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USER'S GUIDE FOR UTCHEM-5.32m
A THREE-DIMENSIONAL CHEMICAL FLOOD SIMULATOR

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Final Report for the Period
September 30, 1992 to December 31, 1995

By
Enhanced Oil and Gas Recovery Research Program
The University of Texas at Austin

July 1996

Performed Under Contract No. DE-AC22-92BC14885

The University of Texas at Austin
Austin, Texas

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Prepared for
U.S. Department of Energy
Assistant Secretary for Fossil Energy

Jerry Casteel, Project Manager
Bartlesville Project Office
P.O. Box 1398
Bartlesville, OK 74005

Prepared by
The Unversity of Texas at Austin
Austin, Texas 78712

User's Guide for

UTCHEM-5.32m

A Three-Dimensional
Chemical Flood Simulator

Enhanced Oil and Gas Recovery Research Program
Center for Petroleum and Geosystems Engineering
The University of Texas at Austin
Austin, Texas 78712

May, 1995

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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
- dilution effects
- adsorption
- interfacial tension
- relative permeability
- 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 adsorption
- polymer properties:
    - shear thinning viscosity
    - permeability reduction
    - inaccessible pore volume
    - adsorption
- gel properties:
    - viscosity
    - adsorption
    - permeability reduction
- tracer properties:
    - partitioning
    - radioactive decay
    - adsorption
    - reaction (ester hydrolization)
- temperature dependent properties:
    - viscosity
    - gel reactions
    - tracer reaction

The following options are available with UTCHEM: isothermal or non-isothermal conditions, a constant or variable time-step, constant pressure or constant rate well conditions, horizontal and vertical wells, and a radial or cartesian geometry. Please refer to the dissertation "Field Scale Simulation of Chemical Flooding" by Naji Saad, August, 1989, for a more detailed discussion of the UTCHEM simulator and its formulation.

2.0 OPERATION OF THE SIMULATOR

The UTCHEM simulator is run on a CRAY Y/MP at the University of Texas High Performance Computing Facility (UNICOS operating system), a number of DEC Alpha systems (DEC 4000/610, 3000/500 & 3000/300X) at the Department of Petroleum and Geosystems Engineering (OSF/1 operating system), and a DEC Alpha system (DEC 3000/500) at the Department of Petroleum and Geosystems Engineering (OpenVMS operating system). The same code is executed on all three systems, except for the use of double precision (64-bit words) on the DEC machines—we differentiate between "Cray" and "DEC" versions of the code by adding a "V" prior to the version number for the "Cray" version and a "D" prior to the version number for the "DEC" (or double-precision) version. Several intrinsic Cray functions need to be implemented when not running on the Cray; these routines are "commented" out in the "Cray" version. Please check the source code for additional information about necessary changes when running on different computers.

2.1 Input and Output Files

UTCHEM requires one input file for non-restart runs. For restart runs, a restart file is required in addition to the original input data file used for the previous run. A detailed input data description is given in section 3.0 and the data in the restart data file is documented in the appendix. A sample input file is given in section 5.0. The number of output files generated by UTCHEM varies depending upon several control flags set by the user in the input file. The number of history plot files depends on the value of the MXW parameter in the source code. The FORTRAN unit number for the history plot file is incremented by one for each well. For example, if MXW is equal to three, then three history plot files would be generated corresponding to FORTRAN unit numbers 19, 20, and 21 even if the run only has two wells. The input and output files are summarized in the following table.

Unit Number	File Name	Contents
1	TEMPL	Analytical temp. profile, created if IENG=1 and IANAL=1
2	ECHO	Echo print of the input file information

3	SUMARY	Summary data
4	PROFIL	Formatted profile data; described in Appendix 6.1
5	INPUT	Input data; described in detail in section 3.0
6	TTABLE	Table of time steps and Courant numbers
7	RESTAR	Stored restart run data; described in Appendix 6.3
8	CONCP	Component concentration profile plotting data, created if IPCTOT>0
9	OVERAL	History of overall properties; described in Appendix 6.5
10	GFILEP	Gel property profile plotting data, created if IREACT=1
11	PRESP	Phase pressure profile plotting data, created if IPPRES>0
12	SATP	Phase saturation profile plotting data, created if IPSAT>0
13	TRACP	Phase tracer concentration profile plotting data, created if IPTRAC>0
14	CAPP	Capacitance property profile plotting data, created if IPCAP>1
15	ALKP	Alkaline option related profile plotting data, created if IREACT>1
16	INPUT2	Restart run data (input file created by an earlier run)
17	WARN	Warning messages
18	TEMPP	Temperature profile, created if IENG =1 and IPTEMP=1
19	HIST01	Well history plotting data for well #1; described in Appendix 6.4
20	HIST02	Well history plotting data for well #2
...		
ℓ	HIST*ℓ*	Well history plotting data for last well
ℓ+1	TRAC01	Aqueous phase tracer concentration at 1st observation point , created if IPOBS>0; described in Appendix 6.6
ℓ+2	TRAC02	Aqueous phase tracer concentration at 2nd observation point
...		
n	TRAC*n*	Aqueous phase tracer concentration at last observation point

2.2 Source Code Array Dimensions

The parameters in the following table are used by the simulator to define array sizes. All the parameter values must be equal to or greater than the size of the grid dimensions specified in the input file, unless otherwise noted. Additionally, all instances of each parameter must be the same throughout the code, so if you want to change the value of one of the parameters, please make sure you make a global substitution.

Parameter	Definition
NNX	Number of grid blocks in X-direction (must be set equal or larger to NX in the input file)

NNY	Number of grid blocks in Y-direction (must be set equal or larger to NY in the input file)
NNZ	Number of grid blocks in Z-direction (must be set equal or larger to NZ in the input file)
MXC	Maximum number of components (cannot be less than 8)
MXP	Number of phases (must be set equal to 3 when there is no gas phase and must be set equal to 4 if gas is present)
MXW	Maximum number of wells
MXWB	Maximum number of well blocks
MXNT	Maximum number of tracers
MXELE	Maximum number of elements
MXFLD	Maximum number of reactive fluid species
MXSLD	Maximum number of solids
MXSORB	Maximum number of adsorbed species
MXACAT	Maximum number of cations associated with surfactant
MXEX	Maximum number of insoluble exchangers

3.0 INPUT DATA DESCRIPTION

The UTCHEM input file 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 six 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 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. 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.

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 alphanumeric characters on a single line (not to exceed 80 characters). This information will be printed as the first line of every output file.

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). Please note that the title must span three lines and that any of those lines can be blank.

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

IMODE - Flag indicating if the problem to be run is a first run or a restart problem.
Possible Values:
1 - First run problem
2 - Restart problem

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 3.5.9 through 3.5.12 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
1 - Chaudhari's method is used (this method is not available if ICOORD = 2)
2 - Two point upstream method is used
3 - Improved total variation diminishing third order method is used (modified in version 5.0)
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 is not used
1 - Capacitance model is used

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 - Alkaline option 1 (no silicon, aluminum, or acid)
3 - Alkaline option 2 (no silicon or aluminum; with acidic crude)
4 - Alkaline option 3 (with silicon and aluminum; no acid)
5 - Alkaline option 4 (with silicon, aluminum, and acidic crude)
6 - Alkaline option 3 and gel reactions are used

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 grid block 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 for the temperature equation option (IENG must be set to 0 on this input line).

ITREAC - Flag indicating if a tracer reaction is used or not.
Possible Values:
0 - Tracer reaction is not used
1 - Tracer reaction is 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

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

Possible Values:

0 - Isothermal simulation
1 - Temperature equation is solved

Note: IENG must be set equal to 0 if the curvilinear grid option (ICOORD=4 on this input line) option is used.

3.1.4 NX, NY, NZ, IDXYZ, IUNIT

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

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

NY - Number of grid blocks 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 grid blocks 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: UTCHEM must be compiled and run with the NX, NY, and NZ input values being equal to or smaller than the NNX, NNY, and NNZ parameters in the code. All 52 occurrences of the NNX, NNY, and NNZ parameters in the code must be set to the same values which must be equal to or larger than the NX, NY, and NZ input values. Additionally, since parameter statements are used for dimensioning arrays in UTCHEM, any time any parameter statement is changed in the FORTRAN source code, all occurrences of that parameter statement must be changed (and set to the same value throughout the code) or the code will not function properly.

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

XCORD - Grid block coordinate of I^{th} corner point in X-direction.

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

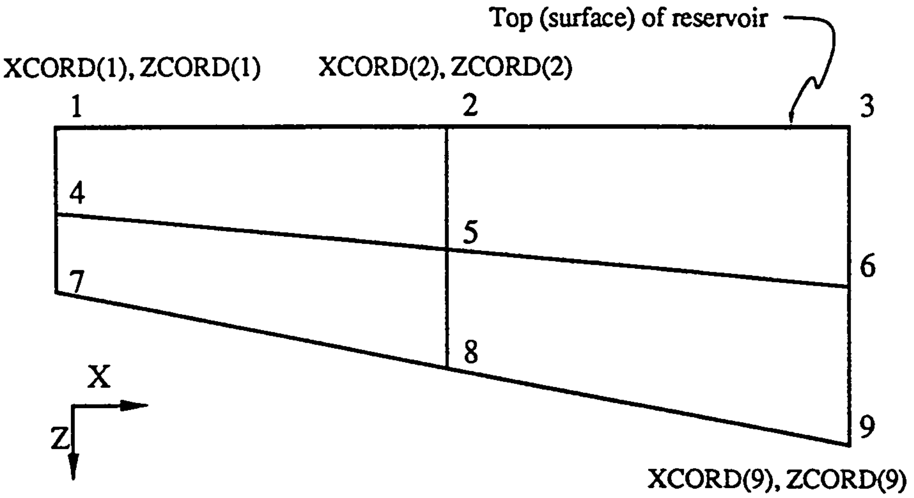
ZCOORD - Grid block coordinate of I^{th} corner point in Z-direction.

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

Note: The coordinates of the corners (or vertices) of the 2-D X-Z cross section grid blocks 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 grid blocks is equal to NX × NZ and the number of coordinate pairs (or nodes) is equal to (NX+1) × (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.

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

DX1 - Grid block size in X direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DY1 - Grid block size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

DZ1 - Grid block 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 - Grid block 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 - Grid block 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 or 3)

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

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

DX1 - Grid block size in X direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NX grid blocks 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 grid blocks in the X direction are 3 feet in size, the fourth through ninth grid blocks in the X direction are 2 feet in size, and the last two grid blocks 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 grid blocks 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 or 3)

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

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

DY1 - Grid block size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY grid blocks 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 or 3)

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

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

DZ1 - Grid block size in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ grid blocks 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.

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

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

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

DZ1 - Grid block size in Z direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NZ grid blocks 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 grid blocks with same size in Y direction.

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

DY1 - Grid block size in Y direction.
Units: feet (IUNIT=0) or m (IUNIT=1)

Note: This line is repeated until sizes for each of the NY grid blocks 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.

3.1.16 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, NTW, NTA, NG

N - Total number of components in the run (including tracers and reactive components).
Possible Values: 1 – 21

NTW - Number of water/oil tracers.
Possible Values: see note

NTA - Number of oil/gas tracers.
Possible Values: see note

NG - Number of gel components.
Possible Values: 4 or 5 when IREACT = 1

4 when IREACT = 6

Note: The combined total number of water/oil and oil/gas tracers (NTW+NTA) must be:

1) less than or equal to MXNT (see section 2.2) and
2) between 0 and 3 (inclusive) if IREACT>1 or between 0 and 13 (inclusive) if IREACT=1.

The components will be listed in the following order for the corresponding values of IREACT:

Index	Component (IREACT = 0)	Component (IREACT = 1)	Component (IREACT = 2)	Component (IREACT = 3)	Component (IREACT = 4)	Component (IREACT = 5)	Component (IREACT = 6)
1	Water	Water	Water	Water	Water	Water	Water
2	Oil	Oil	Oil	Oil	Oil	Oil	Oil
3	Surfactant	Surfactant	Surfactant	Surfactant	Surfactant	Surfactant	Surfactant
4	Polymer	Polymer	Polymer	Polymer	Polymer	Polymer	Polymer
5	Chloride	Chloride	Chloride	Chloride	Chloride	Chloride	Chloride
6	Calcium	Calcium	Calcium	Calcium	Calcium	Calcium	Calcium
7	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1	Alcohol 1
8	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas	Alcohol 2 or Gas
9	Tracer 1	Tracer 1	Tracer 1	Tracer 1	Tracer 1	Tracer 1	Tracer 1
10	Tracer 2	Tracer 2	Tracer 2	Tracer 2	Tracer 2	Tracer 2	Tracer 2
11	Tracer 3	Tracer 3	Tracer 3	Tracer 3	Tracer 3	Tracer 3	Tracer 3
12	Tracer 4	$Na_2Cr_2O_7$	Sodium	Sodium	Sodium	Sodium	Sodium
13	Tracer 5	CSN_2H_4	Hydrogen	Hydrogen	Hydrogen	Hydrogen	Hydrogen
14	Tracer 6	Cr^{3+}	Magnesium	Magnesium	Magnesium	Magnesium	Magnesium
15	Tracer 7	Gel	Carbonate	Carbonate	Carbonate	Carbonate	Carbonate
16	Tracer 8	Hydrogen	—	Acid Comp. of Crude Oil	Aluminum	Aluminum	Aluminum
17	Tracer 9	—	—	—	Silica	Silica	Silica
18	Tracer 10	—	—	—	—	Acid Comp. of Crude Oil	$Na_2Cr_2O_7$
19	Tracer 11	—	—	—	—	—	CSN_2H_4
20	Tracer 12	—	—	—	—	—	Cr^{3+}
21	Tracer 13	—	—	—	—	—	Gel

If IREACT > 0, N must be set to the maximum number of components shown for each case in the above table, whether all the components are present or not. For example, if IREACT = 3, N must be set to 16.

3.1.24 TRNAME(IT), for IT = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

TRNAME(IT) - Name of ITth tracer.

Note: The name of each tracer may not exceed 16 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 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 concentration 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

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 ICOPSM, ICUMTM, ISTOP

ICOPSM - Flag indicating if data will be written to UNIT 3.
Possible Values:
0 - Data will be written to UNIT 3 as directed by CUMHI2 flag
1 - Data will not be written to UNIT 3

ICUMTM - Flag indicating if the output intervals indicated by the CUMPR1, CUMHI1, CUMHI2, WRHPV, WRPRF and RSTC variables on input line 3.5.8 are specified in pore volumes or days.
Possible Values:
0 - Data will be written in pore volume intervals
1 - Data will be written in day intervals
Note: The day interval output option (ICUMTM = 1) is particularly useful if there is a shut in period.

ISTOP - Flag indicating if the maximum and injection times (variables TMAX on input line 3.3.1 and TINJ on input line 3.6.8) 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

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

IPRFLG(KC) - Flag indicating if profile of KCth component should be written to UNIT 8.
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, IPTRAC, IPCAP, IPGEL, IPALK, IPTEMP, IPOBS

IPPRES - Flag indicating if profile of phase pressures should be written to UNIT 11.
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 UNIT 12.
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 UNIT 8.
Possible Values:
0 - Profile of component concentrations will not be written
1 - Profile of component concentrations will be written

IPTRAC - Flag indicating if profile of tracer phase concentrations should be written to UNIT 13.
Possible Values:
0 - Profile of tracer phase concentrations will not be written
1 - Profile of tracer phase concentrations will be written

IPCAP - Flag indicating if profile of capacitance properties should be written to UNIT 14.
Possible Values:
0 - Profile of capacitance properties will not be written
1 - Profile of capacitance properties will be written

IPGEL - Flag indicating if profile of gel properties should be written to UNIT 10.
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 UNIT 15.
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 UNIT 18.
Possible Values:
0 - Profile of temperature will not be written
1 - Profile of temperature will be written

IPOBS - Flag indicating if aqueous phase tracer concentration at observation points should be written to the TRACxx output files.
Possible Values:
0 - Aqueous phase tracer concentrations at observation points will not be written
1 - Aqueous phase tracer concentrations at observation points will be written

3.2.4 IPHP, IADS, ICKL, IVEL, IVIS, IPER, ICNM, IRKF, IPHSE, ICSE

IPHP - Flag indicating if oleic and microemulsion phase pressure data should be printed.
Possible Values:
0 - Oleic and microemulsion phase pressure data will not be printed
1 - Oleic and microemulsion phase pressure data will be printed

IADS - Flag indicating if surfactant, polymer, calcium, gel, chromium, hydrogen, and sodium adsorption data should be printed.
Possible Values:
0 - Adsorption data will not be printed
1 - Adsorption data will be printed

ICKL - Flag indicating if component concentration data in each phase should be printed.
Possible Values:
0 - Component concentration data in each phase will not be printed
1 - Component concentration data in each phase will be printed

IVEL - Flag indicating if X, Y, and Z direction phase fluxes should be printed.
Possible Values:
0 - X, Y, and Z direction phase fluxes will not be printed
1 - X, Y, and Z direction phase fluxes will be printed

IVIS - Flag indicating if phase viscosities should be printed.
Possible Values:
0 - Phase viscosities will not be printed
1 - Phase viscosities will be printed

IPER - Flag indicating if relative permeabilities should be printed.
Possible Values:
0 - Relative permeabilities will not be printed
1 - Relative permeabilities will be printed

ICNM - Flag indicating if phase capillary numbers and interfacial tensions should be printed.
Possible Values:
0 - Capillary numbers and interfacial tensions will not be printed
1 - Capillary numbers and interfacial tensions will be printed

IRKF - Flag indicating if permeability reduction factors should be printed.
Possible Values:
0 - Permeability reduction factors, polymer viscosities, and equivelent shear rate will not be printed
1 - Permeability reduction factors, polymer viscosities, and equivelent shear rate will be printed

IPHSE - Flag indicating if phase environment indexing should be printed.
Possible Values:
0 - Phase environment indexing will not be printed
1 - Phase environment indexing will be printed

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

ICSE - Flag indicating if effective salinity should be printed.
Possible Values:

0 - Effective salinity information will not be printed
1 - Effective salinity will be printed to PROFIL and history data files

Note: These flags give the option of printing a very detailed description (all flags = 1) every CUMPR1 pore volume interval or a very limited description (all flags = 0) to UNIT 4. See the appendix for a list of the values that are written to UNIT 4 automatically.

3.2.5 NOBS (This line is read only if IPOBS > 0)

NOBS - Number of tracer concentration observation points.

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

IOBS(I) - Index of I^{th} tracer concentration observation point in X-direction.

JOBS(I) - Index of J^{th} tracer concentration observation point in Y-direction.

