY1 (This line is read **only if IDXYZ=0 and ICOORD=4**)

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)



3.1.9 II1, II2, DX1 (This line is read only if IDXYZ=1 and ICOORD=1)

II1 - First index for gridblocks with same size in X direction.

II2 - Last index for gridblocks with same size in X direction.

DX1 - Gridblock size in X direction

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NX gridblocks in the X direction have been specified. The first line in the set must have II1=1 and the last line must have II2=NX.

Example: If NX=11 and the first three gridblocks in the X direction are 3 feet in size, the fourth through ninth gridblocks in the X direction are 2 feet in size, and the last two gridblocks in the X direction are 2.5 feet in size, this line would need to be repeated three times to fully describe the X direction gridblocks as follows:

1	3	3.0
4	9	2.0
10	11	2.5

3.1.10 JJ1, JJ2, DY1 (This line is read only if IDXYZ=1 and ICOORD=1)

JJ1 - First index for gridblocks with same size in Y direction.

JJ2 - Last index for gridblocks with same size in Y direction.

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY gridblocks in the Y direction have been specified. The first line in the set must have JJ1=1 and the last line must have JJ2=NY. See the example for input line 3.1.9.

3.1.11 KK1, KK2, DZ1 (This line is read only if IDXYZ=1 and ICOORD=1)

KK1 - First index for gridblocks with same size in Z direction.

KK2 - Last index for gridblocks with same size in Z direction.

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ gridblocks in the Z direction have been specified. The first line in the set must have KK1=1 and the last line must have KK2=NZ. See the example for input line 3.1.9.

3.1.12 R(1) (This line is read only if IDXYZ=1 and ICOORD=2)

R(1) - Wellbore radius.

Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.13 II1, II2, DX1 (This line is read only if IDXYZ=1 and ICOORD=2)

II1 - First index for radial node distances of the same size.

II2 - Last index for radial node distances of the same size.

DX1 - Distance between nodes in radial direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until the NX-1 distances between the NX nodes in the radial direction have been specified. The first line in the set must have II1=1 and the last line must have II2=NX-1.

Example: If NX=35 and the first ten gridblocks in the X direction are 1 foot in size and the rest are 2 feet in size, this line would need to be repeated twice to fully describe the radial direction nodes as follows:

1	10	1.0
11	34	2.0

3.1.14 KK1, KK2, DZ1 (This line is read only if IDXYZ=1 and ICOORD=2)

KK1 - First index for gridblocks with same size in Z direction.

KK2 - Last index for gridblocks with same size in Z direction.

DZ1 - Gridblock size in Z direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ gridblocks in the Z direction have been specified. The first line in the set must have KK1=1 and the last line must have KK2=NZ. See the example for input line 3.1.9.

3.1.15 JJ1, JJ2, DY1 (This line is read only if IDXYZ=1 and ICOORD=4)

JJ1 - First index for gridblocks with same size in Y direction.

JJ2 - Last index for gridblocks with same size in Y direction.

DY1 - Gridblock size in Y direction.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY gridblocks in the Y direction have been specified. The first line in the set must have JJ1=1 and the last line must have JJ2=NY. See the example for input line 3.1.9.

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3.1.16 DX(I), for I=1, NX (This line is read only if IDXYZ=2 and ICOORD=1 or 3)

DX(I) - Grid size of Ith block in X direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.17 DY(J), for J=1, NY (This line is read only if IDXYZ=2 and ICOORD=1 or 4)

DY(J) - Grid size of Jth block in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.18 DY(I), for I=1, NX (This line is read only if IDXYZ=2 and ICOORD=3)

DY(I) - Thickness of Ith block.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.19 DZ(K), for K=1, NZ (This line is read only if IDXYZ=2 and ICOORD=1 or 3)

DZ(K) - Grid size of Kth block in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.20 R(1) (This line is read only if IDXYZ=2 and ICOORD=2)

R(1) - Wellbore radius.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.21 DX(I), for I=1, NX-1 (This line is read only if IDXYZ=2 and ICOORD=2)

DX(I) - Distance between the Ith node and the I+1th node in the radial direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.22 DZ(K), for K=1, NZ (This line is read only if IDXYZ=2 and ICOORD=2)

DZ(K) - Grid size of Kth block in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.1.23 N, NO, NTW, NTA, NGC, NG, NOTH

N - Total number of components in the run (including tracers and reactive components).

Value must be set equal to: $N=8+NO+NTW+NTA+NGC+NG+NOTH$

NO - Total number of NAPL phase organic components in the run.

Note: If IBIO=1, set NO=0 if no NAPL phase is present and all biodegrading species are present only in the aqueous phase; otherwise, set NO to the number of organic species.

NTW - Number of water/oil tracers.

NTA - Number of oil/gas tracers.

NGC - Number of components for geochemistry option.

NG - Number of gel components.

NOTH - Total number of other chemical and biological species that are considered in biodegradation reactions, including products generated by biodegradation reactions, nutrients required for biological growth, electron acceptors, and biological species.

Note: See Appendix D for the component numbering scheme used in UTCHEM and Section 9 of the UTCHEM Technical Documentation for more details on the microbiological population model options.

3.1.24 SPNAME(I), for I=1, N

SPNAME(I) - Name of Ith species.

Note: The name of each component may not exceed 8 characters and each name must be on a separate line of the input file.

3.1.25 ITRU(I), for I=1, NTW (This line is read only if NTW>0 and ITREAC=1)

ITRU(I) - Flag indicating the units of the Ith water tracer.

Possible Values:

1 - Ith tracer units are in volume %

2 - Ith tracer units are in weight %

3.1.26 ICF(KC), for KC=1, N

ICF(KC) - Flag indicating if KCth component is included in the calculations or not.

Possible Values:

0 - The KCth component is not included in the calculations

1 - The KCth component is included in the calculations

Example: If 11 components are considered but Alcohol 2 is not present, this line would appear as follows:

1 1 1 1 1 1 1 0 1 1 1

User notes:

3.2 Output Option Data

The second input section consists of output options. Please remember that

there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

3.2.1 ICUMTM, ISTOP, *IOUTGMS*

ICUMTM - Flag indicating if the output intervals indicated by the CUMPR1, CUMHI1, WRHPV, WRPRF and RSTC variables are specified in pore volumes or days.

Possible Values:

0 - Data will be written in day intervals

1 - Data will be written in pore volume intervals

Note: The day interval output option (ICUMTM=0) is particularly useful if there is a shut in period.

ISTOP - Flag indicating if the maximum and injection times (variables TMAX and TINJ) are specified in pore volumes or days.

Possible Values:

0 - TMAX and TINJ are specified in days

1 - TMAX and TINJ are specified in pore volumes

IOUTGMS - Flag indicating whether or not Ground Water Modeling System (GMS) files will be created.

Possible Values:

0 - GMS files will not be created

1 - GMS files will be created

Note: IOUTGMS must be set to 0 unless you are running GMS.

3.2.2 IPRFLG(KC), for KC=1, N

IPRFLG(KC) - Flag indicating if profile of KCth component should be written to CONCP, COMP_AQ, COMP_OIL, COMP_ME, and GMS concentration output files.

Possible Values:

0 - Profile of KCth component will not be written

1 - Profile of KCth component will be written

Note: If IPCTOT=0, none of the component profiles will be written.

Example: If 11 components are present and only profiles for the oil, surfactant, and polymer components are desired, this line would appear as follows:

0 1 1 1 0 0 0 0 0 0 0

3.2.3 IPPRES, IPSAT, IPCTOT, *IPBIO*, IPCAP, IPGEL, IPALK, IPTEMP, IPOBS

IPPRES - Flag indicating if profile of phase pressures should be written to PRESP output file.

Possible Values:

0 - Profile of phase pressures will not be written

1 - Profile of phase pressures will be written

IPSAT - Flag indicating if profile of phase saturations should be written to SATP output file.

Possible Values:

0 - Profile of phase saturations will not be written

1 - Profile of phase saturations will be written

IPCTOT - Flag indicating if profile of component concentrations should be written to CONCP output file.

Possible Values:

0 - Profile of component concentrations will not be written

1 - Profile of component concentrations will be written

IPBIO - Flag indicating if chemical and biological species concentrations in the aqueous phase and within attached biomass should be written to BIO output file. IPBIO also controls whether aqueous phase concentrations of components 1 through 8 plus oil components should be written to the HIST_{xx} output files.

Possible Values:

0 - Aqueous and intra-biomass concentrations will not be written

1 - Aqueous and intra-biomass concentrations will be written

IPCAP - Flag indicating if profile of capacitance (if ICAP=1) or dual porosity (if ICAP=2) properties should be written to CAPP (capacitance, ICAP=1) or FRAC (dual porosity, ICAP=2) output files.

Possible Values:

0 - Profile of capacitance or dual porosity properties will not be written

1 - Profile of capacitance or dual porosity properties will be written

IPGEL - Flag indicating if profile of gel properties should be written to GFILEP output file.

Possible Values:

0 - Profile of gel properties will not be written

1 - Profile of gel properties will be written

IPALK - Flag indicating if profile of properties related to the alkaline option should be written to ALKP output file.

Possible Values:

0 - Profile of properties related to the alkaline option will not be written

1 - Profile of properties related to the alkaline option will be written

IPTEMP - Flag indicating if profile of reservoir temperature should be written to TEMPP output file.

Possible Values:

0 - Profile of temperature will not be written

1 - Profile of temperature will be written

IPOBS - Flag indicating if aqueous (or gas) phase tracer concentration at observation points should be written to the TRAC_{xx} output files.

Possible Values:

- 0 - Phase tracer concentrations at observation points will not be written
- 1 - Tracer concentrations at observation points will be written

3.2.4 ICKL, IVIS, IPER, ICNM, ICSE, *IHYSTP*, *IFOAMP*, *INONEQ*

ICKL - Flag indicating if component concentration data in each phase should be written to COMP_AQ, COMP_OIL, and COMP_ME output files.

Possible Values:

- 0 - Component concentration data in each phase will not be written
- 1 - Component concentration data in each phase will be written

IVIS - Flag indicating if phase viscosities should be written to VIS output file.

Possible Values:

- 0 - Phase viscosities will not be written
- 1 - Phase viscosities will be written

IPER - Flag indicating if relative permeabilities should be written to RPERM output file.

Possible Values:

- 0 - Relative permeabilities will not be written
- 1 - Relative permeabilities will be written

ICNM - Flag indicating if phase capillary numbers and interfacial tensions should be written to TRAP output file.

Possible Values:

- 0 - Capillary numbers, residual saturations, and interfacial tensions will not be written
- 1 - Capillary numbers, residual saturation, and interfacial tensions will be written

ICSE - Flag indicating if effective salinity should be written to CSE output file.

Possible Values:

- 0 - Effective salinity information will not be written
- 1 - Effective salinity information will be written

IHYSTP - Flag indicating if properties related to the hysteresis option should be written to HYST output file.

Possible Values:

- 0 - Hysteresis data will not be written
- 1 - Hysteresis data will be written

IFOAMP - Flag indicating if properties related to the foam option should be written to FOAM output file.

Possible Values:

- 0 - Foam data will not be written
- 1 - Foam data will be written

INONEQ - Flag indicating if properties related to the rate-limited mass transfer option should be written to DISS output file.

Possible Values:

- 0 - Rate-limited mass transfer data will not be written
- 1 - Rate-limited mass transfer data will be written

3.2.5 IADS, IVEL, IRKF, IPHSE

IADS - Flag indicating if surfactant, polymer, calcium, gel, chromium, hydrogen, and sodium adsorption data should be written to PROF output file.

Possible Values:

0 - Adsorption data will not be written

1 - Adsorption data will be written

IVEL - Flag indicating if X, Y, and Z direction phase fluxes should be written to PROF output file.

Possible Values:

0 - X, Y, and Z direction phase fluxes will not be written

1 - X, Y, and Z direction phase fluxes will be written

IRKF - Flag indicating if permeability reduction factors should be written to PROF output file.

Possible Values:

0 - Permeability reduction factors, polymer viscosities, and equivalent shear rate will not be written

1 - Permeability reduction factors, polymer viscosities, and equivalent shear rate will be written

IPHSE - Flag indicating if phase environment indexing should be written to PROF output file.

Possible Values:

0 - Phase environment indexing will not be written

1 - Phase environment indexing will be written

Note: The indices for the phase environment are as follows:

1 - single phase

2 - two phase oil/water or oil/microemulsion or water/microemulsion

3 - three phase oil/microemulsion/water

4 - lobe II(+) of type III

5 - lobe II(-) of type III

3.2.6 NOBS (This line is read only if IPOBS=1)

NOBS - Number of tracer concentration observation points.

3.2.7 IOBS(I), JOBS(I), KOBS(I), for I=1, NOBS (This line is read only if IPOBS=1 and NOBS>0)

IOBS(I) - Index of Ith observation point in X direction.

JOBS(I) - Index of Ith observation point in Y direction.

KOBS(I) - Index of Ith observation point in Z direction.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM.

3.3. Reservoir Properties

The third input section consists of the reservoir properties. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

3.3.1 TMAX

TMAX - Total injection period (maximum simulation time).

Units: days or pore volumes (dependent on value of ISTOP flag)

3.3.2 COMPR, PSTAND

COMPR - Rock compressibility.

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

PSTAND - Reference pressure at which pore volume and fluid compressibilities are specified.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

Reservoir/Aquifer Properties (input lines 3.1.3-3.1.17)

3.3.3 IPOR1, IPERMX, IPERMY, IPERMZ, IMOD

IPOR1 - Flag indicating constant or variable porosity for reservoir.

Possible Values:

- 0 - Constant porosity for whole reservoir
- 1 - Constant porosity for each layer
- 2 - Variable porosity over reservoir

IPERMX - Flag indicating constant or variable X direction permeability (ICOORD=1 or 3) or radial direction permeability (ICOORD=2) for reservoir.

Possible Values:

- 0 - Constant permeability for whole reservoir
- 1 - Constant permeability for each layer in the X direction (ICOORD=1 or 3) or radial direction (ICOORD=2)
- 2 - Variable permeability over reservoir

IPERMY - Flag indicating constant or variable Y direction permeability for reservoir.

Possible Values:

- 0 - Constant permeability for whole reservoir
- 1 - Constant permeability for each layer in the Y direction
- 2 - Variable permeability over reservoir
- 3 - Y direction permeability is dependent on X direction permeability

IPERMZ - Flag indicating constant or variable Z direction permeability for reservoir.

Possible Values:

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- 0 - Constant permeability for whole reservoir
- 1 - Constant permeability for each layer in the Z direction
- 2 - Variable permeability over reservoir
- 3 - Z direction permeability is dependent on X direction permeability

IMOD - Flag indicating whether the reservoir properties are modified or not.

Possible Values:

- 0 - No property is modified
- 1 - Allow for property modification

Refer to the following table to help determine which input lines should be used to specify the porosity and permeability values for different options:

IPOR1 (porosity flag)	0 (constant porosity for reservoir)	3.3.4
	1 (constant porosity for each layer)	3.3.5
	2 (variable porosity over reservoir)	3.3.6
IPERMX (X or radial direction permeability flag)	0 (constant permeability for reservoir)	3.3.7
	1 (constant permeability for each layer)	3.3.8
	2 (variable permeability over reservoir)	3.3.9
IPERMY (Y direction permeability flag; only if ICOORD≠2)	0 (constant permeability for reservoir)	3.3.10
	1 (constant permeability for each layer)	3.3.11
	2 (variable permeability over reservoir)	3.3.12
	3 (permeability dependent on X direction)	3.3.13
IPERMZ (Z direction permeability flag)	0 (constant permeability for reservoir)	3.3.14
	1 (constant permeability for each layer)	3.3.15
	2 (variable permeability over reservoir)	3.3.16
	3 (permeability dependent on X direction)	3.3.17

3.3.4 PORC1 (This line is read only if IPOR1=0)

PORC1 - Reservoir porosity.

Units: fraction

Note: All elements of the POR array will be set equal to PORC1.

3.3.5 POR(K), for K=1, NZ (This line is read only if IPOR1=1)

POR(K) - Porosity of Kth layer.

Units: fraction

Note: NZ values are actually read into a workspace array (WKSP1) and then the first set of $NX \times NY$ elements (corresponding to layer 1) of the POR array are set equal to WKSP1(1), the second set of $NX \times NY$ elements (corresponding to layer 2) of the POR array are set equal to WKSP1(2), etc.

3.3.6 POR(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IPOR1=2)

POR(I) - Porosity of Ith gridblock

Units: fraction

Note: The three-dimensional grid system is being read into a one-dimensional array. The first index (column) of the three-dimensional system varies fastest, the second index (row) varies next fastest, and the third index (layer) varies slowest.

Example: If you had a $4 \times 3 \times 2$ system (4 columns— $NX=4$, 3 rows— $NY=3$, and 2 layers— $NZ=2$), the values would be read in the following order:

1,1,1	2,1,1	3,1,1	4,1,1
1,2,1	2,2,1	3,2,1	4,2,1
1,3,1	2,3,1	3,3,1	4,3,1
1,1,2	2,1,2	3,1,2	4,1,2
1,2,2	2,2,2	3,2,2	4,2,2
1,3,2	2,3,2	3,3,2	4,3,2

UTCHEM sets the transmissibilities to zero for gridblocks with porosity values less than or equal to 0.01 to specify inactive cells (ICOORD=1).

3.3.7 PERMXC (This line is read only if IPERMX=0)

PERMXC - Permeability of the reservoir in the X direction or in the radial direction (ICOORD=2).

Units: millidarcies = $10^{-3} \mu m^2$

Note: All elements of the PERMX array will be set equal to PERMXC.

Note: In order to specify clay gridblocks, the user should set the permeability for those gridblocks to a value less than or equal to 10^{-5} md. UTCHEM then sets the porosity to 0.01 and water saturation to 1.0 for those gridblocks.

3.3.8 PERMX(K), for K=1, NZ (This line is read only if IPERMX=1)

PERMX(K) - Permeability of the Kth layer in the X direction or in the radial direction (ICOORD=2).

Units: millidarcies = $10^{-3} \mu m^2$

Note: See the note for input line 3.3.5 for information on how the data is read. See the note for input line 3.3.7 for information on specifying clay gridblocks.

3.3.9 PERMX(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IPERMX=2)

PERMX(I) - Permeability of the Ith gridblock in the X direction or in the radial direction (ICOORD=2).

Units: millidarcies = $10^{-3} \mu m^2$

Note: See the note and example for input line 3.3.6 for the order of the permeability values. See the note for input line 3.3.7 for information on specifying clay gridblocks.

3.3.10 PERMYC (This line is read only if IPERMY=0 and ICOORD≠2)

PERMYC - Permeability of the reservoir in the Y direction.

Units: millidarcies = $10^{-3} \mu\text{m}^2$

Note: All elements of the PERMY array will be set equal to PERMYC.

3.3.11 PERMY(K), for K=1, NZ (This line is read only if IPERMY=1 and ICOORD≠2)

PERMY(K) - Permeability of the Kth layer in the Y direction.

Units: millidarcies = $10^{-3} \mu\text{m}^2$

Note: See the note for input line 3.3.5 for information on how the data is read.

3.3.12 PERMY(I), for I=1, NX × NY × NZ (This line is read only if IPERMY=2 and ICOORD≠2)

PERMY(I) - Permeability of the Ith gridblock.

Units: millidarcies = $10^{-3} \mu\text{m}^2$

Note: See the note and example for input line 3.3.6 for the order of the permeability values.

3.3.13 FACTY (This line is read only if IPERMY=3 and ICOORD≠2)

FACTY - Constant permeability multiplier for Y direction permeability.

Units: dimensionless

Note: The X direction permeabilities are multiplied by FACTY to obtain the Y direction permeabilities.

3.3.14 PERMZC (This line is read only if IPERMZ=0)

PERMZC - Permeability of the reservoir in the Z direction.

Units: millidarcies = $10^{-3} \mu\text{m}^2$

Note: All elements of the PERMZ array will be set equal to PERMZC.

3.3.15 PERMZ(K), for K=1, NZ (This line is read only if IPERMZ=1)

PERMZ(K) - Permeability of the Kth layer in the Z direction.

Units: millidarcies = $10^{-3} \mu\text{m}^2$

Note: See the note for input line 3.3.5 for information on how the data is read.

3.3.16 PERMZ(I), for I=1, NX × NY × NZ (This line is read only if IPERMZ=2)

PERMZ(I) - Permeability of the Ith gridblock.

Units: millidarcies ($10^{-3} \mu\text{m}^2$)

Note: See the note and example for input line 3.3.6 for the order of the permeability values.

3.3.17 FACTZ (This line is read only if **IPERMZ=3**)

FACTZ - Constant permeability multiplier for Z direction permeability.

Units: dimensionless

Note: The X direction permeabilities are multiplied by FACTZ to obtain the Z direction permeabilities.

Initial Reservoir/Aquifer Data (input lines 3.3.18-3.3.35)

3.3.18 IDEPTH, IPRESS, ISWI, **ICWI**

IDEPTH - Flag indicating type of depth measurement of the top layer.

Possible Values:

- 0 - Single value for depth of the top layer is specified
- 1 - Depth of top gridblock (1,1,1) and the reservoir dip angles are specified
- 2 - Depth of each gridblock in the top layer is specified

Note: If ICOORD=2, this value is automatically set equal to 0. The depth is specified at the middle of a gridblock.

IPRESS - Flag indicating type of reservoir initial pressure measurement.

Possible Values:

- 0 - Single value for reservoir initial pressure is used for all gridblocks
- 1 - Initial pressure for a point at a specified depth is specified by user
- 2 - Initial pressure for each gridblock is specified by user

ISWI - Flag indicating type of initial water saturation measurement.

Possible Values:

- 0 - Single value for initial water saturation is used for all gridblocks
- 1 - Constant value for water saturation for each layer is specified by user
- 2 - Initial water saturation for each gridblock is specified by user

ICWI - Flag indicating type of initial aqueous phase compositions.

Possible Values:

- 1 - Backward compatibility with previous versions of UTCHEM (only species in aqueous phase are anion and cation)
- 0 - Constant initial aqueous phase concentration for whole reservoir
- 1 - Constant initial aqueous phase concentration for each layer
- 2 - Initial aqueous phase concentration specified for each gridblock

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Refer to the following table to help determine which input lines should be used to specify the initial properties such as depth, pressure, and initial water saturations:

IDEPH (depth flag)	0 (single value for top layer)	3.3.19
	1 (top gridblock and dip angles)	3.3.20
	2 (each gridblock in top layer)	3.3.21
IPRESS (initial pressure flag)	0 (single value for reservoir)	3.3.22
	1 (one point at a specified depth)	3.3.23
	2 (each gridblock)	3.3.24
ISWI (water saturation flag)	0 (single value for reservoir)	3.3.25
	1 (constant value for each layer)	3.3.26
	2 (each gridblock)	3.3.27
ICWI (aqueous phase composition flag)	0 (single value for reservoir)	3.3.32
	1 (constant value for each layer)	3.3.33
	2 (each gridblock)	3.3.34

3.3.19 D111 (This line is read only if IDEPTH=0)

D111 - Depth of the top layer of the reservoir measured from the surface (reference plane), positive downward.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: If IDEPTH=0 and ICOORD=4, D111 is the reference depth of the first gridblock.

3.3.20 D111, THETAX, THETAY (This line is read only if IDEPTH=1)

D111 - Depth of the first gridblock (1,1,1).
Units: feet (IUNIT=0) or m (IUNIT=1)

THETAX - Reservoir dip angle in X direction, positive downward.
Units: radians

THETAY - Reservoir dip angle in Y direction, positive downward.
Units: radians
Note: If ICOORD=4, set THETAY equal to 0 (dip angle in X-Z plane).

3.3.21 EL(I), for I=1, $NX \times NY$ (This line is read only if IDEPTH=2)

EL(I) - Depth of Ith gridblock in the top layer (K=1).
Units: feet (IUNIT=0) or m (IUNIT=1)
Note: See the note and example for input line 3.3.6 for the order of the gridblock depths.

3.3.22 PRESS1 (This line is read only if IPRESS=0)

PRESS1 - Initial reservoir pressure.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

3.3.23 PINIT, HINIT (This line is read only if IPRESS=1)

PINIT - Initial reservoir pressure at HINIT depth.
Units: psia (IUNIT=0) or kPa (IUNIT=1)

HINIT - Depth of the point where PINIT initial pressure is specified.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: Initial pressure is assumed to be the aqueous phase pressure.

3.3.24 P(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IPRESS=2)

P(I) - Initial pressure of each gridblock in the reservoir.
Units: psia (IUNIT=0) or kPa (IUNIT=1)
Note: See the note and example for input line 3.3.6 for the order of the initial pressure values. This is assumed to be the aqueous phase pressure.

3.3.25 SWI (This line is read only if ISWI=0)

SWI - Initial water saturation for all gridblocks of the reservoir.
Units: fraction of pore volume

3.3.26 S(K,1), for K=1, NZ (This line is read only if ISWI=1)

S(K,1) - Initial water saturation for Kth layer.
Units: fraction of pore volume
Note: See the note for input line 3.3.5 for information on how the data is read.