KOBS(I) - Index of K^{th} tracer concentration 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 simulated time).
Units: days or pore volumes (dependent on value of ISTOP flag in line 3.2.1)

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)

3.3.3 IPOR1, IPERMX, IPERMY, IPERMZ

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:
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

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 × NY elements (corresponding to layer 1) of the POR array are set equal to WKSP1(1), the second set of NX × 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 × NY × NZ (This line is read only if IPOR1 = 2)

POR(I) - Porosity of Ith grid block
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 × 3 × 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
```

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

PERMXC - Permeability of the reservoir in the X direction (ICOORD = 1 or 3) 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.

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 (ICOORD = 1 or 3) or in the radial direction (ICOORD = 2).
Units: millidarcies = $10^{-3}\ \mu m^2$
Note: See the note for input line 3.3.5.

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

PERMX(I) - Permeability of the I^{th} grid block in the X direction (ICOORD = 1 or 3) or in the radial direction (ICOORD = 2).
Units: millidarcies = 10^{-3} μm^2
Note: See the note and example for input line 3.3.6 for the order of the permeability values.

3.3.10 PERMYC (This line is read only if IPERMY = 0 and ICOORD = 1 or 3)

PERMYC - Permeability of the reservoir in the Y direction.
Units: millidarcies = 10^{-3} μm^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 = 1 or 3)

PERMY(K) - Permeability of the K^{th} layer in the Y direction.
Units: millidarcies = 10^{-3} μm^2
Note: See note for input line 3.3.5.

3.3.12 PERMY(I), for I = 1, NX × NY × NZ (This line is read only if IPERMY = 2 and ICOORD = 1 or 3)

PERMY(I) - Permeability of the I^{th} grid block.
Units: millidarcies = 10^{-3} μm^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 = 1 or 3)

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} μm^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 K^{th} layer in the Z direction.
Units: millidarcies = 10^{-3} μm^2
Note: See note for input line 3.3.5.

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

PERMZ(I) - Permeability of the I^{th} grid block.

Units: millidarcies (10^{-3} μm^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 and ICOORD = 1 or 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.

3.3.18 IDEPTH, IPRESS, ISWI

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 grid block (1,1,1) and the reservoir dip angles are specified
2 - Depth of each grid block 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 grid blocks
1 - Initial pressure for a point at a specified depth is specified by user
2 - Initial pressure for each grid block 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 grid blocks
1 - Constant value for water saturation for each layer is specified by user
2 - Initial water saturation for each grid block is specified by user

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 grid block.

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

D111 - Depth of the first grid block (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 × NY (This line is read only if IDEPTH = 2)

EL(I) - Depth of I^{th} grid block 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 grid block 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 × NY × NZ (This line is read only if IPRESS = 2)

P(I) - Initial pressure of each grid block 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 grid blocks 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 K^{th} layer.
Units: fraction of pore volume
Note: See the note for input line 3.3.5.

3.3.27 S(I,1), I = 1, NX × NY × NZ (This line is read only if ISWI = 2)

S(I,1) - Initial water saturation for I^{th} 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.

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 for each grid block is specified by user

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

SGI - Initial gas saturation for all grid blocks 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 = 1 and ISGI = 1)

S(K,4) - Initial gas saturation for K^{th} layer.
Units: fraction of pore volume
Note: See the note for input line 3.3.5.

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

S(I,4) - Initial gas saturation for I^{th} block.
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.

3.3.32 C50, C60

C50 - Initial brine salinity.
Units: meq/ml of brine
Note: This is assumed to be all the anions (in equivalents).

C60 - Initial divalent cation concentration of brine.
Units: meq/ml of brine

Note : C50 and C60 are replaced by the input values of C5I and C6I in line 3.5.33 when IREACT>1.

3.4 Physical Property Data

The fourth input section consists of the 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.

3.4.1 C2PLC, C2PRC, EPSME

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

3.4.2 HBNS70, HBNC70, HBNS71, HBNC71, HBNS72, HBNC72

HBNS70 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1—Component 7—associated with surfactant at zero salinity.
Units: volume fraction

HBNC70 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1—Component 7—associated with surfactant at zero salinity.
Units: volume fraction

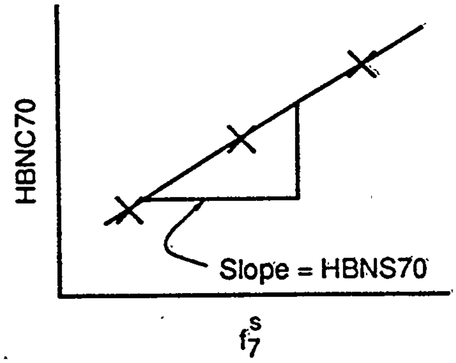
HBNS71 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1—Component 7—associated with surfactant at optimal salinity.
Units: volume fraction

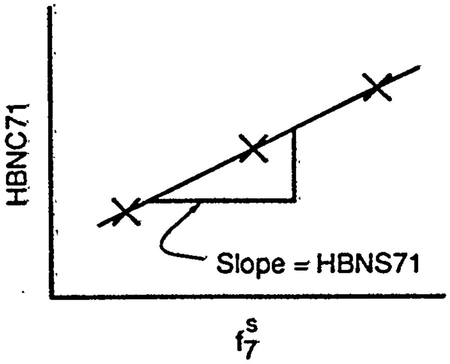
HBNC71 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1—Component 7—associated with surfactant at optimal salinity.
Units: volume fraction

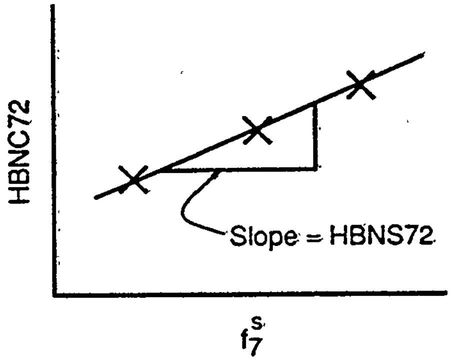
HBNS72 - Slope for maximum height of binodal curve vs. fraction of Alcohol 1—Component 7—associated with surfactant at twice optimal salinity.
Units: volume fraction

HBNC72 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 1—Component 7—associated with surfactant at twice optimal salinity.
Units: volume fraction

Note: These parameters are obtained by matching the volume fraction diagrams corresponding to at least three different total chemical (alcohol + surfactant) compositions. For the first iteration, the slope parameters are set to zero and the intercept parameters are adjusted in order to obtain a reasonable match of the volume fraction diagrams. Then the slope parameters are obtained as follows:







Having obtained the slope parameters, the matching procedure is repeated for further improvements. See Satoh's thesis for example.

3.4.3 HBNS80, HBNC80, HBNS81, HBNC81, HBNS82, HBNC82

HBNS80 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2—Component 8—associated with surfactant at zero salinity.
Units: volume fraction

HBNC80 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2—Component 8—associated with surfactant at zero salinity.
Units: volume fraction

HBNS81 - Slope of maximum height of binodal curve vs. fraction of Alcohol 2—Component 8—associated with surfactant at optimal salinity.
Units: volume fraction

HBNC81 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2—Component 8—associated with surfactant at optimal salinity.
Units: volume fraction

HBNS82 - Slope for maximum height of binodal curve vs. fraction of Alcohol 2—Component 8—associated with surfactant at twice optimal salinity.
Units: volume fraction

HBNC82 - Intercept of maximum height of binodal curve at zero fraction of Alcohol 2—Component 8—associated with surfactant at twice optimal salinity.
Units: volume fraction

Note: See the note for input line 3.4.2 to see how values should be determined.

3.4.4 CSEL7, CSEU7, CSEL8, CSEU8

CSEL7 - Lower effective salinity limit for type III phase region determined when Alcohol 1—Component 7—and calcium approach zero.
Units: meq/ml

CSEU7 - Upper effective salinity limit for type III phase region determined when Alcohol 1—Component 7—and calcium approach zero.
Units: meq/ml

CSEL8 - Lower effective salinity limit for type III phase region determined when Alcohol 2—Component 8—and calcium approach zero.
Units: meq/ml

CSEU8 - Upper effective salinity limit for type III phase region determined when Alcohol 2—Component 8—and calcium approach zero.
Units: meq/ml

Note: The values are calculated as follows:

$$\mathrm{CSEU7} = \lim_{\substack{f_6^s \to 0 \\ f_7^s \to 0}} \left(C_{SEU}\right)$$

$$\mathrm{CSEL7} = \lim_{\substack{f_6^s \to 0 \\ f_7^s \to 0}} \left(C_{SEL}\right)$$

$$\mathrm{CSEU8} = \lim_{\substack{f_6^s \to 0 \\ f_8^s \to 0}} \left(C_{SEU}\right)$$

$$\mathrm{CSEL8} = \lim_{\substack{f_6^s \to 0 \\ f_8^s \to 0}} \left(C_{SEL}\right)$$

and

$$C_{SE} = \frac{C_{51}}{\left(1 - \beta_6 f_6^s\right)\left(1 + \beta_7 f_7^s + \beta_8 f_8^s\right)}$$

3.4.5 BETA6, BETA7, BETA8

BETA6 - The C_{SE} slope parameter, β_6, for calcium.
Units: dimensionless

BETA7 - The C_{SE} slope parameter, β_7, for Alcohol 1—Component 7.
Units: dimensionless

BETA8 - The C_{SE} slope parameter, β_8, for Alcohol 2—Component 8.
Units: dimensionless

Note: See notes for input line 3.4.4.

BETA6 is limited to less than $\frac{1}{f_6^s}$

3.4.6 IALC, OPSK7O, OPSK7S, OPSK8O, OPSK8S

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—Component 7.
Units: dimensionless

OPSK7S - Alcohol partition coefficient (surfactant/water) for Alcohol 1—Component 7.
Units: dimensionless

OPSK8O - Alcohol partition coefficient (oil/water) for Alcohol 2—Component 8.
Units: dimensionless

OPSK8S - Alcohol partition coefficient (surfactant/water) for Alcohol 2—Component 8.
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.

3.4.7 NALMAX, EPSALC

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}.

3.4.8 AKWC7, AKWS7, AKM7, AK7, PT7

AKWC7, AKWS7 - Parameters used to determine partition coefficient of monomeric Alcohol 1—Component 7—between aqueous and oleic pseudophases.
Units: dimensionless

AKM7 - Partition coefficient of monomeric Alcohol 1—Component 7—between surfactant and oleic pseudophases.
Units: dimensionless

AK7 - Self-association constant of Alcohol 1—Component 7—in oleic pseudophase.
Units: dimensionless

PT7 - Ratio of molar volume of Alcohol 1—Component 7—to equivalent molar volume of surfactant.
Units: dimensionless

3.4.9 AKWC8, AKWS8, AKM8, AK8, PT8

AKWC8, AKWS8 - Parameters used to determine partition coefficient of monomeric Alcohol 2—Component 8—between aqueous and oleic pseudophases.
Units: dimensionless

AKM8 - Partition coefficient of monomeric Alcohol 2—Component 8—between surfactant and oleic pseudophases.
Units: dimensionless

AK8 - Self-association constant of Alcohol 2—Component 8—in oleic pseudophase.
Units: dimensionless

PT8 - Ratio of molar volume of Alcohol 2—Component 8—to equivalent molar volume of surfactant.
Units: dimensionless

Note: These values can be calculated using PROPACK and are only required when using Prouvost's model (IALC = 1).

3.4.10 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: For information on the above interfacial tension correlations, please refer to: Healy, R. N. and R. L. Reed: "Physicochemical Aspects of Microemulsion Flooding," *SPE J.* (1975) 87-103 and Huh, C.: "Interfacial Tension and Solubilizing Ability of a Microemulsion Phase that Coexists with Oil and Brine," *J. Colloid Interface Sci.* (1979) **71**, 408-428.

3.4.11 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

Note: The equations used to calculate the interfacial tension parameters are discussed in "Improvements in Physical-Property Models Used in Micellar/Polymer

Flooding" by D. Camilleri, *et. al.* which appeared in the November, 1987 issue of SPE Reservoir Engineering.

3.4.12 CHUH (This line is read only if IFT = 1)

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

3.4.13 XIFTW

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

3.4.14 IMASS

IMASS - Flag indicating the choice of oil solubility in water.
Possible Values
- 0 - No solubility of oil in water in the absence of surfactant (component number 3)
- 1 - Allow for solubility of oil in water in the absence of surfactant or allow for non equilibrium transfer of oil in water

3.4.15 WSOL, CNEM2 (This line is read only if IMASS=1 and IGAS=0 in the presence of surfactant (component no.3))

WSOL - Equilibrium concentration of oil in water in the absence of surfactant.
Units: volume fraction

CNEM2 - Coefficient of non-equilibrium mass transfer of oil in aqueous phase with or without surfactant; M
Units: vol. of water/(bulk vol.-day)

Note: The input value of zero for CNEM2 represents an equilibrium mass transfer. The non-equilibrium mass transfer (CNEM2>0) calculation is valid for type II(-) and lobe II(-) of type III with the plait point in the corner (C2PLC = 0) and in the absence of gas phase (IGAS=0).

$$\frac{\partial(S_\ell C_{2\ell}\phi)}{\partial t} = M\left(C_{2\ell}^{eq} - C_{2\ell}\right), \text{ for } \ell=1 \text{ or } 3$$

$C_{2\ell}^{eq}$ is the computed composition from the hand equations when the surfactant is present and is the input value of WSOL in the absence of surfactant or when the surfactant concentration is below CMC.

3.4.16 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

T11 - Capillary desaturation curve parameter, T_1, for aqueous phase.

T22 - Capillary desaturation curve parameter, T_2, for oleic phase.

T33 - Capillary desaturation curve parameter, T_3, for microemulsion phase.

Note: The expressions for capillary desaturation are:

$$S_{\ell r} - S_{\ell rc} = \frac{S_{\ell rw} - S_{\ell rc}}{1 + T_\ell N_{c\ell}}, \quad \ell = 1,2,3$$

where

$$N_{c\ell} = (2.23\text{x}10^{-5}) \frac{\sqrt{\left(k_x \frac{\partial \Phi}{\partial x}\right)^2 + \left(k_y \frac{\partial \Phi}{\partial y}\right)^2 + \left(k_z \frac{\partial \Phi}{\partial z}\right)^2}}{\sigma_{\ell\ell'}}, \ell = 1,2,3$$

For $\ell = 1$, $\sigma_{\ell\ell'} = \sigma_{wm}$. For $\ell = 2$, $\sigma_{\ell\ell'} = \sigma_{mo}$. For $\ell = 3$, $\sigma_{\ell\ell'} = \sigma_{wm}$ if the aqueous phase is mobile, σ_{mo} otherwise.

T11, T22, and T33 are determined by matching experimental capillary desaturation curves.

3.4.17 IPERM

IPERM - Flag indicating the saturation history direction for relative permeability and capillary pressure calculations
Possible Values:
- 0 - Imbibition Corey
- 1 - First drainage Corey (only for IOW=0 and two phase water/oil flow)

3.4.18 ISRW, IPRW, IEW

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 for each grid block

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 - Constant endpoint relative permeability for each grid block

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 - Constant relative permeability exponent for each grid block

3.4.19 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

3.4.20 S1RWC(K), for K = 1, NZ (This line is read only if ISRW = 1)

S1RWC(K) - Residual saturation of aqueous phase displaced by oil or gas at low capillary number for K^th^ layer.
Units: fraction

3.4.21 S2RWC(K), for K = 1, NZ (This line is read only if ISRW = 1)

S2RWC(K) - Residual saturation of oleic phase displaced by water at low capillary number for K^{th} layer.
Units: fraction

3.4.22 S3RWC(K), for K = 1, NZ (This line is read only if ISRW = 1)

S3RWC(K) - Residual saturation of microemulsion phase displaced by water or oil at low capillary number for K^{th} layer.
Units: fraction

Note: See the note for input line 3.4.42. Additionally, S3RWC(K) must begin a separate line in the input file for each layer.

3.4.23 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 I^{th} grid block.
Units: fraction

3.4.24 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 I^{th} grid block.
Units: fraction

3.4.25 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 grid block.
Units: fraction

3.4.26 P1RWC, P2RWC, P3RWC (This line is read only if 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

3.4.27 P1RWC(K), for K = 1, NZ (This line is read only if IPRW = 1)

P1RWC(K) - Constant endpoint relative permeability of water at low capillary number for Kth layer.
Units: dimensionless

3.4.28 P2RWC(K), for K = 1, NZ (This line is read only if IPRW = 1)

P2RWC(K) - Constant endpoint relative permeability of oil at low capillary number for Kth layer.
Units: dimensionless

3.4.29 P3RWC(K), for K = 1, NZ (This line is read only if IPRW = 1)

P3RWC(K) - Constant endpoint relative permeability of microemulsion at low capillary number for Kth layer.
Units: dimensionless

Note: See the note for input line 3.4.42. Additionally, P1RWC(K) must begin a separate line in the input file for each layer.

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

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

3.4.31 P2RW(I), for I = 1, NX × NY × NZ (This line is read only if IPRW = 2)

P2RWC(K) - Endpoint relative permeability of oil at low capillary number for Ith grid block.

Units: dimensionless

3.4.32 P3RW(I), for I = 1, NX × NY × NZ (This line is read only if IPRW = 2)

P3RW(I) - Endpoint relative permeability of microemulsion at low capillary number for Ith grid block.
Units: dimensionless

3.4.33 E1WC, E2WC, E3WC (This line is read only if 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

3.4.34 E1WC(K), for K = 1, NZ (This line is read only if IEW = 1)

E1WC(K) - Relative permeability exponent of aquesous phase at low capillary number for Kth layer.
Units: dimensionless

3.4.35 E2WC(K), for K = 1, NZ (This line is read only if IEW = 1)

E2WC(K) - Relative permeability exponent of oleic phase at low capillary number for Kth layer.
Units: dimensionless

3.4.36 E3WC(K), for K = 1, NZ (This line is read only if IEW = 1)

E3WC(K) - Relative permeability exponent of microemulsion phase at low capillary number for Kth layer.
Units: dimensionless

Note: See the note for input line 3.4.42. Additionally, E1WC(K) must begin a separate line in the input file for each layer.

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

E1W(I) - Relative permeability exponent of aqueous phase at low capillary number for Ith grid block.
Units: dimensionless

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

E2WC(K) - Relative permeability exponent of oleic phase at low capillary number for I^{th} grid block.
Units: dimensionless

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

E3W(I) - Relative permeability exponent of microemulsion phase at low capillary number for I^{th} grid block.
Units: dimensionless

3.4.40 S1RC, S2RC, S3RC

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

3.4.41 P1RC, P2RC, P3RC

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

3.4.42 E13C, E23C, E31C

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

Note: For IGAS = 0, imbibition Corey relative permeabilities are calculated from:

$$k_{r\ell} = k^{o}_{r\ell} \left(S_{n\ell}\right)^{e_\ell}, \quad \ell = 1, 2, 3$$

where

$$S_{n\ell} = \frac{S_\ell - S_{\ell r}}{1 - S_{1r} - S_{2r} - S_{3r}}$$

$$k^{o}_{r\ell} = k^{o}_{r\ell w} \qquad \text{for ITRAP=0}$$

$$k^{o}_{r\ell} = k^{o}_{r\ell w} + \frac{S_{\ell' rw} - S_{\ell' r}}{S_{\ell' rw} - S_{\ell' rc}}\left(k^{o}_{r\ell c} - k^{o}_{r\ell w}\right) \qquad \text{for ITRAP =1}$$

and

$$e_{\ell} = e_{\ell w} \qquad \text{for ITRAP=0}$$

$$e_{\ell} = e_{\ell w} + \frac{S_{\ell' rw} - S_{\ell' r}}{S_{\ell' rw} - S_{\ell' rc}}\left(e_{\ell c} - e_{\ell w}\right) \qquad \text{for ITRAP=1}$$

The phase indices are assigned values according to the type of flow:

for water/oil: $\ell = 1$, $\ell' = 2$, $e_{\ell c}$ = E13C, $e_{\ell w}$ = E1W
for water/microemulsion: $\ell = 1$, $\ell' = 3$, $e_{\ell c}$ = E23C, $e_{\ell w}$ = E2W
for oil/microemulsion: $\ell = 2$, $\ell' = 3$, $e_{\ell c}$ = E31C, $e_{\ell w}$ = E3W

For two phase oil/water drainage (IPERM =1), S_{2r} is set to 0.0.

3.4.43 VIS1, VIS2, TSTAND

VIS1 - Water viscosity at reference temperature, $\mu_{1,ref}$.
Units: cp = mPa.s

VIS2 - Oil viscosity at reference temperature, $\mu_{2,ref}$.
Units: cp = mPa.s

TSTAND - Reference temperature, T_{ref}.
Units: °F (IUNIT=0) or °C (IUNIT=1)
Note: For IENG=0, If TSAND = 0.0, the water component viscosity will be constant and equal to the input value VIS1. If TSATND > 0.0, water component viscosity will be calculated as a function of reservoir temperature, pressure, and local salinity for each grid block.

3.4.44 VIS4, VSLOPG (This line is read only if IGAS = 1)

VIS4 - Gas viscosity at reference temperature and reference pressure, $\mu_{4,ref}$.
Units: cp = mPa.s

VSLOPG - Slope of gas viscosity, $\mu_{4,s}$.
Units: $(\text{psi})^{-1}$ (IUNIT=0) or $(\text{kPa})^{-1}$ (IUNIT=1)

Note: Gas viscosity is computed from:

$$\mu_4 = \mu_{4,ref}\left(1 + \mu_{4,s}\left(P_1 - \text{PSTAND}\right)\right)$$

3.4.45 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, b_1.
Units: $(°K)^{-1}$

BVI(2) - Parameter for calculating oil viscosity as a function of reservoir temperature, b_2.
Units: $(°K)^{-1}$

Note: The phase viscosities as a function of temperature are calculated from:

$$\mu_\ell = \mu_{\ell,\mathrm{ref}} \exp\left(b_\ell \left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}} \right) \right) \qquad \text{for } \ell = 1,2$$

where T and T_{ref} are in absolute °K.

3.4.46 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, b_4.
Units: $(°K)^{-1}$

Note: Gas viscosity as a function of temperature is computed from:

$$\mu_4 = \mu_{4,\mathrm{ref}}\left(1 + \mu_{4,s}(P - \mathrm{PSTAND})\right) \exp\left(1 + b_4\left(\frac{1}{T} - \frac{1}{T_{\mathrm{ref}}}\right)\right)$$

where T and T_{ref} are in absolute °K.

3.4.47 S2RWC4, S4RWC (This line is read only if IGAS = 1 and ISRW = 0)

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

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

3.4.48 S2RWC4(K), for K = 1, NZ (This line is read only if IGAS = 1 and ISRW = 1)

S2RWC4(K) - Constant residual oil saturation to dispacing gas phase for Kth layer.
Units: fraction

3.4.49 S4RWC(K), for K = 1, NZ (This line is read only if IGAS = 1 and ISRW = 1)

S4RWC(K) - Constant residual gas saturation for Kth layer.
Units: fraction

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

S2RW4(I) - Constant residual oil saturation to dispacing gas phase for Ith grid block.
Units: fraction

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

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

3.4.52 P4RWC (This line is read only if IGAS = 1 and IPRW = 0)

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

3.4.53 P4RWC(K), for K = 1, NZ (This line is read only if IGAS = 1 and IPRW = 1)

P4RWC(K) - Constant gas endpoint relative permeability for Kth layer.
Units: dimensionless

3.4.54 P4RW(I), for I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and IPRW = 2)

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

3.4.55 E4WC (This line is read only if IGAS = 1 and IEW = 0)

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

3.4.56 E4WC(K), for K = 1, NZ (This line is read only if IGAS = 1 and IEW = 1)

E4WC(K) - Constant gas relative permeability exponent for Kth layer.
Units: dimensionless

3.4.57 E4WC(I), for I = 1, NX × NY × NZ (This line is read only if IGAS = 1 and IEW = 2)

E4WC(I) - Constant gas relative permeability exponent for Ith grid block.
Units: dimensionless

3.4.58 S4RC, P4RC, E4C, T44, XIFTG (This line is read only if IGAS = 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

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

3.4.59 ALPHA1, ALPHA2, ALPHA3, ALPHA4, ALPHA5

ALPHA1 - Compositional phase viscosity parameter α_1.

ALPHA2 - Compositional phase viscosity parameter α_2.

ALPHA3 - Compositional phase viscosity parameter α_3.

ALPHA4 - Compositional phase viscosity parameter α_4.

ALPHA5 - Compositional phase viscosity parameter α_5.

Note: Compositional phase viscosity is calculated as:

$$\begin{aligned}\mu_\ell = \; & C_{1\ell}\,\mu_p \exp[\alpha_1 (C_{2\ell} + C_{3\ell})] + \\ & C_{2\ell}\,\mu_o \exp[\alpha_2 (C_{1\ell} + C_{3\ell})] + \\ & C_{3\ell}\,\alpha_3 \exp[\alpha_4 C_{1\ell} + \alpha_5 C_{2\ell}]\end{aligned}$$

Polymer viscosity μ_p is replaced by water viscosity when no polymer is present.

3.4.60 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. %)$^{-3}$

Note: Polymer viscosity at zero shear rate, μ_o, is given by:

$$\mu_o = \mu_w\left[1 + \left(A_{p1}C_{4\ell} + A_{p2}C_{4\ell}^2 + A_{p3}C_{4\ell}^3\right)C_{SEP}^{S_p}\right]$$

A_{p1}, A_{p2}, and A_{p3} are empirical constants for a given polymer and are measured experimentally.

3.4.61 BETAP, CSE1, SSLOPE

BETAP - Parameter, β_P, for calculating the effective divalent salinity, C_{SEP}, used to calculate polymer viscosity (see the note for input line 3.4.60).
Units: dimensionless
Note: C_{SEP} is given by:

$$C_{SEP} = \frac{C_9 + \beta_p C_6}{C_1}$$

CSE1 - Value below which the polymer viscosity is considered to be independent of salinity (minimum value of CSEP—see the note for input line 3.4.60).
Units: meq/ml

SSLOPE - Slope, Sp, of μ_o vs. C_{SEP} on a log-log plot—assumed to be constant (see the note for input line 3.4.60).
Units: dimensionless
Note: This value is usually large and negative for hydrolyzed polyacrylamides and small and positive for polysaccharides.

3.4.62 GAMMAC, GAMHF, POWN

GAMMAC - Coefficient, $\dot{\gamma}_c$, in shear rate equation below.

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

GAMHF - Shear rate, $\dot{\gamma}_{1/2}$, at which polymer viscosity is one half polymer viscosity at zero shear rate.
Units: sec^{-1}

POWN - Exponent, P_α, for calculating shear rate dependence of polymer viscosity.
Units: dimensionless

Note: The shear rate dependence of polymer viscosity is modeled by Meter's equation:

$$\mu_p = \mu_\infty + \frac{\mu_o - \mu_\infty}{1 + \left[\frac{\dot{\gamma}_{eq}}{\dot{\gamma}_{1/2}}\right]^{P_\alpha - 1}}$$

where the equivalent shear rate $\dot{\gamma}_{eq}$ is calculated as:

$$\dot{\gamma}_{eq} = \left(\frac{3n+1}{4n}\right)^{\frac{n}{n-1}} \frac{4uc}{\sqrt{8kk_{rw}\phi s_w}} = \dot{\gamma}_c \frac{u}{\sqrt{kk_{rw}\phi s_w}}$$

where u is in ft/day, k is in Darcies, and $\dot{\gamma}_{eq}$ is in 1/sec. Using n = 0.8 and with the unit conversion we have $\dot{\gamma}_c$ = 3.94 C. The value of shear rate coefficient C can be calculated as:

$$C = \left(4.8 \; N_v^{0.167}\right)^{\frac{1}{1-P_\alpha}}$$

where N_v is in cm/sec. N_v is a dimensional group called viscosity number computed as:

$$N_v = \frac{\sqrt{k\,k_{rw}\,\phi\,s_w}}{\Theta_o\,u^{n-1}}$$

Please refer to the following sources for more detail:

Wreath, Dana G.: "A Study of Polymerflooding and Residual Oil Saturation," M.S. Thesis, U. of Texas, Austin (Dec. 1989).

Wreath, Dana G., G. A. Pope, and K. Sepehrnoori: "Dependence of Polymer Apparent Viscosity of the Permeable Media and Flow Conditions," In Situ, 14(3), 263-284 (1990).

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

CRK - Parameter for calculating permeability reduction factor R_k.
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 R_k.

3.4.64 DEN1, DEN2, DEN3, DEN7, DEN8, IDEN

DEN1 - Specific weight, γ_1, or density of water—Component 1.
Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN2 - Specific weight, γ_2, or density of oil—Component 2.
Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN3 - Specific weight, γ_3, or density of surfactant—Component 3.
Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN7 - Specific weight, γ_7, or density of Alcohol 1—Component 7.
Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

DEN8 - Specific weight, γ_8, or density of Alcohol 2 (when IGAS = 0) or gas (when IGAS = 1) —Component 8.
Units: psi/ft (IUNIT=0) or g/cm^3 (IUNIT=1)

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

Note: Specific weight for pure water is 0.433 psi/ft (density of 1 g/cm^3)

3.4.65 ISTB

ISTB - Flag indicating the units to be used when printing injection and production rates.
Possible Values:
0 - Rates printed at bottomhole condition in ft^3 or m^3
1 - Rates printed at surface condition in BBLS

3.4.66 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/ft^3

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

3.4.67 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.

3.4.68 ICPC, IEPC, IOW

ICPC - Flag indicating type of capillary pressure endpoint, c_{pc}.
Possible Values:
0 - Constant capillary pressure endpoint for entire reservoir
1 - Constant capillary pressure endpoint for each layer
2 - Capillary pressure endpoint for each grid block

IEPC - Flag indicating type of capillary pressure exponent, n_{pc}.
Possible Values:
0 - Constant capillary pressure exponent for entire reservoir
1 - Constant capillary pressure exponent for each layer
2 - Capillary pressure exponent for each grid block

IOW - Flag indicating the wettability for capillary pressure calculations.
Possible Values:
0 - The capillary pressure curve is for water-wet rock
1 - The capillary pressure curve is for oil-wet rock (zero at residual water saturations)

3.4.69 CPC0 (This line is read only if ICPC = 0)

CPC0 - Capillary pressure endpoint for entire reservoir, c_{pc}.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

3.4.70 CPC(K), for K = 1, NZ (This line is read only if ICPC = 1)

CPC(K) - Capillary pressure endpoint for K^th layer, c_{pc}.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

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

CPC(I) - Capillary pressure endpoint for I^th gridblock, c_{pc}.
Units: $\text{psi}\sqrt{\text{darcies}}$ (IUNIT=0) or $\text{kPa}\sqrt{\mu\text{m}^2}$ (IUNIT=1)

3.4.72 EPC0 (This line is read only if IEPC = 0)

EPC0 - Capillary pressure exponent for entire reservoir, n_{pc}.
Units: dimensionless

3.4.73 EPC(K), for K = 1, NZ (This line is read only if IEPC = 1)

EPC(K) - Capillary pressure exponent for K^{th} layer, n_{pc}.
Units: dimensionless

3.4.74 EPC(I), for I = 1, NX × NY × NZ (This line is read only if IEPC = 2)

EPC(I) - Capillary pressure exponent for I^{th} gridblock, n_{pc}.
Units: dimensionless

Note: The CPC and EPC values are determined by curve fitting a plot of water-oil capillary pressure vs. normalized water saturation (see the note for input line 3.4.42). For imbibition two phases:

$$P_{C\ell\ell'} = c_{pc}\sqrt{\frac{\phi}{k_a}}\,\frac{\sigma_{\ell\ell'}}{\sigma_{wo}}(1-S_{n\ell})^{n_{pc}}$$

For three phases:

$$P_{C13} = P_{Cwm} = c_{pc}\sqrt{\frac{\phi}{k_a}}\,\frac{\sigma_{wm}}{\sigma_{wo}}(1-S_{n1})^{n_{pc}}$$

and

$$P_{C32} = P_{Cmo} = c_{pc}\sqrt{\frac{\phi}{k_a}}\,\frac{\sigma_{mo}}{\sigma_{wo}}\left(\frac{S_{n2}}{S_{n3}+S_{n2}}\right)^{n_{pc}}$$

For two phase oil/water drainage (IPERM =1):

$$P_{Cow} = c_{pc}\sqrt{\frac{\phi}{k_a}}\left(\frac{S_w - S_{wr}}{1-S_{wr}}\right)^{n_{pc}}$$

The value for n_{pc} <u>must</u> be non-zero.

3.4.75 D(KC,1), for KC = 1, N

D(KC,1) - Molecular diffusion coefficient of KC^{th} component in aqueous phase.
Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.76 D(KC,2), for KC = 1, N

D(KC,2) - Molecular diffusion coefficient of KC^{th} component in oleic phase.

Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.77 D(KC,3), for KC = 1, N

D(KC,3) - Molecular diffusion coefficient of KCth component in microemulsion phase.
Units: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.78 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: ft^2/day (IUNIT=0) or m^2/day (IUNIT=1)

3.4.79 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)

3.4.80 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)

3.4.81 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)

3.4.82 ALPHAL(4), ALPHAT(4) (This line is read only if IGAS = 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)

3.4.83 AD31, AD32, B3D, AD41, AD42, B4D

AD31 - Surfactant adsorption parameter, a_{31}.
Units: dimensionless

AD32 - Surfactant adsorption parameter, a_{32}.
Units: ml/meq

B3D - Surfactant adsorption parameter, b_3.
Units: dimensionless

AD41 - Polymer adsorption parameter, a_{41}.
Units: dimensionless

AD42 - Polymer adsorption parameter, a_{42}.
Units: ml/meq

B4D - Polymer adsorption parameter, b_4.
Units: $\frac{\text{volume of water}}{\text{weight\% polymer}}$

Note: Langmuir-type isotherms are used to model surfactant and polymer adsorption. Surfactant adsorption is irreversible with respect to surfactant concentration:

$$\overline{C}_3 = \frac{a_3 C_3^*}{1 + b_3 C_3^*}$$

$$\text{Units: } \frac{\text{volume of adsorbed surfactant}}{\text{volume of water}}$$

$$\text{where } C_3^* = \frac{\tilde{C}_3 - \overline{C}_3}{C_1} \text{ and } a_3 = a_{31} + a_{32}\, C_{SE}$$

When $a_{32} = 0$, there will be no salinity dependence.

A Langmuir-type isotherm is used to describe the adsorption level of polymer, component 4, as a function of the concentration of polymer in the water as:

$$\overline{C}_4 = \frac{a_4 C_4^*}{1 + b_4 C_4^*}$$

$$\text{Units: } \frac{\text{weight\% adsorbed polymer}}{\text{volume of water}}$$

$$\text{where } C_4^* = \frac{\tilde{C}_4 - \overline{C}_4}{C_1} \text{ and } a_4 = a_{41} + a_{42}\, C_{SEP}$$

3.4.84 QV, XKC, XKS, EQW

QV - Cation exchange capacity of clays.
Units: meq/ml of pore volume

XKC - Cation exchange constant, β^C, for clays.
Units: $(\text{meq/ml})^{-1}$

XKS - Cation exchange constant, β^S, for surfactant.
Units: $(\text{meq/ml})^{-1}$

EQW - Equivalent weight of surfactant.

Note: The cation exchange model is:

$$\frac{(\bar{C}_9)^2}{\bar{C}_6} = \beta^C Q_v \frac{(C_9^o)^2}{C_6^o} \quad \text{for clay}$$

$$\frac{(C_9^s)^2}{C_6^s} = \beta^C C_3 \frac{(C_9^o)^2}{C_6^o} \quad \text{for micelles}$$

EQW must be non-zero.

3.4.85 TK(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

TK(I) - Tracer partitioning coefficient, $K_{\kappa,\text{ref}}$, for I$^{\text{th}}$ water/oil tracer at initial chloride (C_{50}) concentration and reference temperature (TSTAND). A value of 0.0 indicates a water or gas tracer and a value of -1.0 indicates an oil tracer.
Units: fraction

Note: $K_{\kappa,\text{ref}} = \frac{C_{\kappa o}}{C_{\kappa w}}$ for oil/water tracer

$K_{\kappa,\text{ref}} = \frac{C_{\kappa o}}{C_{\kappa g}}$ for oil/gas tracer

3.4.86 TKS(I), for I = 1, NTW (This line is read only if NTW > 0)

TKS(I) - Parameter for calculating water/oil tracer partitioning coefficient, K_κ, for I$^{\text{th}}$ tracer as a function of salinity, TKS_k.
Units: $(\text{meq/ml})^{-1}$

Note: $K_\kappa = K_{\kappa,\text{ref}}\left(1 + TKS_\kappa (C_{51} - C_{50})\right)$

3.4.87 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, K_κ, for I$^{\text{th}}$ tracer as a function of reservoir temperature, TKT_k.
Units: $(°F)^{-1}$ (IUNIT=0) or $(°C)^{-1}$ (IUNIT=1)

Note: $K_\kappa = K_{\kappa,\text{ref}}\left(1 + TKT_\kappa (T - T_{\text{ref}})\right)$

3.4.88 RDC(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

RDC(I) - Radioactive decay coefficient, λ_K, for Ith tracer. A value of 0.0 indicates a non–radioactive tracer.
Units: 1/days

Note: $C = C_0 e^{-\lambda_K (t - t_0)}$

where

$$\lambda_k = -\frac{\ln(0.5)}{t_{1/2,k}}$$

$t_{1/2,k}$ = half life of radioactive tracer, day

3.4.89 RET(I), for I = 1, NTW+NTA (This line is read only if NTW+NTA > 0)

RET(I) - Tracer retardation factor D_S—adsorbed concentration/flowing concentration. A value of 0.0 indicates no retardation.
Units: dimensionless

Note: The retardation factor is defined as:

$$D_s = \frac{\overline{C}}{C} = \frac{(1-\phi)\rho_r a_T}{\phi \rho_\ell C_{T\ell}}$$

where $\ell = 1$ for oil/water tracer and $\ell = 4$ for gas/water tracer.

This factor causes a reduction in tracer velocity:

$$V_t = \frac{u/\phi}{1 + D_S}$$

3.4.90 FFL(1), FFH(1), CM(I,1), for I = 1, NTW (This line is read only if NTW > 0 and ICAP = 1)

FFL(1) - Value of flowing fraction for phase 1 when fractional flow = 0.0.
Units: dimensionless

FFH(1) - Value of flowing fraction for phase 1 when fractional flow = 1.0.
Units: dimensionless

CM(I,1) - Mass transfer coefficients for Ith tracer in phase 1.
Units: 1/sec

3.4.91 FFL(2), FFH(2), CM(I,2), for I = 1, NTW (This line is read only if NTW > 0 and ICAP = 1)

FFL(2) - Value of flowing fraction for phase 2 when fractional flow = 0.0.

Units: dimensionless

FFH(2) - Value of flowing fraction for phase 2 when fractional flow = 1.0.
Units: dimensionless

CM(I,2) - Mass transfer coefficients for I^{th} tracer in phase 2.
Units: 1/sec

3.4.92 FFL(3), FFH(3), CM(I,3), for I = 1, NTW (This line is read only if NTW > 0 and ICAP = 1)

FFL(3) - Value of flowing fraction for phase 3 when fractional flow = 0.0.
Units: dimensionless

FFH(3) - Value of flowing fraction for phase 3 when fractional flow = 1.0.
Units: dimensionless

CM(I,3) - Mass transfer coefficients for I^{th} tracer in phase 3.
Units: 1/sec

3.4.93 TAK1 (This line is read only if NTW > 0 and ITREAC = 1)

TAK1 - Rate constant for a first-order aqueous phase reaction at reference temperature (T_{ref}) in which Tracer 2 (component 10) hydrolyzes to form Tracer 3 (component 11) according to $C_{11,1} = \text{TAK1}\ C_{10,1}$.
Units: days^{-1}

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

TMW(I) - Molecular weight of the I^{th} 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.

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

TDEN(I) - Density of the I^{th} tracer.
Units: g/cm^3

3.4.96 TAKT (This line is read only if NTW > 0 and ITREAC = 1 and IENG = 1)

TAKT - Parameter for calculating rate constant for a first-order aqueous phase reaction as a function of reservoir temperature.
Units: $(^{\circ}K)^{-1}$

Note: $$\text{TAK} = \text{TAK1}\ \exp\left(\text{TAKT}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$$

3.4.97 AK1, AK2, SCR, X4, X14, X16, WM4 (This line is read only if NG>0)

AK1 - Kinetic rate coefficient for Cr^{3+} at reference temperature (T_{ref}), $AK1_{ref}$.
Units: ppm^{-1} $days^{-1}$

AK2 - Kinetic rate coefficient for gel at reference temperature (T_{ref}), $AK2_{ref}$.
Units: $(mole/liter)^{1-X4-X14+X16}$ $days^{-1}$
Note: In order to achieve the same results achieved in versions previous to UTCHEM-V-5.0, please use the following conversion:

$$AK2_{new} = \frac{SCR \times M_{Cr^{3+}} \times M^2_{polymer} \times 10^9}{(1+SCR)} AK2_{old}$$

SCR - Stoichiometric ratio in mass between Cr^{3+} and polymer.
Units: dimensionless

Note: $SCR = \dfrac{n \times M_{Cr^{3+}}}{M_{polymer}}$

X4 - Exponent to be used for polymer component of gelation reaction.
Units: dimensionless

X14 - Exponent to be used for chromium component of gelation reaction.
Units: dimensionless

X16 - Exponent to be used for hydrogen ion component of gelation reaction.
Units: dimensionless

WM4 - Molecular weight of polymer.
Units: g/mole

3.4.98 AK1T, AK2T (This line is read only if NG>0 and IENG = 1)

AK1T - Parameter for calculating Kinetic rate coefficient for Cr^{3+} as a function of reservoir temperature.
Units: $(^{\circ}K)^{-1}$

AK2T - Parameter for calculating Kinetic rate coefficient for gel as a function of reservoir temperature.
Units: $(^{\circ}K)^{-1}$

Note: The kinetic rate coefficients as a function of temperature are computed from:

$$AK1 = AK1_{ref} \exp\left(AK1T\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$$

$$AK2 = AK2_{ref} \exp\left(AK2T\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$$

3.4.99 AG1, AG2, CRG, AGK, BGK (This line is read only if NG>0)

AG1 - Flory-Huggins parameter for gel viscosity, A_{g1}.
Units: cp ppm^{-1} = mPa.s ppm^{-1}

AG2 - Flory-Huggins parameter for gel viscosity, A_{g2}.
Units: cp ppm^{-2} = mPa.s ppm^{-2}

CRG - Constant, C_δ, 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, A_{15} and B_{15}, for Langmuir correlation with gel concentration.
Units: dimensionless

Note: Dimensionless pore radius reduction group:

$$N_\delta = C\delta \frac{[\mu]^{1/3}}{\left[\sqrt{k_x k_y}/\phi\right]^{1/2}}$$

$$C_\delta = 3.9 \times 10^{-3} N_g M_{\text{polymer}}^{1/3}$$

$$[\mu] = \lim_{\substack{C_{4\ell}\to 0\\ \dot{\gamma}\to 0}} \left(\frac{\mu_p - \mu_w}{\mu_w C_{4\ell}}\right)$$

From this the permeability reduction factor for idealized case is expressed as:

$$RRF_{\max} = \frac{k_w\text{, before gel treatment}}{k_w\text{, after gel treatment}} = \left(1 - N_\delta\right)^{-4}$$

The "Langmuir-type" isotherm for permeability reduction as a function of gel concentration is:

$$RRF = 1 + \frac{(RRF_{\max} - 1)A_{15}\, C_{15,1}}{1 + B_{15}\, C_{15,1}}$$

Note: Gel viscosity is calculated from

$$\mu_{gel} = \mu_w\left[1 + A_{g1}C_{15,1} + A_{g2}C_{15,1}^2\right]$$

if there is flowing polymer concentration, add μ_{gel} to the μ_p calculation. See note for input line 3.4.62.

3.4.100 A15D, B15D, ICREX, A14D, B14D, CRNAK, HNAK, C160 (This line is read only if 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 "Langmuir-type" isotherm for chromium and gel adsorption is expressed as:

$$\overline{C}_\kappa = \frac{a_\kappa\ C_{\kappa,1}}{1 + b_\kappa\ C_{\kappa,1}},\ \kappa = \begin{cases} 14 \text{ for chromium} \\ 15 \text{ for gel} \end{cases}$$

The input values of CRNAK, HNAK, and C160 are ignored for IREACT=6

3.4.101 IP1, IP2 (This line is read only if NG>0, NY = 1 and NZ = 1)

IP1, IP2 - Grid block 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.

3.4.102 TEMPI (This line is read only if IENG = 1)

TEMPI- Constant initial reservoir temperature.
Units : °F (IUNIT=0) or °C (IUNIT=1)

3.4.103 DENS, CRTC, CVSPR, CVSPL(L), L=1,MXP (This line is read only if IENG = 1)

DENS - Reservoir rock density.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)

CRTC - Reservoir thermal conductivity.
Units: Btu $(day\text{-}ft\text{-}°F)^{-1}$ (IUNIT=0) or kJ $(day\text{-}m\text{-}°K)^{-1}$ (IUNIT=1)

CVSPR - Reservoir rock heat capacity.

Units: Btu $(lb\text{-}^\circ F)^{-1}$ (IUNIT=0) or kJ $(kg\text{-}^\circ K)^{-1}$ (IUNIT=1)

CVSPL(L) - Phase L heat capacity (MXP is equal to 3 (IGAS=0) or 4 (IGAS=1)).
Units: Btu $(lb\text{-}^\circ F)^{-1}$ (IUNIT=0) or kJ $(kg\text{-}^\circ K)^{-1}$ (IUNIT=1)

3.4.104 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. Heat flux into the reservoir from the overbuden/underburden is calculated from the model of Vinsome and Westerveld, *J. Can, Pet. Tech.*, July-Sept. 1980, pp. 87-90
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 soluion is considered

3.4.105 TCONO, DENO, CVSPO, TCONU, DENU, CVSPU (This line is read only if IENG = 1 and IHLOS = 1)

TCONO - Thermal conductivity of overburden rock.
Units: Btu $(day\text{-}ft\text{-}^\circ F)^{-1}$ (IUNIT=0) or kJ $(day\text{-}m\text{-}^\circ K)^{-1}$ (IUNIT=1)

DENO - Density of overburden rock.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)

CVSPO - Heat capacity of overburden rock.
Units: Btu $(lb\text{-}^\circ F)^{-1}$ (IUNIT=0) or kJ $(kg\text{-}^\circ K)^{-1}$ (IUNIT=1)

TCONU - Thermal conductivity of underburden rock.
Units: Btu $(day\text{-}ft\text{-}^\circ F)^{-1}$ (IUNIT=0) or kJ $(day\text{-}m\text{-}^\circ K)^{-1}$ (IUNIT=1)

DENU - Density of underburden rock.
Units: lb/ft^3 (IUNIT=0) or g/cm^3 (IUNIT=1)

CVSPU - Heat capacity of underburden rock.
Units: Btu $(lb\text{-}^\circ F)^{-1}$ (IUNIT=0) or kJ $(kg\text{-}^\circ K)^{-1}$ (IUNIT=1)

3.5 Physical Property Data for Geochemical Options

The fifth input section consists of physical property data that is read 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 not preceeded by the usual seven comment lines and individual data lines are not preceeded by three comment lines. Sections 6.6 through 6.9 of the Appendix give a list of elements, fluid species, solid species, and adsorbed species for geochemical options.

3.5.1 IRSPS, IPHAD (This line is read only if IREACT > 1)

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 IREACT > 1 and 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 or 5)

CSELP - Lower optimum salinity limit for generated surfactant.
Units: meq/ml

CSEUP - Upper optimum salinity limit for generated surfactant.
Units: meq/ml

3.5.4 NELET, NFLD, NSLD, NSORB, NACAT, ICHRGE (This line is read only if IREACT > 1)

NELET - Total number of elements less non reacting element.
Maximum Value: 9

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.

ICHRGE - 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 SiO_2 is considered, the oxygen balance must be used.

3.5.5 NIAQ, NEX, NSLEL, NSURF1 (This line is read only if IREACT > 1)

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 or 4.

3.5.6 NH, NNA, NCA, NMG, NCARB (This line is read only if IREACT > 1)

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.
Note: If magnesium is not considered, NMG must be set equal to 0.

NCARB - Position number corresponding to the carbonate pseudo-element in the element array ELEMNT.

3.5.7 NALU, NSILI, NOXY (This line is read only if IREACT > 3)

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.

3.5.8 NACD (This line is read only if IREACT = 3 or 5)

NACD - Position number corresponding to the petroleum acid pseudo-element in the element array ELEMNT.

3.5.9 ELEMNT(I), for I = 1, NELET (This line is read only if IREACT > 1)

ELEMNT(I) - Name of the Ith element.
Note: The name of each element may not exceed 32 characters and each name must be on a separate line of the input file.

3.5.10 FLDSPS(I), for I = 1, NFLD (This line is read only if IREACT > 1)

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 or 5, the last fluid species must be HA_w (petroleum acid in water).

3.5.11 SLDSPS(I), for I = 1, NSLD (This line is read only if IREACT > 1 and 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.

3.5.12 SORBSP(I), for I = 1, NSORB (This line is read only if IREACT > 1 and NSORB > 0)

SORBSP(I) - Name of the Ith adsorbed cation.
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.

3.5.13 ACATSP(I), for I = 1, NACAT (This line is read only if IREACT > 1 and 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.

3.5.14 NSORBX(I), for I = 1, NEX (This line is read only if IREACT > 1 and NSORB > 0)

NSORBX(I) - Number of cations for Ith exchanger.

3.5.15 AR(I,J), for J = 1, NFLD, for I = 1, NELET << or >>
AR(I,J), for J = 1, NFLD, for I = 1, NELET-1 (This line is read only if IREACT > 1)

AR(I,J) - Stoichiometric coefficient of Ith element in Jth fluid species.

Note: If ICHRGE = 0, then NFLD × NELET values are required by the program. If ICHRGE = 1, then NFLD × (NELET-1) values are required by the program.

3.5.16 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 IREACT > 1 and NSLD > 0)

BR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} solid species.

Note: If ICHRGE = 0, then NSLD × NELET values are required by the program. If ICHRGE = 1, then NSLD × (NELET-1) values are required by the program.

3.5.17 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 IREACT > 1 and NSORB > 1)

DR(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} sorbed species.

Note: If ICHRGE = 0, then NSORB × NELET values are required by the program. If ICHRGE = 1, then NSORB × (NELET-1) values are required by the program.

3.5.18 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 IREACT > 1 and NACAT > 1)

ER(I,J) - Stoichiometric coefficient of I^{th} element in J^{th} surfactant associated cation.

Note: If ICHRGE = 0, then NACAT × NELET values are required by the program. If ICHRGE = 1, then NACAT × (NELET-1) values are required by the program.

3.5.19 BB(I,J), for J = 1, NIAQ+NSORB+NACAT, for I = 1, NFLD+NSORB+NACAT (This line is read only if IREACT > 1)

BB(I,J) - Exponent of the J^{th} independent fluid species concentration when the I^{th} fluid species is expressed in terms of independent species concentrations.

3.5.20 EXSLD(I,J), for J = 1, NIAQ, for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD ≥ 1)

EXSLD(I,J) - Exponent of the J^{th} independent fluid species concentration in the solubility product definition of the I^{th} solid.

3.5.21 CHARGE(I), for I = 1, NFLD (This line is read only if IREACT > 1)

CHARGE(I) - Charge of the I^{th} fluid species.

3.5.22 SCHARG(I,J), for J = 1, NSORBX(I), for I = 1, NEX (This line is read only if IREACT > 1 and NSORB ≥ 1)

SCHARG(I,J) - Charge of the J^{th} sorbed species on the I^{th} exchanger.

3.5.23 EQK(I), for I = 1, NFLD (This line is read only if IREACT > 1)

EQK(I) - Equilibrium constant for I^{th} fluid species when expressed in independent species concentrations only.

3.5.24 EXK(I,J), for J = 1, NSORBX(I)-1, for I = 1, NEX (This line is read only if IREACT > 1 and NEX > 0)

EXK(I,J) - Exchange equilibrium constant for J^{th} exchange equilibrium of the I^{th} insoluble exchanger.

3.5.25 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 IREACT > 1 and NEX > 0)

EXEX(I,J,K) - Exponent of K^{th} independent species in J^{th} equilibrium relation of the I^{th} exchanger

3.5.26 REDUC(I,J), for J = 1, NSORBX(I)-1, for I = 1, NEX (This line is read only if IREACT > 1 and 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.

3.5.27 EXCAI(I), for I = 1, NEX (This line is read only if IREACT > 1 and NEX >0)

EXCAI(I) - Exchange capacity of I^{th} insoluble exchanger.
Units: meq/ml pore volume

3.5.28 SPK(I), for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD ≥ 1)

SPK(I) - Solubility product of I^{th} solid defined in terms of independent fluid species concentrations only.

3.5.29 CHACAT(I), for I = 1, NACAT (This line is read only if IREACT > 1 and NACAT ≥ 1)

CHACAT(I) - Charge of I^{th} surfactant associated cation.

3.5.30 ACATK(I), for I = 1, NACAT-1 (This line is read only if IREACT > 1 and NACAT ≥ 1)

ACATK(I) - Equilibrium constant for I^{th} exchange equilibrium for cation exchanges on surfactant.

3.5.31 EXACAT(I,J) for J = 1, NIAQ+NSORB+NACAT, for I = 1, NACAT-1 (This line is read only if IREACT > 1 and NACAT ≥ 1)

EXACAT(I,J) - Exponent of J^{th} independent species in I^{th} equilibrium for cation exchange on surfactant.

3.5.32 CI(J), for J = 1, NACAT (This line is read only if IREACT > 1 and NACAT ≥ 1)

CI(J) - Initial concentration of J^{th} surfactant associated cation.
Units: moles/liter pore volume

3.5.33 C5I, C6I (This line is read only if IREACT > 1)

C5I - Initial concentration of non reacting anions.
Units: equivalents/liter

C6I - Initial concentration of calcium in aqueous phase.
Units: equivalents/liter

3.5.34 CELAQI(J), for J = 1, N-NO6 (This line is read only if IREACT > 1)

CELAQI(J) - Initial concentrations of $(J+11)^{th}$ component.
Units: equivalents/liter

Note : NO6 = 11 for 1< IREACT<6
NO6 = 15 for IREACT = 6

3.5.35 CAC2I (This line is read only if IREACT = 3 or 5)

CAC2I - Initial concentration of acid in oil.
Units: moles/liter oil

3.5.36 CAQI(J), for J = 1, NIAQ (This line is read only if IREACT > 1)

CAQI(J) - Initial guesses for J^{th} independent species concentration.
Units: moles/liter water

3.5.37 CSLDI(I), for I = 1, NSLD (This line is read only if IREACT > 1 and NSLD ≥ 1)

CSLDI(I) - Initial concentration of I^{th} solid.
Units: moles/liter pore volume

3.5.38 CSORBI(I), for I = 1, NSORB (This line is read only if IREACT > 1 and NSORB ≥ 1)

CSORBI(I) - Initial concentration of I^{th} adsorbed cation.
Units: moles/liter pore volume

3.5.39 C1I, C2I (This line is read only if IREACT = 3 or 5)

C1I - Initial concentration of water in aqueous phase.
Units: volume fraction

C2I - Initial concentration of oil in oleic phase.
Units: volume fraction

3.5.40 ACIDIS, EQWPS (This line is read only if IREACT = 3 or 5)

ACIDIS - Dissociation constant of the petroleum acid, K_a.

EQWPS - Equivalent weight of petroleum acid.

3.6 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.

3.6.1 IBOUND

IBOUND - The flag to specify if constant potential boundaries at the left and right sides of the simulation model are specified.
Possible Values:
0 : No boundary is specified
1 : Boundary is specified

3.6.2 IBL, IBR (This line is read only if IBOUND = 1)

IBL - The flag to specify if the left hand side constant potential boundary is specified.
Possible Values:
0 : No boundary is specified
1 : Boundary is specified

IBR - The flag to specify if the right hand side constant potential boundary is specified.
Possible Values:
0 : No boundary is specified
1 : Boundary is specified

3.6.3 PBL, C1BL, C5BL, C6BL (This line is read only if IBOUND = 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

C6BL - Concentration of calcium in aqueous phase at the left boundary.
Units : meq/ml

3.6.4 PBR, C1BR, C5BR, C6BR (This line is read only if IBOUND = 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

C6BR - Concentration of calcium in aqueous phase at the right boundary.
Units : meq/ml

3.6.5 NWELL, IRO, ITIME

NWELL - Maximum number of wells used for the simulation.
Note: If ICOORD = 2, NWELL must be equal to 1 and the MXW parameter in the source code 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
Note: This model (IRO=1) does not work for ICOORD = 4.
2 - Peaceman model is used (this was the default in versions previous to UTCHEM-V-5.0)
Note: For information on the Babu and Odeh well radius model, please refer to: Babu, D. K, and A. S. Odeh: "Productivity of a Horizontal Well," *SPE Reser. Eng.* (November 1989) **4**, 417-421 and Appendices A and B, paper SPE 18334, SPE Publ., Richardson, TX.

ITIME - 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 is not a shut-in period. If IMES = 1, this flag is ignored. For a shut-in period you need to use ITIME = 0

Note: The Courant number is defined as:

$$C = \frac{Q \ \Delta t}{\Delta x \ \Delta y \ \Delta z \ \phi}$$

The following values for minimum and maximum Courant numbers are recommended for different simulations as follows:

Process	Min. Courant #	Max. Courant #
Waterflood/tracer	0.04	0.4
Polymerflood	0.02	0.2
Surfactant/polymerflood	0.01	0.1
Geochemical process	0.01	0.1

3.6.6 The data on input lines 3.6.6.a through 3.6.6.d are repeated for M = 1 to NWELL times.

3.6.6.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. The history profile data for the well indicated by IDW(M) will be written to FORTRAN UNIT number 18 + IDW(M).

IW(M) - First index of the reservoir grid block containing the M^th^ well.
Possible Values: Between 1 and the number of grid blocks in the pertinent direction, inclusive
Note: If the M^th^ 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 grid block containing the M^th^ well.
Possible Values: Between 1 and the number of grid blocks in the pertinent direction, inclusive
Note: If the M^th^ 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(1) = JW(1) = 1.

IFLAG(M) - Flag indicating type of well constraint specification for M^th^ 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 M^th^ well.
Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(M) - Skin factor for M^th^ well.
Units: dimensionless

IDIR(M) - Flag indicating the direction in which the M^th^ 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.

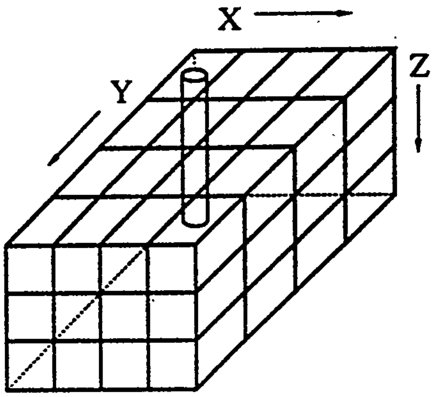
IFIRST(M) - Index of the first block in which the M^th^ well is completed.
Possible Values: Between 1 and the number of grid blocks in the pertinent direction, inclusive

ILAST(M) - Index of the last block in which the M^th^ well is completed.
Possible Values: Between IFIRST(M) and the number of grid blocks in the pertinent direction, inclusive

IPRF(M) - Flag indicating if partial completion of the well is considered.

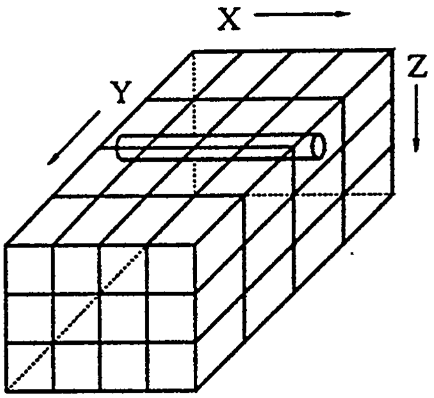
Possible Values:
- 0 - The well is fully completed
- 1 - The well is partially completed

Example: For a vertical well (completed through all the layers) as illustrated in the 4 × 4 × 3 example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



IDIR(M) = 3
IW(M) = 1
JW(M) = 1
IFIRST(M) = 1
ILAST(M) = 3

For a horizontal well (completed from the first to last grid block in the X direction and parallel to the X-axis) as illustrated in the 4 × 4 × 3 example below, note the values of IDIR(M), IW(M), JW(M), IFIRST(M), and ILAST(M):



IDIR(M) = 1
IW(M) = 2
JW(M) = 1
IFIRST(M) = 1
ILAST(M) = 4

Note: Horizontal wells can be used for 2-D X-Y or 3-D simulations.

3.6.6.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

3.6.6.c WELNAM(M)

WELNAM(M) - Name of the Mth well.

Note: The name can consist of any combination of up to 18 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(M)—at the beginning of the history output files.

3.6.6.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 M^{th} 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 M^{th} well.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

PWFMAX(M) - Maximum flowing bottom hole pressure (specified at the top layer) for the M^{th} well.
Units: psi (IUNIT=0) or kPa (IUNIT=1)

QTMIN(M) - Minimum total flow rate (specified at the top layer) for the M^{th} well.
Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

QTMAX(M) - Maximum total flow rate (specified at the top layer) for the M^{th} well.
Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: 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 M^{th} pressure constraint injector or producer produces at total rate less than QTMIN(M), the M^{th} 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 M^{th} 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).

3.6.7 The data on input lines 3.6.7.a, 3.6.7.b, 3.6.7.c, and 3.6.7.d are repeated for M = 1 to NWELL times.

Note 1: 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.

Note 2: 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).

3.6.7.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 M^th^ 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 3.6.6.a.

QI(M,L) - Injection rate of L^th^ phase in M^th^ well (see note).
Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

C(M,KC,L) - Concentration of KC^th^ component in L^th^ phase in M^th^ well.
Units: vary according to component (see note)

Note: 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 in. MXP is equal to 3 (IGAS = 0) or 4 (IGAS = 1).

The following values for L correspond to the indicated phase:
1 - Aqueous phase
2 - Oleic phase
3 - Microemulsion phase
4 - Gas phase

The following values for KC correspond to the indicated component (corresponding concentration units are in parentheses):
For all values of IREACT:
1 - Water (volume fraction)
2 - Oil (volume fraction)
3 - Surfactant (volume fraction)
4 - Polymer (weight percent)
5 - Total nonsorbing anions concentration, assumed to all be chloride anions (meq/ml)
6 - Divalent cations, assumed to all be calcium for IREACT<2 (meq/ml)
7 - Alcohol 1 (volume fraction)
8 - Alcohol 2 (volume fraction) or Gas (volume fraction)
9 - Tracer 1
10 - Tracer 2
11 - Tracer 3
For IREACT = 0:
12 - Tracer 4

13 - Tracer 5
...
20 - Tracer 12
21 - Tracer 13

For IREACT = 1:
12 - $Na_2Cr_2O_7$ (ppm)
13 - CSN_2H_4 (ppm)
14 - Cr^{3+} (ppm)
15 - Gel (ppm)
16 - Hydrogen (meq/ml)

For IREACT = 2, 3, 4, 5, or 6:
12 - Sodium (meq/ml)
13 - Hydrogen (meq/ml)
14 - Magnesium (meq/ml)
15 - Carbonate (meq/ml)

For IREACT = 3:
16 - Acid component of crude oil (meq/ml)

For IREACT = 4 , 5, or 6:
16 - Aluminum (meq/ml)
17 - Silica (meq/ml)

For IREACT = 5:
18 - Acid component of crude oil (meq/ml)

For IREACT = 6
18 - $Na_2Cr_2O_7$ (ppm)
19 - CSN_2H_4 (ppm)
20 - Cr^{3+} (ppm)
21 - Gel (ppm)

3.6.7.b ID(M), PWF(M) (This line is read only if IFLAG(M) = 2 or 3)

ID(M) - Well I.D. number for the M^th 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 3.6.6.a.

PWF(M) - Flowing bottom hole pressure for the M^th well.
Units: psia (IUNIT=0) or kPa (IUNIT=1)

3.6.7.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 M^th 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 3.6.6.a.

TEMINJ(M) - Injection temperature for M^th well.
Units: °F (IUNIT=0) or °C (IUNIT=1)

3.6.7.d ID(M), QI(M,1) (This line is read only if IFLAG(M) = 4)

ID(M) - Well I.D. number for the M^th 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 3.6.6.a.

QI(L) - Total production rate for M^{th} well.
Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)
Note: This value needs to be input as a negative number

3.6.8 TINJ, CUMPR1, CUMHI1, CUMHI2, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.
Units: days or pore volumes (dependent on value of ISTOP flag on input line 3.2.1)

CUMPR1 - Indicates interval at which profiles should be written to UNIT 4.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

CUMHI1 - Indicates interval at which production data should be written to UNIT 4.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

CUMHI2 - Indicates interval at which production data should be written to UNIT 3.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

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 on input line 3.2.1)
Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed. The unit number of the file to be written to starts at 19 and continues upward. For example, for a run with three producers, UNITS 19, 20 and 21 would be used. The history of reservoir properities and overall rates from all the producing wells is written to UNIT 9.

WRPRF - Indicates interval at which concentration, pressure, saturation, tracer phase concentration, capacitance property, gel property, alkaline property , and temperature profiles should be written to UNITS 8, 11, 12, 13, 14, 10, 15, and 18 respectively.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)
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 UNIT 7.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

3.6.9 DT (This line is read only if IMES = 1 and ITIME = 0)

DT - Time step size for constant time step option.

Units: days

3.6.10 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES = 2 and ITIME = 0)

DT - Initial time step size, Δt_i.
Units: days

DCLIM - Tolerance for concentration change for the first three components, ΔC_{lim}.
Units: volume fraction

DTMAX - Maximum time step size, Δt_{max}.
Units: days

DTMIN - Minimum time step size, Δt_{min}.
Units: days

Note: The time step selection is based on the method of relative changes for the first three components (water, oil, and surfactant) as:

$$\Delta t^{n+1} = \Delta t^{n} \min \left(\frac{\Delta C_{lim}}{\max\limits_{i=1}^{NBL} \left| \Delta C_{i,\kappa} \right|} \right) \qquad \kappa = 1, 2, 3$$

Δt^{n+1} is limited to: $\Delta t_{min} \leq \Delta t^{n+1} \leq \Delta t_{max}$

3.6.11 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES = 2, ITIME = 1, and at least one well is not shut-in.)

DT - Initial time step size, Δt_i.
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

Note: The minimum and maximum time steps in days are computed based on the minimum and maximum Courant number as:

$$\Delta t_{min} = \frac{CNMIN}{\min\limits_{M=1}^{nwell} \left(\max\limits_{i=1}^{nwbc} \frac{Q_i}{\Delta x_i \ \Delta y_i \ \Delta z_i \ \phi_i} \right)}$$

and

$$\Delta t_{max} = \frac{CNMAX}{\min\limits_{M=1}^{nwell}\left(\max\limits_{i=1}^{nwbc} \frac{Q_i}{\Delta x_i \ \Delta y_i \ \Delta z_i \ \phi_i}\right)}$$

3.6.12 DT, (DCLIM(KC), for KC = 1, N), DTMAX, DTMIN (This line is read only if IMES = 3 or 4 and ITIME = 0)

DT - Initial time-step size, Δt_i.
Units: days

DCLIM(KC) - Tolerance for concentration change, $\Delta C_{lim,\kappa}$, of KC^th component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, 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 3.6.7.a)
IMES = 4: dimensionless

DTMAX - Maximum time step size, Δt_{max}.
Units: days

DTMIN - Minimum time step size, Δt_{min}.
Units: days

Note: For IMES = 3, the method of relative changes is applied to all the components in the simulation run:

$$\Delta t^{n+1} = \Delta t^n \min\left(\frac{\Delta C_{lim}}{\max\limits_{i=1}^{NBL}\left|\Delta C_{i,\kappa}\right|}\right) \qquad \kappa = 1, ..., n_c$$

Δt^{n+1} is limited to: $\Delta t_{min} \leq \Delta t^{n+1} \leq \Delta t_{max}$

$\Delta C_{lim,\kappa}$ is a fraction of the initial or injected concentration (whichever is larger) of the KC^th component. For example: $\Delta C_{lim,3} = 0.1 \times C_3$ where C_3 is the total concentration of component 3. If $\Delta C_{lim,\kappa}$ of the KC^th component is entered as zero, that component is not considered in the time-step size selection.

For IMES = 4, the new time-step size is calculated according to:

$$\Delta t^{n+1} = \Delta t^n \min\left(\frac{R_{lim,\kappa}}{\max\limits_{i=1}^{NBL}\left|\frac{\Delta C_{i,\kappa}}{C_{i,\kappa}}\right|}\right) \qquad \kappa = 1, ..., n_c$$

Δt^{n+1} is limited to: $\Delta t_{min} \leq \Delta t^{n+1} \leq \Delta t_{max}$

$R_{lim,\kappa}$ is the dimensionless relative change in concentration. For example: $R_{lim,3} = 0.1$ indicates a 10% change in concentration of component 3.

3.6.13 DT, (DCLIM(KC), for KC = 1, N), CNMAX, CNMIN (This line is read only if IMES = 3 or 4, ITIME = 1, and reservoir is not shut-in.)

DT - Initial time step size, Δt_i.
Units: days

DCLIM(KC) - Tolerance for concentration change, $\Delta C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, 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 3.6.7.a)
IMES = 4: dimensionless

CNMAX - Maximum Courant number.
Units: dimensionless

CNMIN - Minimum Courant number.
Units: dimensionless

Note: See note for input lines 3.6.11 and 3.6.12 for time step calculation information.

IMPORTANT NOTE: The data on lines 3.6.14 through 3.6.23 describe the changes in boundary conditions and are repeated until the injected time (TINJ on input line 3.6.8) is greater than or equal to the maximum simulation time (TMAX on input line 3.3.1).

3.6.14 IRO, ITIME, IFLAG(M), 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 (this was the default in versions previous to UTCHEM-V-5.0)
Note: For information on the Babu and Odeh well radius model, please refer to: Babu, D. K, and A. S. Odeh: "Productivity of a Horizontal Well," *SPE Reser. Eng.* (November 1989) **4**, 417-421 and Appendices A and B, paper SPE 18334, SPE Publ., Richardson, TX.

ITIME - 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.

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

3.6.15 NWEL1

NWEL1 - Number of wells with changes in location (IW(M), JW(M)), skin, direction, perforation, name, or minimum and maximum bottomhole pressure or mimimum or maximum rate.

3.6.16 The data on input lines 3.6.16.a through 3.6.16.d are repeated for M = 1 to NWEL1 times.

3.6.16.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 grid block containing the ID^{th} well.
Possible Values: Between 1 and the number of grid blocks in the pertinent direction, inclusive
Note: See note for input line 3.6.6.a.

JW(ID) - Second index of the reservoir grid block containing the ID^{th} well.
Possible Values: Between 1 and the number of grid blocks in the pertinent direction, inclusive
Note: See note for input line 3.6.6.a.

RW(ID) - Radius of ID^{th} well.
Units: feet (IUNIT=0) or m (IUNIT=1)

SWELL(ID) - Skin factor for ID^{th} well.
Units: dimensionless

IDIR(ID) - Flag indicating the direction in which the ID^{th} 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 ID^{th} well is completed.
Possible Values: Between 1 and the number of grid blocks in the pertinent direction, inclusive

ILAST(ID) - Index of the last block in which the ID^{th} well is completed.
Possible Values: Between IFIRST(ID) and the number of grid blocks in the pertinent direction, inclusive
Note: At this time, UTCHEM assumes the well is completed continuously between IFIRST(ID) and ILAST(ID).

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

3.6..16.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

3.6.16.c WELNAM(ID)

WELNAM(ID) - Name of the IDth well.
Note: The name can consist of any combination of up to 18 alphanumeric characters. This information will be printed—along with the well I.D. number, IDW(ID)—at the beginning of the history output files.

3.6.16.d ICHEK, PWFMIN(ID), PWFMAX(ID), QTMIN(ID), QTMAX(ID)

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 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: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

QTMAX(ID) - Maximum total flow rate (specified at the top layer) for the IDth well.
Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)

Note: See the note for input line 3.6.6.d.

3.6.17 NWEL2, (ID(J), for J = 1, NWEL2)

NWEL2 - Number of wells with changes in rate, concentration or bottomhole pressure.

ID(J) - ID number for J^{th} well with changes.

3.6.18 The data on input lines 3.6.18.a through 3.6.18.d are repeated for M = 1 to NWEL2 times.

3.6.18.a ID, (QI(ID,L), for L = 1, MXP), (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 L^{th} phase in ID^{th} well (see note for input line 3.6.7.a).
Units: ft^3/day (IUNIT=0) or m^3/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 line 3.6.7.a)

Note: If IGAS = 0, then MXP = 3. If IGAS = 1, then MXP = 4.

3.6.18.b ID(ID), PWF(ID) (This line is read only if IFLAG(ID) = 2 or 3)

ID(ID) - Well ID number with changes from the previous slug injection period.

PWF(ID) - Flowing bottom hole pressure for the ID^{th} well.
Units: psia (IUNIT=0) or kPa (IUNIT=1)

3.6.18.c ID(ID), TEMINJ(ID) (This line is read only if IENG = 1 and IFLAG(ID) = 1or 3)

ID(ID) - Well ID number with changes from the previous slug injection period.

TEMINJ(ID) - Injection temperature for the ID^{th} well.
Units: °F (IUNIT=0) or °C (IUNIT=1)

3.6.18.d ID(ID), QI(ID,1) (This line is read only if IFLAG(ID) = 4)

ID(ID) - Well ID number with changes from the previous slug injection period.

QI(ID,1) - Total production rate for ID^{th} well.
Units: ft^3/day (IUNIT=0) or m^3/day (IUNIT=1)
Note: This value needs to be input as a negative number.

3.6.19 TINJ, CUMPR1, CUMHI1, CUMHI2, WRHPV, WRPRF, RSTC

TINJ - Cumulative injection time.
Units: days or pore volumes (dependent on value of ISTOP flag on input line 3.2.1)

CUMPR1 - Indicates interval at which profiles should be written to UNIT 4.

Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

CUMHI1 - Indicates interval at which production data should be written to UNIT 4.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

CUMHI2 - Indicates interval at which production data should be written to UNIT 3.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

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 on input line 3.2.1)
Note: If WRHPV > total pore volume injected or maximum simulation time, the data will not be printed. The unit number of the file to be written to starts at 19 and continues upward. For example, for a run with three producers, UNITS 19, 20, and 21 would be used. The history of reservoir properties and the total rate from all the producing wells is written to UNIT 9.

WRPRF - Indicates interval at which concentration, pressure, saturation, tracer phase concentration, capacitance property, pressure difference, gel property, alkaline property , and temperature profiles should be written to UNITS 8, 11, 12, 13, 14, 10, 15 and 18 respectively.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)
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 UNIT 7.
Units: pore volumes or days (dependent on value of ICUMTM flag on input line 3.2.1)

3.6.20 DT (This line is read only if IMES = 1 and ITIME = 0)

DT - Time step size for constant time step option.
Units: days

3.6.21 DT, DCLIM, DTMAX, DTMIN (This line is read only if IMES = 2 and ITIME = 0)

DT - Initial time step size, Δt_i.
Units: days

DCLIM - Tolerance for concentration change for the first three components, ΔC_{lim}.
Units: volume fraction

DTMAX - Maximum time step size, Δt_{max}.
Units: days

DTMIN - Minimum time step size, Δt_{min}.
Units: days

Note: See note for input line 3.6.10.

3.6.22 DT, DCLIM, CNMAX, CNMIN (This line is read only if IMES = 2, ITIME = 1, and at least one well is not shut-in.)

DT - Initial time step size, Δt_i.
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

Note: See note for input line 3.6.11.

3.6.23 DT, (DCLIM(KC), for KC = 1, N), DTMAX, DTMIN (This line is read only if IMES = 3 or 4 and ITIME = 0)

DT - Initial time-step size, Δt_i.
Units: days

DCLIM(KC) - Tolerance for concentration change, $\Delta C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, 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 3.6.7.a)
IMES = 4: dimensionless

DTMAX - Maximum time step size, Δt_{max}.
Units: days

DTMIN - Minimum time step size, Δt_{min}.
Units: days

Note: See note for input line 3.6.12.

3.6.24 DT, (DCLIM(KC), for KC = 1, N), CNMAX, CNMIN (This line is read only if IMES = 3 or 4, ITIME = 1, and reservoir is not shut-in.)

DT - Initial time step size, Δt_i.
Units: days

DCLIM(KC) - Tolerance for concentration change, $\Delta C_{lim,\kappa}$, of KCth component (IMES = 3) or relative tolerance for concentration change, $R_{lim,\kappa}$, 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 3.6.7.a)

IMES = 4: dimensionless

CNMAX - Maximum Courant number.
Units: dimensionless

CNMIN - Minimum Courant number.
Units: dimensionless

Note: See note for input lines 3.6.11 and 3.6.12 for time step calculation information.

4.0 NOMENCLATURE

The nomenclature consists of the names of the variables as they appear in equations in this text (and related reports) and descriptions of those variables. FORTRAN names of the variables as they appear in the UTCHEM simulator appear in parenthesis where applicable.

a_T = Adsorbed tracer amount per unit mass of rock.

a_3 = Surfactant adsorption parameter

a_{31} = Surfactant adsorption parameter (AD31)

a_{32} = Surfactant adsorption parameter (AD32)

a_{31} = Surfactant adsorption parameter (AD31)

a_4 = Polymer adsorption parameter

a_{42} = Polymer adsorption parameter (AD42)

a_κ = Adsorption parameter for κ^{th} component (A14D, A15D)

A_{p1} = Polymer viscosity parameter (AP1)

A_{p2} = Polymer viscosity parameter (AP2)

A_{p3} = Polymer viscosity parameter (AP3)

A_{15} = Permeability reduction parameter for Langmuir correlation with gel concentration (AGK)

B_{15} = Permeability reduction parameter for Langmuir correlation with gel concentration (BGK)

b_3 = Surfactant adsorption parameter (B3D)

b_4 = Polymer adsorption parameter (B4D)

b_κ = Adsorption parameter for κ^{th} component (B14D, B15D)

c_{pc} = Capillary pressure parameter (CPC)

C = Shear rate coefficient

$C_{i,\kappa}$ = Total concentration of component κ in grid block i

$\Delta C_{i,\kappa}$ = Change in total concentration of component κ in grid block i over the current time-step

$\Delta C_{lim,\kappa}$ = Tolerance for concentration change of component κ

C_o = Initial condition for tracer used in radioactive decay equation

C_{SE} = Effective salinity for phase behavior and surfactant adsorption

C_{SEL} = Type II(–)/III phase boundary or effective salinity limit (CSEL7 for Alcohol 1—Component 7 and CSEL8 for Alcohol 2—Component 8)

C_{SEP} = Effective salinity (ion strength) for polymer properties

C_{SEU} = Type III/II(+) phase boundary or effective salinity limit (CSEU7 for Alcohol 2—Component 7 and CSEU8 for Alcohol 2—Component 8)

C_{T1} = Concentration of tracer in phase 1

C_6^o = Concentration of free calcium cations

C_9^o = Concentration of free sodium cations

C_δ = Permeability reduction parameter for gel (CRG)

C_κ = Overall concentration of component κ in the mobile phases

$\overline{C}_\kappa$ = Adsorbed concentration of component κ

$C_{\kappa o}$ = Concentration of tracer component κ in oil

$C_{\kappa w}$ = Concentration of tracer component κ in water

$\tilde{C}_\kappa$ = Overall concentration of component κ in the mobile and stationary phases

$C_{\kappa\ell}$ = Concentration of component κ in phase ℓ

CNMAX = Maximum Courant number

CNMIN = Minimum Courant number

D_S = Retardation factor for tracer (RET)

e_ℓ = Relative permeability exponent for phase ℓ

$e_{\ell c}$ = Relative permeability exponent for phase ℓ at low interfacial tension (E13C, E23C, and E31C)

$e_{\ell w}$ = Relative permeability exponent for phase ℓ at high interfacial tension (E1W, E2W, and E3W)

f_κ^s = Amount of component κ associated with surfactant

k = Permeability at 100% brine saturation

k_a = Apparent permeability used in capillary pressure calculations

$k_{r\ell}$ = Relative permeability of phase ℓ

$k_{r\ell}^o$ = End point relative permeability of phase ℓ

$k_{r\ell c}^o$ = End point relative permeability of phase ℓ at low interfacial tension (P1RC for phase 1, P2RC for phase 2, and P3RC for phase 3)

$k_{r\ell w}^o$ = End point relative permeability of phase ℓ at high interfacial tension (P1RW for phase 1, P2RW for phase 2, and P3RW for phase 3)

k_x = Absolute permeability in the x-direction (PERMX)

k_y = Absolute permeability in the y-direction (PERMY)

k_z = Absolute permeability in the z-direction (PERMZ)

K_κ = Tracer κ partition coefficient (TK)

L = Length of the core, or reservoir length

$M_{Cr^{3+}}$ = Molecular weight of chromium component

$M_{polymer}$ = Molecular weight of polymer component

n = Cr^{3+}/polymer mass stoichiometric ratio

n_{pc} = Capillary pressure exponent (EPC)

$N_{c\ell}$ = Capillary number of phase ℓ

N_v = Viscosity number

N_δ = Dimensionless number representing the reduction of the pore radius due to adsorption of gel

$P_{C\ell\ell'}$ = Capillary pressure between phases ℓ and ℓ'

P_α = Exponent for calculating shear rate dependence of polymer viscosity (POWN)

Q_i = Maximum injection/production flow rate inwell block i

Q_v = Cation exchange capacity of clay (QV)

R_k = Permeability reduction factor

RRF = Residual resistance factor for gel

RRF_{max} = Maximum residual resistance factor for gel

$S_{n\ell}$ = Normalized mobile saturation of phase ℓ used in relative permeability and capillary pressure calculations

S_p = Exponent for calculating salinity dependence of polymer viscosity (SSLOPE)

S_ℓ = Saturation of phase ℓ

$S_{\ell r}$ = Residual saturation of phase ℓ

$S_{\ell' rc}$ = Residual saturation of phase ℓ' at low interfacial tension (S1RWC, S2RWC, and S3RWC for phases 1, 2 and 3)

$S_{\ell' rw}$ = Residual saturation of phase ℓ' at high interfacial tension (S1RW, S2RW, and S3RW for phases 1, 2 and 3)

SCR = Stoichiometric ratio between Cr^{3+} and polymer

t = A time variable in the radioactive decay of tracer equation

Δt_i = Initial time-step size (DT)

Δt_{max} = Maximum time-step size (DTMAX)

Δt_{min} = Minimum time-step size (DTMIN)

Δt^n = Time-step size at n^{th} time level

Δt^{n+1} = Time-step size at $n+1^{th}$ time level

t_o = An initial time at which the tracer concentration C_o is known; used in the radioactive decay equation

T_1 = Capillary desaturation parameter for aqueous phase (T11)

T_2 = Capillary desaturation parameter for oleic phase (T22)

T_3 = Capillary desaturation parameter for microemulsion phase (T33)

T_4 = Capillary desaturation parameter for gas phase (T44)

u = Flux

V_t = Tracer velocity

Δx_i = Size of grid block i in x direction

x_4 = Exponent used in gelation reaction

x_{14} = Exponent used in gelation reaction

x_{16} = Exponent used in gelation reaction

Δy_i = Size of grid block i in y direction

Δz_i = Size of grid block i in z direction

Greek Symbols

α_1 = Compositional microemulsion phase viscosity parameter (ALPHA1)

α_2 = Compositional microemulsion phase viscosity parameter (ALPHA2)

α_3 = Compositional microemulsion phase viscosity parameter (ALPHA3)

α_4 = Compositional microemulsion phase viscosity parameter (ALPHA4)

α_5 = Compositional microemulsion phase viscosity parameter (ALPHA5)

β^C = Cation exchange constant for clay (XKC)

β_P = Effective salinity parameter for polymer viscosity (BETAP)

β^S = Cation exchange constant for surfactant (XKS)

β_6 = Effective salinity parameter for calcium—Component 6 (BETA6)

β_7 = Effective salinity parameter for Alcohol 1—Component 7 (BETA7)

β_8 = Effective salinity parameter for Alcohol 2—Component 8 (BETA8)

$\dot{\gamma}_{eq}$ = Equivalent shear rate for porous medium

$\dot{\gamma}_c$ = Coefficient in equivalent shear rate equation (GAMMAC)

$\dot{\gamma}_{1/2}$ = Shear rate at which polymer viscosity is one-half the polymer viscosity at zero shear rate (GAMHF)

γ_1 = Specific weight of brine—Component 1 (DEN1)

γ_2 = Specific weight of oil—Component 2 (DEN2)

γ_3 = Specific weight of surfactant—Component 3 (DEN3)

γ_7 = Specific weight of Alcohol 1—Component 7 (DEN7)

γ_8 = Specific weight of Alcohol 2 or gas—Component 8 (DEN8)

λ_κ = Radioactive decay coefficient for κ^{th} tracer (RDC)

$[\mu]$ = Intrinsic viscosity of a gel solution

μ_o = Polymer viscosity at zero shear rate

μ_p = Polymer viscosity

μ_w = Water viscosity

μ_ℓ = Viscosity of phase ℓ (VIS1 for phase 1, VIS2 for phase 2, and VIS4 for phase 4)

$\mu_{4,ref}$ = Viscosity of gas phase at reference pressure

$\mu_{4,s}$ = Slope of gas viscosity function

μ_∞ = Viscosity at infinite shear rate

ρ_g = Rock density

ρ_s = Solution density

ρ_ℓ = Density of phase ℓ

σ_{wo} = Interfacial tension between oil and water

$\sigma_{\ell\ell'}$ = Interfacial tension between phases ℓ and ℓ'

ϕ = Porosity (POR)

ϕ_i = Porosity of gridblock i

Φ = Potential

Θo = Relaxation time coefficient

Subscripts

κ = Component number

For all values of IREACT:
1 = Water
2 = Oil
3 = Surfactant
4 = Polymer
5 = Chloride
6 = Calcium
7 = Alcohol 1
8 = Alcohol 2 or Gas
9 = Tracer 1
10 = Tracer 2
11 = Tracer 3

For IREACT = 0:
12 = Tracer 4
13 = Tracer 5
.
.
.
20 = Tracer 12
21 = Tracer 13

For IREACT = 1:
12 = Sodium dichromate ($Na_2Cr_2O_7$)
13 = Thiourea (CSN_2H_4)
14 = Trivalent chromium (Cr^{3+})
15 = Gel
16 = Hydrogen

For IREACT = 2, 3, 4, 5, or 6:

12 = Sodium
13 = Hydrogen
14 = Magnesium
15 = Carbonate

For IREACT = 3:

16 = Acid component of crude oil

For IREACT = 4, 5, or 6:

16 = Aluminum
17 = Silica

For IREACT = 5:

18 = Acid component of crude oil

For IREACT = 6

18 = Sodium dichromate ($Na_2Cr_2O_7$)
19 = Thiourea (CSN_2H_4)
20 = Trivalent chromium (Cr^{3+})
21 = Gel

ℓ = Phase number

1 = Aqueous
2 = Oleic
3 = Microemulsion
4 = Gas

r = Residual

w = Low capillary number values

c = High capillary number values

5.0 SAMPLE INPUT FILE

The following material is a sample input file for UTCHEM-5.32m. Each input section (except for 3.5 — see the note at the beginning of section 3.5) is set apart by a header and each data line has three comment lines containing information about the input variables including: the user's manual input line number, a brief comment, and the FORTRAN variable names used in the FORTRAN source code. We strongly recommend that the user take the time to update the comment lines when modifying the input file in order to reduce confusion when running the simulator.