3.3.27 S(I,1), for I=1, $NX \times NY \times NZ$ (This line is read only if ISWI=2)

S(I,1) - Initial water saturation for Ith block.
Units: fraction of pore volume
Note: See the note and example for input line 3.3.6 for the order of the initial water saturation values.

Initial Gas Saturations (input lines 3.3.28-3.3.31) — This section is **required only if** gas is present (**IGAS**≥1).

3.3.28 ISGI (This line is read only if IGAS≥1)

ISGI - Flag indicating type of initial gas saturation.
Possible Values:
0 - Constant initial gas saturation for whole reservoir
1 - Constant initial gas saturation for each layer
2 - Initial gas saturation specified for each gridblock

3.3.29 SGI (This line is read only if IGAS \geq 1 and ISGI=0)

SGI - Initial gas saturation for all gridblocks of the reservoir.
Units: fraction of pore volume

3.3.30 S(K,4), for K=1, NZ (This line is read only if IGAS \geq 1 and ISGI=1)

S(K,4) - Initial gas saturation for Kth layer.
Units: fraction of pore volume
Note: See the note for input line 3.3.5 for information on how the data is read.

3.3.31 S(I,4), for I=1, NX \times NY \times NZ (This line is read only if IGAS \geq 1 and ISGI=2)

S(I,4) - Initial gas saturation for Ith gridblock.
Units: fraction of pore volume
Note: See the note and example for input line 3.3.6 for the order of the initial gas saturation values.

Initial Aqueous Phase Compositions (input lines 3.3.32-3.3.34)

Note: Please see the example following input line 3.3.34 for more information on how UTCHEM uses the ICF flag to control exactly how many values are read on input lines 3.3.32-3.3.34.

3.3.32 **CWI(KW)**, for KW=1, N << or >>
CWI(KW), for KW=1, 8+NO (This line is read only if ICWI=0)

CWI(KW) - Initial concentration of species KW in the aqueous phase.
Units: volume fraction

Note: If N \leq 8, at most N values are required by the program. If N>8, at most 8+NO values are required by the program. Please see example following input line 3.3.34.

3.3.33 **CWI(K,KW)**, for K=1, NZ, for KW=1, N << or >>
CWI(K,KW), for K=1, NZ, for KW=1, 8+NO (This line is read only if ICWI=1)

CWI(K, KW) - Initial concentration of species KW in the aqueous phase at Kth layer.
Units: volume fraction

Note: If N \leq 8, at most N \times NZ values are required by the program. If N>8, at most (8+NO) \times NZ values are required by the program. Please see example following input line 3.3.34.

3.3.34 **CWI(I,KW)**, for I=1, $NX \times NY \times NZ$, for KW=1, N << or >>

CWI(I,KW), for I=1, $NX \times NY \times NZ$, for KW=1, 8+NO (This line is read only if ICWI=2)

CWI(I,KW) - Initial concentration of species KW in the aqueous phase at Ith gridblock.

Units: volume fraction

Note: If $N \leq 8$, at most $N \times NX \times NY \times NZ$ values are required by the program. If $N > 8$, at most $(8+NO) \times NX \times NY \times NZ$ values are required by the program. Please see the example below.

Example:

Values are only read for the 8 "basic" components (water, oil, surfactant, polymer, anion, cation, alcohol 1, alcohol 2) and any multiple organic components present. See Appendix D for more information on UTCHEM components.

In addition, values are only read for a component if the ICF flag for that component has been set to 1.

In this example, we are providing initial concentrations for the water, oil, and anion components for a case with 5 components and $5 \times 3 \times 2$ gridblocks where the ICF array has been initialized as:

1 1 0 0 1

For ICWI=0:

```
CC
CC
*-- Initial water conc. in aq. phase
    0.999
CC
CC
*-- Initial oil conc. in aq. phase
    0.001
CC
CC
*-- Initial chloride conc. in aq. phase
    0.4
```

For ICWI=1:

```
CC
CC
*-- Initial water conc. in aq. phase in each layer
    0.999  0.999
CC
CC
*-- Initial oil conc. in aq. phase in each layer
    0.001  0.001
CC
```

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```
CC
*-- Initial chloride conc. in aq. phase in each layer
    0.4  0.4
```

For ICWI=2:

```
CC
CC
*-- Initial water conc. in aq. phase in each gridblock
    30*0.999
CC
CC
*-- Initial oil conc. in aq. phase in each gridblock
    30*0.001
CC
CC
*-- Initial chloride conc. in aq. phase in each gridblock
    15*0.4  15*0.3
```

Initial Organic Concentrations (input lines 3.3.35-3.3.38) — This section is required only if the multiple organic option is used (NO>1).

3.3.35 ICOI (This line is read only if NO>1)

ICOI - Flag indicating type of initial oil phase compositions.

Possible Values:

- 0 - Constant initial oil phase concentration for whole reservoir
- 1 - Constant initial oil phase concentration for each layer
- 2 - Initial oil phase concentration specified for each gridblock

3.3.36 COI(KO), for KO=1, NO (This line is read only if NO>1 and ICOI=0)

COI(KO) - Initial oil phase concentration for oil component KO for the reservoir.

Units: volume fraction

3.3.37 COI(K,KO), for K=1, NZ, for KO=1, NO (This line is read only if NO>1 and ICOI=1)

COI(K, KO) - Initial oil phase concentration for oil component KO at Kth layer.

Units: volume fraction

3.3.38 COI(I,KO), for I=1, NX × NY × NZ, for KO=1,NO (This line is read only if NO>1 and ICOI=2)

COI(I,KO) - Initial oil phase concentration for oil component KO at Ith gridblock.

Units: volume fraction

Reservoir Property Modification Data (input lines 3.3.39-3.3.49) — This section is **required only if IMOD=1**.

3.3.39 IMPOR, IMKX, IMKY, IMKZ, IMSW (This line is read only if IMOD=1)

IMPOR - Flag indicating whether the porosity is modified or not.

Possible Values:

0 - No modification is considered in porosity values

1 - Allow modification in porosity

IMKX- Flag indicating whether the permeability in the X direction is modified or not.

Possible Values:

0 - No modification is considered in X permeability

1 - Allow modification in X permeability

IMKY- Flag indicating whether the permeability in the Y direction is modified or not.

Possible Values:

0 - No modification is considered in Y permeability

1 - Allow modification in Y permeability

IMKZ- Flag indicating whether the permeability in the Z direction is modified or not.

Possible Values:

0 - No modification is considered in Z permeability

1 - Allow modification in Z permeability

IMSW- Flag indicating whether the initial water saturation is modified or not.

Possible Values:

0 - No modification is considered in initial water saturation values

1 - Allow modification in initial water saturation

3.3.40 NMOD0 (This line is read only if IMOD=1 and IMPOR=1)

NMOD0 - Number of regions with modified porosity.

3.3.41 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD>0)

IMIN - The first index in X direction.

IMAX - The last index in X direction.

JMIN - The first index in Y direction.

JMAX - The last index in Y direction.

KMIN - The first index in Z direction.

KMAX - The last index in Z direction.

IFACT - Flag indicating how porosity is modified.

Possible Values:

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- 1 - Replace porosity with FACTX
- 2 - Multiply porosity by FACTX
- 3 - Add FACTX to porosity

FACTX - The constant used to modify the porosity value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD0 times.

3.3.42 NMOD1 (This line is read only if IMOD=1 and IMKX=1)

NMOD1 - Number of regions with modified X permeability.

3.3.43 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD1>0)

IMIN - The first index in X direction.

IMAX - The last index in X direction.

JMIN - The first index in Y direction.

JMAX - The last index in Y direction.

KMIN - The first index in Z direction.

KMAX - The last index in Z direction.

IFACT - Flag indicating how X permeability is modified.

Possible Values:

- 1 - Replace X permeability with FACTX
- 2 - Multiply X permeability by FACTX
- 3 - Add FACTX to X permeability

FACTX - The constant used to modify the X permeability value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD1 times.

3.3.44 NMOD2 (This line is read only if IMOD=1 and IMKY=1)

NMOD2 - Number of regions with modified Y permeability.

3.3.45 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD2>0)

IMIN - The first index in direction.

IMAX - The last index in X direction.

JMIN - The first index in Y direction.

JMAX - The last index in Y direction.

KMIN - The first index in Z direction.

KMAX - The last index in Z direction.

IFACT - Flag indicating how Y permeability is modified.

Possible Values:

- 1 - Replace Y permeability with FACTX
- 2 - Multiply Y permeability by FACTX
- 3 - Add FACTX to Y permeability

FACTX - The constant used to modify the Y permeability value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD2 times.

3.3.46 NMOD3 (This line is read only if IMOD=1 and IMKZ=1)

NMOD3 - Number of regions with modified Z permeability.

3.3.47 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD3>0)

IMIN - The first index in X direction.

IMAX - The last index in X direction.

JMIN - The first index in Y direction.

JMAX - The last index in Y direction.

KMIN - The first index in Z direction.

KMAX - The last index in Z direction.

IFACT - Flag indicating how Z permeability is modified.

Possible Values:

- 1 - Replace Z permeability with FACTX
- 2 - Multiply Z permeability by FACTX
- 3 - Add FACTX to Z permeability

FACTX - The constant used to modify the Z permeability value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD3 times.

3.3.48 NMOD4 (This line is read only if IMOD=1 and IMSW=1)

NMOD4 - number of regions with modified initial water saturation.

3.3.49 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD4>0)

IMIN - The first index in X direction.

IMAX - The last index in X direction.

JMIN - The first index in Y direction.

JMAX - The last index in Y direction.

KMIN - The first index in Z direction.

KMAX - The last index in Z direction.

IFACT - Flag indicating how initial water saturation is modified.

Possible Values:

1 - Replace initial water saturation with FACTX

2 - Multiply initial water saturation by FACTX

3 - Add FACTX to initial water saturation

FACTX - The constant used to modify the initial water saturation value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD4 times.

3.3.50 NMOD5 (This line is read only if IMOD=1, IMSW=1, and IGAS \geq 1)

NMOD5 - number of regions with modified initial gas saturation.

3.3.51 IMIN, IMAX, JMIN, JMAX, KMIN, KMAX, IFACT, FACTX (This line is read only if IMOD=1 and NMOD5 $>$ 0)

IMIN - The first index in X direction.

IMAX - The last index in X direction.

JMIN - The first index in Y direction.

JMAX - The last index in Y direction.

KMIN - The first index in Z direction.

KMAX - The last index in Z direction.

IFACT - Flag indicating how initial gas saturation is modified.

Possible Values:

1 - Replace initial gas saturation with FACTX

2 - Multiply initial gas saturation by FACTX

3 - Add FACTX to initial gas saturation

FACTX - The constant used to modify the initial gas saturation value.

Note: See the note for input line 3.3.6 for a description of how the gridblocks are ordered in UTCHEM. This line is repeated NMOD5 times.

3.3.52 C50, C60 (This line is read only if ICWI=-1)

C50 - Constant initial brine salinity.

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Units: meq/ml of water

Note: This is assumed to be all the anions (in equivalents).

C60 - Initial divalent cation concentration of brine.

Units: meq/ml of water

Note: C50 and C60 are replaced by the input values of C5I and C6I when IREACT>1.

User notes:

3.4 General Physical Property Data

The fourth input section consists of the general physical property data. Please remember that there are seven comment lines at the beginning of this section and that each data line is preceded by three comment lines.

Surfactant/Cosolvent Phase Behavior Data (input lines 3.4.1-3.4.21)

3.4.1 C2PLC, C2PRC, EPSME, IHAND

C2PLC - Oil concentration at plait point in type II(+) region.
Units: volume fraction

C2PRC - Oil concentration at plait point in type II(-) region.
Units: volume fraction

EPSME - Critical micelle concentration (CMC)—minimum surfactant concentration for the formation of micelles.
Units: volume fraction

IHAND - Flag to specify whether modified Hand's rule is considered or not.
Possible Values:
0 - Original Hand's rule is considered for phase behavior (default)
1 - Modified Hand's rule is considered for Phase behavior
Note: The option of IHAND=1 is available only for oil/microemulsion, Type II(-) phase behavior, and IMASS=1.

3.4.2 IFGHBN

IFGHBN - Flag indicating type of phase behavior parameters.
Possible Values:
0 - Input height of binodal curve (default)
1 - Input solubilization ratio (new option)

Note: The input solubilization parameter (IFGHBN=1) is currently only available for the multiple organic option (NO>1). The effect of temperature or alcohol on phase behavior is not currently modeled for IFGHBN=1. See [Sections 2 & 11 of the UTCHEM Technical Documentation](#) for more details on the input height of binodal curve option and [Section 7 of the UTCHEM Technical Documentation](#) for more details on the input solubilization ratio option.

Binodal Curve Input Option (input lines 3.4.3-3.4.11) — This section is required only if **IFGHBN=0**.

3.4.3 HBNS70, HBNC70, HBNS71, HBNC71, HBNS72, HBNC72 (This line is read only if IFGHBN=0)

HBNS70 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1 associated with surfactant at zero salinity.

Units: volume fraction

HBNC70 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1 (associated with surfactant at zero salinity).

Units: volume fraction

HBNS71 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1 associated with surfactant at optimal salinity.

Units: volume fraction

HBNC71 - Intercept of maximum height of binodal curve at zero fraction of Alcohol associated with surfactant at optimal salinity.

Units: volume fraction

HBNS72 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1 associated with surfactant at twice optimal salinity.

Units: volume fraction

HBNC72 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1 associated with surfactant at twice optimal salinity.

Units: volume fraction

Note: If alcohol is not present, the maximum height of binodal curves at three different salinities are the only parameters used in the phase behavior calculations.

3.4.4 HBNT0, HBNT1, HBNT2, CSET (This line is read only if IFGHBN=0 and IENG=1)

HBNT0 - Slope of height of binodal curve versus temperature at zero salinity

Units: volume fraction/(°F) (IUNIT=0) or volume fraction/°C (IUNIT=1)

HBNT1 - Slope of height of binodal curve versus temperature at optimal salinity

Units: volume fraction/(°F) (IUNIT=0) or volume fraction/°C (IUNIT=1)

HBNT2 - Slope of height of binodal curve versus temperature at twice optimal salinity

Units: volume fraction/(°F) (IUNIT=0) or volume fraction/°C (IUNIT=1)

CSET - The Slope parameter, β_T , for temperature dependency of the three-phase window

Units: (°F)⁻¹ (IUNIT=0) or (°C)⁻¹ (IUNIT=1)

3.4.5 HBNS80, HBNC80, HBNS81, HBNC81, HBNS82, HBNC82 (This line is read only if IFGHBN=0)

HBNS80 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2 associated with surfactant at zero salinity.

Units: volume fraction

HBNC80 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2 associated with surfactant at zero salinity.

Units: volume fraction

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- HBNS81 - Slope of maximum height of binodal curve vs. fraction of Alcohol 2 associated with surfactant at optimal salinity.
Units: volume fraction
- HBNC81 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2 associated with surfactant at optimal salinity.
Units: volume fraction
- HBNS82 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2 associated with surfactant at twice optimal salinity.
Units: volume fraction
- HBNC82 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2 associated with surfactant at twice optimal salinity.
Units: volume fraction
- 3.4.6 CSEL7, CSEU7, CSEL8, CSEU8 (This line is read only if IFGHBN=0)
- CSEL7 - Lower effective salinity limit for type III phase region determined when Alcohol 1 and calcium approach zero.
Units: meq/ml water
- CSEU7 - Upper effective salinity limit for type III phase region determined when Alcohol 1 and calcium approach zero.
Units: meq/ml water
- CSEL8 - Lower effective salinity limit for type III phase region determined when Alcohol 2 and calcium approach zero.
Units: meq/ml water
- CSEU8 - Upper effective salinity limit for type III phase region determined when Alcohol 2 and calcium approach zero.
Units: meq/ml water
- 3.4.7 BETA6, BETA7, BETA8 (This line is read only if IFGHBN=0)
- BETA6 - The effective salinity slope parameter for calcium.
Units: dimensionless
- BETA7 - The effective salinity slope parameter for Alcohol 1.
Units: dimensionless
- BETA8 - The effective salinity slope parameter for Alcohol 2.
Units: dimensionless
- 3.4.8 IALC, OPSK7O, OPSK7S, OPSK8O, OPSK8S (This line is read only if IFGHBN=0)
- IALC - Flag indicating choice of alcohol partition model to use.
Possible Values:
0 - Hirasaki's model will be used
1 - Prouvost's model will be used
- OPSK7O - Alcohol partition coefficient (oil/water) for Alcohol 1.

Units: dimensionless

OPSK7S - Alcohol partition coefficient (surfactant/water) for Alcohol 1.

Units: dimensionless

OPSK8O - Alcohol partition coefficient (oil/water) for Alcohol 2.

Units: dimensionless

OPSK8S - Alcohol partition coefficient (surfactant/water) for Alcohol 2.

Units: dimensionless

Note: If IALC=0 then OPSK7O, OPSK7S, OPSK8O, and OPSK8S remain fixed. If OPSK7O, OPSK7S, OPSK8O, and OPSK8S are equal to zero and IALC=0, then alcohol is lumped with surfactant as a single component (total chemical). OPSK7O, OPSK7S, OPSK8O, and OPSK8S are only used when Hirasaki's model is chosen. See Section 11 of the UTCHEM Technical Documentation for more details on the alcohol partition models.

3.4.9 NALMAX, EPSALC (This line is read only if IFGHBN=0)

NALMAX - Maximum number of iterations for alcohol partitioning for two alcohol system.

Note: The suggested value is 20 and a value of zero would result in no iterations.

EPSALC - Tolerance for convergence of iterations for two alcohol system.

Note: Suggested values are 10^{-3} and 10^{-4} .

3.4.10 AKWC7, AKWS7, AKM7, AK7, PT7 (This line is read only if IFGHBN=0)

AKWC7, AKWS7 - Parameters used to determine partition coefficient of monomeric Alcohol 1 between aqueous and oleic pseudophases.

Units: dimensionless

AKM7 - Partition coefficient of monomeric Alcohol 1 between surfactant and oleic pseudophases.

Units: dimensionless

AK7 - Self-association constant of Alcohol 1 in oleic pseudophase.

Units: dimensionless

PT7 - Ratio of molar volume of Alcohol 1 to equivalent molar volume of surfactant.

Units: dimensionless

3.4.11 AKWC8, AKWS8, AKM8, AK8, PT8 (This line is read only if IFGHBN=0)

AKWC8, AKWS8 - Parameters used to determine partition coefficient of monomeric Alcohol 2 between aqueous and oleic pseudophases.

Units: dimensionless

AKM8 - Partition coefficient of monomeric Alcohol 2 between surfactant and oleic pseudophases.

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Units: dimensionless

AK8 - Self-association constant of Alcohol 2 in oleic pseudophase.

Units: dimensionless

PT8 - Ratio of molar volume of Alcohol 2 to equivalent molar volume of surfactant.

Units: dimensionless

Solubilization Ratio Input Option (input lines 3.4.12-3.4.21) — These lines are **required only** if the phase behavior calculation is based on the solubilization ratio (**IFGHBN=1**).

3.4.12 IOD (This line is read only if IFGHBN=1 and NO>1)

IOD - Flag indicating whether phase behavior depends on organic composition

Possible Values:

0 - Phase behavior and properties depend on organic composition

1 - Phase behavior and properties are independent of organic composition (default)

3.4.13 NCOMP (This line is read only if IFGHBN=1 and IOD=0)

NCOMP - Number of organic components in the first solubility measurement.

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3.4.14 ONAME(I) for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

ONAME(I) - Name of organic species in the first solubility measurement.
Currently the values in the following table can be specified.

ONAME Value	Formula	Name	Molecular Weight	Equivalent Alkane Carbon No. (EACN)
DECANE	C ₁₀ H ₂₂	Decane	142	10
OCTANE	C ₈ H ₁₈	Octane	114	8
HEXANE	C ₆ H ₁₄	Hexane	86	6
PCE	C ₂ Cl ₄	Tetrachloro-ethylene	165.8	2.9
PXYLEN		P-xylene	106	2
TOLUEN		Toluene	92	1
CCL4	CCl ₄	Carbon tetrachloride	153.8	-0.06
TCE	C ₂ HCl ₃	Trichloro-ethylene	131.4	-3.81
DCB	1,2-C ₆ H ₄ Cl ₂	1,2-dichloro-benzene	146.9	-4.89
TCA	CH ₃ CCl ₃	1,1,1-trichloro-ethene	133.35	-2.5
DCE	1,2-C ₂ H ₄ Cl ₂		98.9	-12.1
CHCL3	CHCl ₃		119.4	-13.67
CH2CL2	CH ₂ Cl ₂		84.9	-13.79
C2CL4	1,1,2,2-C ₂ H ₂ Cl ₄		167.8	-22.15

Note: Each organic species name must appear on a separate line of the input file.

3.4.15 OCOMP(I), for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

OCOMP(I) - Concentration of Ith organic component in the first solubility measurement.
Units: mole fraction

3.4.16 CS0, SCS0, CS1, SCS1, CS2, SCS2, DCS20 (This line is read only if IFGHBN=1)

CS0 - Effective salinity which is between the lower and optimal effective salinity limits for type III phase region in the first solubility measurement;
CSEL<CS0<CSEOP.
Units: meq/ml

SCS0 - Solubilization parameter at CS0 in the first solubility measurement.
Units: volume fraction

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CS1 - Optimal effective salinity in the first solubility measurement (CSEOP).
Units: meq/ml

SCS1 - Solubilization parameter at CS1.
Units: volume fraction

CS2 - Effective salinity which is between the optimal and the upper effective salinity limits for type III phase region in the first solubility measurement; $CSEOP < CS2 < CSEU$.
Units: meq/ml

SCS2 - Solubilization parameter at CS2 in the first solubility measurement.
Units: volume fraction

DCS20 - The difference of the upper and the lower effective salinity limits for type III phase region in the first solubility measurement; $CSEU - CSEL$.

3.4.17 NCOMP (This line is read only if IFGHBN=1 and IOD=0)

NCOMP - Number of organic components in the second solubility measurement.

3.4.18 ONAME(I), for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

ONAME(I) - Name of organic species in the second solubility measurement.
Note: See input line 3.4.14 for a list of available species names. Each organic species name must appear on a separate line of the input file.

3.4.19 OCOMP(I), for I=1, NCOMP (This line is read only if IFGHBN=1 and IOD=0)

OCOMP(I) - Concentration of Ith organic component in the second solubility measurement.
Units: mole fraction

3.4.20 CS0, SCS0, CS1, SCS1, CS2, SCS2, DCS20 (This line is read only if IFGHBN=1 and IOD=0)

CS0 - Effective salinity which is between the lower and optimal effective salinity limits for type III phase region in the second solubility measurement; $CSEL < CS0 < CSEOP$.
Units: meq/ml

SCS0 - Solubilization parameter at CS0 in the second solubility measurement.
Units: volume fraction

CS1 - Optimal effective salinity in the second solubility measurement.
Units: meq/ml

SCS1 - Solubilization parameter at CS1 in the second solubility measurement.
Units: volume fraction

CS2 -Effective salinity which is between the optimal and the upper effective salinity limits for type III phase region in the second solubility measurement; CSEOP<CS2<CSEU.
Units: meq/ml

SCS2 - Solubilization parameter at CS2 in the second solubility measurement.
Units: volume fraction

DCS20 - The difference of the upper and the lower effective salinity limits for type III phase region in the second solubility measurement; CSEU - CSEL.

3.4.21 BETA6 (This line is read only if IFGHBN=1)

BETA6 - The effective salinity slope parameter for calcium.
Units: dimensionless

Interfacial Tension Data (input lines 3.4.22-3.4.25)

3.4.22 **IFT**

IFT - This flag indicates which interfacial tension correlation is used.
Possible Values:
0 - Healy and Reed's correlation will be used
1 - Huh's correlation will be used

Note: See Section 2 of the UTCHEM Technical Documentation for more details on the interfacial tension model options.

3.4.23 G11, G12, G13, G21, G22, G23 (This line is read only if IFT=0)

G11, G12, G13 - Interfacial tension parameters for water-microemulsion interface.

G21, G22, G23 - Interfacial tension parameters for oil-microemulsion interface.
Units: Dimensionless

3.4.24 CHUH, AHUH (This line is read only if IFT=1)

CHUH - Constant in modified Huh's interfacial tension correlation.
Typical Values: 0.1 - 0.35

AHUH - Constant in modified Huh's interfacial tension correlation
Typical values: 5 - 20

3.4.25 XIFTW

XIFTW - $\log_{10} \sigma_{wo}$ where σ_{wo} is the interfacial tension of the water-oil interface.
Units: dynes/cm = mN/m

Organic Mass Transfer Data (input lines 3.4.26-3.4.30)

3.4.26 IMASS, ICOR

IMASS - Flag indicating the choice of oil solubility in water.

Possible Values

- 0 - No solubility of oil in water in the absence of surfactant
- 1 - Allow for solubility of oil in water in the absence of surfactant
- 2 - Allow for non-equilibrium solubility of oil in water

ICOR - Flag indicating whether mass transfer coefficient is constant or calculated.

Possible Values

- 0 - Mass transfer coefficient in constant
- 1 - Mass transfer coefficient in calculated using correlation

Note: See Section 12 of the UTCHEM Technical Documentation for more details on the organic dissolution model used in UTCHEM.

3.4.27 WSOL (This line is read only if $NO \leq 1$ and $IMASS > 0$)

WSOL - Equilibrium concentration of oil in water in the absence of surfactant.

Units: volume fraction

3.4.28 WSOLK(K), for K=1, NO (This line is read only if $NO > 1$ and $IMASS > 1$)

WSOLK(K) - Water/oil equilibrium partition coefficient for oil component K in the absence of surfactant

Units: volume fraction

Note: See Section 7 of the UTCHEM Technical Documentation for more details on the rate limited multiple organic dissolution model.

3.4.29 ISOL, CNEM (This line is read only if $IMASS = 2$ and $ICOR = 0$)

ISOL - Flag indicating the solution scheme for the non-equilibrium mass transfer calculations

Possible Values

- 0 - Implicit method is used
- 1 - Explicit method is used

Note: The explicit method ($ISOL = 1$) is the only option available when gas is present ($IGAS \geq 1$).

CNEM - Coefficient of non-equilibrium mass transfer of oil in aqueous phase with or without surfactant.

Units: vol. of water/(bulk vol.-day)

Note: The non-equilibrium mass transfer calculation is valid for type II(-) with the plait point in the corner ($C2PLC = 0$) and in the absence of gas phase ($IGAS = 0$).

3.4.30 ISOL, EQB0, EQB1, EQB2, EQB3 (This line is read only if $IMASS = 2$ and $ICOR = 1$)

ISOL - Flag indicating the solution scheme for the non-equilibrium mass transfer calculations

Possible Values

- 0 - Implicit method is used
- 1 - Explicit method is used

Note: The explicit method (ISOL=1) is the only option available when gas is present (IGAS \geq 1).

EQB0 - Sherwood number constant.

EQB1 - Reynold's number exponent.

EQB2 - Oil content exponent.

EQB3 - Schmidt number exponent.

3.4.31 ITRAP, T11, T22, T33

ITRAP - Flag indicating whether residual saturations and relative permeabilities are dependent on capillary number or not.

Possible Values:

- 0 - Residual saturations are not dependent on capillary number; endpoint and exponent of relative permeability curves are constant
- 1 - Residual saturations and relative permeabilities are dependent on capillary number
- 2 - Residual saturations and relative permeabilities are dependent on trapping number

Note: ITRAP=2 is currently not available with the curvilinear grid option (ICOORD=4) or when gas is present (IGAS \geq 1)

T11 - Capillary desaturation curve parameter for aqueous phase.

T22 - Capillary desaturation curve parameter for oleic phase.

T33 - Capillary desaturation curve parameter for microemulsion phase.

Note: Options ITRAP=1 and ITRAP=2 are identical for 1-d displacement in the vertical direction with zero capillary pressure. See [Section 2 of the UTCHEM Technical Documentation](#) for more information on the capillary and trapping number options.

Relative Permeability Data (input lines 3.4.32-3.4.60)

3.4.32 IPERM

IPERM - Flag indicating which relative permeability and capillary pressure model is used.

Possible Values:

- 0 - Imbibition Corey
- 1 - First drainage Corey (only for two phase water/oil flow)
- 2 - Parker and Lenhard's model for water-wet porous media with hysteresis option
- 3 - Lenhard's model for mixed-wet porous media including hysteresis

Note: Lenhard's model (IPERM=3) is for two phase oil/water only. See [Section 14 of the UTCHEM Technical Documentation](#) for more details on this option.

3.4.33 IHYST (This line is read only if IPERM=2)

IHYST - Flag indicating whether the hysteresis is used with Parker and Lenhard's model (IPERM=2)

Possible Values:

0 - Hysteretic model is not used

1 - Hysteretic model is used

Note: See [Section 3 of the UTCHEM Technical Documentation](#) for more details on this option.

3.4.34 IPARK (This line is read only if IPERM=2 and IHYST=1)

IPARK - Flag indicating the model used to calculate the oil trapping for hysteretic model

Possible Values:

0 - Kalurachchi and Parker's model is used

1 - Parker and Lenhard's model is used

Low Capillary Number Data (input lines 3.4.35-3.4.57)

3.4.35 ISRW, IPRW, IEW (This line is read only for IPERM< 2)

ISRW - Flag indicating type of residual saturation.

Possible Values:

0 - Constant residual saturation for entire reservoir

1 - Constant residual saturation for each layer

2 - Residual saturation specified for each gridblock

IPRW - Flag indicating type of endpoint relative permeability.

Possible Values:

0 - Constant endpoint relative permeability for entire reservoir

1 - Constant endpoint relative permeability for each layer

2 - Endpoint relative permeability specified for each gridblock

IEW - Flag indicating type of relative permeability exponent.

Possible Values:

0 - Constant relative permeability exponent for entire reservoir

1 - Constant relative permeability exponent for each layer

2 - Relative permeability exponent specified for each gridblock

3.4.36 ISRW (This line is read only if IPERM=2 or 3)

ISRW - Flag indicating type of residual saturation.

Possible Values:

0 - Constant residual saturation for entire reservoir

1 - Constant residual saturation for each layer

2 - Residual saturation specified for each gridblock

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Refer to the following table to help determine which input lines should be used to specify the relative permeability parameters for different options:

IPERM = 0 or 1 (imbibition Corey or first drainage Corey)	ISRW [residual saturation]	
	0 (constant for reservoir)	3.4.37
	1 (constant for each layer)	3.4.38-3.4.40
	2 (each gridblock)	3.4.41-3.4.43
	IPRW [endpoint rel. perm.]	
	0 (constant for reservoir)	3.4.44
	1 (constant for each layer)	3.4.45-3.4.47
	2 (each gridblock)	3.4.48-3.4.50
	IEW [rel. perm. exponent]	
	0 (constant for reservoir)	3.4.51
	1 (constant for each layer)	3.4.52-3.4.54
	2 (each gridblock)	3.4.55-3.4.57
IPERM = 2 or 3 (Parker and Lenhard for water-wet or Lenhard for mixed-wet)	ISRW [residual saturation]	
	0 (constant for reservoir)	3.4.37
	1 (constant for each layer)	3.4.38-3.4.40
	2 (each gridblock)	3.4.41-3.4.43

3.4.37 S1RWC, S2RWC, S3RWC (This line is read only if ISRW=0)

S1RWC - Residual saturation of aqueous phase displaced by oil at low capillary number for entire reservoir.
Units: fraction

S2RWC - Residual saturation of oleic phase displaced by water at low capillary number for entire reservoir.
Units: fraction

S3RWC - Residual saturation of microemulsion phase displaced by water at low capillary number for entire reservoir.
Units: fraction

3.4.38 S1RW(K), for K=1, NZ (This line is read only if ISRW=1)

S1RW(K) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for Kth layer.
Units: fraction

Note: S1RW(K) must begin a separate line in the input file for each layer. See the note for input line 3.3.5 for information on how the data is read.

3.4.39 S2RW(K), for K=1, NZ (This line is read only if ISRW=1)

S2RW(K) - Residual saturation of oleic phase displaced by water at low capillary number for Kth layer.

Units: fraction

Note: S2RW(K) must begin a separate line in the input file for each layer. See the note for input line 3.3.5 for information on how the data is read.

3.4.40 S3RW(K), for K=1, NZ (This line is read only if ISRW=1)

S3RW(K) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for Kth layer.

Units: fraction

Note: S3RW(K) must begin a separate line in the input file for each layer. See the note for input line 3.3.5 for information on how the data is read.

3.4.41 S1RW(I), for I=1, NX × NY × NZ (This line is read only if ISRW=2)

S1RW(I) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for Ith gridblock.

Units: fraction

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.42 S2RW(I), for I=1, NX × NY × NZ (This line is read only if ISRW=2)

S2RWC(K) - Residual saturation of oleic phase displaced by water at low capillary number for Ith gridblock.

Units: fraction

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.43 S3RW(I), for I=1, NX × NY × NZ (This line is read only if ISRW=2)

S3RW(I) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for Ith gridblock.

Units: fraction

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

Relative Permeability Endpoint and Exponent Data (input lines 3.4.44-3.4.57) — These lines are **required only if** Corey function (**IPERM<2**) is used.

3.4.44 P1RWC, P2RWC, P3RWC (This line is read only if IPERM<2 and IPRW=0)

P1RWC - End point relative permeability of water at low capillary number for entire reservoir.
Units: dimensionless

P2RWC - End point relative permeability of oil at low capillary number for entire reservoir.
Units: dimensionless

P3RWC - End point relative permeability of microemulsion at low capillary number for entire reservoir.
Units: dimensionless

3.4.45 P1RW(K), for K=1, NZ (This line is read only if IPERM<2 and IPRW=1)

P1RW(K) - Constant endpoint relative permeability of water at low capillary number for Kth layer.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.46 P2RW(K), for K=1, NZ (This line is read only if IPERM<2 and IPRW=1)

P2RW(K) - Constant endpoint relative permeability of oil at low capillary number for Kth layer.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.47 P3RW(K), for K=1, NZ (This line is read only if IPERM<2 and IPRW=1)

P3RW(K) - Constant endpoint relative permeability of microemulsion at low capillary number for Kth layer.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.48 P1RW(I), for I=1, NX × NY × NZ (This line is read only if IPERM<2 and IPRW=2)

P1RW(I) - Endpoint relative permeability of water at low capillary number for Ith gridblock.
Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

- 3.4.49 P2RW(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IPERM<2 and IPRW=2)

P2RW(I) - Endpoint relative permeability of oil at low capillary number for Ith gridblock.

Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

- 3.4.50 P3RW(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IPERM<2 and IPRW=2)

P3RW(I) - Endpoint relative permeability of microemulsion at low capillary number for Ith gridblock.

Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

- 3.4.51 E1WC, E2WC, E3WC (This line is read only if IPERM<2 and IEW=0)

E1WC - Phase relative permeability exponent for aqueous phase at low capillary number for entire reservoir.

Units: dimensionless

E2WC - Phase relative permeability exponent for oleic phase at low capillary number for entire reservoir.

Units: dimensionless

E3WC - Phase relative permeability exponent for microemulsion phase at low capillary number system for entire reservoir.

Units: dimensionless

- 3.4.52 E1W(K), for K=1, NZ (This line is read only if IPERM<2 and IEW=1)

E1W(K) - Relative permeability exponent of aqueous phase at low capillary number for Kth layer.

Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

- 3.4.53 E2W(K), for K=1, NZ (This line is read only if IPERM<2 and IEW=1)

E2W(K) - Relative permeability exponent of oleic phase at low capillary number for Kth layer.

Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.54 E3W(K), for K=1, NZ (This line is read only if IPERM<2 and IEW=1)

E3W(K) - Relative permeability exponent of microemulsion phase at low capillary number for Kth layer.

Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.55 E1W(I), for I=1, NX × NY × NZ (This line is read only if IPERM<2 and IEW=2)

E1W(I) - Relative permeability exponent of aqueous phase at low capillary number for Ith gridblock.

Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.56 E2W(I), for I=1, NX × NY × NZ (This line is read only if IPERM<2 and IEW=2)

E2W(I) - Relative permeability exponent of oleic phase at low capillary number for Ith gridblock.

Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.57 E3W(I), for I=1, NX × NY × NZ (This line is read only if IPERM<2 and IEW=2)

E3W(I) - Relative permeability exponent of microemulsion phase at low capillary number for Ith gridblock.

Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

High Capillary Number Data (input lines 3.4.58-3.4.60) — These lines are required only if ITRAP=1 or ITRAP=2.

3.4.58 S1RC, S2RC, S3RC (This line is read only if ITRAP=1 or 2)

S1RC - Residual saturation of aqueous phase at high capillary number.

Units: fraction

S2RC - Residual saturation of oleic phase at high capillary number.

Units: fraction

S3RC - Residual saturation of microemulsion phase at high capillary number.

Units: fraction

Note: The residual saturations at high capillary number can not be set equal to those at low capillary number.

3.4.59 P1RC, P2RC, P3RC (This line is read only for ITRAP=1 or 2 and IPERM< 2)

P1RC - End point relative permeability of aqueous phase at high capillary number condition.
Units: dimensionless

P2RC - End point relative permeability of oleic phase at high capillary number condition.
Units: dimensionless

P3RC - End point relative permeability of microemulsion phase at high capillary number condition.
Units: dimensionless

3.4.60 E13C, E23C, E31C (This line is read only for ITRAP=1 or 2 and IPERM< 2)

E13C, E23C, E31C - Parameters used for calculating exponents for relative permeability calculations at high capillary number.
Units: dimensionless

Viscosity Data (input lines 3.4.61-3.4.66)

3.4.61 VIS1, VIS2, TSTAND

VIS1 - Water viscosity at reference temperature.
Units: cp = mPa.s

VIS2 - Oil viscosity at reference temperature.
Units: cp = mPa.s

TSTAND - Reference temperature
Units: °F (IUNIT=0) or °C (IUNIT=1)

3.4.62 IOVIS (This line is read only if NO>1)

IOVIS - Flag indicating whether the viscosity is a function of organic composition.
Possible Values:

0 - Viscosity does not depend on the organic species concentration.

1 - Viscosity depends on the organic species concentration.

Note: See Section 2 of the UTCHEM Technical Documentation for more information on the IOVIS=0 option and Section 7 of the UTCHEM Technical Documentation for more information on the IOVIS=1 option.

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3.4.64 OVIS(K), for K=1, NO (This line is read only if NO>1 and IOVIS=1)

OVIS(K) - Viscosity for organic component K at reference temperature.
Units: cp = mPa.s

3.4.64 VIS4, VSLOPG (This line is read only if IGAS≥1)

VIS4 - Gas viscosity at reference temperature and reference pressure.
Units: cp = mPa.s

VSLOPG - Slope of gas viscosity.
Units: (psi)⁻¹ (IUNIT=0) or (kPa)⁻¹ (IUNIT=1)

3.4.65 BVI(1), BVI(2) (This line is read only if IENG=1)

BVI(1) - Parameter for calculating water viscosity as a function of reservoir temperature.
Units: (°K)⁻¹

BVI(2) - Parameter for calculating oil viscosity as a function of reservoir temperature.
Units: (°K)⁻¹

3.4.66 BVI(4) (This line is read only if IGAS≥1 and IENG=1)

BVI(4) - Parameter for calculating gas viscosity as a function of reservoir temperature.
Units: (°K)⁻¹

Corey Option Gas Relative Permeability Data (input lines 3.4.67-3.4.78)

— These lines are **required only if IGAS≥1 and IPERM=0.**

Refer to the following table to help determine which input lines should be used to specify the gas relative permeability parameters for different options:

ISRW (residual saturation flag)	0 (constant for reservoir)	3.4.67
	1 (constant for each layer)	3.4.68-3.4.69
	2 (variable over reservoir)	3.4.70-3.4.71
IPRW (endpoint relative permeability flag)	0 (constant for reservoir)	3.4.72
	1 (constant for each layer)	3.4.73
	2 (variable over reservoir)	3.4.74
IEW (relative permeability exponent flag)	0 (constant for reservoir)	3.4.75
	1 (constant for each layer)	3.4.76
	2 (variable over reservoir)	3.4.77

3.4.67 S2RWC4, S4RWC (This line is read only if ISRW=0)

S2RWC4 - Constant residual oil saturation to displacing gas phase for entire reservoir.
Units: fraction

S4RWC - Constant residual gas saturation for entire reservoir.
Units: fraction

3.4.68 S2RW4(K), for K=1, NZ (This line is read only if ISRW=1)

S2RW4(K) - Constant residual oil saturation to displacing gas phase for Kth layer.
Units: fraction

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.69 S4RW(K), for K=1, NZ (This line is read only if ISRW=1)

S4RW(K) - Constant residual gas saturation for Kth layer.
Units: fraction

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.70 S2RW4(I), for I=1, NX × NY × NZ (This line is read only if ISRW=2)

S2RW4(I) - Constant residual oil saturation to displacing gas phase for Ith gridblock.
Units: fraction

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.71 S4RW(I), for I=1, NX × NY × NZ (This line is read only if ISRW=2)

S4RW(I) - Residual gas saturation for Ith gridblock.
Units: fraction

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.72 P4RWC (This line is read only if IPRW=0)

P4RWC - Constant gas endpoint relative permeability for entire reservoir.
Units: dimensionless

3.4.73 P4RW(K), for K=1, NZ (This line is read only if IPRW=1)

P4RW(K) - Constant gas endpoint relative permeability for Kth layer.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.74 P4RW(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IPRW=2)

P4RW(I) - Constant gas endpoint relative permeability for Ith gridblock.
Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.75 E4WC (This line is read only if IEW=0)

E4WC - Constant gas relative permeability exponent for entire reservoir.
Units: dimensionless

3.4.76 E4W(K), for K=1, NZ (This line is read only if IEW=1)

E4W(K) - Constant gas relative permeability exponent for Kth layer.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

3.4.77 E4W(I), for I=1, $NX \times NY \times NZ$ (This line is read only if IEW=2)

E4W(I) - Constant gas relative permeability exponent for Ith gridblock.
Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.78 S4RC, P4RC, E4C, T44 (This line is read only if ITRAP=1)

S4RC - Residual gas saturations at high capillary number.
Units: fraction

P4RC - Gas endpoint relative permeability at high capillary number.
Units: dimensionless

E4C - Gas relative permeability exponent at high capillary number.
Units: dimensionless

T44 - Gas phase trapping parameter.
Units: dimensionless

3.4.79 XIFTG, XIFTGW (This line is read only if IGAS \geq 1 or IPERM=2)

XIFTG - Log of interfacial tension between gas and oil.
Units: dyne/cm = mN/m

XIFTGW - Log of interfacial tension between gas and water.
Units: dyne/cm = mN/m

Microemulsion Viscosity Data (input line 3.4.80)

3.4.80 ALPHAV(I), for I=1, 5

ALPHAV(I) - Compositional phase viscosity parameters.

Units: dimensionless

Note: All five viscosity parameters must be positive values.

Note: See Section 2 of the UTCHEM Technical Documentation for more information on the compositional viscosity model.

Polymer Property Data (input lines 3.4.81-3.4.84) — See Section 2 of the UTCHEM Technical Documentation for information on the polymer property models.

3.4.81 AP1, AP2, AP3

AP1, AP2, AP3 - Parameters used for calculating polymer viscosity at zero shear rate as a function of polymer and electrolyte concentrations.

Units: (wt. %)⁻¹, (wt. %)⁻², (wt. %)⁻³

3.4.82 BETAP, CSE1, SSLOPE

BETAP - Parameter for calculating the effective divalent salinity used to calculate polymer viscosity.

Units: dimensionless

CSE1 - Value below which the polymer viscosity is considered to be independent of salinity.

Units: meq/ml

SSLOPE - Slope of viscosity vs. effective salinity on a log-log plot—assumed to be constant.

Units: dimensionless

Note: This value is usually large and negative for hydrolyzed polyacrylamides and small and positive for polysaccharides.

3.4.83 GAMMAC, GAMHF, POWN

GAMMAC - Coefficient in shear rate equation below.

Units: $\frac{\text{day(darcy)}^{1/2}}{\text{ft} - \text{sec}}$ (IUNIT=0) or $\frac{\text{day}(\mu\text{m}^2)^{1/2}}{\text{m} - \text{sec}}$ (IUNIT=1)



GAMHF - Shear rate at which polymer viscosity is one half polymer viscosity at zero shear rate.

Units: sec⁻¹

POWN - Exponent for calculating shear rate dependence of polymer viscosity.

Units: dimensionless

3.4.84 IPOLYM, EPHI3, EPHI4, BRK, CRK

IPOLYM - Flag indicating type of polymer partitioning.

Possible Values:

0 - All polymer exists in aqueous phase if aqueous phase exists;
otherwise, it exists completely in microemulsion phase

1 - Partitioning of polymer to water component is constant

EPHI3 - Effective porosity for surfactant—ratio of apparent porosity for surfactant to actual porosity.

Units: dimensionless

EPHI4 - Effective porosity for polymer—ratio of apparent porosity for polymer to actual porosity.

Units: dimensionless

BRK - Parameter for calculating permeability reduction factor.

Units: $\frac{\text{volume of polymer} - \text{rich phase}}{\text{weight\% polymer}}$

CRK - Parameter for calculating permeability reduction factor.

Units: $(\text{darcy})^{1/2} (100 \text{ g/g})^{-1/3} = (\mu\text{m}^2)^{1/2} (100 \text{ g/g})^{-1/3}$

Note: EPHI3 and EPHI4 are used to account for inaccessible pore volume in the case of surfactant and polymer.

$$\phi_{\text{surfactant}} = \phi \times \text{EPHI3}$$

$$\phi_{\text{polymer}} = \phi \times \text{EHPI4}$$

The effect of permeability reduction or residual resistance is to reduce the mobility of the polymer rich phase. This is accounted for by multiplying the viscosity of the phase by BRK.

Component Density Data (input lines 3.4.85-3.4.92)

3.4.85 DEN1, DEN2, DEN23, DEN3, DEN7, DEN8, IDEN (This line is read only if NO≤1)

DEN1 - Specific weight or density of water (Component 1).

Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN2 - Specific weight or density of oil (Component 2).

Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN23 - Coefficient of oil in microemulsion phase density calculations.

Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN3 - Specific weight or density of surfactant (Component 3).

Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN7 - Specific weight or density of Alcohol 1 (Component 7).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN8 - Specific weight or density of Alcohol 2 (when IGAS=0) or gas (when IGAS≥1) (Component 7).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

IDEN - Flag indicating if gravity effect should be considered.
Possible Values:
1 - Do not consider gravity effect
2 - Consider gravity effect

3.4.86 **DEN1, DEN2, DEN3, DEN7, DEN8, IDEN, IODEN** (This line is read only if NO>1)

DEN1 - Specific weight or density of water (Component 1).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN2 - Specific weight or density of oil (Component 2).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN3 - Specific weight or density of surfactant (Component 3).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN7 - Specific weight or density of Alcohol 1 (Component 7).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

DEN8 - Specific weight or density of Alcohol 2 (when IGAS=0) or gas (when IGAS≥1) (Component 7).
Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

IDEN - Flag indicating if gravity effect should be considered.
Possible Values:
1 - Do not consider gravity effect
2 - Consider gravity effect

IODEN - Flag indicating if specific weight/density is a function of organic species concentration.

Possible Values:
0 - Does not depend on organic species concentration
1 - Depends on organic species concentration

Note: See Section 2 of the UTCHEM Technical Documentation for information on the IODEN=0 option or Section 7 of the UTCHEM Technical Documentation for information on the IODEN=1 option.

Note: Specific weight for pure water is 0.433 psi/ft (density of 1 g/cm³). IODEN must be set to 1 if any non-aqueous phase species (those with indices < (8+NO)) participate in biodegradation equations.

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Multiple Organic Density Data (input lines 3.4.87-3.4.88) — These lines are **required only if IODEN=1 and NO>1**.

3.4.87 DNOILC(K), for K=1, NO (This line is read only if IODEN=1 and NO>1)

DNOILC(K) - Specific weight or density of organic component K for oleic phase.

Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

3.4.88 DNAME(K), for K=1, NO (This line is read only if IODEN=1 and NO>1)

DNAME(K) - Specific weight or density of organic component K for microemulsion phase.

Units: psi/ft (IUNIT=0) or g/cm³ (IUNIT=1)

Multiple Organic Data (input lines 3.4.89-3.4.92) — These lines are **required only if NO>1**. Furthermore, if (**IFGHBN=1 and IOD=0**) or **IOVIS=1**.

3.4.89 INAME (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)))

INAME - Flag indicating whether name of the organic components will be provided by user.

Possible Values:

0 - Name of the organic components will be provided; the molecular weight and equivalent alkane carbon number will be obtained from the built-in database

1 - Molecular weight and equivalent alkane carbon number for each organic components will be provided.

3.4.90 ONAME(K), for K=1, NO (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)) and INAME=0)

ONAME(K) - Name of organic component K. See input line 3.4.14 for a list of valid component names.

3.4.91 OMWT(K), for K=1, NO (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)) and INAME=1)

OMWT(K) - Molecular weight for organic component K.

3.4.92 OEACN(K), for K=1, NO (This line is read only if NO>1 and ((IFGHBN=1 and IOD=0) or IOVIS=1)) and INAME=1)

OEACN(K) - equivalent alkane carbon number for organic component K.

Note: See Section 7 of the UTCHEM Technical Documentation for information on the equivalent alkane carbon number.

3.4.93 ISTB

ISTB - Flag indicating the units to be used when printing injection and production rates.

Possible Values:

0 - Rates printed at bottomhole condition in ft³ or m³

1 - Rates printed at surface condition in bbls

3.4.94 FVF(L), for L=1, MXP (This line is read only if ISTB=1 and IUNIT=0)

FVF(L) - Formation volume factor for Lth phase.

Units: SCF/ft³

Note: MXP=3 when IGAS=0 and MXP=4 when IGAS≥1.

Fluid Compressibility Data (input lines 3.4.95-3.4.97)

3.4.95 COMPC(1), COMPC(2), COMPC(3), COMPC(7), COMPC(8)

COMPC(1) - Compressibility of brine (Component 1).

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

COMPC(2) - Compressibility of oil (Component 2).

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

COMPC(3) - Compressibility of surfactant (Component 3).

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

COMPC(7) - Compressibility of Alcohol 1 (Component 7).

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

COMPC(8) - Compressibility of Alcohol 2 (when IGAS=0) or gas (when IGAS≥1) (Component 8).

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

Note: For incompressible fluids, values of zero should be used for the COMPC values listed above.

3.4.96 ICOMPO (This line is read only if NO>1)

ICOMPO - Flag indicating whether each organic component has different compressibility.

Possible Values:

0 - All organic components have the same compressibility as COMPC(2)

1 - Each organic component has different compressibility

3.4.97 COMPC(KC), for KC=1, NO (This line is read only if NO>1 and ICOMPO=1)

COMPC(KC) - Compressibility of organic component KC.

Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

Capillary Pressure Data (input lines 3.4.98-3.4.116) — See Sections 2, 3, and 14 of the UTCHEM Technical Documentation for capillary pressure information.

3.4.98 ENTP, CLAMDA, ALPDS, ALPWS, VNDS, VNWS, PNEG (This line is read only if IPERM=3)

ENTP - Brooks-Corey entry pressure.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

CLAMDA - Exponent of Brooks-Corey capillary pressure function.

ALPDS - Alpha parameter in the van Genuchten capillary pressure function for drying path (water saturation is decreasing).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

ALPWS - Alpha parameter in the van Genuchten capillary pressure function for wetting path (water saturation is increasing).
Units: 1/psi (IUNIT=0) or 1/kPa (IUNIT=1)

VNDS - Exponent n in the van Genuchten capillary pressure function for drying path.

VNWS - Exponent n in the van Genuchten capillary pressure function for wetting path.

PNEG - Maximum negative capillary pressure.
Units: psi (IUNIT=0) or kPa (IUNIT=1)
Note: The value for PNEG must be a negative number.

3.4.99 ICPC, IEPC, IOW (This line is read only if IPERM≤2)

ICPC - Flag indicating type of capillary pressure endpoint.
Possible Values:
0 - Constant capillary pressure endpoint for entire reservoir
1 - Constant capillary pressure endpoint for each layer
2 - Capillary pressure endpoint specified for each gridblock

IEPC - Flag indicating type of capillary pressure exponent.
Possible Values:
0 - Constant capillary pressure exponent for entire reservoir
1 - Constant capillary pressure exponent for each layer
2 - Capillary pressure exponent specified for each gridblock

IOW - Flag indicating the wettability for two-phase oil/water capillary pressure calculations using imbibition Corey function (IPERM=0).
Possible Values:
0 - The capillary pressure curve is for strongly water-wet rock (default)
1 - The capillary pressure curve is for strongly oil-wet rock
2 - The capillary pressure curve is for mixed-wet rocks
Note: IOW=1 and 2 are only available with the imbibition Corey function (IPERM=0).

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Refer to the following table to help determine which input lines should be used to specify the capillary pressure data for different values of IPERM:


If IPERM = 0		
IOW=0 or 1 (strongly water- or oil-wet)	ICPC [capillary pressure endpoint] 0 (constant for reservoir) 1 (constant for each layer) 2 (variable over reservoir)	3.4.100
		3.4.101
		3.4.102
	IEPC [capillary pressure exponent] 0 (constant for reservoir) 1 (constant for each layer) 2 (variable over reservoir)	3.4.103
		3.4.104
		3.4.105
IOW = 2 (mixed-wet)	ICPC [capillary pressure endpoint] 0 (constant for reservoir) 1 (constant for each layer) 2 (variable over reservoir)	3.4.106
		3.4.107-3.4.111
		3.4.112-3.4.116
If IPERM = 1 or 2		
IOW=0 (strongly water-wet)	ICPC [capillary pressure endpoint] 0 (constant for reservoir) 1 (constant for each layer) 2 (variable over reservoir)	3.4.100
		3.4.101
		3.4.102
	IEPC [capillary pressure exponent] 0 (constant for reservoir) 1 (constant for each layer) 2 (variable over reservoir)	3.4.103
		3.4.104
		3.4.105
If IPERM=3 go to input line 3.4.117		

Capillary Pressure Data for Strongly Water- or Oil-Wet Rocks (input lines 3.4.100-3.4.105) — These lines are **required only if IPERM≤2 and IOW<2**.

3.4.100 CPC0 (This line is read only if IPERM≤2 and IOW<2 and ICPC=0)

CPC0 - Capillary pressure endpoint for entire reservoir (if IPERM<2) or van Genuchten capillary pressure parameter, α , for entire reservoir (if IPERM=2).

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Units:	<u>if IUNIT=0</u>	<u>if IUNIT=1</u>
if IPERM<2:	psi $\sqrt{\text{darcies}}$	kPa $\sqrt{\mu\text{m}^2}$ 
if IPERM=2:	$(\text{psi} \sqrt{\text{darcies}})^{-1}$	$\sqrt{\mu\text{m}^2} / \text{kPa}$

3.4.101 CPC(K), for K=1, NZ (This line is read only if IPERM≤2 and IOW<2 and ICPC=1)

CPC(K) - Capillary pressure endpoint for Kth layer (if IPERM<2) or van Genuchten capillary pressure parameter, α, for Kth layer (if IPERM=2).

Units:	<u>if IUNIT=0</u>	<u>if IUNIT=1</u>
if IPERM<2:	psi $\sqrt{\text{darcies}}$	kPa $\sqrt{\mu\text{m}^2}$
if IPERM=2:	$(\text{psi} \sqrt{\text{darcies}})^{-1}$	$\sqrt{\mu\text{m}^2} / \text{kPa}$

3.4.102 CPC(I), for I=1, NX × NY × NZ (This line is read only if IPERM≤2 and IOW<2 and ICPC=2)

CPC(I) - Capillary pressure endpoint for Ith gridblock (if IPERM<2) or van Genuchten capillary pressure parameter, α, for Ith gridblock (if IPERM=2).

Units:	<u>if IUNIT=0</u>	<u>if IUNIT=1</u>
if IPERM<2:	psi $\sqrt{\text{darcies}}$	kPa $\sqrt{\mu\text{m}^2}$
if IPERM=2:	$(\text{psi} \sqrt{\text{darcies}})^{-1}$	$\sqrt{\mu\text{m}^2} / \text{kPa}$

3.4.103 EPC0 (This line is read only if IPERM≤2 and IOW<2 and IEPC=0)

EPC0 - Capillary pressure exponent for entire reservoir (if IPERM<2) or van Genuchten capillary pressure parameter, n, for entire reservoir (if IPERM=2).

Units: dimensionless

3.4.104 EPC(K), for K=1, NZ (This line is read only if IPERM≤2 and IOW<2 and IEPC=1)

EPC(K) - Capillary pressure exponent for Kth layer (if IPERM<2) or van Genuchten capillary pressure parameter, n, for Kth layer (if IPERM=2).

Units: dimensionless

3.4.105 EPC(I), for I=1, NX × NY × NZ (This line is read only if IPERM≤2 and IOW<2 and IEPC=2)

EPC(I) - Capillary pressure exponent for Ith gridblock (if IPERM<2) or van Genuchten capillary pressure parameter, n, for Ith gridblock (if IPERM=2).

Units: dimensionless

Capillary Pressure Data for Mixed-Wet Rocks using Corey's option (input lines 3.4.106-3.4.116) — These lines are **required only if IPERM=0 and IOW=2**.

- 3.4.106 CPCW, EPCW, CPCO, EPCO, SSTAR (This line is read only if IPERM=0 and IOW=2 and ICPC=0)

CPCW - Capillary pressure endpoint for entire reservoir for positive branch.

Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

EPCW - Capillary pressure exponent for entire reservoir for positive branch.

Units: dimensionless

CPCO - Capillary pressure endpoint for entire reservoir for negative branch.

Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

EPCO - Capillary pressure exponent for entire reservoir for negative branch.

Units: dimensionless

SSTAR - Water saturation where the capillary pressure is zero.

Units: dimensionless

- 3.4.107 CPC(K,1), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

CPC(K,1) - Capillary pressure endpoint for Kth layer for positive branch.

Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

Note: See the note for input line 3.3.5 for information on how the data is read.

- 3.4.108 EPC(K,1), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

EPC(K,1) - Capillary pressure exponent for Kth layer for positive branch.

Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

- 3.4.109 CPC(K,2), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

CPC(K,2) - Capillary pressure endpoint for Kth layer for negative branch.

Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

Note: See the note for input line 3.3.5 for information on how the data is read.

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- 3.4.110 EPC(K,2), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

EPC(K,2) - Capillary pressure exponent for Kth layer for negative branch.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

- 3.4.111 SSTAR(K), for K=1, NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=1)

SSTAR(K) - Water saturation for Kth layer where the capillary pressure is zero.
Units: dimensionless

Note: See the note for input line 3.3.5 for information on how the data is read.

- 3.4.112 CPC(I,1), for I=1, NX × NY × NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

CPC(I,1) - Capillary pressure endpoint for Ith gridblock for positive branch.
Units: psi√darcies (IUNIT=0) or kPa√μm² (IUNIT=1)

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

- 3.4.113 EPC(I,1), for I=1, NX × NY × NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

EPC(I,1) - Capillary pressure exponent for Ith gridblock for positive branch.
Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

- 3.4.114 CPC(I,2), for I=1, NX × NY × NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

CPC(I,2) - Capillary pressure endpoint for Ith gridblock for negative branch.
Units: psi√darcies (IUNIT=0) or kPa√μm² (IUNIT=1)

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

- 3.4.115 EPC(I,2), for I=1, NX × NY × NZ (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

EPC(I,2) - Capillary pressure exponent for Ith gridblock for negative branch.
Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

3.4.116 SSTAR(I), for I= 1, $NX \times NY \times NZ$ (This line is read only if IPERM=0 and IOW=2 and ICPC=2)

SSTAR(I) - Water saturation in Ith gridblock where the capillary pressure is zero.
Units: dimensionless

Note: See the note for input line 3.3.6 for information on how this data should be ordered.

Diffusion and Dispersion Data (input lines 3.4.117-3.4.124)

3.4.117 D(KC,1), for KC=1, N

D(KC,1) - Molecular diffusion coefficient of KCth component in aqueous phase.

Units: ft²/day (IUNIT=0) or m²/day (IUNIT=1)

Note: The input diffusion coefficient should be divided by tortuosity (D/τ) where the value of tortuosity is greater than one.

3.4.118 D(KC,2), for KC=1, N

D(KC,2) - Molecular diffusion coefficient of KCth component in oleic phase.

Units: ft²/day (IUNIT=0) or m²/day (IUNIT=1)

Note: The input diffusion coefficient should be divided by tortuosity (D/τ) where the value of tortuosity is greater than one.

3.4.119 D(KC,3), for KC=1, N

D(KC,3) - Molecular diffusion coefficient of KCth component in microemulsion phase.

Units: ft²/day (IUNIT=0) or m²/day (IUNIT=1)

Note: The input diffusion coefficient should be divided by tortuosity (D/τ) where the value of tortuosity is greater than one.

3.4.120 D(KC,4), for KC=1, N (This line is read only if IGAS≥1)

D(KC,4) - Molecular diffusion coefficient of KCth component in gas phase.

Units: ft²/day (IUNIT=0) or m²/day (IUNIT=1)

Note: The input diffusion coefficient should be divided by tortuosity (D/τ) where the value of tortuosity is greater than one.

3.4.121 ALPHAL(1), ALPHAT(1)

ALPHAL(1) - Longitudinal dispersivity of aqueous phase.

Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(1) - Transverse dispersivity of aqueous phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.4.122 ALPHAL(2), ALPHAT(2)

ALPHAL(2) - Longitudinal dispersivity of oleic phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(2) - Transverse dispersivity of oleic phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.4.123 ALPHAL(3), ALPHAT(3)

ALPHAL(3) - Longitudinal dispersivity of microemulsion phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(3) - Transverse dispersivity of microemulsion phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

3.4.124 ALPHAL(4), ALPHAT(4) (This line is read only if IGAS \geq 1)

ALPHAL(4) - Longitudinal dispersivity of gas phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

ALPHAT(4) - Transverse dispersivity of gas phase.
Units: feet (IUNIT=0) or m (IUNIT=1)

Adsorption Data (input lines 3.4.125-3.4.130)

3.4.125 IADSO

IADSO - Organic adsorption calculation flag.

Possible Values

- 0 - Organic adsorption is not considered
- 1 - Organic adsorption calculated using linear adsorption model
- 2 - Organic adsorption calculated using Langmuir isotherm
- 3 - Organic adsorption calculated using Freundlich isotherm

Note: See Section 13 of the UTCHEM Technical Documentation for information on the organic adsorption isotherm models.

3.4.126 IREV, DENS, IKADS (This line is read only if IADSO>0)

IREV - Flag indicating if organic adsorption is reversible or not.

Possible Values:

- 0 - Irreversible organic adsorption
- 1 - Reversible organic adsorption

DENS - Grain soil density

Units: lb/ft³ (IUNIT=0), g/cc (IUNIT=1)

IKADS - Flag indicating constant or variable organic adsorption parameter for reservoir.

Possible Values:

- 0 - Constant organic adsorption parameter for entire reservoir
- 1 - Constant organic adsorption parameter for each layer
- 2 - Organic adsorption parameter specified for each gridblock

3.4.127 AD21(1,KO), AD22(1,KO), for KO=1, NO (This line is read only if IADSO>0 and IKADS=0)

AD21(1,KO) - Adsorption parameter for KOth organic component.

AD22(1,KO) - Adsorption parameter for KOth organic component.

Note: This line is read at least once even if NO=0.

All elements of the AD21(n,KO) array will be set equal to AD21(1,KO) and all elements of the AD22(n,KO) array will be set equal to AD22(1,KO).

Example: If there are two organic components (NO=2) with adsorption parameters of 0.6 & 1.0 for the first component and 0.3 & 1.0 for the second component, this line will be repeated twice (once for each component) as follows:

```
0.6    1.0
0.3    1.0
```

3.4.128 AD21(K,KO), AD22(K,KO), for K=1, NZ, for KO=1, NO (This line is read only if IADSO>0 and IKADS=1)

AD21(K,KO) - Adsorption parameter for KOth organic component in the Kth layer.

AD22(K,KO) - Adsorption parameter for KOth organic component in the Kth layer.

Note: This line is read at least once even if NO=0. See the note for input line 3.3.5 for information on how the data is read.

The user should provide NO sets (1 per organic component) of NZ lines of data (1 per layer in the Z direction) of adsorption parameter pairs. Each of these adsorption parameter sets is preceded by 3 comment lines.

Example: If there are two organic components (NO=2), and three layers (NZ=3), the input data would appear as follows:

```
CC
CC
*----AD21    AD22    (1st organic component)
          0.6    1.0
          0.6    1.0
          0.6    1.0
CC
```

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```

CC
*----AD21      AD22  (2nd organic component)
      0.3      1.0
      0.3      1.0
      0.3      1.0

```

3.4.129 The data on input lines 3.4.129.a and 3.4.129.b are repeated for KO=1 to NO times. See note following input line 3.4.129.b for more information.

3.4.129.a AD21(I,KO), for I=1, $NX \times NY \times NZ$ (This line is read only if IADSO>0 and IKADS=2)

AD21(I,KO) - Adsorption parameter for KO^{th} organic component in I^{th} gridblock.

3.4.129.b AD22(I,KO), for I=1, $NX \times NY \times NZ$ (This line is read only if IADSO>0 and IKADS=2)

AD22(I,KO) - Adsorption parameter for KO^{th} organic component in I^{th} gridblock.

Note: This line is read at least once even if NO=0. See the note for input line 3.3.6 for information on how this data should be ordered.

The user should provide NO sets (1 per organic component) of $NX \times NY \times NZ$ adsorption parameters (1 per gridblock). Each set consists of a separate input line for the AD21 and AD22 parameters.

Example: If there are two organic components (NO=2), $NX=2$, $NY=2$, and $NZ=1$, the input data would appear as follows:

```

CC
CC
*----AD21      (1st organic component)
      0.6      0.6      0.6      0.6
CC
CC
*----AD22      (1st organic component)
      1.0      1.0      1.0      1.0
CC
CC
*----AD21      (2nd organic component)
      4*0.3
CC
CC
*----AD22      (2nd organic component)
      4*1.0

```

Note: This example also shows an input convention allowing the user to specify multiple occurrences of the same value. Using

4*0.3

is equivalent to using

0.3 0.3 0.3 0.3

3.4.130 AD31, AD32, B3D, AD41, AD42, B4D, IADK, IADS1, FADS, **REFK**

AD31 - Surfactant adsorption parameter.
Units: dimensionless

AD32 - Surfactant adsorption parameter.
Units: ml/meq

B3D - Surfactant adsorption parameter.
Units: $\frac{\text{volume of water}}{\text{volume of surfactant}}$

AD41 - Polymer adsorption parameter.
Units: dimensionless

AD42 - Polymer adsorption parameter.
Units: ml/meq

B4D - Polymer adsorption parameter.
Units: $\frac{\text{volume of water}}{\text{weight\% polymer}}$

IADK - Permeability dependent adsorption flag
Possible Values:
0 - Surfactant and polymer adsorption is independent of permeability
1 - Surfactant and polymer adsorption is dependent on permeability

IADS1 - Flag to specify the competitive surfactant adsorption in the presence of polymer
Possible Values:
0 - Surfactant and polymer adsorption are independent
1 - Competitive surfactant and polymer adsorption is considered

FADS - Parameter to adjust the competitive adsorption calculation

REFK - The reference permeability at which the surfactant and polymer adsorption input parameters are measured.
Units: md

Note: See [Section 2 of the UTCHEM Technical Documentation](#) for information on the surfactant and polymer adsorption model.

3.4.131 QV, XKC, XKS, EQW

QV - Cation exchange capacity of clays.
Units: meq/ml of pore volume

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XKC - Cation exchange constant for clays.

Units: (meq/ml)⁻¹

XKS - Cation exchange constant for surfactant.

Units: (meq/ml)⁻¹

EQW - Equivalent weight of surfactant.

Note: See Section 2 of the UTCHEM Technical Documentation for information on the cation exchange model.

Tracer Data (input lines 3.4.132-3.4.144) — These lines are **required only if NTW+NTA>0**. See Section 4 of the UTCHEM Technical Documentation for more details on tracer modeling in UTCHEM.

3.4.132 TK(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0)

TK(I) - Tracer partition coefficient for Ith water/oil tracer at initial chloride concentration and reference temperature. A value of 0.0 indicates a water or gas nonpartitioning tracer and a value of -1.0 indicates a nonpartitioning oil tracer.

Units: fraction

3.4.133 TKS(I), for I=1, NTW, **C5INI** (This line is read only if NTW>0)

TKS(I) - Parameter for calculating water/oil tracer partition coefficient for Ith tracer as a function of salinity.

Units: (meq/ml)⁻¹

C5INI - Reference salinity at which the partition coefficients are measured.

Units: meq/ml water

3.4.134 TKT(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and IENG=1)

TKT(I) - Parameter for calculating tracer partitioning coefficient for Ith tracer as a function of reservoir temperature.

Units: (°F)⁻¹ (IUNIT=0) or (°C)⁻¹ (IUNIT=1)

3.4.135 RDC(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0)

RDC(I) - Radioactive decay coefficient for Ith tracer. A value of 0.0 indicates a non-radioactive tracer.

Units: 1/days

3.4.136 RET(I), for I=1, NTW+NTA (This line is read only if NTW+NTA>0)

RET(I) - Tracer adsorption parameter (adsorbed concentration/flowing concentration). A value of 0.0 indicates no retardation.

Units: dimensionless

Dead-end Pore Model Data (input lines 3.4.137-3.4.140) — These lines are required only if **NTW+NTA>0** and **ICAP=1**.

3.4.137 FFL(1), FFH(1), CM(I,1), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1)

FFL(1) - Water phase flowing fraction at fractional flow = 0.0.
Units: dimensionless

FFH(1) - Water phase flowing fraction at fractional flow = 1.0.
Units: dimensionless

CM(I,1) - Mass transfer coefficients for Ith tracer in water phase.
Units: 1/sec

3.4.138 FFL(2), FFH(2), CM(I,2), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1)

FFL(2) - Oil phase flowing fraction at fractional flow = 0.0.
Units: dimensionless

FFH(2) - Oil phase flowing fraction at fractional flow = 1.0.
Units: dimensionless

CM(I,2) - Mass transfer coefficients for Ith tracer in oil phase.
Units: 1/sec

3.4.139 FFL(3), FFH(3), CM(I,3), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1)

FFL(3) - Microemulsion phase flowing fraction at fractional flow = 0.0.
Units: dimensionless

FFH(3) - Microemulsion phase flowing fraction for at fractional flow = 1.0.
Units: dimensionless

CM(I,3) - Mass transfer coefficients for Ith tracer in microemulsion phase.
Units: 1/sec

3.4.140 FFL(4), FFH(4), CM(I,4), for I=1, NTW+NTA (This line is read only if NTW+NTA>0 and ICAP=1 and IGAS≥1)

FFL(4) - Value of flowing fraction for gas phase when fractional flow = 0.0.
Units: dimensionless

FFH(4) - Value of flowing fraction for gas phase when fractional flow = 1.0.
Units: dimensionless

CM(I,4) - Mass transfer coefficients for Ith tracer in gas phase.
Units: 1/sec

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Reacting Tracer Data (input lines 3.4.141-3.4.144) — The following lines are required only if **NTW>0** and **ITREAC=1**.

3.4.141 NRT, TAK(I), for I=1, NRT (This line is read only if NTW>0 and ITREAC=1)

NRT - Number of reacting tracers.
Possible Values: 1 or 2

TAK(I) - Rate constant for a first-order aqueous phase reaction at reference temperature for reacting tracer I
Units: days⁻¹

Note: First reacting tracer is tracer 2 hydrolyzes to form tracer 3. The second reacting tracer if present is tracer 4 hydrolyzes to form tracer 5.

3.4.142 TMW(I), for I=1, NTW (This line is read only if NTW>0 and ITREAC=1)

TMW(I) - Molecular weight of the Ith tracer.
Units: The user can specify the molecular weight in any unit as long as the units are the same for all the tracers. It is assumed that the reaction of 1 mole of primary tracer produces 1 mole of secondary tracer. If not, use "equivalent" molecular weights.

3.4.143 TDEN(I), for I=1, NTW (This line is read only if NTW>0 and ITREAC=1)

TDEN(I) - Density of the Ith tracer.
Units: g/cm³

3.4.144 TAKT(I), for I=1, NRT (This line is read only if NTW>0 and ITREAC=1 and IENG=1)

TAKT(I) - Parameter for calculating rate constant for a first-order aqueous phase reaction as a function of reservoir temperature for reacting tracer I.
Units: (°K)⁻¹

Dual Porosity Data (input lines 3.4.145-3.4.163) — This section is **required for dual porosity option (ICAP=2) only**. This option works only with English unit (IUNIT=0) and the Cartesian coordinate (ICOORD=1). See [Section 5 of the UTCHEM Technical Documentation](#) for more details on this option. The capability of dual porosity option at this time is limited to single phase water and one tracer component. Restart capability (IMODE=2) is not currently available for the dual porosity option.

3.4.145 NSUB, MSUB, ISUB (This line is read only if ICAP=2)

NSUB - Number of subgrids in lateral direction.

MSUB - Number of subgrids in vertical direction.

ISUB - Mode of subgridding
Possible Values:
0 - Uniform matrix block dimension

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1 - Variable matrix block size dimension in each direction

2 - Variable matrix block dimension in whole reservoir

3.4.146 DXL(1), DYL(1), DZL(1) (This line is read only if ICAP=2 and ISUB=0)

DXL(1), DYL(1), DZL(1) - Uniform matrix block sizes in x y, and z directions.

Units: feet

Note: All values of the DXL, DYL, and DZL arrays are set to DXL(1), DYL(1), and DZL(1), respectively.

3.4.147 II1, II2, XL1 (This line is read only if ICAP=2 and ISUB=1)

II1, II2 - First and last index for gridblocks with same size in X direction.

XL1 - Matrix block size in X direction.

Units: feet

3.4.148 JJ1, JJ2, YL1 (This line is read only if ICAP=2 and ISUB=1)

JJ1, JJ2 - First and last index for gridblocks with same size in Y direction.

YL1 - Matrix block size in Y direction.

Units: feet

3.4.149 KK1, KK2, ZL1 (This line is read only if ICAP=2 and ISUB=1)

KK1, KK2 - First and last index for gridblocks with same size in Z direction

ZL1 - Matrix block size in Z direction.

Units: feet

3.4.150 DXL(I), for I=1, $NX \times NY \times NZ$ (This line is read only if ICAP=2 and ISUB=2)

DXL(I) - Matrix block size in X direction for Ith reservoir gridblock.

Units: feet

3.4.151 DYL(I), for I=1, $NX \times NY \times NZ$ (This line is read only if ICAP=2 and ISUB=2)

DYL(I) - Matrix block size in Y direction for Ith reservoir gridblock.

Units: feet

3.4.152 DZL(I), for I=1, $NX \times NY \times NZ$ (This line is read only if ICAP=2 and ISUB=2)

DZL(I), - Matrix block size in Z direction for Ith reservoir gridblock.

Units: feet

3.4.153 VFRACM(I), for I=1, NSUB (This line is read only if ICAP=2)

VFRACM(I) - Volume fraction of Ith subgrid. These values are used to generate subgrids in the lateral direction.