```
CC*******************************************************************
CC                                                                  *
CC     BRIEF DESCRIPTION OF DATA SET : UTCHEM (VERSION 5.32m)       *
CC                                                                  *
CC*******************************************************************
CC                                                                  *
CC  SURFACTANT/POLYMER FLOOD TEST (EX01), 11X11X2                   *
CC                                                                  *
CC  LENGTH (FT) : 250               PROCESS : SURFACTANT/POLYMER    *
CC  THICKNESS (FT) : 10             INJ. RATE (FT3/DAY) : 112.3     *
CC  WIDTH (FT) : 250                COORDINATES : CARTISIAN         *
CC  POROSITY : 0.20                                                 *
CC  GRID BLOCKS : 11X11X2                                           *
CC  DATE : 2/16/95                                                  *
CC                                                                  *
CC*******************************************************************
CC
CC*******************************************************************
CC                                                                  *
CC    RESERVOIR DESCRIPTION                                         *
CC                                                                  *
CC*******************************************************************
CC
CC
*----RUNNO
ex01 surfactant/polymer flood
CC
CC
*----HEADER
ex01
TESTING  UTCHEM VERSION 5.32  ON  3/27/95 (DEC 3000/500)
SURFACTANT/POLYMER, SALINITY GRADIENT RUN (.4 -> .3 -> .1).
CC
CC SIMULATION FLAGS
*---- IMODE IMES IDISPC ICWM ICAP IREACT ICOORD ITREAC ITC IGAS IENG
        1    2    3      0    0     0      1     0     0    0   0
CC
CC NO. OF GRIDBLOCKS,FLAG SPECIFIES CONSTANT OR VARIABLE GRID SIZE, UNIT
*----NX   NY  NZ  IDXYZ   IUNIT
     11   11  2,  0        0
CC
CC  CONSTANT GRID BLOCK SIZE IN X, Y, AND Z
*----DX1      DY1       DZ1
     22.727   22.727  5.0
```

```
CC
CC TOTAL NO. OF COMPONENTS, NO. OF TRACERS, NO. OF GEL COMPONENTS
*----N   NTW NTA  NG
   11   3   0   0
CC
CC  IF THERE IS TRACER, NAME OF THE TRACERS
*---- TRNAME(IT) FOR IT=1,NT
TRACER 1
TRACER 2
TRACER 3
CC
CC FLAG INDICATING IF THE COMPONENT IS INCLUDED IN CALCULATIONS OR NOT
*----ICF(KC) FOR KC=1,N
    1  1  1  1  1  1  1  0  1  1  1
CC
CC*******************************************************************
CC                                                                  *
CC    OUTPUT OPTIONS                                                *
CC                                                                  *
CC*******************************************************************
CC
CC
CC FLAG TO WRITE TO UNIT 3,FLAG FOR PV OR DAYS TO PRINT OR TO STOP THE RUN
*----ICOPSM ICUMTM  ISTOP
    0      0         0
CC
CC FLAG INDICATING IF THE PROFILE OF KCTH COMPONENT SHOULD BE WRITTEN
*----IPRFLG(KC),KC=1,N
    0  0  0  0  0  0  0  0  0  0  0
CC
CC FLAG FOR PRES,SAT.,TOTAL CONC.,TRACER CONC.,CAP.,GEL, ALKALINE PROFILES
*----IPPRES IPSAT IPCTOT IPTRAC IPCAP IPGEL IPALK IPTEMP IPOBS
     1      1      1      1      0     0     0     0      0
CC
CC FLAG FOR WRITING SEVERAL PROPERTIES TO UNIT 4 (PROFIL)
*----IPHP IADS ICKL IVEL IVIS IPER ICNM IRKF IPHSE ICSE
     0     0    0    0    0    0    0    0    0     0
CC
CC*******************************************************************
CC                                                                  *
CC    RESERVOIR PROPERTIES                                          *
CC                                                                  *
CC*******************************************************************
CC
CC
CC MAX. SIMULATION TIME ( DAYS)
*---- TMAX
     1500
CC
CC ROCK COMPRESSIBILITY (1/PSI), STAND. PRESSURE(PSIA)
*----COMPR   PSTAND
     0.      0.
CC
CC FLAGS INDICATING CONSTANT OR VARIABLE POROSITY, X,Y,AND Z PERMEABILITY
*----IPOR1 IPERMX IPERMY IPERMZ
      0      1     1      0
CC
CC CONSTANT POROSITY
*----PORC1
    .20
CC
CC CONSTANT X-PERMEABILITY (MILIDARCY) FOR LAYER K = 1,NZ
*----PERMX(1)  PERMX(2)
    500.      100.
```