3.4.154 ZLSUB(1,I), for I=1, MSUB (This line is read only if ICAP=2)

ZLSUB(1,I) - Thickness fraction of Ith vertical subgrid. These values are used to generate subgrids in the vertical direction.

3.4.155 KPH, KKX, KKZ (This line is read only if ICAP=2)

KPH - Flag for matrix porosity distribution.

Possible Values:

- 0 - Uniform matrix porosity
- 1 - Variable matrix porosity

KKX - Flag for diffusion coefficient distribution in lateral direction in matrix.

Possible Values:

- 0 - Uniform matrix diffusion coefficient
- 1 - Uniform matrix diffusion coefficient in each reservoir layer
- 2 - Variable matrix diffusion coefficient at each reservoir node

KKZ - Flag for diffusion coefficient distribution in vertical direction in matrix.

Possible Values:

- 0 - Uniform matrix diffusion coefficient
- 1 - Uniform matrix diffusion coefficient in each reservoir layer
- 2 - Variable matrix diffusion coefficient at each reservoir node

3.4.156 PHIC (This line is read only if ICAP=2 and KPH=0)

PHIC - Matrix porosity.

3.4.157 PORCM(I,1,1), for I=1, NX × NY × NZ (This line is read only if ICAP=2 and KPH=1)

PORCM(I,1,1) - Matrix porosity of the Ith reservoir node.

3.4.158 DMC (This line is read only if ICAP=2 and KKX=0)

DMC - Matrix diffusion coefficient in lateral direction.

Units: ft²/day

3.4.159 DMX(K), for K=1, NZ (This line is read only if ICAP=2 and KKX=1)

DMX(K) - Matrix diffusion coefficient in Kth reservoir layer in lateral direction.

Units: ft²/day

3.4.160 DMX(I), for I=1, NX × NY × NZ (This line is read only if ICAP=2 and KKX=2)

DMX(I) - Matrix diffusion coefficient at Ith reservoir node in lateral direction.

Units: ft²/day

3.4.161 DMC (This line is read only if ICAP=2 and KKZ=0)

DMC - Matrix diffusion coefficient in vertical direction.

Units: ft²/day

3.4.162 DMZ(K), for K=1, NZ (This line is read only if ICAP=2 and KKZ=1)

DMZ(K) - Matrix diffusion coefficient in Kth reservoir layer in vertical direction.

Units: ft²/day

3.4.163 DMZ(I), for I=1, NX × NY × NZ (This line is read only if ICAP=2 and KKZ=2)

DMZ(I) - Matrix diffusion coefficient at Ith reservoir node in vertical direction.

Units: ft²/day

Gel Reaction Data (input lines 3.4.164-3.4.168) — These lines are **required only if IREACT=1 or IREACT=4 and NG>0**. Refer to Section 6 of the UTCHEM Technical Documentation for more details on this option.

3.4.164 KGOPT, AK1, AK2, SCR, X4, X13, X14, X16, WM4 (This line is read only if IREACT=1 or 4 and NG>0)

KGOPT - Flag to specify the gelation type used.

Possible Values:

- 1 - Polymer/chromium chloride gel
- 2 - Polymer/chromium malonate gel
- 3 - Silicate gel

AK1 - Kinetic rate coefficient for NG1 and NG2 at reference temperature (KGOPT=1).

Units: ppm⁻¹ days⁻¹

AK2 - Kinetic rate coefficient for gel at reference temperature .

Units: (mole/liter)^{1-X4-X14+X16} days⁻¹ for KGOPT=1
(mole/liter)^{1-X4-X13+X16} days⁻¹ for KGOPT=2
(mole/liter)^{1-X4+X14} days⁻¹ for KGOPT=3

SCR - Stoichiometric ratio in mass between Cr³⁺ and polymer.

Units: dimensionless

X4 - Exponent to be used for polymer or silicate in gelation reaction.

Units: dimensionless

X13 - Exponent to be used for component (NG2) in gelation reaction for KGOPT=2.

Units: dimensionless

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X14 - Exponent to be used for the third gel option component (NG3) in gelation reaction.

Units: dimensionless

X16 - Exponent to be used for hydrogen ion component (NG5) of gelation reaction.

Units: dimensionless

WM4 - Molecular weight of polymer (KGOPT=1 or 2) or silicate (KGOPT=3).

Units: g/mole

Note: The following tables define different gelation options and corresponding gel components.

For IREACT=1:

Component No.	KGOPT=1	KGOPT=2	KGOPT=3
4	Polymer	Polymer	Silicate
NG1	Na ₂ Cr ₂ O ₇	-	-
NG2	CSN ₂ H ₄	Malonate ion	-
NG3	Cr(III)	Cr(III)	OH ⁻
NG4	Gel	Gel	Gel
NG5	Hydrogen	Hydrogen	-

For IREACT=4:

Component NO.	KGOPT=1	KGOPT=2
4	Polymer	Polymer
NGC1	Sodium	Sodium
NGC2	Hydrogen	Hydrogen
NGC3	Magnesium	Magnesium
NGC4	Carbonate	Carbonate
NGC5	Chromium*	Chromium*
NGC6	Silica	Silica
NG1	Na ₂ Cr ₂ O ₇	-
NG2	CSN ₂ H ₄	Malonate ion
NG3	Cr(III)**	Cr(III)**
NG4	Gel	Gel

Where NG and NGC are the gel option and geochemistry option species.

3.4.165 AK1T, AK2T (This line is read only if IREACT=1 or 4 and NG>0 and IENG=1)

AK1T - Parameter for calculating Kinetic rate coefficient for Cr³⁺ as a function of reservoir temperature.

Units: (°K)⁻¹

AK2T - Parameter for calculating Kinetic rate coefficient for gel as a function of reservoir temperature.

Units: (°K)⁻¹

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3.4.166 AG1, AG2, CRG, AGK, BGK (This line is read only if IREACT=1 or 4 and NG>0)

AG1 - Flory-Huggins parameter for gel viscosity.

Units: $\text{cp ppm}^{-1} = \text{mPa.s ppm}^{-1}$

AG2 - Flory-Huggins parameter for gel viscosity.

Units: $\text{cp ppm}^{-2} = \text{mPa.s ppm}^{-2}$

CRG - Constant in the dimensionless pore radius reduction group. This constant depends on the gel type.

Units: $\sqrt{\text{darcy}}(\text{wt}\%)^{1/3} = \sqrt{\mu\text{m}^2}(\text{wt}\%)^{1/3}$

AGK, BGK - Permeability reduction parameters for Langmuir correlation with gel concentration.

Units: dimensionless

3.4.167 A15D, B15D, ICREX, A14D, B14D, CRNAK, HNAK, C160 (This line is read only if IREACT=1 or 4 and NG>0)

A15D, B15D - Gel adsorption parameters.

Units: vol. of water / ppm gel

ICREX - Flag indicating if Cr^{3+} will be allowed to exchange with clays.

Possible Values:

0 - Cr^{3+} exchange with clays is not allowed

1 - Cr^{3+} exchange with clays is allowed

A14D, B14D - Chromium adsorption parameters.

Units: vol. of water / ppm chromium

CRNAK - Chromium-sodium exchange reaction equilibrium constant.

HNAK - Hydrogen-sodium exchange reaction equilibrium constant.

C160 - Initial hydrogen ion concentration.

Units: meq/ml

Note: The input values of CRNAK, HNAK, and C160 are ignored for IREACT=4

3.4.168 IP1, IP2 (This line is read only if IREACT=1 or 4 and NG>0 and NY=1 and NZ=1)

IP1, IP2 - Gridblock locations where calculated pressure values should be printed to UNIT 19.

Note: These values are intended to be used for comparison with pressure tab data of 1-D experiments.

Temperature Data (input lines 3.4.169-3.4.172) — These lines are **required only if** temperature variation is considered in the simulation for **IENG=1**.

3.4.169 TEMPI (This line is read only if IENG=1)

TEMPI- Constant initial reservoir temperature.

Units: °F (IUNIT=0) or °C (IUNIT=1)

3.4.170 DENS, CRTC, CVSPR, (CVSPL(L), for L=1, MXP) (This line is read only if IENG=1)

DENS - Reservoir rock density.

Units: lb/ft³ (IUNIT=0) or g/cm³ (IUNIT=1)

CRTC - Reservoir thermal conductivity.

Units: Btu (day-ft-°F)⁻¹ (IUNIT=0) or kJ (day-m-°K)⁻¹ (IUNIT=1)

CVSPR - Reservoir rock heat capacity.

Units: Btu (lb-°F)⁻¹ (IUNIT=0) or kJ (kg-°K)⁻¹ (IUNIT=1)

CVSPL(L) - Phase L heat capacity (MXP is equal to 3 (IGAS=0) or 4 (IGAS≥1)).

Units: Btu (lb-°F)⁻¹ (IUNIT=0) or kJ (kg-°K)⁻¹ (IUNIT=1)

3.4.171 IHLOS, IANAL (This line is read only if IENG=1)

IHLOS - Flag indicating if the heatloss calculation to overburden and underburden rock is considered or not.

Possible Values:

0 - Heatloss is not considered

1 - Heatloss is considered

IANAL - Flag indicating if the temperature profile is calculated from analytical solution (only 1-D).

Possible Values:

0 - Analytical solution is not considered

1 - Analytical solution is considered

3.4.172 TCONO, DENO, CVSPO, TCONU, DENU, CVSPU (This line is read only if IHLOS=1 and if IENG=1)

TCONO - Thermal conductivity of overburden rock.

Units: Btu (day-ft-°F)⁻¹ (IUNIT=0) or kJ (day-m-°K)⁻¹ (IUNIT=1)

DENO - Density of overburden rock.

Units: lb/ft³ (IUNIT=0) or g/cm³ (IUNIT=1)

CVSPO - Heat capacity of overburden rock.

Units: Btu (lb-°F)⁻¹ (IUNIT=0) or kJ (kg-°K)⁻¹ (IUNIT=1)

TCONU - Thermal conductivity of underburden rock.

Units: Btu (day-ft-°F)⁻¹ (IUNIT=0) or kJ (day-m-°K)⁻¹ (IUNIT=1)

DENU - Density of underburden rock.

Units: lb/ft³ (IUNIT=0) or g/cm³ (IUNIT=1)

CVSPU - Heat capacity of underburden rock.

Units: Btu (lb-°F)⁻¹ (IUNIT=0) or kJ (kg-°K)⁻¹ (IUNIT=1)

Foam Model Data (input lines 3.4.173 and 3.4.174) — These lines are required only if the foam option is considered (**IGAS=2**).

3.4.173 RFMAX, SOSTAR, CSTAR, EPXLO, SHRTN, VELGR (This line is read only if IGAS=2)

RFMAX- Maximum foam "R" parameter.

Units: dimensionless

SOSTAR - Critical oil saturation above which foam is not generated.

Units: dimensionless

CSSTAR - Critical surfactant concentration below which foam is not generated.

Units: volume fraction

EPXLO - Water saturation tolerance parameter in foam model.

Units: dimensionless

SHRTN - Gas shear thinning exponent.

Units: dimensionless

VELGR - Reference gas velocity.

Units: ft/day (IUNIT=0) or m/day (IUNIT=1)

3.4.174 SWSTAR(I), for I=1, NX × NY × NZ (This line is read only if IGAS=2)

SWSTAR(I)- Water saturation at critical capillary pressure for Ith gridblock.

Units: dimensionless

Note: SWSTAR(I) is assumed to be corrected for the permeability used in the simulation.

User notes:

3.5 Physical Property Data for Geochemical Options

The fifth input section consists of physical property data for geochemistry option and it is **required only** if **IREACT>1**. The data for this section is generated by a preprocessor program (EQBATCH) and does not have the same format as the rest of the input data for UTCHEM. This input section is read by a separate routine called GEOREAD not preceded by the usual seven comment lines and individual data lines are not preceded by three comment lines. Appendix B gives an example for the list of elements, fluid species, solid species, and adsorbed species for geochemical options. See Section 8 of the UTCHEM Technical Documentation for information on the geochemical model.

3.5.1 IRSPS, IPHAD

IRSPS - Flag indicating if the reactive species concentrations should be printed.

Possible Values:

- 0 - Reactive species concentrations will not be printed
- 1 - Independent aqueous reactive species, solid species, and sorbed species concentrations will be printed
- 2 - All aqueous species, solid species, and sorbed species concentrations will be printed

IPHAD - Flag indicating whether surfactant adsorption is pH dependent or not.

Possible Values:

- 0 - Surfactant adsorption is not pH dependent
- 1 - Surfactant adsorption is pH dependent

3.5.2 PHC, PHT, PHT1, HPHAD (This line is read only if IPHAD>0)

PHC - Critical pH above which surfactant adsorption is pH dependent.

PHT - Extrapolated pH value at zero surfactant adsorption.

PHT1 - pH value above which surfactant adsorption is constant.

HPHAD - Fraction of the low-pH adsorption plateau retained at a pH above PHT1.

3.5.3 CSELP, CSEUP (This line is read only if IREACT=3)

CSELP - Lower optimum salinity limit for generated surfactant.

Units: meq/ml water

CSEUP - Upper optimum salinity limit for generated surfactant.

Units: meq/ml water

3.5.4 NELET, NFLD, NSLD, NSORB, NACAT, ICHARGE

NELET - Total number of elements less nonreacting element.

NFLD - Total number of fluid species.

NSLD - Total number of solid species.

NSORB - Total number of sorbed species.

NACAT - Total number of surfactant associated cations.

ICHARGE - Flag indicating whether an oxygen balance or a charge balance will be used.

Possible Values:

0 - Oxygen balance used

1 - Charge balance in solution used

Note: If solid SiO₂ is considered, the oxygen balance must be used.

3.5.5 NIAQ, NEX, NSLEL, NSURF1

NIAQ - Total number of independent fluid species.

NEX - Total number of insoluble exchangers.

NSLEL - Total number of elements comprising the solid species.

NSURF1 - Position number corresponding to the insitu generated surfactant anion in the fluid species array FLDSPS.

Note: NSURF1 is automatically set to 0 by the program if IREACT=2.

3.5.6 NH, NNA, NCA, NMG, NCARB

NH - Position number corresponding to the hydrogen element in the element array ELEMNT.

NNA - Position number corresponding to the sodium element in the element array ELEMNT.

NCA - Position number corresponding to the calcium element in the element array ELEMNT.

NMG - Position number corresponding to the magnesium element in the element array ELEMNT.

NCARB - Position number corresponding to the carbonate pseudo-element in the element array ELEMNT.

Note: A value of zero is required if the element is not considered.

3.5.7 NALU, NSILI, NOXY

NALU - Position number corresponding to the aluminum element in the element array ELEMNT.

NSILI - Position number corresponding to the silicon element in the element array ELEMNT.

NOXY - Position number corresponding to the oxygen element in the element array ELEMNT.

Note: A value of zero is required if the element is not considered.

3.5.8 NACD (This line is read only if IREACT=3)

NACD - Position number corresponding to the petroleum acid pseudo-element in the element array ELEMNT.

3.5.9 NCR, NHFD, NCRFD (This line is read only if IREACT=4)

NCR - Position number corresponding to the chromium element in the element array ELEMNT.

NHFD - Position number corresponding to the hydrogen ion element in the fluid species array FLDSPS.

NCRFD - Position number corresponding to the CR(III) ion in the fluid species array FLDSPS.

3.5.10 ELEMNT(I), ELCRG(I) for I=1, NELET

ELEMNT(I) - Name of the Ith element.

ELCRG(I) - Charge for Ith element

Note: The name of each element may not exceed 32 characters. Each name and its charge must be on a separate line of the input file. The order in which these elements must be listed corresponds to the order in which the component names are specified on input line 3.1.24 with the exceptions of calcium and chloride (if they exist) since Components 5 and 6 are reserved for these elements.

3.5.11 FLDSPS(I), for I=1, NFLD

FLDSPS(I) - Name of the Ith fluid species.

Note: The name of each fluid species may not exceed 32 characters and each name must be on a separate line of the input file. If IREACT=3, the last fluid species must be HA_w (petroleum acid in water).

3.5.12 SLDSPS(I), for I=1, NSLD (This line is read only if NSLD>0)

SLDSPS(I) - Name of the Ith solid species.

Note: The name of each solid may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.13 SORBSP(I), for I=1, NSORB (This line is read only if NSORB>0)

SORBSP(I) - Name of the Ith adsorbed cation.

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Note: The name of each adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.14 ACATSP(I), for I=1, NACAT (This line is read only if NACAT>0)

ACATSP(I) - Name of the Ith surfactant adsorbed cation.

Note: The name of each surfactant adsorbed cation may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.15 NSORBX(I), for I=1, NEX (This line is read only if NSORB>0)

NSORBX(I) - Number of cations for Ith exchanger.

3.5.16 AR(I,J), for J=1, NFLD, for I=1, NELET or >>
AR(I,J), for J=1, NFLD, for I=1, NELET-1

AR(I,J) - Stoichiometric coefficient of Ith element in Jth fluid species.

Note: If ICHRG=0, then NFLD × NELET values are required by the program.
If ICHRG=1, then NFLD × (NELET-1) values are required by the program.

3.5.17 BR(I,J), for J=1, NSLD, for I=1, NELET << or >>
BR(I,J), for J=1, NSLD, for I=1, NELET-1 (This line is read only if NSLD>0)

BR(I,J) - Stoichiometric coefficient of Ith element in Jth solid species.

Note: If ICHRG=0, then NSLD × NELET values are required by the program.
If ICHRG=1, then NSLD × (NELET-1) values are required by the program.

3.5.18 DR(I,J), for J=1, NSORB, for I=1, NELET << or >>
DR(I,J), for J=1, NSORB, for I=1, NELET-1 (This line is read only if NSORB>0)

DR(I,J) - Stoichiometric coefficient of Ith element in Jth sorbed species.

Note: If ICHRG=0, then NSORB × NELET values are required by the program. If ICHRG=1, then NSORB × (NELET-1) values are required by the program.

3.5.19 ER(I,J), for J=1, NACAT, for I=1, NELET << or >>
ER(I,J), for J=1, NACAT, for I=1, NELET-1 (This line is read only if NACAT>0)

ER(I,J) - Stoichiometric coefficient of Ith element in Jth surfactant associated cation.

Note: If ICHRGE=0, then $NACAT \times NELET$ values are required by the program. If ICHRGE=1, then $NACAT \times (NELET-1)$ values are required by the program.

3.5.20 BB(I,J), for J=1, NIAQ+NSORB+NACAT, for I=1, NFLD+NSORB+NACAT

BB(I,J) - Exponent of the Jth independent fluid species concentration when the Ith fluid species is expressed in terms of independent species concentrations.

3.5.21 EXSLD(I,J), for J=1, NIAQ, for I=1, NSLD (This line is read only if NSLD>0)

EXSLD(I,J) - Exponent of the Jth independent fluid species concentration in the solubility product definition of the Ith solid.

3.5.22 CHARGE(I), for I=1, NFLD

CHARGE(I) - Charge of the Ith fluid species.

3.5.23 SCHARG(I,J), for J=1, NSORBX(I), for I=1, NEX (This line is read only if NSORB>0)

SCHARG(I,J) - Charge of the Jth sorbed species on the Ith exchanger.

3.5.24 EQK(I), for I=1, NFLD

EQK(I) - Equilibrium constant for Ith fluid species when expressed in independent species concentrations only.

3.5.25 EXK(I,J), for J=1, NSORBX(I)-1, for I=1, NEX (This line is read only if NEX>0)

EXK(I,J) - Exchange equilibrium constant for Jth exchange equilibrium of the Ith insoluble exchanger.

3.5.26 EXEX(I,J,K), for K=1, NIAQ+NSORB+NACAT, for J=1, NSORBX(I)-1, for I=1, NEX (This line is read only if NEX>0)

EXEX(I,J,K) - Exponent of Kth independent species in Jth equilibrium relation of the Ith exchanger

3.5.27 REDUC(I,J), for J=1, NSORBX(I)-1, for I=1, NEX (This line is read only if NEX>0)

REDUC(I,J) - Valence difference of the two cations involved in the exchange reaction J on exchanger I.

Note: This value is positive if the higher valence cation bulk concentration has a positive exponent in EXEX(I,J) definition and is negative otherwise.

- 3.5.28 EXCAI(I), for I=1, NEX (This line is read only if NEX>0)
EXCAI(I) - Exchange capacity of Ith insoluble exchanger.
Units: meq/ml pore volume
- 3.5.29 SPK(I), for I=1, NSLD (This line is read only if NSLD≥1)
SPK(I) - Solubility product of Ith solid defined in terms of independent fluid species concentrations only.
- 3.5.30 CHACAT(I), for I=1, NACAT (This line is read only if NACAT≥1)
CHACAT(I) - Charge of Ith surfactant associated cation.
- 3.5.31 ACATK(I), for I=1, NACAT-1 (This line is read only if NACAT≥1)
ACATK(I) - Equilibrium constant for Ith exchange equilibrium for cation exchanges on surfactant.
- 3.5.32 EXACAT(I,J) for J=1, NIAQ+NSORB+NACAT, for I=1, NACAT-1 (This line is read only if NACAT≥1)
EXACAT(I,J) - Exponent of Jth independent species in Ith equilibrium for cation exchange on surfactant.
- 3.5.33 CI(J), for J=1, NACAT (This line is read only if NACAT≥1)
CI(J) - Initial concentration of Jth surfactant associated cation.
Units: moles/liter pore volume
- 3.5.34 C5I, C6I
C5I - Initial concentration of nonreacting anions.
Units: equivalents/liter
C6I - Initial concentration of calcium in aqueous phase.
Units: equivalents/liter
- 3.5.35 CELAQI(J), for J=1, NGC
CELAQI(J) - Initial concentrations of Jth geochemistry component.
Units: equivalents/liter
- 3.5.36 CAC2I (This line is read only if IREACT=3)
CAC2I - Initial concentration of acid in oil.
Units: moles/liter oil
- 3.5.37 CAQI(J), for J=1, NIAQ
CAQI(J) - Initial guesses for Jth independent species concentration.
Units: moles/liter water

3.5.38 CSLDI(I), for I=1, NSLD (This line is read only if NSLD>0)

CSLDI(I) - Initial concentration of Ith solid.
Units: moles/liter pore volume

3.5.39 CSORBI(I), for I=1, NSORB (This line is read only if NSORB>0)

CSORBI(I) - Initial concentration of Ith adsorbed cation.
Units: moles/liter pore volume

3.5.40 C1I, C2I (This line is read only if IREACT=3)

C1I - Initial concentration of water in aqueous phase.
Units: volume fraction

C2I - Initial concentration of oil in oleic phase.
Units: volume fraction

3.5.41 ACIDIS, EQWPS (This line is read only if IREACT=3)

ACIDIS - Dissociation constant of the petroleum acid.

EQWPS - Equivalent weight of petroleum acid.

User notes:

3.6 Data for Biodegradation Option

The sixth input section consists of physical property data that is **required only if IBIO=1**. This section includes the biodegradation and mass transfer parameters required to model the biodegradation of chemical species. This section is read only if IBIO=1. The data is read by a separate subroutine called BIOREAD, and is input in the standard UTCHEM format. Section 9 of the UTCHEM Technical Documentation gives more details on this option.

3.6.1 DENBLK

DENBLK - Bulk density of the porous medium (mass of porous medium per unit total volume).
Units: g/cm³

3.6.2 CMIN, EPSBIO, IBTIM

CMIN - Minimum concentration of substrate and electron acceptor that is of interest. This parameter is used for two purposes. First, if concentrations of all substrates and electron acceptors in a gridblock are below CMIN, then biodegradation reactions are assumed negligible at the gridblock and are not modeled. Second, when the concentration of all substrates and electron acceptors fall below CMIN during solution of the biodegradation reaction expressions, further biodegradation reactions are assumed to be negligible and program execution returns to the main program.
Units: mg/L

EPSBIO - Convergence tolerance for solution of the biodegradation equations.

Note: Values of 10⁻⁴ to 10⁻⁶ are recommended, although larger values can also result in accurate simulations. Small values ensure accurate solutions of the biodegradation equations but increase run times, while larger values decrease run times at the expense of some accuracy.

IBTIM - Flag indicating type of time step control for solution of biodegradation equations.

Possible Values:

- 0 - No time step control; biodegradation equations are solved at every transport time step
- 1 - Manual time step control; biodegradation time step is specified by user
- 2 - Automatic time step control; biodegradation time step is controlled by UTCHEM based on an acceptable error specified by the user

3.6.3 BTMIN, BTMAX (This line is read only if IBTIM=1)

BTMIN - Minimum time step for solution of biodegradation equations.

BTMAX - Maximum potential biodegradation time step.

Note: If the transport time step is smaller than BTMIN, the biodegradation equations will be solved at intervals of BTMIN. If the transport time step falls between BTMIN and BTMAX, the biodegradation equations will be solved at every transport time step. BTMAX should be set to a value greater than BTMIN and is only used to initialize variables in this option.

3.6.4 BIORME, BTMAX (This line is read only if IBTIM=2)

BIORME - The maximum acceptable error in terms of the mass of substrate in the system resulting from a biodegradation time step being larger than the transport time step.

BTMAX - Maximum biodegradation time step allowed.