```
CC
CC CONSTANT Y-PERMEABILITY (MILIDARCY) FOR LAYER K = 1,NZ
*----PERMY(1)  PERMY(2)
     500.       100.
CC
CC CONSTANT Z-PERMEABILITY
*----PERMZC (MILIDARCY)
     50.
CC
CC FLAG FOR CONSTANT OR VARIABLE DEPTH, PRESSURE, WATER SATURATION
*----IDEPTH  IPRESS  ISWI
      0        0       0
CC
CC CONSTANT DEPTH (FT)
*----D111
      0.
CC
CC CONSTANT PRESSURE (PSIA)
*----PRESS1
     1.
CC
CC CONSTANT INITIAL WATER SATURATION
*----SWI
     .65
CC
CC CONSTANT CHLORIDE AND CALCIUM CONCENTRATIONS (MEQ/ML)
*----C50       C60
    0.4       .003
CC
CC*********************************************************************
CC                                                                    *
CC    PHYSICAL PROPERTY DATA                                          *
CC                                                                    *
CC*********************************************************************
CC
CC
CC OIL CONC. AT PLAIT POINT FOR TYPE II(+) AND TYPE II(-), CMC
*---- C2PLC   C2PRC  EPSME
      0.       1.      .0001
CC SLOPE AND INTERCEPT OF BINODAL CURVE AT ZERO, OPT., AND 2XOPT SALINITY
CC FOR ALCOHOL 1
*----HBNS70 HBNC70 HBNS71 HBNC71 HBNS72 HBNC72
     0.131   .1     .191   .026   .363   .028
CC SLOPE AND INTERCEPT OF BINODAL CURVE AT ZERO, OPT., AND 2XOPT SALINITY
CC FOR ALCOHOL 2
*----HBNS80 HBNC80 HBNS81 HBNC81 HBNS82 HBNC82
     0.      0.     0.     0.     0.     0.
CC
CC LOWER AND UPPER EFFECTIVE SALINITY FOR ALCOHOL 1 AND ALCOHOL 2
*----CSEL7  CSEU7  CSEL8  CSEU8
     .177   .344   0.     0.
CC
CC THE CSE SLOPE PARAMETER FOR CALCIUM AND ALCOHOL 1 AND ALCOHOL 2
*----BETA6  BETA7  BETA8
     .8     -2.    0.
CC
CC FLAG FOR ALCOHOL PART. MODEL AND PARTITION COEFFICIENTS
*----IALC  OPSK7O  OPSK7S  OPSK8O  OPSK8S
     1     0.      0.      0.      0.
CC
CC NO. OF ITERATIONS, AND TOLERANCE
*----NALMAX   EPSALC
     20       .0001
CC
```

```
CC ALCOHOL 1 PARTITIONING PARAMETERS IF IALC=1
*----AKWC7   AKWS7  AKM7  AK7     PT7
     4.671   1.79   48.   35.31   .222
CC
CC ALCOHOL 2 PARTITIONING PARAMETERS IF IALC=1
*----AKWC8   AKWS8  AKM8  AK8     PT8
     0.      0.     0.    0.      0.
CC
CC
*---- IFT MODEL FLAG
      0
CC
CC INTERFACIAL TENSION PARAMETERS
*----G11  G12     G13   G21   G22    G23
     13.  -14.8   .007  13.   -14.5  .010
CC
CC LOG10 OF OIL/WATER INTERFACIAL TENSION
*----XIFTW
     1.3
CC
CC MASS TRANSFER FLAG
*----IMASS
     0
CC
CC CAPILLARY DESATURATION PARAMETERS FOR PHASE 1, 2, AND 3
*----ITRAP   T11        T22        T33
     1       1865.      59074      364.2
CC
CC RELATIVE PERM. FLAG (0:IMBIBITION COREY,1:FIRST DRAINAGE COREY)
*----IPERM
     0
CC
CC FLAG FOR CONSTANT OR VARIABLE REL. PERM. PARAMETERS
*----ISRW  IPRW  IEW
     0     0     0
CC
CC CONSTANT RES. SATURATION OF PHASES 1,2,AND 3 AT LOW CAPILLARY NO.
*----S1RWC  S2RWC  S3RWC
     .37    .35    .37
CC
CC CONSTANT ENDPOINT REL. PERM. OF PHASES 1,2,AND 3 AT LOW CAPILLARY NO.
*----P1RW  P2RW  P3RW
     .11   .95   .11
CC
CC CONSTANT REL. PERM. EXPONENT OF PHASES 1,2,AND 3 AT LOW CAPILLARY NO.
*----E1W  E2W  E3W
     1.   2.16  1.
CC
CC  RES. SATURATION OF PHASES 1,2,AND 3 AT HIGH CAPILLARY NO.
*----S1RC  S2RC  S3RC
     .0    .0    .0
CC
CC ENDPOINT REL. PERM. OF PHASES 1,2,AND 3 AT HIGH CAPILLARY NO.
*----P1RC  P2RC  P3RC
     1.    1.    1.
CC
CC REL. PERM. EXPONENT OF PHASES 1,2,AND 3 AT HIGH CAPILLARY NO.
*----E13C  E23C  E31C
     1.     2.16   1.
CC
CC WATER AND OIL VISCOSITY , RESERVOIR TEMPERATURE
*----VIS1   VIS2  TEMPV
     0.86   4.    0.
CC
```

```
CC VISCOSITY PARAMETERS
*----ALPHA1 ALPHA2  ALPHA3  ALPHA4  ALPHA5
     4.     5.      -30.    .9      .7
CC
CC PARAMETERS TO CALCULATE POLYMER VISCOSITY AT ZERO SHEAR RATE
*----AP1     AP2     AP3
     81.     2700.   2500.
CC
CC PARAMETER TO COMPUTE CSEP,MIN. CSEP, AND SLOPE OF LOG VIS. VS. LOG CSEP
*----BETAP CSE1  SSLOPE
     10.    .01   .17
CC
CC PARAMETER FOR SHEAR RATE DEPENDENCE OF POLYMER VISCOSITY
*----GAMMAC  GAMHF  POWN
     20.      10.    1.8
CC
CC FLAG FOR POLYMER PARTITIONING, PERM. REDUCTION PARAMETERS
*----IPOLYM EPHI3 EPHI4 BRK    CRK
     1      1.    0.8    1000.  0.0186
CC
CC SPECIFIC WEIGHT FOR COMPONENTS 1,2,3,7,AND 8 , AND GRAVITY FLAG
*----DEN1  DEN2  DEN3 DEN7 DEN8 IDEN
     .433  .368  .42  .346  0.  2
CC
CC  FLAG FOR CHOICE OF UNITS ( 0:BOTTOMHOLE CONDITION , 1: STOCK TANK)
*-----ISTB
      0
CC
CC COMPRESSIBILITY FOR VOL. OCCUPYING COMPONENTS 1,2,3,7,AND 8
*----COMPC(1)  COMPC(2)  COMPC(3)  COMPC(7)  COMPC(8)
     0.        0.        0.        0.        0.
CC
CC CONSTANT OR VARIABLE PC PARAM., WATER-WET OR OIL-WET PC CURVE FLAG
*----ICPC   IEPC  IOW
     0      0     0
CC
CC CAPILLARY PRESSURE PARAMETER, CPC0
*----CPC0
     9.
CC
CC CAPILLARY PRESSURE PARAMETER, EPC0
*---- EPC0
      2.
CC
CC MOLECULAR DIFFUSION COEF. KCTH COMPONENT IN PHASE 1 (D(KC),KC=1,N)
*----D(1) D(2) D(3) D(4) D(5) D(6) D(7) D(8) D(9) D(10) D(11)
     0.   0.   0.   0.   0.   0.   0.   0.   0.   0.    0.
CC
CC MOLECULAR DIFFUSION COEF. OF KCTH COMPONENT IN PHASE 2 (D(KC),KC=1,N)
*----D(1) D(2) D(3) D(4) D(5) D(6) D(7) D(8) D(9)  D(10)  D(11)
     0.   0.   0.   0.   0.   0.   0.   0.   0.    0.     0.
CC
CC MOLECULAR DIFFUSION COEF. OF KCTH COMPONENT IN PHASE 3 (D(KC),KC=1,N)
*----D(1) D(2) D(3) D(4) D(5) D(6) D(7) D(8) D(9) D(10)  D(11)
     0.   0.   0.   0.   0.   0.   0.   0.   0.   0.     0.
CC
CC LONGITUDINAL AND TRANSVERSE DISPERSIVITY OF PHASE 1
*----ALPHAL(1)     ALPHAT(1)
     12.          .4
CC
CC LONGITUDINAL AND TRANSVERSE DISPERSIVITY OF PHASE 2
*----ALPHAL(2)     ALPHAT(2)
     12.           .4
CC
```

```
CC LONGITUDINAL AND TRANSVERSE DISPERSIVITY OF PHASE 3
*----ALPHAL(3)     ALPHAT(3)
     12.           .4
CC
CC SURFACTANT AND POLYMER ADSORPTION PARAMETERS
*----AD31  AD32  B3D    AD41   AD42  B4D
     1.5    .5    1000.  0.7    0.    100.
CC
CC PARAMETERS FOR CATION EXCHANGE OF CLAY AND SURFACTANT
*----QV     XKC   XKS  EQW
     0.044  .25   .2   419.
CC
CC TRACER PARTITIONING COEFFICIENT (TK(IT),IT=1,NT)
*---- TK(1)  TK(2)  TK(3)
      .0     1.     0.
CC
CC SALINITY DEPENDENCE PART. COEFF.
*---- TKS(1)  TKS(2)  TKS(3)
      0.      0.      0.
CC
CC RADIACTIVE DECAY COEFFICIENT (RDC(IT),IT=1,NT)
*---- RDC(1)  RDC(2)   RDC(3)
      .0    > .0       .0
CC
CC TRACER RETARDATION COEFFICIENT (RET(IT),IT=1,NT)
*---- RET(1)   RET(2)  RET(3)
      .0       0.      0.
CC
CC******************************************************************
CC                                                                 *
CC    WELL DATA                                                    *
CC                                                                 *
CC******************************************************************
CC
CC
CC FLAG FOR RIGHT AND LEFT BOUNDARY
*---- IBOUND
      0
CC
CC TOTAL NUMBER OF WELLS, WELL RADIUS FLAG, FLAG FOR TIME OR COURANT NO.
*----NWELL   IRO   ITIME
      2      2      0
CC
CC WELL ID,LOCATIONS,AND FLAG FOR SPECIFYING WELL TYPE, WELL RADIUS, SKIN
*----IDW    IW    JW     IFLAG    RW     SWELL  IDIR    IFIRST  ILAST  IPRF
      1     1     1      1        .5     0.      3      1        2     0
CC
CC WELL NAME
*---- WELNAM
INJECTOR
CC
CC ICHEK, MAX. AND MIN. ALLOWABLE BOTTOMHOLE PRESSURE AND RATE
*----ICHEK PWFMIN   PWFMAX  QTMIN   QTMAX
      2     0.0      5000.   0.0     1000.
CC
CC WELL ID, LOCATION, AND FLAG FOR SPECIFYING WELL TYPE, WELL RADIUS, SKIN
*----IDW   IW    JW    IFLAG    RW     SWELL  IDIR  IFIRST   ILAST    IPRF
     2     11    11    2        .5      0.     3     1         2        0
CC
CC WELL NAME
*---- WELNAM
PRODUCER
CC
CC ICHEK , MAX. AND MIN. ALLOWABLE BOTTOMHOLE PRESSURE AND RATE
```