Note: A warning message is presented if the biodegradation time step computed from the automatic time step controller is smaller than the transport time step. See [Section 9 of the UTCHEM Technical Documentation](#) for more information.

3.6.5 NBC, NMET, IBKIN, IBPP

NBC - Total number of chemical and biological species that are considered in biodegradation reactions, including oil components, surfactants, products generated by abiotic and biodegradation reactions, nutrients required for biological growth, electron acceptors, and biological species.

NMET - Number of substrate/electron acceptor/biological species metabolic combinations. Include combinations of biodegrading products/electron acceptor/biological species for each product that also biodegrades.

IBKIN - Flag specifying the type of biodegradation kinetics.

Possible Values:

- 0 - No reaction; biodegradation parameters are read, but biodegradation equations are never solved (useful for restart runs)
- 1 - Monod kinetics with external mass transfer resistances
- 2 - Monod kinetics with no external mass transfer resistances
- 3 - Instantaneous kinetics (stoichiometric reactions)
- 4 - Monod kinetics with automatic control of external mass transfer resistances

Note: First order kinetics with biomass growth can be also be modeled by adjusting the values of the Monod parameters. See input line 3.6.12 below.

IBPP - Flag indicating whether or not porosity and permeability are affected by biological growth.

Possible Values:

- 0 - Porosity and permeability are not affected by biomass growth

1 - Porosity and permeability are affected by biomass growth

3.6.6 IMTVAR (This line is read only if IBKIN=4)

IMTVAR - Flag indicating type of mass transfer control.

Possible Values:

- 1 - Mass transfer is considered in each gridblock at each time step only when the Damkohler number is greater than the user-specified value
- 2 - Mass transfer is considered in each gridblock at each time step only when the effectiveness factor is less than the user-specified value

3.6.7 DAMX (This line is read only if IBKIN=4 and IMTVAR=1)

DAMX - Value of Damkohler number used to control mass transfer in biodegradation calculations.

Recommended value: 0.1

3.6.8 EFMIN (This line is read only if IBKIN=4 and IMTVAR=2)

EFMIN - Value of effectiveness factor used to control mass transfer in biodegradation calculations.

Recommended value: greater than 0.95

3.6.9 KC(I), ITYPE(I), CINIT(I), RABIO(I), NPABIO(I), for I=1, NBC

Note: One line is required for each chemical and biological species that participates in biodegradation reactions.

KC(I) - Index of the Ith chemical or biological species.

ITYPE(I) - Flag indicating whether the Ith component is a chemical or biological species.

Possible values:

- 1 - The Ith component is a chemical species
- 2 - The Ith component is a biological species

CINIT(I) - Initial concentration of chemical or free-floating (unattached) biological species I in the aqueous phase.

Units: mg/ℓ

Note: Although a value of CINIT must be entered for organic species that participate in biodegradation reactions, these values are ignored by the program. Initial concentrations of these components are input on input lines 3.3.32 through 3.3.35.

RABIO(I) - First-order abiotic reaction rate constant.

Units: 1/days

Note: Although a value of RABIO can be specified for biological as well as chemical species, biomass decay should not be controlled with RABIO. Instead, use the parameters ENDOG and ENDOGB to control endogenous decay of unattached and attached biomass,

respectively. RABIO should normally be set to 0.0 for biological species.

NPABIO(I) - Number of products generated by a first-order abiotic reaction of chemical species I.

Note: A value must be entered for biological species as well, although the value is ignored by the program because generation of products from decay of biomass is not allowed.

3.6.10 KC(I), DENBIO(I), RCOL(I), TCOL(I), COLNUM(I), ENDOG(I), ENDOGB(I), CBI(I), CBIOMN(I), ADSBIO(I), for I=1, NBS

Note: One line is required for each biological species.

KC(I) - Index of the biological species.

DENBIO(I) - density of attached biological species I (biofilm density).

Units: g cells / cm³ biomass

RCOL(I) - radius of an attached microcolony of biological species I.

Units: cm

Note: The parameter RCOL is used to calculate the surface area of a single attached microcolony. Although microcolonies are assumed to be disk-shaped by the model, the user may specify any desired surface area per microcolony using RCOL. TCOL can then be adjusted to obtain the desired volume of the microcolony since the thickness of the microcolony does not affect external mass transfer into the attached biomass.

TCOL(I) - Thickness of a single attached microcolony of biological species I.

Units: cm

COLNUM(I) - Number of bacterial cells per microcolony of biological species I.

Units: cells/colony

ENDOG(I) - endogenous decay coefficient of *unattached* cells of biological species I.

Units: 1/days

ENDOGB(I) - endogenous decay coefficient of *attached* cells of biological species I.

Units: 1/days

CBI(I) - Number of attached bacterial cells of biological species I per gram of dry soil.

Units: cells/gram of solid

CBIOMN(I) - Lower limit of number of attached bacterial cells of biological species I.

Units: cells/gram of solid

Note: A population of attached microorganisms, sustained by naturally occurring organic matter, is assumed to exist in the porous medium regardless of the concentration of other chemical species. This

concentration is CBIOMN, and the concentration of biomass is not allowed to fall below this value.

ADSBIO(I) - Biomass partitioning coefficient.

Units: $\frac{\text{mass of attached microorganisms}}{\text{mass of unattached microorganisms}}$

3.6.11 ISUB(I), IEA(I), IBS(I), BRMAX(I), BRMAXB(I), YXS(I), AKS(I), AKA(I), FEA(I), for I=1, NMET

Note: One line is read for each metabolic combination. Values of all parameters on this line must be supplied by the user even if instantaneous kinetics or abiotic reactions are used to describe loss of substrate.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

BRMAX(I) - maximum specific growth rate of *unattached* microorganisms for metabolic combination I.

Units: 1/days

BRMAXB(I) - Maximum specific growth rate of *attached* microorganisms for metabolic combination I.

Units: 1/days

YXS(I) - Yield coefficient for metabolic combination I.

Units: biomass produced per mass of substrate biodegraded

AKS(I) - Substrate half-saturation coefficient for metabolic combination I.

Units: mg/ℓ

AKA(I) - Electron acceptor half-saturation coefficient for metabolic combination I.

Units: mg/ℓ

FEA(I) - Electron acceptor utilization coefficient.

Units: mass of electron acceptor consumed per mass of substrate biodegraded

3.6.12 ISUB(I), IEA(I), IBS(I), NCOMPS(I), NIHB(I), NPROD(I), NNUT(I), ICOMET(I), for I=1, NMET

Note: One line is read for each metabolic combination.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

NCOMPS(I) - Number of other substrates competing with substrate ISUB in metabolic combination I.

NIHB(I) - Number of other chemical species that inhibit metabolic combination I.

NPROD(I) - Number of products generated from metabolic combination I.

NNUT(I) - Number of nutrients that limit the biodegradation rate through Monod terms for metabolic combination I.

ICOMET(I) - Flag indicating whether or not the substrate in metabolic combination I is biodegraded through aerobic cometabolism.

Possible Values:

0 - Substrate ISUB(I) serves as a primary substrate

1 - Substrate ISUB(I) is biodegraded through aerobic cometabolism

Note: Users may specify multiple competing substrates, nutrients, and inhibiting constituents for each metabolic combination. Substrate competition, inhibition and cometabolism cannot be modeled if instantaneous kinetics are selected. However, values for the biodegradation rate parameters must be specified even if instantaneous kinetics are specified.

First-order biodegradation kinetics can be modeled by using a very large value of K_S , and adjusting the ratio of μ_{\max}/K_S to be equal to the desired first-order biodegradation rate coefficient.

3.6.13 ISUB(I), IEA(I), IBS(I), (ICSUB(I,J), for J=1, Number of competing substrates), for I=1, NMET (This line is read only if there are competing substrates)

Note: One line is read for each metabolic combination for which there is substrate competition between two or more substrates.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

ICSUB(J) - Indices of other substrates that compete with substrate ISUB(I) in metabolic combination I.

Note: The number of input lines required must equal the number of species that are competing, since complementary lines are required to fully describe the competition. For example, if substrate 12 in metabolic combination 12-15-16 must compete with substrates 13 and 14 that are also biodegraded by biological species 16 using electron acceptor 15, then the required input lines are:

12	15	16	13	14
13	15	16	12	14
14	15	16	12	13

- 3.6.14 ISUB(I), IEA(I), IBS(I), IHB(I), BSIHB(I), for I=1, Number of metabolic combination and inhibiting compound associations (This line is only read if there are metabolic combination and inhibiting compound associations)

Note: One input line is read for each association of metabolic combination and inhibiting compound.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

IHB(I) - Index of chemical species that inhibits metabolic combination I.

BSIHB(I) - Inhibition constant for metabolic combination I.

Units: mg/ℓ

Note: The total number of lines are

$$I = \sum_{J=1}^{N_{MET}} NIHB(J).$$

For example, suppose there are two substrate-electron acceptor-biological species metabolic combinations: 9-10-12 and 9-11-12. Metabolic combination 9-10-12 is inhibited by the substrate itself (9) and electron acceptor 11, while metabolic combination 9-11-12 is inhibited by only the substrate. Assuming that the imbibition constant for each combination is 0.001, the input lines for this scenario would be:

9	10	12	9	0.001
9	10	12	11	0.001
9	11	12	9	0.001

- 3.6.15 ISUB(I), IEA(I), IBS(I), IPR(I), FPR(I), for I=1, Number of biodegradation product formation and metabolic combination associations (This line is read only if there are biodegradation product formation described with Monod kinetics and metabolic combination associations)

Note: One line is read for each association of product formation and metabolic combination.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

IPR(I) - Index of product generated by metabolic combination I.

FPR(I) - Product generation coefficient (stoichiometric ratio - mass of product generated per mass of substrate biodegraded).

Note: Number of lines are

$$I = \sum_{J=1}^{N_{MET}} N_{PROD}(J).$$

For example, if metabolic combination 9-14-15 generates products 10 and 11, and metabolic combination 12-14-15 generates product 13, then the input lines would be (assuming a values of 0.5 for FPR(I)):

9	14	15	10	0.5
9	14	15	11	0.5
12	14	15	13	0.5

Parameters for generation of products through first-order reactions are described on input line 3.6.16.

- 3.6.16 ISUB(I), IPR(I), FPR(I), for I=1, Number of products generated by first-order reactions of the biodegradation species. (This line is read only if there are products of first-order reactions of biological species)

ISUB(I) - Index of chemical species that reacts abiotically to generate a product.

IPR(I) - Index of product generated by abiotic reaction of ISUB(I).

FPR(I) - Product generation coefficient (stoichiometric ratio - mass of product generated per mass of reactant reacted).

Note: Number of lines are

$$I = \sum_{J=1}^{N_{BC}} N_{PABIO}(J).$$

For example, if the abiotic products 11, 12 and 13 were generated from the first-order reaction of biodegradation species 9, the input lines would be:

9	11	1.0
9	12	1.0
9	13	1.0

- 3.6.17 ISUB(I), IEA(I), IBS(I), INUT(I), AKN(I), FN(I), for I=1, Number of metabolic combination and limiting nutrient associations (This line is read only if there are metabolic combination and limiting nutrient associations)

Note: One line is read for each association of metabolic combination and limiting nutrient.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

INUT(I) - Index of nutrient limiting the rate of biodegradation through a Monod term in metabolic combination I.

AKN(I) - Nutrient half-saturation coefficient for metabolic combination I.

Units: mg/ℓ

FN(I) - Nutrient utilization coefficient (mass of nutrient consumed per mass of substrates biodegraded) for metabolic combination I.

Note: Number of lines are $I = \sum_{J=1}^{N_{MET}} NNUTT(J)$.

3.6.18 ISUB(I), IEA(I), IBS(I), TC(I), IRLIM(I), for I=1, Number of cometabolic combinations for which aerobic cometabolism exists (This line is read only if there are cometabolic combinations for which aerobic cometabolism exists for at least one metabolic combination specified on input line 3.6.12)

Note: One input line is required for each cometabolic combination for which aerobic cometabolism exists.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

TC(I) - Transformation capacity for cometabolism of substrate ISUB(I) (mass of substrate utilized per mass of biomass destroyed).

IRLIM(I) - Flag indicating whether reducing power limitations are considered for cometabolic combination I.

Possible Values:

0 - No reducing power limitations are considered

1 - Cometabolic reaction consumes reducing power

Note: Reducing power limits the biodegradation rate through Monod terms in the manner of Chang and Alvarez-Cohen, 1995. The loss of a biological species' reducing power reduces its activity toward all substrates, not just the cometabolite.

Note: The total number of lines are $I = \sum_{J=1}^{N_{MET}} COMET(J)$.

3.6.19 ISUB(I), IEA(I), IBS(I), IGROW(I), REDI(I), AKR(I), FRP(I), FRC(I), for I=1, Number of cometabolic biodegradation reactions in which reducing power limitations are considered (This line is read only if there are cometabolic biodegradation reactions in which reducing power limitations are considered and IRLIM(I)>0 for at least one metabolic combination specified on input line 3.6.17)

Note: One line is required for each cometabolic biodegradation reaction in which reducing power limitations are considered.

ISUB(I) - Substrate index for metabolic combination I.

IEA(I) - Electron acceptor index for metabolic combination I.

IBS(I) - Biological species index for metabolic combination I.

IGROW(I) - Index of growth substrate for cometabolism of substrate ISUB(I).

REDI(I) - Initial intracellular reducing power (NADH) concentration.
Units: mmol/mg of biomass

AKR(I) - Reducing power half-saturation coefficient.
Units: mmol/mg of biomass

FRP(I) - Reducing power generation coefficient for metabolic combination (IGROW(I), IEA(I), IBS(I)) (mmol reducing power generated per mg of growth substrate consumed).

FRC(I) - Reducing power consumption coefficient for cometabolic combination (ISUB(I), IEA(I), IBS(I)) (mmol reducing power consumed per mg of substrate consumed by cometabolism).

Note: The total number of lines are

$$I = \sum_{J=1}^K \text{IRLIM}(J)$$

where

$$K = \sum_{J=1}^{\text{NMET}} \text{COMET}(J).$$

3.7 Recurrent Injection/Production Data Set

The sixth input section consists of the recurrent injection/production well data. Please remember that there are seven comment lines at the beginning of this section and that each line is preceded by three comment lines.

3.7.1 IBOUND, IZONE

IBOUND - Flag indicating if constant potential boundaries at the top, left, and right sides of the simulation model are specified.

Possible Values:

- 0 - No boundary is specified
- 1 - Boundary is specified

IZONE - Flag indicating the aquifer zone to be modeled.

Possible Values:

- 0 - Saturated zone is modeled
- 1 - Vadose zone is modeled
- 2 - Both saturated and vadose zones are modeled

Note: See Section 2 of the UTCHEM Technical Documentation for more information.

3.7.2 IBL, IBR, IBT, WTABL, WTABR (This line is read only if IBOUND=1)

IBL - Flag indicating if the left hand side constant potential boundary is specified.

Possible Values:

- 0 - No boundary is specified
- 1 - Boundary is specified

IBR - Flag indicating if the right hand side constant potential boundary is specified.

Possible Values:

- 0 - No boundary is specified
- 1 - Boundary is specified

IBT - Flag indicating if the top constant pressure boundary of the vadose zone is specified.

Possible Values:

- 0 - Top boundary is closed
- 1 - Top boundary is open

WTABL - The depth to the water table at the left boundary.

Units: feet (IUNIT=0) or m (IUNIT=1)

WTABR - The depth to the water table at the right boundary.

Units: feet (IUNIT=0) or m (IUNIT=1)

Note: The depth to the water table is only used if IZONE=2.

3.7.3 PBL, C1BL, C5BL, C6BL (This line is read only if IBOUND=1 and IZONE≠1 and IBL=1)

PBL - Pressure at the center of the top layer at the left boundary.
Units: psia (IUNIT=0) or kPa (IUNIT=1)

C1BL - Concentration of water in aqueous phase at the left boundary.
Units: volume fraction

C5BL - Concentration of chloride in aqueous phase at the left boundary.
Units: meq/ml water

C6BL - Concentration of calcium in aqueous phase at the left boundary.
Units: meq/ml water

3.7.4 PBR, C1BR, C5BR, C6BR (This line is read only if IBOUND=1 and IZONE≠1 and IBR=1)

PBR - Pressure at the center of the top layer at the right boundary.
Units: psia (IUNIT=0) or kPa (IUNIT=1)

C1BR - Concentration of water in aqueous phase at the right boundary.
Units: volume fraction

C5BR - Concentration of chloride in aqueous phase at the right boundary.
Units: meq/ml water

C6BR - Concentration of calcium in aqueous phase at the right boundary.
Units: meq/ml water

Note: For the biodegradation option (IBIO=1), the concentrations of all species considered at the boundary are set to the initial concentrations. If the variation in temperature is considered (IENG=1), the temperatures at the boundaries are set to the initial temperature.

3.7.5 NWELL, IRO, ITSTEP, NWREL

NWELL - Number of wells used for the simulation including the pseudowells to mimic an open boundary.

Note: If ICOORD=2, NWELL must be equal to 1 and the NWELL input file in the HEAD file must be set equal to 2.

IRO - Flag indicating the equivalent well radius model to be used.
Possible Values:

- 1 - Babu and Odeh model is used
- 2 - Peaceman model is used

Note: The Babu and Odeh model (IRO=1) does not work for ICOORD=4.

ITSTEP - Flag indicating the units to be used when specifying the minimum and maximum time step.

Possible Values:

- 0 - Minimum and maximum time steps are input in days

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1 - Minimum and maximum time steps are input as Courant numbers

Note: This option is only used if IMES>1 and is not a shut-in period. If IMES=1, this flag is ignored. For a shut-in period you need to use ITSTEP=0

NWREL - Number of actual wells used for the simulation excluding the pseudowells.

Note: The history data are written only for NWREL wells.

Note: See Appendix E for more details on the Courant number and time step selection options.

The following values for minimum and maximum Courant numbers are recommended for different simulations as follows:

<u>Process</u>	<u>Min. Courant #</u>	<u>Max. Courant #</u>
Waterflood/tracer	0.04	0.4
Polymerflood	0.02	0.2
Surfactant/polymerflood	0.01	0.1
Geochemical process	0.01	0.1

See Section 10 of the UTCHEM Technical Documentation for well model information.

3.7.6 The data on input lines 3.7.6.a through 3.7.6.d are repeated for M=1 to NWELL times.

Important note: Input the actual wells first (NWREL) and then the pseudowells.

3.7.6.a IDW(M), IW(M), JW(M), IFLAG(M), RW(M), SWELL(M), IDIR(M), IFIRST(M), ILAST(M), IPRF(M)

IDW(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: This number is used by UTCHEM to keep track of which well is being described in the recurrent injection/production well section.

IW(M) - First index of the reservoir gridblock containing the Mth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: If the Mth well is completed parallel to the X-axis, IW(M) is the Y direction index—if the well is completed parallel to the Y- or Z-axis, IW(M) is the X direction index. See example below.
If ICOORD=2, IW(1)=JW(1)=1.

JW(M) - Second index of the reservoir gridblock containing the Mth well.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

Note: If the Mth well is completed parallel to the X- or Y-axis, JW(M) is the Z direction index—if the well is completed parallel to the Z-axis, JW(M) is the Y direction index. See example below.
If ICOORD=2, IW(M)=JW(M)=1.

IFLAG(M) - Flag indicating type of well constraint specification for Mth well.

Possible Values:

- 1 - Rate constrained injection well
- 2 - Pressure constrained production well (This option is available only if ICOORD=1 or 3)
- 3 - Pressure constrained injection well (This option is available only if ICOORD=1 or 3)
- 4 - Rate constrained production well

RW(M) - Radius of Mth well.

Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(M) - Skin factor for Mth well.

Units: dimensionless

IDIR(M) - Flag indicating the direction in which the Mth well is completed.

Possible Values:

- 1 - Well completed parallel to the X-axis
- 2 - Well completed parallel to the Y-axis
- 3 - Well completed parallel to the Z-axis

Note: If ICOORD=2, IDIR(M) must be equal to 3.

IFIRST(M) - Index of the first block in which the Mth well is completed.

Possible Values: Between 1 and the number of gridblocks in the pertinent direction, inclusive

ILAST(M) - Index of the last block in which the Mth well is completed.

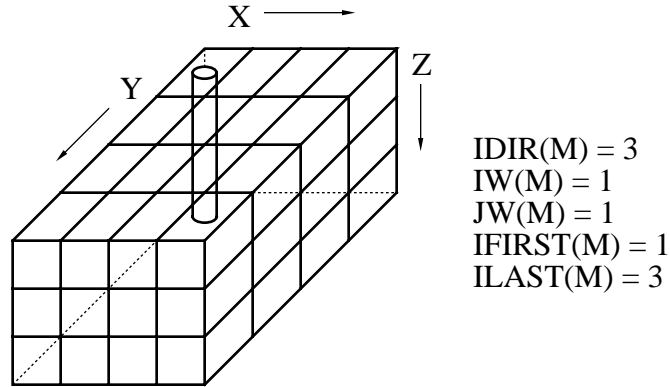
Possible Values: Between IFIRST(M) and the number of gridblocks in the pertinent direction, inclusive

IPRF(M) - Flag indicating if partial completion of the well is considered.

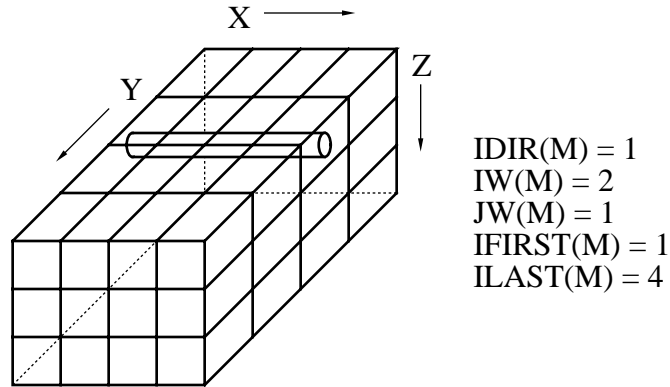
Possible Values:

- 0 - The well is fully completed
- 1 - The well is partially completed

Example: For a vertical well (completed through all the layers) as illustrated in the $4 \times 4 \times 3$ example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



For a horizontal well (completed from the first to last gridblock in the X direction and parallel to the X-axis) as illustrated in the $4 \times 4 \times 3$ example below, note the values of $IDIR(M)$, $IW(M)$, $JW(M)$, $IFIRST(M)$, and $ILAST(M)$:



Note: Horizontal wells can be used for 2-D X-Y or 3-D simulations.

3.7.6.b KPRF(M,IWB), for IWB=1, NWBC (This line is read only if IPRF=1)

KPRF(M,IWB) - Flag indicating if the IWBth well block of the Mth well is perforated or not.

Possible Values:

- 0 - The well block is not perforated
- 1 - The well block is perforated

3.7.6.c WELNAM(M)

WELNAM(M) - Name of the Mth well.

Note: The name can consist of any combination of up to 8 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(M)—at the beginning of the history output files.

3.7.6.d ICHEK(M), PWFMIN(M), PWFMAX(M), QTMIN(M), QTMAX(M)

ICHEK(M) - The flag to specify whether to check the rate or pressure caps for the Mth well.

Possible Values:

- 0 - There will be no check on the rate or pressure limits and no automatic shut in for the pressure constraint injector
- 1 - There will be no automatic shut in for the pressure constraint injector but the pressure or rate limits are checked
- 2 - There will be both the automatic shut in and the check on the pressure or rate limits

PWFMIN(M) - Minimum flowing bottom hole pressure (specified at the top layer) for the Mth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(M) - Maximum flowing bottom hole pressure (specified at the top layer) for the Mth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(M) - Minimum total flow rate (specified at the top layer) for the Mth well.

Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

QTMAX(M) - Maximum total flow rate (specified at the top layer) for the Mth well.

Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

Note: QTMIN(M) and QTMAX(M) need to be input as negative values for production wells (IFLAG=2 or 4).

PWFMIN(M) and PWFMAX(M) are the pressure caps for a rate constraint injector or producer well. QTMIN(M) and QTMAX(M) are the total rate caps for a pressure constraint injector or producer well. If the Mth pressure constraint injector or producer produces at total rate less than QTMIN(M), the Mth well will be switched to a rate constraint well with total rate of QTMIN(M) for the rest of the injector or production period. On the other hand, if the total rate is greater than the QTMAX(M), the Mth well then will be switched to a rate constraint well with the total rate of QTMAX(M). The similar concept is applied to a rate constraint injector or producer.

The user can skip the well control calculation by specifying very small values for QTMIN(M) and PWFMIN(M) and very large values for QTMAX(M) and PWFMAX(M).

The code still has the automatic option for shut in of a pressure constraint injector injecting at a rate of less than QTMIN(M).

- 3.7.7 The data on input lines 3.7.7.a, 3.7.7.b, 3.7.7.c, and 3.7.7.d are **repeated** for M=1 to NWELL times.

Note: For injection wells that are on rate constraint only injection rates and concentrations for each phase are listed. For injection wells that are on pressure constraint the injection pressure is also specified. In this case the injection rates are treated as phase cuts in the injected fluid. For producer pressure constraint only the bottom hole pressure is specified. For producer rate constraint only the total production rate is specified.

The user can shut in a pressure constraint well by specifying a negative bottom hole pressure or a rate constraint well by specifying a value of zero for rate (QI).

- 3.7.7.a ID(M), (QI(M,L), (C(M,KC,L), for KC=1, N), for L=1, MXP) (This set of data is read only if IFLAG(M)=1 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 3.7.6.a.

QI(M,L) - Injection rate of Lth phase in Mth well (see note below).

Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

C(M,KC,L) - Concentration of KCth component in Lth phase in Mth well.

Units: vary according to component (see note below)

Note: See Appendix D for component and phase numbering scheme and the concentration units for each species.

The KC index changes the fastest, the L index changes the next fastest, and the M index changes the slowest. A separate data line should be in the input file for each phase—that is, M × L lines will be read by the program. MXP is equal to 3 (IGAS=0) or 4 (IGAS≥1).

- 3.7.7.b ID(M), PWF(M) (This line is read only if IFLAG(M)=2 or 3)

ID(M) - Well I.D. number for the Mth well.

Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)

Note: See note for IDW(M) on input line 3.7.6.a. For IFLAG(M)=3, the rates (QI(M,L)) are used as an injected volume fraction for each phase.

PWF(M) - Flowing bottom hole pressure for the Mth well.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

- 3.7.7.c ID(M), TEMINJ(M) (This line is read only if IENG=1 and IFLAG(M)=1 or 3)

ID(M) - Well I.D. number for the Mth well.

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Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)
Note: See note for IDW(M) on input line 3.7.6.a.

TEMINJ(M) - Injection temperature for Mth well.
Units: °F (IUNIT=0) or °C (IUNIT=1)

3.7.7.d ID(M), QI(M,1) (This line is read only if IFLAG(M)=4)

ID(M) - Well I.D. number for the Mth well.
Possible Values: Must be between 1 and MXW (the source code parameter indicating the maximum number of wells)
Note: See note for IDW(M) on input line 3.7.6.a.

QI(L) - Total production rate for Mth well.
Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)
Note: This value needs to be input as a negative number.

3.7.8 TINJ, CUMPR1, CUMHI1, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.
Units: days or pore volumes (dependent on value of ISTOP flag)

CUMPR1 - Indicates interval at which profiles should be written to the PROF output file.
Units: pore volumes or days (dependent on value of ICUMTM flag)

CUMHI1 - Indicates interval at which production data should be written to the PROF output file.
Units: pore volumes or days (dependent on value of ICUMTM flag)

WRHPV - Indicates interval at which production histories should be written to output file(s) for history plotting.
Units: pore volumes or days (dependent on value of ICUMTM flag)
Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed.

WRPRF - Indicates interval at which information should be written to the output files controlled by the flags listed on input lines 3.2.3 and 3.2.4.
Units: pore volumes or days (dependent on value of ICUMTM flag)
Note: If WRPRF > total pore volume injected or maximum simulation time, the data will not be written.

RSTC - Indicates the interval at which restart data should be written to the RESTAR output file.
Units: pore volumes or days (dependent on value of ICUMTM flag)

Time Step Selection Data (input lines 3.7.9-3.7.13)

See Appendix E for more details on the time step selection options.

3.7.9 DT (This line is read only if IMES=1 and ITSTEP=0)

DT - Time step size for constant time step option.
Units: days

3.7.10 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES=2 and ITSTEP=0)

DT - Initial time step size.
Units: days

DCLIM - Tolerance for concentration change for the first three components.
Units: volume fraction

DTMAX - Maximum time step size.
Units: days

DTMIN - Minimum time step size.
Units: days

3.7.11 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES=2, ITSTEP=1, and at least one well is not shut-in.)

DT - Initial time step size.
Units: days

DCLIM - Tolerance for concentration changes for the first three components.
Units: volume fraction

CNMAX - Maximum Courant number.
Units: dimensionless

CNMIN - Minimum Courant number.
Units: dimensionless

3.7.12 DT, (DELC(KC), for KC=1, N), DTMAX, DTMIN (This line is read only if IMES=3 or 4 and ITSTEP=0)

DT - Initial time-step size.
Units: days

DELC(KC) - Tolerance for concentration change of KCth component (IMES=3) or relative tolerance for concentration change of KCth component (IMES=4).
Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)
IMES=4: dimensionless

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Note: DELC(KC) is the dimensionless relative change in concentration.
For example: DELC(3)=0.1 indicates a 10% change in concentration of component 3.

DTMAX - Maximum time step size.
Units: days

DTMIN - Minimum time step size.
Units: days

3.7.13 DT, (DELC(KC), for KC=1, N), CNMAX, CNMIN (This line is read only if IMES=3 or 4, ITSTEP=1, and all the wells are not shut-in)

DT - Initial time step size.
Units: days

DELC(KC) - Tolerance for concentration change of KCth component (IMES=3) or relative tolerance for concentration change of KCth component (IMES=4).
Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)
IMES=4: dimensionless

CNMAX - Maximum Courant number.
Units: dimensionless

CNMIN - Minimum Courant number.
Units: dimensionless

IMPORTANT NOTE: The data on input lines 3.7.14 through 3.7.29 describe the changes in boundary conditions and are repeated until the injected time (TINJ) is greater than or equal to the maximum simulation time (TMAX).

3.7.14 IBMOD

IBMOD - Flag to indicate if there are changes to the boundary conditions in this set of recurrent data.
Possible Values:
0 - There are no changes to the boundary conditions
1 - There are changes to the boundary conditions

3.7.15 IBOUND (This line is read only if IBMOD=1)

IBOUND - Flag indicating if constant potential boundaries at the top, left, and right sides of the simulation model are specified.
Possible Values:
0 - No boundary is specified
1 - Boundary is specified

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3.7.16 IBL, IBR, IBT, WTABL, WTABR (This line is read only if IBMOD=1 and IBOUND=1)

IBL - Flag indicating if the left hand side constant potential boundary is specified.

Possible Values:

0 - No boundary is specified

1 - Boundary is specified

IBR - Flag indicating if the right hand side constant potential boundary is specified.

Possible Values:

0 - No boundary is specified

1 - Boundary is specified

IBT - Flag indicating if the top constant pressure boundary of the vadose zone is specified.

Possible Values:

0 - Top boundary is closed

1 - Top boundary is open

WTABL - The depth to the water table at the left boundary.

Units: feet (IUNIT=0) or m (IUNIT=1)

WTABR - The depth to the water table at the right boundary.

Units: feet (IUNIT=0) or m (IUNIT=1)

3.7.17 PBL, C1BL, C5BL, C6BL (This line is read only if IBMOD=1 and IBOUND=1 and IZONE≠1 and IBL=1)

PBL- Pressure at the center of the top layer at the left boundary.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

C1BL- Concentration of water in aqueous phase at the left boundary.

Units: volume fraction

C5BL - Concentration of chloride in aqueous phase at the left boundary.

Units: meq/ml water

C6BL - Concentration of calcium in aqueous phase at the left boundary.

Units: meq/ml water

3.7.18 PBR, C1BR, C5BR, C6BR (This line is read only if IBMOD=1 and IBOUND=1 and IZONE≠1 and IBR=1)

PBR - Pressure at the center of the top layer at the right boundary.

Units: psia (IUNIT=0) or kPa (IUNIT=1)

C1BR - Concentration of water in aqueous phase at the right boundary.

Units: volume fraction

C5BR - Concentration of chloride in aqueous phase at the right boundary.

Units: meq/ml water

C6BR - Concentration of calcium in aqueous phase at the right boundary.

Units: meq/ml water

Note: For the biodegradation option (IBIO=1), the concentrations of all species considered at the boundary are set to the initial concentrations. If the variation in temperature is considered (IENG=1), the temperatures at the boundaries are set to the initial temperature.

3.7.19 IRO, ITSTEP, (IFLAG(M), for M=1, NWELL)

IRO - Flag indicating the equivalent well radius model to be used.

Possible Values:

1 - Babu and Odeh model is used

2 - Peaceman model is used

Note: The Babu and Odeh model (IRO=1) does not work for ICOORD=4.

ITSTEP - Flag indicating the units to be used when specifying the minimum and maximum time step.

Possible Values:

0 - Minimum and maximum time steps are input in days

1 - Minimum and maximum time steps are input as Courant numbers

Note: This option is only used if IMES>1 and it is not a shut-in period. If IMES=1, this flag is ignored. For a shut-in period of time, set ITSTEP=0.

IFLAG(M) - Flag indicating type of well constraint specification for Mth well.

Possible Values:

1 - Rate constrained injection well

2 - Pressure constrained production well (This option is available only if ICOORD=1 or 3)

3 - Pressure constrained injection well (This option is available only if ICOORD=1 or 3)

4 - Rate constrained production well

3.7.20 NWEL1

NWEL1 - Number of wells with changes in location (IW(M), JW(M)), skin, direction, perforation, name, or minimum and maximum bottomhole pressure or minimum or maximum rate.

3.7.21 The data on input lines 3.7.21.a through 3.7.21.d are repeated for M=1 to NWEL1 times.

3.7.21.a ID, IW(ID), JW(ID), RW(ID), SWELL(ID), IDIR(ID), IFIRST(ID), ILAST(ID), IPRF(ID)

ID - Well ID number with changes from the previous slug injection period.

IW(ID) - First index of the reservoir gridblock containing the IDth well.

Note: See note for input line 3.7.6.a.

JW(ID) - Second index of the reservoir gridblock containing the IDth well.

Note: See note for input line 3.7.6.a.

RW(ID) - Radius of IDth well.

Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(ID) - Skin factor for IDth well.

Units: dimensionless

IDIR(ID) - Flag indicating the direction in which the IDth well is completed.

Possible Values:

1 - Well completed parallel to the X-axis

2 - Well completed parallel to the Y-axis

3 - Well completed parallel to the Z-axis

Note: If ICOORD=2, IDIR(1) must be equal to 3.

IFIRST(ID) - Index of the first block in which the IDth well is completed.

ILAST(ID) - Index of the last block in which the IDth well is completed.

IPRF(ID) - Flag indicating if partial completion of the well is considered.

Possible Values:

0 - The well is fully completed

1 - The well is partially completed

3.7.21.b KPRF(ID,IWB), for IWB=1, NWBC (This line is read only if IPRF=1)

KPRF(ID,IWB) - Flag indicating if the IWBth well block of the IDth well is perforated or not.

Possible Values:

0 - The well block is not perforated

1 - The well block is perforated

3.7.21.c WELNAM(ID)

WELNAM(ID) - Name of the IDth well.

3.7.21.d ICHEK(ID), PWFMIN(ID), PWFMAX(ID), QTMIN(ID), QTMAX(ID)

ICHEK(ID) - The flag to specify whether to check the rate or pressure caps for the IDth well.

Possible Values:

0 - There will be no check on the rate or pressure limits and no automatic shut in for the pressure constraint injector

1 - There will be no automatic shut in for the pressure constraint injector but the user specified pressure or rate limits are checked

2 - There will be both the automatic shut in and the check on the user specified pressure or rate limits

PWFMIN(ID) - Minimum flowing bottom hole pressure (specified at the top layer) for the IDth well.

Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(ID) - Maximum flowing bottom hole pressure (specified at the top layer) for the IDth well.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(ID) - Minimum total flow rate (specified at the top layer) for the IDth well.
Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

QTMAX(ID) - Maximum total flow rate (specified at the top layer) for the IDth well.
Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

Note: See the note for input line 3.7.6.d.

3.7.22 NWEL2, (IDWW(J), for J=1, NWEL2)

NWEL2 - Number of wells with changes in rate, concentration or bottomhole pressure.

IDWW(J) - ID number for Jth well with changes.

3.7.23 The data on input lines 3.7.23.a through 3.7.23.d are repeated for M=1 to NWEL2 times.

3.7.23.a ID, QI(ID,L), (C(ID,KC,L), for KC=1,N), for L=1, MXP (This set of data is read only if IFLAG(ID)=1 or 3)

ID - Well ID number with changes from the previous slug injection period.

QI(ID,L) - Injection rate of Lth phase in IDth well (see note for input line 3.7.7.a).
Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

C(ID,KC,L) - Concentration of KCth component in Lth phase for IDth well.
Units: vary according to component (see note for input line 3.7.7.a)

Note: If IGAS=0, then MXP=3. If IGAS≥1, then MXP=4.

3.7.23.b ID, PWF(ID) (This line is read only if IFLAG(ID)=2 or 3)

ID - Well ID number with changes from the previous slug injection period.

PWF(ID) - Flowing bottom hole pressure for the IDth well.
Units: psia (IUNIT=0) or kPa (IUNIT=1)

3.7.23.c ID, TEMINJ(ID) (This line is read only if IENG=1 and IFLAG(ID)=1 or 3)

ID - Well ID number with changes from the previous slug injection period.

TEMINJ(ID) - Injection temperature for the IDth well.
Units: °F (IUNIT=0) or °C (IUNIT=1)

3.7.23.d ID, QI(ID,1) (This line is read only if IFLAG(ID)=4)

ID - Well ID number with changes from the previous slug injection period.

QI(ID,1) - Total production rate for IDth well.

Units: ft³/day (IUNIT=0) or m³/day (IUNIT=1)

Note: This value needs to be input as a negative number.

3.7.24 TINJ, CUMPR1, CUMHI1, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.

Units: days or pore volumes (dependent on value of ISTOP flag)

CUMPR1 - Indicates interval at which profiles should be written to the PROF output file.

Units: pore volumes or days (dependent on value of ICUMTM flag)

CUMHI1 - Indicates interval at which production data should be written to the PROF output file.

Units: pore volumes or days (dependent on value of ICUMTM flag)

WRHPV - Indicates interval at which production histories should be written to output file(s) for history plotting.

Units: pore volumes or days (dependent on value of ICUMTM flag)

Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed.

WRPRF - Indicates interval at which information should be written to the output files controlled by the flags listed on input lines 3.2.3 and 3.2.4.

Units: pore volumes or days (dependent on value of ICUMTM flag)

Note: If WRPRF > total pore volume injected or maximum simulation time, the data will not be written.

RSTC - Indicates the interval at which restart data should be written to the RESTAR output file.

Units: pore volumes or days (dependent on value of ICUMTM flag)

3.7.25 DT (This line is read only if IMES=1 and ITSTEP=0)

DT - Time step size for constant time step option.

Units: days

3.7.26 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES=2 and ITSTEP=0)

DT - Initial time step size.

Units: days

DCLIM - Tolerance for concentration change for the first three components.

Units: volume fraction

DTMAX - Maximum time step size.

Units: days

DTMIN - Minimum time step size.

Units: days

- 3.7.27 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES=2, ITSTEP=1, and at least one well is not shut-in)

DT - Initial time step size.

Units: days

DCLIM - Tolerance for concentration changes for the first three components.

Units: volume fraction

CNMAX - Maximum Courant number.

Units: dimensionless

CNMIN - Minimum Courant number.

Units: dimensionless

- 3.7.28 DT, (DELC(KC), for KC=1, N), DTMAX, DTMIN (This line is read only if IMES=3 or 4 and ITSTEP=0)

DT - Initial time-step size.

Units: days

DELC(KC) - Tolerance for concentration change, $\Delta C_{\text{lim},K}$, of KC^{th} component (IMES=3) or relative tolerance for concentration change of KC^{th} component (IMES=4).

Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)

IMES=4: dimensionless

DTMAX - Maximum time step size.

Units: days

DTMIN - Minimum time step size.

Units: days

- 3.7.29 DT, (DELC(KC), for KC=1, N), CNMAX, CNMIN (This line is read only if IMES=3 or 4, ITSTEP=1, and reservoir is not shut-in)

DT - Initial time step size.

Units: days

DELC(KC) - Tolerance for concentration change of KC^{th} component (IMES=3) or relative tolerance for concentration change of KC^{th} component (IMES=4).

Units: IMES=3: volume fraction, weight percent, meq/ml, or ppm (depending on which component the tolerance is for—see note for input line 3.7.7.a)

IMES=4: dimensionless

CNMAX - Maximum Courant number.
Units: dimensionless

CNMIN - Minimum Courant number.
Units: dimensionless

User notes:

A OUTPUT FILES

The following sections describe: (A.1) data that is written to the profile data file, (A.2) restart run procedure, (A.3) data written to stored restart data file, (A.4) data written to history files for each well, (A.5) data written to history of reservoir properties and overall injection and production rates from all the wells, (A.6) data written to aqueous phase tracer concentration data files, and (A.7) output files created when running GMS.

A.1 Data Written to Profile Data File

The information in the following lists is written to the profile data file (PROF).

Printed for each well at each CUMHI1 interval:

- Time, number of time steps
- Time step size
- Courant number
- Cumulative pore volume injected
- Original in place for each component
- Cumulative injection for each component
- Cumulative production for each component
- Amount retained for each component
- Relative error for each component
- Fraction of oil recovered
- If IREACT ≥ 2 :
 - Average number of iterations, computation time
- For each well:
 - Position of the well, first and last well block completed
 - Cumulative injection/production
 - Bottomhole pressure for each well block
 - All well related information (such as pressure for each phase, phase concentration, phase cut, etc.)
 - Producer wellbore temperature and phase cut and concentration

Printed for each gridblock at each CUMPR1 interval:

- Phase flux in each direction if IVEL=1
- Permeability reduction factor if IRKF=1
- Surfactant, polymer, or organic adsorbed concentration if IADS=1
- Index of surfactant phase environment if IPHSE=1

A.2 Restart Run Procedure

The restart procedure is available with UTCHEM. This enables a user to continue a run past the initial time period or to break a large run up into smaller segments. Each time you run UTCHEM, a file called RESTAR is created. This file (described in section 6.3) contains all the information necessary to continue the run at a later time. In order to do so, the user needs to:

- 1.- Rename the output file RESTAR from the previous run to INPUT2
- 2.- Set the variable IMODE equal to 2 on input line 3.1.3 of file INPUT
- 3.- Change the value of TMAX on input line 3.3.1 of file INPUT to the new injection period being simulated in the restart run
- 4.- Change the value of TINJ on input line 3.7.8 of file INPUT if appropriate
- 5.- Add additional information for input lines 3.7.14 through 3.7.29 of file INPUT if the well conditions are different for the new injection period

Note: Make sure the source code you run the restart problem (IMODE=2) has the same values for the array sizes in the parameter statement as the one used in original run (IMODE=1).

A.3 Data Written to Stored Restart Run Data File

The information in the following list is always written to the stored restart data file (RESTAR). If the user is running a RESTART run, this data file needs to be renamed to correspond to the INPUT2 input file. The values in parentheses are the FORTRAN variable names as they appear in the code.

Printed at the end of each run:

- Values in the PARAM.INC file (see the table in Section 2.2 for a comprehensive list)

- Time (T), injection time (TINJ), time step size (DT), number of time steps (ICNT)

- New slug injection or restart flag (IINJ), number of time step reduction (INEC), cumulative pore volume injection (CUMPV), number of blocks in X-direction minus 1 (NXM1)

- Cumulative injection (CUMI), cumulative production (CUMP), original in place (OIP) for each component

- Cumulative injection/production (CUMQI and CUMQP) for each well

- Phase concentration (C), phase saturation (S), effective salinity (CSE), overall concentration (CTOT), number of phases (NPHASE)

- If ICOORD=2:

 - Boundary concentration (CE), boundary pressure (PE)

- Viscosity (VIS), relative permeability (RPERM), injection rate (QI), total rate for each well (QT), phase rate (Q), bottomhole pressure (PWF)

- Pressure (P)

- If IADSO>1:

 - Organic adsorption (C2ADSS)

- If LMO=1:

 - Multiple organic adsorption (C2ADSK)

- Surfactant adsorption (C3ADSS), surfactant adsorption parameter (A3DS), polymer adsorption (C4ADSS)

- Permeability reduction factor (RKF), calcium concentration (C6JO), calcium adsorbed by clay (C6ADSS), calcium adsorbed by surfactant (C6HATS)

- Alcohol 7 partitioning coefficient (X7OLD), alcohol 8 partitioning coefficient (X8OLD)

- Oil breakthrough (BTO), tracer breakthrough (TBT), tracer injection concentration (CINJT), tracer retardation factor (TRD)

- Lower effective salinity (CSEL), upper effective salinity (CSEU)

- Density (DEN), capillary pressure (PRC)

- Total surfactant (TSURF)

- If IPERM=2 and IHYST=1:

 - Minimum water saturation (SWMIN)

- If IPERM=3:

 - Minimum water saturation (SWMIN), last time step water saturation (SWOLD), water saturation at reversal point (SWREV), last time step capillary pressure (PCOLD), capillary pressure at reversal point (PCREV)

 - Flag to define the scanning path (IPATH), saturation reversal flag (ISWREV)

- If ICAP=1:

Dendritic concentration (CD), dendritic saturation (SD), flowing saturation (SF), total flowing concentration (CTF)

If NG≠0:
Chromium adsorption (C14ADS), gel adsorption (C15ADS), cation exchange capacity of clay (QW)

If IENG=1:
Cum. heat inj. (CUMHI), cum. heat prod. (CUMHP), temperature (TEM), total volumetric heat capacity (TVHC)

If IENG=1 and IHLOS=1:
Cum. heat loss (TQLOS), integral for overburden and underburden heatloss calculations (RINO, RINU), time of change of overburden temp. from the reservoir block (TTCHG), overburden temperature (TEMPOB), underburden temperature (TEMPUB)

If IENG =1 and ICOORD =2:
Boundary enthalpy (ENTHE)

If IREACT >1:
Solid concentration (CSLDT), adsorbed concentration (CSORBT), species concentration (CAQSP), surf. associated cation concentration (CACATT), cation concentration (CACAT)
Cumulative no. of iteration for geochem option (ITCUM)

If IBIO =1:
Concentrations of attached biomass and intra-biomass concentrations of chemical species (CB)
Concentrations of reducing power in aqueous phase biomass (RED) and attached biomass (REDB)

A.4 Data Written to Well History Plotting Data File(s)

The information in the following list is always written to the well history plotting data files (HIST01-HISTxx) for each production well.

Printed at each WRHPV interval:

Cumulative pore volume, time [days], cumulative production [ft³, m³, or STB], water oil ratio, cumulative oil recovery, total production rate [ft³/day, m³/day, or STB/day]

If IGAS =1: Water cut, oil cut, microemulsion cut, gas cut

Wellbore pressure for each well block [psi or kPa]

If IENG =1: Wellbore temperature [°F or °C]

For I=1, N:

If ICF(I) =1: phase concentration for component N (C(I,L), L=1,MXP), total concentration of component N (CTOT(I))

If IREACT>1 or ICF(3)=1: Lower effective salinity, upper effective salinity, effective salinity

If IBIO =1 and IBPR =1:

Aqueous phase concentrations of components 1 through 8 and oil components in units of mg/L

If IBIO=1, IBPR=1, and there are cometabolic biodegradation reactions in which reducing power limitations are considered:

Concentrations of reducing power (NADH) in aqueous phase and attached biomass

If IREACT >1:

Independent species concentration (CAQSP(KK), KK=1, NIAQ) [mole/liter of water]

If IRSPS >0: Dependent species concentration (CAQSP(KK), KK=NIAQ+1,NFLD) [mole/liter of water]

If IREACT =3: Phase concentration of injected + generated surfactant (PSURF(I,L), L=1,3), total concentration of injected + generated surfactant (TSURF)

If NSLD >0: Concentration of solid components (CSLDT(KK), KK=1, NSLD) [mole/liter of pore volume]

If ICNM >0: Log₁₀ of interfacial tension between water/microemulsion and oil/microemulsion (XIFT1, XIFT2) [dyne/cm]

The information in the following list is always written to the well history plotting data files for each injection well.

Printed at each WRHPV interval:

Cumulative pore volume, time in days, cumulative injection [ft³, m³, or STB], injection rate [ft³/day, m³/day, or STB/day]

Wellbore pressure for each well block [psi or kPa]

Pressure drop between the wells (for the specific case of one injector and one producer only) or pressure drop between the pressure tabs (when NG>0, NY=1, NZ=1, see input line 3.4.168) [psi or kPa]

A.5 Data Written to Overall History Plotting Data File

The information in the following list is always written to the overall history plotting data file (OVERAL).

Printed at each WRHPV interval:

Cumulative pore volume, time in days, volumetric averaged reservoir pressure (psi or kPa), cumulative oil produced (%OOIP), cumulative oil produced (bbls or m³), volumetric averaged reservoir temperature (°F or °C) (only if IENG=1)

Total injection rate (B/D or m³/day), total production rate (B/D or m³/day), total fluid injected (1000 bbls or m³), total fluid produced (1000 bbls or m³) [Note: The fluid injected and produced values are calculated for the last time step before the print interval.]

Overall production rate for each phase (QBAR(L) for L=1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1) (B/D or m³/day)

Average cut for each phase (FBAR(L) for L=1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1)

Average saturation for each phase (SBAR(L) for L=1, MXP where MXP=3 if IGAS=0 and MXP=4 if IGAS =1)

If ICF(3)=1: Cumulative surfactant injected (bbls or m³), Cumulative surfactant produced (bbls or m³), adsorbed surfactant (bbls or m³), retained surfactant (bbls or m³), adsorbed surfactant (ml/ml PV)

If ICF(4)=1: Cumulative polymer injected (wt%), Cumulative polymer produced (wt%), adsorbed polymer (wt%), retained polymer (wt%), adsorbed polymer (wt. % / PV)

A.6 Data Written to Tracer Concentration Observation Point Data File(s)

The information in the following list is written to the tracer observation history plotting data files (TRAC01-TRAC n) for each tracer (if IPOBS=0).