```
*----ICHEK PWFMIN   PWFMAX  QTMIN   QTMAX
      2    0.0     5000.   0.0     50000.
CC
CC ID,INJ. RATE AND INJ. COMP. FOR RATE CONS. WELLS FOR EACH PHASE (L=1,3)
*----ID  QI(M,L)  C(M,KC,L)
     1    112.3     .94  0.  0.03  .05  0.3  0.001  0.03  0.  1. 1.  1.
     1     0.        0.   0.  0.    0.   0.   0.     0.     0.  0. 0.  0.
     1     0.        0.   0.  0.    0.   0.   0.     0.     0.  0. 0.  0.
CC
CC ID, BOTTOM HOLE PRESSURE FOR PRESSURE CONSTRAINT WELL (IFLAG=2 OR 3)
*----ID   PWF
     2    1.
CC
CC CUM. INJ. TIME , AND INTERVALS (PV OR DAY) FOR WRITING TO OUTPUT FILES
*----TINJ    CUMPR1   CUMHI1   CUMHI2   WRHPV   WRPRF      RSTC
     111.3   0.09     0.09      0.09    0.005  0.09      0.25
CC
CC FOR IMES=2 ,THE INI. TIME STEP,CONC. TOLERANCE,MAX.,MIN. TIME STEPS
*----DT      DCLIM   DTMAX   DTMIN
     0.05    0.003   0.5     0.05
CC
CC IRO, ITIME, NEW FLAGS FOR ALL THE WELLS
*---- IRO ITIME IFLAG
       2   0     1  2
CC
CC NUMBER OF WELLS CHANGES IN LOCATION OR SKIN OR PWF
*----NWEL1
      0
CC
CC NUMBER OF WELLS WITH RATE CHANGES, ID
*----NWEL1    ID
     1        1
CC
CC ID,INJ. RATE AND INJ. COMP. FOR RATE CONS. WELLS FOR EACH PHASE (L=1,3)
*----ID  QI(M,L)  C(M,KC,L)
     1    112.3     1.  0.  0.  0.05  0.1  0.001  0.  0.  0. 0. 0.
     1    0.        0.  0.  0.  0.    0.   0.     0.  0.  0. 0. 0.
     1    0.        0.  0.  0.  0.    0.   0.     0.  0.  0. 0. 0.
CC
CC CUM. INJ. TIME , AND INTERVALS (PV) FOR WRITING TO OUTPUT FILES
*----TINJ    CUMPR1  CUMHI1  CUMHI2   WRHPV     WRPRF   RSTC
     3300    0.25      0.25    0.25      0.005    .5     0.75
CC
CC FOR IMES=2 ,THE INI. TIME STEP,CONC. TOLERANCE,MAX.,MIN. TIME STEPS
*----DT      DCLIM   DTMAX   DTMIN
     0.05    0.003   0.5     0.05
```

6.0 APPENDIX

The following sections describe: (1) data that is automatically written to the profile data file, (2) restart run procedure, (3) data written to stored restart data file, (4) data written to history files for each well, (5) data written to history of reservoir properties and overall injection and production rates from all the wells, (6) data written to aqueous phase tracer concentration data files, (7) list of elements and reactions for IREACT=2, (8) list of elements and reactions for IREACT=3, (9) list of elements and reactions for IREACT=4 or 6, (10) list of elements and reactions for IREACT=5, and (11) main program flow outline.

6.1 Default Data Written to Profile Data File

The information in the following lists is always written to the profile data file (PROFIL) and is not controlled by the various print control flags in the input files.

Printed 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 at each CUMPR1 interval:

- Reservoir temperature if IENG = 1
- Phase saturation profile for each phase
- Aqueous phase pressure profile

Concentration of each component in the fluid
If tracers are present and ICAP≠0:
    Flowing concentration
    Dendiritic concentration
    Flowing saturation
    Dendiritic saturation

6.2 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 line 3.1.3 of input 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 3.5.8 of file INPUT if appropriate

5.- Add additional information for input lines 3.5.14 through 3.5.24 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).

6.3 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:

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 (CUMQ) 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)
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)
Variables for writing profiles to UNIT 4 (CUMPRO), histories to UNIT 4 (CUMHIS), histories to UNIT 3 (CUMHCP)
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 ICAP>0:
    Dendiritic concentration (CD), dendiritic 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)

6.4 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-HISTℓ) for each production well.

Printed at each WRHPV interval:

Cumulative pore volume, time in days, cumulative production (ft^3, m^3, or STB), water oil ratio, cumulative oil recovery, total production rate (ft^3/day, m^3/day, or STB/day)
Water cut, oil cut, microemulsion cut, gas cut (only if IGAS = 1)
Wellbore pressure for each well block (psi or kPa)
Wellbore temperature (°F or °C) (only if IENG=1)
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))
Lower effective salinity, upper effective salinity, effective salinity (only if ICSE = 1)
For IREACT >1
    Independent species concentration, mole/liter of water (CAQSP(KK), KK = 1, NIAQ)
    Dependent species concentration, mole/liter of water (CAQSP(KK), KK = NIAQ+1,NFLD) (only if IRSPS>0)
    Phase Concentration of (inj.+genereated) surfactant (PSURF(I,L), L = 1,3), total concentration of (inj.+ generated) surfactant (TSURF) (only if IREACT = 3 or 5)
    Concentration of solid components, mole/liter of pore volume (CSLDT(KK), KK = 1, NSLD) (only if NSLD>0)
    Log_{10} of interfacial tension between water/microemulsion and oil/microemulsion (XIFT1, XIFT2) (only if ICNM>0) (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 (ft^3, m^3, or STB), injection rate (ft^3/day, m^3/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 line 3.4.93) (psi or kPa)

6.5 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 m^3), volumetric averaged reservoir temperature (°F or °C) (only if IENG=1)

Total injection rate (B/D or m^3/day), total production rate (B/D or m^3/day), total fluid injected (1000 bbls or m^3), total fluid produced (1000 bbls or m^3)

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 m^3/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 m^3), Cumulative surfactant produced (bbls or m^3), adsorbed surfactant (bbls or m^3), retained surfactant (bbls or m^3)

If ICF(4) = 1: Cumulative polymer injected (wt%), Cumulative polymer produced (wt%), adsorbed polymer (wt%), retained polymer (wt%)

6.6 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
Aqueous phase tracer concentration at NOBS observation locations

6.7 List of Elements and Reactive Species for IREACT = 2

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Chlorine, Oxygen, S (inj. surfactant)
Independent aqueous or oleic species:	H^+, Na^+, Ca^{2+}, Mg^{2+}, CO_3^{2-}, Cl^-, S^-, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^+$, $Mg(OH)^+$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, OH^-, HCO_3^-, H_2CO_3, $CaCO_3^o$, $MgCO_3^o$
Solid species:	$CaCO_3$ (Calcite), $Ca(OH)_2$ (Calcium hydroxide), $MgCO_3$ (Magnesite), $Mg(OH)_2$ (Magnesium hydroxide)
Adsorbed cations:	$\overline{H}^+$, $\overline{Na}^+$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^+$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftarrows} H^+ + OH^-$	$K_1^{eq} = [H^+]\,[OH^-]$
$H^+ + CO_3^{2-} \overset{K_2^{eq}}{\rightleftarrows} HCO_3^-$	$K_2^{eq} = \dfrac{[HCO_3^-]}{[H^+]\,[CO_3^{2-}]}$
$Ca^{2+} + H_2O \overset{K_3^{eq}}{\rightleftarrows} Ca(OH)^+ + H^+$	$K_3^{eq} = \dfrac{[Ca(OH)^+]\,[H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_4^{eq}}{\rightleftarrows} Mg(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Mg(OH)^+]\,[H^+]}{[Mg^{2+}]}$
$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_5^{eq}}{\rightleftarrows} Ca(HCO_3)^+$	$K_5^{eq} = \dfrac{[Ca(HCO_3)^+]}{[Ca^{2+}]\,[CO_3^{2-}]\,[H^+]}$

$$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_6^{eq}}{\rightleftarrows} Mg(HCO_3)^+$$

$$K_6^{eq} = \frac{\left[Mg(HCO_3)^+\right]}{\left[Mg^{2+}\right]\left[CO_3^{2-}\right]\left[H^+\right]}$$

$$2H^+ + CO_3^{2-} \overset{K_7^{eq}}{\rightleftarrows} H_2CO_3$$

$$K_7^{eq} = \frac{\left[H_2CO_3\right]}{\left[CO_3^{2-}\right]\left[H^+\right]^2}$$

$$Ca^{2+} + CO_3^{2-} \overset{K_8^{eq}}{\rightleftarrows} CaCO_3^o$$

$$K_8^{eq} = \frac{\left[CaCO_3^o\right]}{\left[Ca^{2+}\right]\left[CO_3^{2-}\right]}$$

$$Mg^{2+} + CO_3^{2-} \overset{K_9^{eq}}{\rightleftarrows} MgCO_3^o$$

$$K_9^{eq} = \frac{\left[MgCO_3^o\right]}{\left[Mg^{2+}\right]\left[CO_3^{2-}\right]}$$

Dissolution reactions	Solubility product
$CaCO_3 \overset{K_1^{sp}}{\rightleftarrows} Ca^{2+} + CO_3^{2-}$	$K_1^{sp} = \left[Ca^{2+}\right]\left[CO_3^{2-}\right]$
$MgCO_3 \overset{K_2^{sp}}{\rightleftarrows} Mg^{2+} + CO_3^{2-}$	$K_2^{sp} = \left[Mg^{2+}\right]\left[CO_3^{2-}\right]$
$Ca(OH)_2 \overset{K_3^{sp}}{\rightleftarrows} Ca^{2+} + 2OH^-$	$K_3^{sp} = \left[Ca^{2+}\right]\left[H^+\right]^{-2}$
$Mg(OH)_2 \overset{K_4^{sp}}{\rightleftarrows} Mg^{2+} + 2OH^-$	$K_4^{sp} = \left[Mg^{2+}\right]\left[H^+\right]^{-2}$

Exchange reactions (on clay)	Exchange equilibrium constant
$2\overline{Na}^+ + Ca^{2+} \overset{K_1^{ex}}{\rightleftarrows} 2Na^+ + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{\left[\overline{Ca}^{2+}\right]\left[Na^+\right]^2}{\left[Ca^{2+}\right]\left[\overline{Na}^+\right]^2}$
$2\overline{Na}^+ + Mg^{2+} \overset{K_2^{ex}}{\rightleftarrows} 2Na^+ + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{\left[\overline{Mg}^{2+}\right]\left[Na^+\right]^2}{\left[Mg^{2+}\right]\left[\overline{Na}^+\right]^2}$

$$\bar{H}^+ + Na^+ + OH^- \overset{K_3^{ex}}{\rightleftarrows} \overline{Na}^+ + H_2O$$

$$K_3^{ex} = \frac{[Na^+]\left[\bar{H}^+\right]}{\left[\overline{Na}^+\right][H^+]}$$

Exchange reactions (on micelle)

Exchange equilibrium constant

$$2\overline{\overline{Na}}^+ + Ca^{2+} \overset{K_1^{exm}}{\rightleftarrows} 2Na^+ + \overline{\overline{Ca}}^{2+}$$

$$K_1^{exm} = \frac{\left[\overline{\overline{Ca}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Ca^{2+}]}$$

where $K_1^{exm} = \beta_1^{exm}\,[S^-]$

$$2\overline{\overline{Na}}^+ + Mg^{2+} \overset{K_2^{exm}}{\rightleftarrows} 2Na^+ + \overline{\overline{Mg}}^{2+}$$

$$K_2^{exm} = \frac{\left[\overline{\overline{Mg}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Mg^{2+}]}$$

where $K_2^{exm} = \beta_2^{exm}\,[S^-]$

6.8 List of Elements and Reactive Species for IREACT = 3

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, A (from acid HA), Oxygen, Chlorine, S (Injected surfactant)
Independent aqueous or oleic species:	H^+, Na^+, Ca^{2+}, Mg^{2+}, CO_3^{2-}, HA_o, Cl^-, S^-, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^+$, $Mg(OH)^+$, $Ca(HCO_3)^+$, HA_w, $Mg(HCO_3)^+$, OH^-, HCO_3^-, A^-, H_2CO_3, $CaCO_3^o$, $MgCO_3^o$
Solid species:	$CaCO_3$ (Calcite), $Ca(OH)_2$ (Calcium hydroxide), $MgCO_3$ (Magnesite), $Mg(OH)_2$ (Magnesium hydroxide)
Adsorbed cations:	$\overline{H}^+$, $\overline{Na}^+$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^+$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftarrows} H^+ + OH^-$	$K_1^{eq} = [H^+]\,[OH^-]$
$HA_w + OH^- \overset{K_2^{eq}}{\rightleftarrows} A^- + H_2O$	$K_2^{eq} = \dfrac{[A^-]\,[H^+]}{[HA_w]}$
$H^+ + CO_3^{2-} \overset{K_3^{eq}}{\rightleftarrows} HCO_3^-$	$K_3^{eq} = \dfrac{[HCO_3^-]}{[H^+]\,[CO_3^{2-}]}$
$Ca^{2+} + H_2O \overset{K_4^{eq}}{\rightleftarrows} Ca(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Ca(OH)^+]\,[H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_5^{eq}}{\rightleftarrows} Mg(OH)^+ + H^+$	$K_5^{eq} = \dfrac{[Mg(OH)^+]\,[H^+]}{[Mg^{2+}]}$

$$\mathrm{Ca^{2+} + H^+ + CO_3^{2-}} \overset{K_6^{eq}}{\rightleftarrows} \mathrm{Ca(HCO_3)^+} \qquad K_6^{eq} = \frac{\left[\mathrm{Ca(HCO_3)^+}\right]}{\left[\mathrm{Ca^{2+}}\right]\left[\mathrm{CO_3^{2-}}\right]\left[\mathrm{H^+}\right]}$$

$$\mathrm{Mg^{2+} + H^+ + CO_3^{2-}} \overset{K_7^{eq}}{\rightleftarrows} \mathrm{Mg(HCO_3)^+} \qquad K_7^{eq} = \frac{\left[\mathrm{Mg(HCO_3)^+}\right]}{\left[\mathrm{Mg^{2+}}\right]\left[\mathrm{CO_3^{2-}}\right]\left[\mathrm{H^+}\right]}$$

$$\mathrm{2H^+ + CO_3^{2-}} \overset{K_8^{eq}}{\rightleftarrows} \mathrm{H_2CO_3} \qquad K_8^{eq} = \frac{\left[\mathrm{H_2CO_3}\right]}{\left[\mathrm{CO_3^{2-}}\right]\left[\mathrm{H^+}\right]^2}$$

$$\mathrm{Ca^{2+} + CO_3^{2-}} \overset{K_9^{eq}}{\rightleftarrows} \mathrm{CaCO_3^o} \qquad K_9^{eq} = \frac{\left[\mathrm{CaCO_3^o}\right]}{\left[\mathrm{Ca^{2+}}\right]\left[\mathrm{CO_3^{2-}}\right]}$$

$$\mathrm{Mg^{2+} + CO_3^{2-}} \overset{K_{10}^{eq}}{\rightleftarrows} \mathrm{MgCO_3^o} \qquad K_{10}^{eq} = \frac{\left[\mathrm{MgCO_3^o}\right]}{\left[\mathrm{Mg^{2+}}\right]\left[\mathrm{CO_3^{2-}}\right]}$$

Partitioning of HA

Partition coefficient

$$\mathrm{HA_o} \overset{K_D}{\rightleftarrows} \mathrm{HA_w} \qquad K_D = \frac{\left[\mathrm{HA_w}\right]_{water}}{\left[\mathrm{HA_o}\right]_{oil}}$$

Dissolution reactions

Solubility product

$$\mathrm{CaCO_3} \overset{K_1^{sp}}{\rightleftarrows} \mathrm{Ca^{2+} + CO_3^{2-}} \qquad K_1^{sp} = \left[\mathrm{Ca^{2+}}\right]\left[\mathrm{CO_3^{2-}}\right]$$

$$\mathrm{MgCO_3} \overset{K_2^{sp}}{\rightleftarrows} \mathrm{Mg^{2+} + CO_3^{2-}} \qquad K_2^{sp} = \left[\mathrm{Mg^{2+}}\right]\left[\mathrm{CO_3^{2-}}\right]$$

$$\mathrm{Ca(OH)_2} \overset{K_3^{sp}}{\rightleftarrows} \mathrm{Ca^{2+} + 2OH^-} \qquad K_3^{sp} = \left[\mathrm{Ca^{2+}}\right]\left[\mathrm{H^+}\right]^{-2}$$

$$\mathrm{Mg(OH)_2} \overset{K_4^{sp}}{\rightleftarrows} \mathrm{Mg^{2+} + 2OH^-} \qquad K_4^{sp} = \left[\mathrm{Mg^{2+}}\right]\left[\mathrm{H^+}\right]^{-2}$$

Exchange reactions (on matrix)	Exchange equilibrium constant
$2\overline{Na}^+ + Ca^{2+} \overset{K_1^{ex}}{\rightleftarrows} 2Na^+ + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{[\overline{Ca}^{2+}][Na^+]^2}{[Ca^{2+}][\overline{Na}^+]^2}$
$2\overline{Na}^+ + Mg^{2+} \overset{K_2^{ex}}{\rightleftarrows} 2Na^+ + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{[\overline{Mg}^{2+}][Na^+]^2}{[Mg^{2+}][\overline{Na}^+]^2}$
$\overline{H}^+ + Na^+ + OH^- \overset{K_3^{ex}}{\rightleftarrows} \overline{Na}^+ + H_2O$	$K_3^{ex} = \dfrac{[Na^+][\overline{H}^+]}{[\overline{Na}^+][H^+]}$

Exchange reactions (on micelle)	Exchange equilibrium constant
$2\overline{\overline{Na}}^+ + Ca^{2+} \overset{K_1^{exm}}{\rightleftarrows} 2Na^+ + \overline{\overline{Ca}}^{2+}$	$K_1^{exm} = \dfrac{[\overline{\overline{Ca}}^{2+}][Na^+]^2}{[\overline{\overline{Na}}^+]^2[Ca^{2+}]}$ where $K_1^{exm} = \beta_1^{exm}\{[A^-] + [S^-]\}$
$2\overline{\overline{Na}}^+ + Mg^{2+} \overset{K_2^{exm}}{\rightleftarrows} 2Na^+ + \overline{\overline{Mg}}^{2+}$	$K_2^{exm} = \dfrac{[\overline{\overline{Mg}}^{2+}][Na^+]^2}{[\overline{\overline{Na}}^+]^2[Mg^{2+}]}$ where $K_2^{exm} = \beta_2^{exm}\{[A^-] + [S^-]\}$

6.9 List of Elements and Reactive Species for IREACT = 4 or 6

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Aluminum, Silicon, Oxygen, Chlorine, S (Injected surfactant)
Independent aqueous or oleic species:	H^+, Na^+,Ca^{2+}, Mg^{2+}, Al^{3+}, CO_3^{2-}, Cl^-, S^-, H_4SiO_4, H_2O
Dependent aqueous or oleic species:	$Ca(OH)^+$, $Mg(OH)^+$, $Al(OH)^{2-}$,$Al(OH)_2^-$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, OH^-, HCO_3^-, $H_3SiO_4^-$, $H_2SiO_4^{2-}$, $HSi_2O_6^{3-}$, $Si_2O_5^{2-}$, $Al(OH)_4^-$, H_2CO_3, $CaCO_3^o$, $MgCO_3^o$
Solid species:	$CaCO_3$ (Calcite), $Al_2Si_2O_5(OH)_4$ (Kaolinite), $MgCO_3$ (Magnesite), $NaAlSi_2O_6.H_2O$ (Analcite), SiO_2 (Silica), $Mg(OH)_2$ (Magnesium Hydroxide)
Adsorbed cations on rock surface:	$\overline{H}^+$, $\overline{Na}^+$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^+$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftarrows} H^+ + OH^-$	$K_1^{eq} = [H^+]\ [OH^-]$
$H^+ + CO_3^{2-} \overset{K_2^{eq}}{\rightleftarrows} HCO_3^-$	$K_2^{eq} = \dfrac{[HCO_3^-]}{[H^+]\ [CO_3^{2-}]}$
$Ca^{2+} + H_2O \overset{K_3^{eq}}{\rightleftarrows} Ca(OH)^+ + H^+$	$K_3^{eq} = \dfrac{[Ca(OH)^+]\ [H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_4^{eq}}{\rightleftarrows} Mg(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Mg(OH)^+]\ [H^+]}{[Mg^{2+}]}$
$Al^{3+} + H_2O \overset{K_5^{eq}}{\rightleftarrows} Al(OH)^{2+} + H^+$	$K_5^{eq} = \dfrac{[Al(OH)^{2+}][H^+]}{[Al^{3+}]}$

$$Al^{3+} + 2H_2O \overset{K_6^{eq}}{\rightleftarrows} Al(OH)_2^+ + 2H^+ \qquad K_6^{eq} = \frac{[Al(OH)_2^+][H^+]^2}{[Al^{3+}]}$$

$$Al^{3+} + 4H_2O \overset{K_7^{eq}}{\rightleftarrows} Al(OH)_4^- + 4H^+ \qquad K_7^{eq} = \frac{[Al(OH)_4^-][H^+]^4}{[Al^{3+}]}$$

$$H_4SiO_4 \overset{K_8^{eq}}{\rightleftarrows} H^+ + H_3SiO_4^- \qquad K_8^{eq} = \frac{[H^+][H_3SiO_4^-]}{[H_4SiO_4]}$$

$$H_4SiO_4 \overset{K_9^{eq}}{\rightleftarrows} 2H^+ + H_2SiO_4^{2-} \qquad K_9^{eq} = \frac{[H^+]^2[H_2SiO_4^{2-}]}{[H_4SiO_4]}$$

$$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_{10}^{eq}}{\rightleftarrows} Ca(HCO_3)^+ \qquad K_{10}^{eq} = \frac{[Ca(HCO_3)^+]}{[Ca^{2+}]\,[CO_3^{2-}][H^+]}$$

$$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_{11}^{eq}}{\rightleftarrows} Mg(HCO_3)^+ \qquad K_{11}^{eq} = \frac{[Mg(HCO_3)^+]}{[Mg^{2+}]\,[CO_3^{2-}][H^+]}$$

$$2H^+ + CO_3^{2-} \overset{K_{12}^{eq}}{\rightleftarrows} H_2CO_3 \qquad K_{12}^{eq} = \frac{[H_2CO_3]}{[CO_3^{2-}][H^+]^2}$$

$$2H_4SiO_4 \overset{K_{13}^{eq}}{\rightleftarrows} 2H_2O + 3H^+ + HSi_2O_6^{3-} \qquad K_{13}^{eq} = \frac{[H^+]^3[HSi_2O_6^{3-}]}{[H_4SiO_4]^2}$$

$$2H_4SiO_4 \overset{K_{14}^{eq}}{\rightleftarrows} 2H^+ + 3H_2O + Si_2O_5^{2-} \qquad K_{14}^{eq} = \frac{[H^+]^2[Si_2O_5^{2-}]}{[H_4SiO_4]^2}$$

Solid species	Solubility product
$CaCO_3$	$K_1^{sp} = [Ca^{2+}]\,[CO_3^{2-}]$
$MgCO_3$	$K_2^{sp} = [Mg^{2+}]\,[CO_3^{2-}]$
SiO_2	$K_3^{sp} = [H_4SiO_4]$

$Al_2Si_2O_5(OH)_4$	$K_4^{sp} = [H^+]^{-6}[Al^{3+}]^2[H_4SiO_4]^2$
$NaAlSi_2O_6.H_2O$	$K_5^{sp} = [H^+]^{-4}[Na^+][Al^{3+}][H_4SiO_4]^2$
$Mg(OH)_2$	$K_6^{sp} = [Mg^{2+}]\,[H^+]^{-2}$

Exchange reactions (on matrix)	Exchange equilibrium constant
$2\overline{Na}^+ + Ca^{2+} \overset{K_1^{ex}}{\rightleftarrows} 2Na^+ + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{\left[\overline{Ca}^{2+}\right][Na^+]^2}{[Ca^{2+}]\left[\overline{Na}^+\right]^2}$
$2\overline{Na}^+ + Mg^{2+} \overset{K_2^{ex}}{\rightleftarrows} 2Na^+ + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{\left[\overline{Mg}^{2+}\right][Na^+]^2}{[Mg^{2+}]\left[\overline{Na}^+\right]^2}$
$\overline{H}^+ + Na^+ + OH^- \overset{K_3^{ex}}{\rightleftarrows} \overline{Na}^+ + H_2O$	$K_3^{ex} = \dfrac{[Na^+]\left[\overline{H}^+\right]}{\left[\overline{Na}^+\right][H^+]}$

Exchange reactions (on micelle)	Exchange equilibrium constant
$2\overline{\overline{Na}}^+ + Ca^{2+} \overset{K_1^{exm}}{\rightleftarrows} 2Na^+ + \overline{\overline{Ca}}^{2+}$	$K_1^{exm} = \dfrac{\left[\overline{\overline{Ca}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Ca^{2+}]}$ where $K_1^{exm} = \beta_1^{exm}\,[S^-]$
$2\overline{\overline{Na}}^+ + Mg^{2+} \overset{K_2^{exm}}{\rightleftarrows} 2Na^+ + \overline{\overline{Mg}}^{2+}$	$K_2^{exm} = \dfrac{\left[\overline{\overline{Mg}}^{2+}\right][Na^+]^2}{\left[\overline{\overline{Na}}^+\right]^2[Mg^{2+}]}$ where $K_2^{exm} = \beta_2^{exm}\,[S^-]$

6.10 List of Elements and Reactive Species for IREACT = 5

Elements or pseudo-element:	Hydrogen (reactive), Sodium, Calcium, Magnesium, Carbonate, Aluminum, Silicon, A (from acid HA), Oxygen, Chlorine, S (InjectedSurfactant)
Independent aqueous or oleic species:	H^+, Na^+, Ca^{2+}, Mg^{2+}, Al^{3+}, CO_3^{2-}, H_4SiO_4, HA_o, H_2O
Dependent aqueous species:	$Ca(OH)^+$, $Mg(OH)^+$, $Al(OH)^{2-}$, $Al(OH)_2^-$, $Ca(HCO_3)^+$, $Mg(HCO_3)^+$, A^-, OH^-, HCO_3^-, $H_3SiO_4^-$, $H_2SiO_4^{2-}$, $HSi_2O_6^{3-}$, $Si_2O_5^{2-}$, $Al(OH)_4^-$, H_2CO_3, HA_w
Solid species:	$CaCO_3$ (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)
Adsorbed cations on rock surface:	$\overline{H}^+$, $\overline{Na}^+$, $\overline{Ca}^{2+}$, $\overline{Mg}^{2+}$
Adsorbed cations on micelles:	$\overline{\overline{Na}}^+$, $\overline{\overline{Ca}}^{2+}$, $\overline{\overline{Mg}}^{2+}$

Aqueous reactions	Equilibrium constant
$H_2O \overset{K_1^{eq}}{\rightleftarrows} H^+ + OH^-$	$K_1^{eq} = [H^+]\,[OH^-]$
$HA_w + OH^- \overset{K_2^{eq}}{\rightleftarrows} A^- + H_2O$	$K_2^{eq} = \dfrac{[A^-]\,[H^+]}{[HA_w]}$
$H^+ + CO_3^{2-} \overset{K_3^{eq}}{\rightleftarrows} HCO_3^-$	$K_3^{eq} = \dfrac{[HCO_3^-]}{[H^+]\,[CO_3^{2-}]}$
$Ca^{2+} + H_2O \overset{K_4^{eq}}{\rightleftarrows} Ca(OH)^+ + H^+$	$K_4^{eq} = \dfrac{[Ca(OH)^+]\,[H^+]}{[Ca^{2+}]}$
$Mg^{2+} + H_2O \overset{K_5^{eq}}{\rightleftarrows} Mg(OH)^+ + H^+$	$K_5^{eq} = \dfrac{[Mg(OH)^+]\,[H^+]}{[Mg^{2+}]}$

$$Al^{3+} + H_2O \overset{K_6^{eq}}{\rightleftarrows} Al(OH)^{2+} + H^+ \qquad K_6^{eq} = \frac{[Al(OH)^{2+}][H^+]}{[Al^{3+}]}$$

$$Al^{3+} + 2H_2O \overset{K_7^{eq}}{\rightleftarrows} Al(OH)_2^{+} + 2H^+ \qquad K_7^{eq} = \frac{[Al(OH)_2^{+}][H^+]^2}{[Al^{3+}]}$$

$$Al^{3+} + 4H_2O \overset{K_8^{eq}}{\rightleftarrows} Al(OH)_4^{-} + 4H^+ \qquad K_8^{eq} = \frac{[Al(OH)_4^{-}][H^+]^4}{[Al^{3+}]}$$

$$H_4SiO_4 \overset{K_9^{eq}}{\rightleftarrows} H^+ + H_3SiO_4^{-} \qquad K_9^{eq} = \frac{[H^+][H_3SiO_4^{-}]}{[H_4SiO_4]}$$

$$H_4SiO_4 \overset{K_{10}^{eq}}{\rightleftarrows} 2H^+ + H_2SiO_4^{2-} \qquad K_{10}^{eq} = \frac{[H^+]^2[H_2SiO_4^{2-}]}{[H_4SiO_4]}$$

$$Ca^{2+} + H^+ + CO_3^{2-} \overset{K_{11}^{eq}}{\rightleftarrows} Ca(HCO_3)^+ \qquad K_{11}^{eq} = \frac{\left[Ca(HCO_3)^+\right]}{[Ca^{2+}]\left[CO_3^{2-}\right][H^+]}$$

$$Mg^{2+} + H^+ + CO_3^{2-} \overset{K_{12}^{eq}}{\rightleftarrows} Mg(HCO_3)^+ \qquad K_{12}^{eq} = \frac{\left[Mg(HCO_3)^+\right]}{[Mg^{2+}]\left[CO_3^{2-}\right][H^+]}$$

$$2H^+ + CO_3^{2-} \overset{K_{13}^{eq}}{\rightleftarrows} H_2CO_3 \qquad K_{13}^{eq} = \frac{[H_2CO_3]}{\left[CO_3^{2-}\right][H^+]^2}$$

$$2H_4SiO_4 \overset{K_{14}^{eq}}{\rightleftarrows} 2H_2O + 3H^+ + HSi_2O_6^{3-} \qquad K_{14}^{eq} = \frac{[H^+]^3[HSi_2O_6^{3-}]}{[H_4SiO_4]^2}$$

$$2H_4SiO_4 \overset{K_{15}^{eq}}{\rightleftarrows} 2H^+ + 3H_2O + Si_2O_5^{2-} \qquad K_{15}^{eq} = \frac{[H^+]^2[Si_2O_5^{2-}]}{[H_4SiO_4]^2}$$

Partitioning of HA

Partition coefficient

$$HA_o \overset{K_D}{\rightleftarrows} HA_w \qquad K_D = \frac{[HA_w]_{water}}{[HA_o]_{oil}}$$

Solid species	Solubility product
$CaCO_3$	$K_1^{sp} = [Ca^{2+}]\,[CO_3^{2-}]$
$MgCO_3$	$K_2^{sp} = [Mg^{2+}]\,[CO_3^{2-}]$
SiO_2	$K_3^{sp} = [H_4SiO_4]$
$Al_2Si_2O_5(OH)_4$	$K_4^{sp} = [H^+]^{-6}[Al^{3+}]^2[H_4SiO_4]^2$
$NaAlSi_2O_6.H_2O$	$K_5^{sp} = [H^+]^{-4}[Na^+][Al^{3+}][H_4SiO_4]^2$
$Mg(OH)_2$	$K_6^{sp} = [Mg^{2+}]\,[H^+]^{-2}$

Exchange reactions (on matrix)	Exchange equilibrium constant
$2\overline{Na}^{+} + Ca^{2+} \overset{K_1^{ex}}{\rightleftarrows} 2Na^{+} + \overline{Ca}^{2+}$	$K_1^{ex} = \dfrac{[\overline{Ca}^{2+}]\,[Na^+]^2}{[Ca^{2+}]\,[\overline{Na}^{+}]^2}$
$2\overline{Na}^{+} + Mg^{2+} \overset{K_2^{ex}}{\rightleftarrows} 2Na^{+} + \overline{Mg}^{2+}$	$K_2^{ex} = \dfrac{[\overline{Mg}^{2+}]\,[Na^+]^2}{[Mg^{2+}]\,[\overline{Na}^{+}]^2}$
$\overline{H}^{+} + Na^{+} + OH^{-} \overset{K_3^{ex}}{\rightleftarrows} \overline{Na}^{+} + H_2O$	$K_3^{ex} = \dfrac{[Na^+]\,[\overline{H}^{+}]}{[\overline{Na}^{+}]\,[H^+]}$

Exchange reactions (on micelle)	Exchange equilibrium constant

$$2\bar{\bar{Na}}^{+} + Ca^{2+} \overset{K^{exm}_{1}}{\rightleftarrows} 2Na^{+} + \bar{\bar{Ca}}^{2+}$$

$$K^{exm}_{1} = \frac{\left[\bar{\bar{Ca}}^{2+}\right]\left[Na^{+}\right]^{2}}{\left[\bar{\bar{Na}}^{+}\right]^{2}\left[Ca^{2+}\right]}$$

where $K^{exm}_{1} = \beta^{exm}_{1}\{[A^{-}] + [S^{-}]\}$

$$2\bar{\bar{Na}}^{+} + Mg^{2+} \overset{K^{exm}_{2}}{\rightleftarrows} 2Na^{+} + \bar{\bar{Mg}}^{2+}$$

$$K^{exm}_{2} = \frac{\left[\bar{\bar{Mg}}^{2+}\right]\left[Na^{+}\right]^{2}}{\left[\bar{\bar{Na}}^{+}\right]^{2}\left[Mg^{2+}\right]}$$

where $K^{exm}_{2} = \beta^{exm}_{2}\{[A^{-}] + [S^{-}]\}$

6.11 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) if IREACT=0 or 1.

I. INOUT
   A. FILE1
   B. PRINTS
   C. PRINTI
   D. READIN (called only if IREACT>1)
   E. METRIC (called only if IUNIT=1)
   F. WELLIX
      1. RADIUS
   G. FILE3
   H. FILE2
   I. GRDFAC

II. RSTART (called only if IMODE=2)
   A. NSLUG
   B. WELLIX
      1. RADIUS

III. TIME0
   A. DENSTY

IV. TRAN1

V. ASIGN1

VI. TRANS (Transmissibilities)

VII. SOLMAT (Pressure Eq.)
   A. WELL
   B. JCG
   C. BUNDRY (called only if IBOUND=1)

VIII. QRATE

IX. CONEQ (Concentration Eq.)

X. ADSORB

XI. REACTR (called only if IREACT>1)
   A. RENAM1
   B. TOTALS
   C. MANIPL
   D. JACUP
      1. GAUSS
      2. SOLVE
   E. RENAM2

XII. CSECAL
  A. ALCPTN (called only if IALC=1)
    1. TWOALC
    2. CUBIC
  B. IONCNG
  C. PHASC (called only if surfactant is not present and IREACT<1)
  D. PHCOMP (called only if surfactant is present or IREACT>1)
    1. TIELIN
      a. TRY
    2. REVISE
    3. VGAMMA
    4. SINGLE

XIII. TCAP (called only if ICAP=1)

XIV. DENSTY

XV. ASIGN2

XVI. ENGBAL (called only if IENG=1)

XVII. LAWER (called only if IENG=1 and IANAL=1)

XVIII. CAPNUM

XIX. TRAP (called only if IGAS=0)

XX. TRAPG (called only if IGAS=1)

XXI. VISCOS

XXII. WELLCK

XXIII. OUTDT1

XXIV. OUTDT2
  A. PRINTI
  B. PRINTS

XXV. NSLUG
  A. WELLIX
    1. RADIUS

XXVI. RSTART

XXVII. Go to step V (ASIGN1) if not done

XXVIII. SUMTAB

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