Printed at each WRHPV interval:

Time in days, cumulative pore volume

For NTW tracers:

Aqueous phase tracer concentration at NOBS observation locations

For NTA tracers:

Gas phase tracer concentration at NOBS observation locations

A.7 Output Files Created When Running GMS

The following binary output files are created when running GMS. The "*file*" prefix for the file names comes from the prefix of the input file name. For example, if the input file is named run1.dat, all GMS output file names will start with "run1" in place of "*file*" in the table below. For the component concentration files, *spname*(#) refers to the value of SPNAME on input line 3.1.24.

Output file name	Contents
<i>file_spname(1).dat</i>	Total concentration of component 1, created if IPCTOT=1 and ICF(1)≠0 and IPRFLG(1)≠1
<i>ile_spname(2).dat</i>	Total concentration of component 2, created if IPCTOT=1 and ICF(2)≠0 and IPRFLG(2)≠1
...	...
<i>ile_spname(xx).dat</i>	Total concentration of last component, created if IPCTOT=1 and ICF(xx)≠0 and IPRFLG(xx)≠1
<i>file_p001.dat</i>	Water pressure data, created if IPRESS=1
<i>file_p002.dat</i>	Oil pressure data, created if IPRESS=1
<i>file_p003.dat</i>	Microemulsion pressure data, created if IPRESS=1
<i>file_p004.dat</i>	Gas pressure data, created if IPRESS=1 and IGAS>0
<i>file_s001.dat</i>	Water saturation data, created if IPSAT=1
<i>file_s002.dat</i>	Oil saturation data, created if IPSAT=1
<i>file_s003.dat</i>	Microemulsion saturation data, created if IPSAT=1
<i>file_s004.dat</i>	Gas saturation data, created if IPSAT=1 and IGAS>0
<i>file_t001.dat</i>	Temperature data, created if IENG=1 and IPTEMP=1

B GEOCHEMISTRY OPTION (IREACT>1)

This section gives an example list of elements and reactive species for the geochemistry options of IREACT=2 or IREACT=4.

<u>Elements or pseudo-element:</u>	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Aluminum, Silicon, Oxygen, Chlorine, S (Injected surfactant)
<u>Independent aqueous or oleic species:</u>	H^+ , Na^+ , Ca^{2+} , Mg^{2+} , Al^{3+} , CO_3^{2-} , Cl^- , S^- , H_4SiO_4 , H_2O
<u>Dependent aqueous or oleic species:</u>	$Ca(OH)^+$, $Mg(OH)^+$, $Al(OH)^{2-}$, $Al(OH)_2^-$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, OH^- , HCO_3^- , $H_3SiO_4^-$, $H_2SiO_4^{2-}$, $HSiO_6^{3-}$, $Si_2O_5^{2-}$, $Al(OH)_4^-$, H_2CO_3 , $CaCO_3^0$, $MgCO_3^0$
<u>Solid species:</u>	$CaCO_3$ (Calcite), $Al_2Si_2O_5(OH)_4$ (Kaolinite), $MgCO_3$ (Magnesite), $NaAlSi_2O_6 \cdot H_2O$ (Analcite), SiO_2 (Silica), $Mg(OH)_2$ (Magnesium Hydroxide)
<u>Adsorbed cations on rock surface:</u>	\bar{H}^+ , \bar{Na}^+ , \bar{Ca}^{2+} , \bar{Mg}^{2+}
<u>Adsorbed cations on micelles:</u>	$\bar{\bar{Na}}^+$, $\bar{\bar{Ca}}^{2+}$, $\bar{\bar{Mg}}^{2+}$

<u>Aqueous reactions</u>	<u>Equilibrium constant</u>
$H_2O \xrightleftharpoons{K_1^{eq}} H^+ + OH^-$	$K_1^{eq} = [H^+] [OH^-]$
$H^+ + CO_3^{2-} \xrightleftharpoons{K_2^{eq}} HCO_3^-$	$K_2^{eq} = \frac{[HCO_3^-]}{[H^+] [CO_3^{2-}]}$
$Ca^{2+} + H_2O \xrightleftharpoons{K_3^{eq}} Ca(OH)^+ + H^+$	$K_3^{eq} = \frac{[Ca(OH)^+] [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \xrightleftharpoons{K_4^{eq}} Mg(OH)^+ + H^+$	$K_4^{eq} = \frac{[Mg(OH)^+] [H^+]}{[Mg^{2+}]}$
$Al^{3+} + H_2O \xrightleftharpoons{K_5^{eq}} Al(OH)^{2+} + H^+$	$K_5^{eq} = \frac{[Al(OH)^{2+}] [H^+]}{[Al^{3+}]}$
$Al^{3+} + 2H_2O \xrightleftharpoons{K_6^{eq}} Al(OH)_2^+ + 2H^+$	$K_6^{eq} = \frac{[Al(OH)_2^+] [H^+]^2}{[Al^{3+}]}$

Aqueous reactions (cont.)	Equilibrium constant (cont.)
$\text{Al}^{3+} + 4\text{H}_2\text{O} \xrightleftharpoons{K_7^{\text{eq}}} \text{Al}(\text{OH})_4^- + 4\text{H}^+$	$K_7^{\text{eq}} = \frac{[\text{Al}(\text{OH})_4^-][\text{H}^+]^4}{[\text{Al}^{3+}]}$
$\text{H}_4\text{SiO}_4 \xrightleftharpoons{K_8^{\text{eq}}} \text{H}^+ + \text{H}_3\text{SiO}_4^-$	$K_8^{\text{eq}} = \frac{[\text{H}^+][\text{H}_3\text{SiO}_4^-]}{[\text{H}_4\text{SiO}_4]}$
$\text{H}_4\text{SiO}_4 \xrightleftharpoons{K_9^{\text{eq}}} 2\text{H}^+ + \text{H}_2\text{SiO}_4^{2-}$	$K_9^{\text{eq}} = \frac{[\text{H}^+]^2[\text{H}_2\text{SiO}_4^{2-}]}{[\text{H}_4\text{SiO}_4]}$
$\text{Ca}^{2+} + \text{H}^+ + \text{CO}_3^{2-} \xrightleftharpoons{K_{10}^{\text{eq}}} \text{Ca}(\text{HCO}_3)^+$	$K_{10}^{\text{eq}} = \frac{[\text{Ca}(\text{HCO}_3)^+]}{[\text{Ca}^{2+}][\text{CO}_3^{2-}][\text{H}^+]}$
$\text{Mg}^{2+} + \text{H}^+ + \text{CO}_3^{2-} \xrightleftharpoons{K_{11}^{\text{eq}}} \text{Mg}(\text{HCO}_3)^+$	$K_{11}^{\text{eq}} = \frac{[\text{Mg}(\text{HCO}_3)^+]}{[\text{Mg}^{2+}][\text{CO}_3^{2-}][\text{H}^+]}$
$2\text{H}^+ + \text{CO}_3^{2-} \xrightleftharpoons{K_{12}^{\text{eq}}} \text{H}_2\text{CO}_3$	$K_{12}^{\text{eq}} = \frac{[\text{H}_2\text{CO}_3]}{[\text{CO}_3^{2-}][\text{H}^+]^2}$
$2\text{H}_4\text{SiO}_4 \xrightleftharpoons{K_{13}^{\text{eq}}} 2\text{H}_2\text{O} + 3\text{H}^+ + \text{HSi}_2\text{O}_6^{3-}$	$K_{13}^{\text{eq}} = \frac{[\text{H}^+]^3[\text{HSi}_2\text{O}_6^{3-}]}{[\text{H}_4\text{SiO}_4]^2}$
$2\text{H}_4\text{SiO}_4 \xrightleftharpoons{K_{14}^{\text{eq}}} 2\text{H}^+ + 3\text{H}_2\text{O} + \text{Si}_2\text{O}_5^{2-}$	$K_{14}^{\text{eq}} = \frac{[\text{H}^+]^2[\text{Si}_2\text{O}_5^{2-}]}{[\text{H}_4\text{SiO}_4]^2}$

Solid species	Solubility product
CaCO_3	$K_1^{\text{sp}} = [\text{Ca}^{2+}][\text{CO}_3^{2-}]$
MgCO_3	$K_2^{\text{sp}} = [\text{Mg}^{2+}][\text{CO}_3^{2-}]$
SiO_2	$K_3^{\text{sp}} = [\text{H}_4\text{SiO}_4]$
$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$	$K_4^{\text{sp}} = [\text{H}^+]^{-6}[\text{Al}^{3+}]^2[\text{H}_4\text{SiO}_4]^2$
$\text{NaAlSi}_2\text{O}_6 \cdot \text{H}_2\text{O}$	$K_5^{\text{sp}} = [\text{H}^+]^{-4}[\text{Na}^+][\text{Al}^{3+}][\text{H}_4\text{SiO}_4]^2$
$\text{Mg}(\text{OH})_2$	$K_6^{\text{sp}} = [\text{Mg}^{2+}][\text{H}^+]^{-2}$

Exchange reactions (on matrix)	Exchange equilibrium constant
$2\overline{\text{Na}}^+ + \text{Ca}^{2+} \xrightleftharpoons{K_1^{\text{ex}}} 2\text{Na}^+ + \overline{\text{Ca}}^{2+}$	$K_1^{\text{ex}} = \frac{[\overline{\text{Ca}}^{2+}] [\text{Na}^+]^2}{[\text{Ca}^{2+}] [\overline{\text{Na}}^+]^2}$
$2\overline{\text{Na}}^+ + \text{Mg}^{2+} \xrightleftharpoons{K_2^{\text{ex}}} 2\text{Na}^+ + \overline{\text{Mg}}^{2+}$	$K_2^{\text{ex}} = \frac{[\overline{\text{Mg}}^{2+}] [\text{Na}^+]^2}{[\text{Mg}^{2+}] [\overline{\text{Na}}^+]^2}$
$\overline{\text{H}}^+ + \text{Na}^+ + \text{OH}^- \xrightleftharpoons{K_3^{\text{ex}}} \overline{\text{Na}}^+ + \text{H}_2\text{O}$	$K_3^{\text{ex}} = \frac{[\text{Na}^+] [\overline{\text{H}}^+]}{[\overline{\text{Na}}^+] [\text{H}^+]}$

Exchange reactions (on micelle)	Exchange equilibrium constant
$2\overline{\overline{\text{Na}}}^+ + \text{Ca}^{2+} \xrightleftharpoons{K_1^{\text{exm}}} 2\text{Na}^+ + \overline{\overline{\text{Ca}}}^{2+}$	$K_1^{\text{exm}} = \frac{[\overline{\overline{\text{Ca}}}^{2+}] [\text{Na}^+]^2}{[\overline{\overline{\text{Na}}}^+]^2 [\text{Ca}^{2+}]}$ <p style="text-align: center;">where $K_1^{\text{exm}} = \beta_1^{\text{exm}} [\text{S}^-]$</p>
$2\overline{\overline{\text{Na}}}^+ + \text{Mg}^{2+} \xrightleftharpoons{K_2^{\text{exm}}} 2\text{Na}^+ + \overline{\overline{\text{Mg}}}^{2+}$	$K_2^{\text{exm}} = \frac{[\overline{\overline{\text{Mg}}}^{2+}] [\text{Na}^+]^2}{[\overline{\overline{\text{Na}}}^+]^2 [\text{Mg}^{2+}]}$ <p style="text-align: center;">where $K_2^{\text{exm}} = \beta_2^{\text{exm}} [\text{S}^-]$</p>

User notes:

C MAIN PROGRAM FLOW OUTLINE

The following outline represents the basic flow through the main program of UTCHEM (that is, the order in which major subroutines are called).

- I. INOUT
 - A. FILE1
 - B. PRINTS
 - C. PRINTI
 - D. RESREAD
 - E. INNAME (called only if NO>1 and IOD is not equal to 1)
 - F. MOPPST (called only if NO>1)
 - 1. SLV2EQ
 - G. PRINTO (called only if NO>1)
 - H. WMEACN (called only if NO>1 and IOD is not equal to 1)
 - I. DPREAD (called only if ICAP=2 and NTW>0)
 - J. GEOREAD (called only if IREACT>1)
 - K. BIOREAD (called only if IBIO=1)
 - L. WELREAD
 - M. METRIC (called only if IUNIT=1)
 - N. INIT
 - 1. WELLIX
 - a. RADIUS
 - O. FILE3
 - P. FILE2
 - Q. GRDFAC
 - R. GMSINI (called only if IOUTGMS=1)
- II. RSTART (called only if IMODE=2)
 - A. NSLUG
 - B. WELLIX
 - 1. RADIUS
- III. TIME0
 - A. OMOFR (called only if NO>1)
 - B. DENSTY
 - C. RPERM0
 - D. ADS0 (called only if ICWI≥0)
 - E. VIS0
- IV. TRAN1
- V. ASIGN1
- VI. TRANS (Transmissibilities)
- VII. SOLMAT (Pressure Eq.)
 - A. WELL
 - B. BUNDRY (called only if IBOUND=1)
 - C. JCG
- VIII. QRATE

- IX. CONEQ (Conservation Eq.)
 - A. GEL
- X. ADOIL (called only if IADSO>0)
- XI. ADSORB
- XII. REACTR (called only if IREACT>1)
 - A. RENAM1
 - B. TOTALS
 - C. MANIPL
 - D. JACUP
 - 1. GAUSS
 - 2. SOLVE
 - E. RENAM2
- XIII. CSECAL
 - A. ALCPTN (called only if IALC=1)
 - 1. TWOALC
 - 2. CUBIC
 - B. CSEOD (called only if NO>1 and IOD is not equal to 1)
 - C. IONCNG
 - D. PHASC (called only if surfactant is not present and IREACT<1)
 - 1. MAYER (called only if IMASS=2 and ICOR=1)
 - a. FLUX (called only if IMASS=2 and ICOR=1)
 - 2. NONEQ
 - 3. ODISWO (called only if NO>1)
 - a. NONEQK
 - E. PHCOMP (called only if surfactant is present or IREACT>1)
 - 1. MAYER (called only if IMASS=2 and ICOR=1)
 - a. FLUX (called only if IMASS=2 and ICOR=1)
 - 2. NONEQ
 - 3. ODISWO
 - 4. TIELIN
 - a. TRY
 - 5. REVISE
 - 6. VGAMMA
 - 7. SINGLE
 - 8. ODISTM (called only if IHAND=0)
 - 9. ODISTM1 (called only if IHAND=1)
- XIV. BIOSOLVE (called only if IBIO=1)
 - A. FLUX
 - B. PHABIO (called only if IBPP=1)
 - C. THIRDD
 - D. INST (called only if IBKIN =3)
 - E. SDRIV2 (called only if IBKIN = 1 or 2 and running Cray version of code)
 - 1. F
 - 2. G
 - F. DDRIV2 (called only if IBKIN = 1 or 2 and running double precision version of code)
 - 1. F

2. G

- XV. OMOFR (called only if NO>1)
- XVI. TCAP (called only if ICAP=1)
- XVII. TDIFFU (called only if ICAP=2)
- XVIII. DENSTY
- XIX. ASIGN2
- XX. ENGBAL (called only if IENG=1)
- XXI. LAUWER (called only if IENG=1 and IANAL=1)
- XXII. CAPNUM (called only if ITRAP=1)
- XXIII. TRAPNO (called only if ITRAP=2 and IGAS=0)
- XXIV. TRAP (called only if IPERM<2 and IGAS=0)
- XXV. TRAPG (called only if IPERM<2 and IGAS≥1)
- XXVI. HYSWWG (called only if IPERM=2 and ICF(3)=0)
- XXVII. HYSWWS (called only if IPERM=2 and ICF(3)=1)
- XXVIII. HYSTMW (called only if IPERM=3)
 - A. CUBIC2
- XXIX. UTFOAM (called only if IGAS=2)
- XXX. VISCOS
- XXXI. WELLCK (called only if ICHEK>0)
- XXXII. OUTDT1
- XXXIII. OUTDT3
- XXXIV. OUTDT2
 - A. PRINTI
 - B. PRINTS
- XXXV. NSLUG
 - A. WELLIX
 - 1. RADIUS
- XXXVI. RSTART
- XXXVII. Go to step V (ASIGN1) if not done
- XXXVIII. SUMTAB

User notes:

D PHASES AND SPECIES IN UTCHEM

This section gives the component numbering scheme in UTCHEM and the unit for each component.

The following values for L correspond to the indicated phase:

<u>L</u>	<u>Phase</u>
1	Aqueous phase
2	Oleic phase
3	Microemulsion phase
4	Gas phase

The following indices correspond to the indicated components [corresponding concentration units are listed in square brackets]:

For all values of IREACT:

<u>Index</u>	<u>Component [conc. units]</u>
1	Water [volume fraction]
2	Oil [volume fraction]
3	Surfactant [volume fraction]
4	Polymer or silicate (KGOPT=3) [weight percent]
5	Total nonsorbing anions concentration, assumed to all be chloride anions [meq/ml water]
6	Divalent cations, assumed to all be calcium for IREACT<2 [meq/ml water]
7	Alcohol 1 [volume fraction]
8	Alcohol 2 or Gas [volume fraction]

Organic species (IBIO=0 and NO>1):

<u>Index</u>	<u>Component [conc. units]</u>
9	First organic species [volume fraction]
8+NO	Last organic species [volume fraction]

Tracers (NT>0):

<u>Index</u>	<u>Component [conc. units]</u>
9+NO	First tracer [<i>dependent on user input</i>]
8+NO+NTW+NTA	Last tracer [<i>dependent on user input</i>]

Geochemistry option species (IREACT=2 or IRECAT=3):

<u>Index</u>	<u>Component [conc. units]</u>
9+NO+NTW+NTA	First geochemistry component [meq/ml]
8+NO+NTW+NTA+NGC	Last geochemistry component [meq/ml]

Gel model species (IREACT=1 and NG>0):

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	KGOPT=1	KGOPT=2	KGOPT=3
<u>Index</u>	<u>Component</u> <u>[conc. units]</u>	<u>Component</u> <u>[conc. units]</u>	<u>Component</u> <u>[conc. units]</u>
NG1*	Na ₂ Cr ₂ O ₇ [ppm]	—	—
NG2	CSN ₂ H ₄ [ppm]	Malonate ion [ppm]	—
NG3	Cr ³⁺ [ppm]	Cr ³⁺ [ppm]	OH ⁻ [ppm]
NG4	Gel [ppm]	Gel [ppm]	Gel [ppm]
NG5	Hydrogen [meq/ml]	Hydrogen [meq/ml]	—

*where NG1 = 9+NO+NTW+NTA

Geochemistry/Gel option species (IREACT=4 and NG>0):

<u>Index</u>	<u>Component [conc. units]</u>
9+NO+NTW+NTA	First geochemistry component [meq/ml]
8+NO+NTW+NTA+NGC	Last geochemistry component [meq/ml]

	KGOPT=1	KGOPT=2
<u>Index</u>	<u>Component [conc. units]</u>	<u>Component [conc. units]</u>
NG1*	Na ₂ Cr ₂ O ₇ [ppm]	—
NG2	CSN ₂ H ₄ [ppm]	Malonate ion [ppm]
NG3	Cr ³⁺ [ppm]	Cr ³⁺ [ppm]
NG4	Gel [ppm]	Gel [ppm]

*where NG1 = 9+NO+NTW+NTA+NGC

Biological model species (IBIO=1):

<u>Index</u>	<u>Component</u> <u>[conc. units]</u>
9+NO+NTW+NTA+NGC+NG	First biological species [mg/ℓ]
8+NO+NTW+NTA+NGC+NG+NOTH	Last biological species [mg/ℓ]

E TIME-STEP SELECTION

This section discusses the automatic time-step selection options available in UTCHEM: (E.1) selector based on method of relative changes for the first three components, (E.2) selector based on method of relative changes for all the components, and (E.3) selector based on changes in dimensionless concentration for all the components.

The Courant number, C , is defined as:

$$C = \frac{Q \Delta t}{\Delta x \Delta y \Delta z \phi}$$

where Q is maximum injection/production per wellblock.

E.1 Method of Relative Changes for First Three Components (IMES=2)

Minimum and maximum time step in days (option ITSTEP=0):

The time step selection is based on the method of relative changes for the first three components (water, oil, and surfactant) as:

$$\Delta t^{n+1} = \Delta t^n \min \left(\frac{\Delta C_{\text{lim}}}{\max_{i=1}^{\text{NBL}} |\Delta C_{i,\kappa}|} \right) \quad \kappa = 1, 2, 3 \quad (\text{E.1})$$

where Δt^{n+1} is limited to: $\Delta t_{\text{min}} \leq \Delta t^{n+1} \leq \Delta t_{\text{max}}$. Δt_{min} and Δt_{max} are the input time step values and ΔC_{lim} is the input value for concentration tolerance (DCLIM).

Minimum and maximum time step in days (option ITSTEP=1):

The minimum and maximum time steps in days are computed based on the minimum and maximum Courant number as:

$$\Delta t_{\text{min}} = \frac{\text{CNMIN}}{\min_{M=1}^{\text{nwell}} \left(\max_{i=1}^{\text{nwbc}} \frac{Q_i}{\Delta x_i \Delta y_i \Delta z_i \phi_i} \right)}$$

and

$$\Delta t_{\max} = \frac{\text{CNMAX}}{\min_{M=1}^{\text{nwell}} \left(\max_{i=1}^{\text{nwbc}} \frac{Q_i}{\Delta x_i \Delta y_i \Delta z_i \phi_i} \right)}$$

where Courant number (C) is limited to: $\text{CNMIN} \leq C \leq \text{CNMAX}$. CNMIN and CNMAX are the input Courant number values in input line 3.7.11. The time step is then calculated from Eq. E.1.

E.2 Method of Relative Changes for All Components (IMES=3)

For IMES=3, the method of relative changes is applied to all the components in the simulation run:

$$\Delta t^{n+1} = \Delta t^n \min \left(\frac{\Delta C_{\text{lim},\kappa}}{\max_{i=1}^{\text{NBL}} |\Delta C_{i,\kappa}|} \right) \quad \kappa = 1, \dots, n_c$$

where Δt^{n+1} is limited to: $\Delta t_{\text{min}} \leq \Delta t^{n+1} \leq \Delta t_{\text{max}}$. $\Delta C_{\text{lim},\kappa}$ is a fraction of the initial or injected concentration (whichever is larger) of the KC^{th} component, DELC(KC) in input lines 3.7.12 or 3.7.13. For example: $\Delta C_{\text{lim},3} = 0.1 \times C_3$ where C_3 is the total concentration of component 3. If $\Delta C_{\text{lim},\kappa}$ of the KC^{th} component is entered as zero, that component is not considered in the time-step size selection.

E.3 Method of Relative Changes Using Dimensionless Concentration for All Components (IMES=4)

For IMES=4, the method of relative changes is applied to all the components in the simulation run:

$$\Delta t^{n+1} = \Delta t^n \min \left(\frac{R_{\text{lim},\kappa}}{\max_{i=1}^{\text{NBL}} \left| \frac{\Delta C_{i,\kappa}}{C_{i,\kappa}} \right|} \right) \quad \kappa = 1, \dots, n_c$$

where Δt^{n+1} is limited to: $\Delta t_{\text{min}} \leq \Delta t^{n+1} \leq \Delta t_{\text{max}}$. $R_{\text{lim},\kappa}$ is the input dimensionless relative change in concentration of component κ (DELC(KC)) on input lines 3.7.12 or 3.7.13. For example $R_{\text{lim},3}=0.1$ indicates a 10% change in concentration of Component 3.

F CHANGES TO USER'S GUIDE

This section is designed to point out the major modifications to the UTCHEM user's guide (as opposed to the code) that occurred between versions 7.0 and 9.0. This list is not comprehensive.

F.1 New Variables

This section lists new input variables introduced to UTCHEM with version 7.0. The variables are also flagged within the body of the user's guide by being printed in *italicized boldface*.

Variable(s)	Line number(s)
IOUTGMS	3.2.1
IPBIO	3.2.3
IHYSTP, IFOAMP, INONEQ	3.2.4
ICWI	3.3.18
CWI	3.3.32-3.3.34
REFK	3.4.130
C5INI	3.4.133

F.2 Modified Variables

This section lists deleted input variables and variables whose definitions were modified or expanded in version 9.0.

Variable(s)	Line number(s)	Modification
RUNNO	3.1.1	Restricted size and expanded usage
IPTRAC, IPBR	3.2.3 (in 7.0 guide)	Variable deleted
IPHP	3.2.4 (in 7.0 guide)	Variable deleted
IADS, IVEL, IRFK, IPHSE	3.2.5	Moved to new input line

F.3 Other Changes

This section lists additional changes made to the user's guide for version 9.0.

Change	Section number (s)
Updated Input and Output file discussion to include HEAD file	2.1
Changed "Source Code Array Dimensions" section to "Description of HEAD File" - major overhaul of this section	2.2
Updated compilation instructions	2.3 and 2.4
Removed Cray compilation information	Previously Section 2.5
Updated information	A.1
Updated main program flow outline	C
Moved work . job description	2.4, removed old Appendix F

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