Pore-Scale Network Model User Manual

The pore-scale network model is written in C++ and uses a keyword based input file. Most keywords are optional and there is no necessary order to them. Comments in the data file are indicated by '%', resulting in the rest of the line being discarded. All keywords should be terminated by '#'. The input data file can be supplied as an argument to the executable.

C:\path_to_executable\poreflow.exe default.dat

Required keywords

NETWORK

This specifies the files containing data such as inscribed radii, volumes and the connection list defining the network topology.

- 1. Are the files in binary format? Binary files take up less disk space and load substantially quicker than ASCII files. However binary files can not be interchanged between different computer platforms (e.g. Windows and Solaris).
- 2. The network data are located in four files when using ASCII format (filename_node1.dat, filename_node2.dat, filename_link1.dat, filename_link2.dat) and two files when using binary format (filename_node.bin and filename_link.bin). Only the prefix filename is to be specified.

```
NETWORK
F ../data/berea
#
```

SAT TARGET

Each line represents a separate flooding cycle (e.g. primary oil flooding, secondary water flooding etc.).

- 1. Final water saturation target after the flooding cycle (fraction). The actual value might not actually be reached due to trapping or water retained in corners.
- 2. The cycle can also be terminated when a capillary pressure (Pa) is reached.
- 3. Target water saturation interval (fraction) between reporting results. The state of the model will be evaluated at the first possible configuration after the incremental target has been reached.

- 4. Target capillary pressure interval (Pa) between reporting results.
- 5. Should relative permeability be calculated? If this is not of primary interest it can be very time saving to set this option to false ('F') as most of the CPU time is spent solving the pressure field, required for relative permeability calculations.
- 6. Calculate resistivity index? CPU time required for this is the same as for relative permeability calculations.

```
SAT_TARGET
0.00
                     0.02
         66380.0
                                5000.0
                                                F
1.00
         -1.0E21
                     0.02
                              10000.0
                                           Т
                                                Т
0.00
          1.0E21
                     0.05
                                5000.0
                                           Т
                                                Т
```

EQUIL_CON_ANG

Once invaded by oil the wettability of a pore element will typically change. Advancing and receding contact angles are defined in terms of an intrinsic contact angle, either distributed according to a truncated weibull distribution

$$\theta i = (\theta i, \max - \theta i, \min) \left(-\delta \ln \left[x(1 - e^{-1/\delta}) + e^{-1/\delta} \right] \right)^{1/\gamma} + \theta i, \min, \tag{1}$$

where δ and γ are parameters defining the shape of the distribution and x is a random number between 0 and 1, or alternatively distributed uniformly by setting δ and γ to less than 0 in the input file.

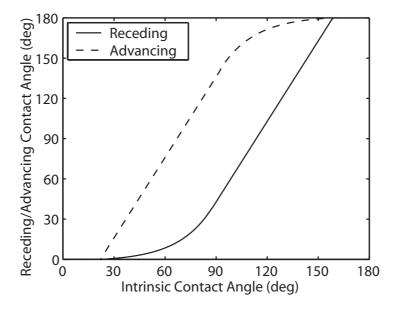


Figure 1: Relationship between receding and advancing contact angles on a rough surface, as a function of intrinsic contact angle measured at rest on a smooth surface [Morrow, 1975].

- 1. What model should be used for determining receding and advancing contact angles? Model 1 sets $\theta_i = \theta_r = \theta_a$. Model 2 separates θ_r and θ_a by a constant angle, with $\theta_a(\theta_i = 0^\circ) = 0^\circ$ and $\theta_r(\theta_i = 180^\circ) = 180^\circ$. With a separation angle of 25.2° this corresponds to the Class II model defined by Morrow [1975]. Model 3 corresponds to the Class III model defined by Morrow [1975] and is illustrated in Figure 1.
- 2. Minimum intrinsic contact angle (degrees)
- 3. Maximum intrinsic contact angle (degrees)
- 4. δ exponent (set this to a negative number for uniform distribution).
- 5. γ exponent (set this to a negative number for uniform distribution).
- 6. How are the contact angles distributed on the pore-scale? 'rMax' associates the larger pores (in terms of inscribed radius) with the larger angles, 'rMin' associates the larger pores with the smaller angles and 'rand' distributes the angles randomly. Throats are assigned the angle of either connecting pore based on equal probability.
- 7. The separation angle for intrinsic contact angle model 2.

```
EQUIL_CON_ANG
2  30.0  60.0  -1.0  -1.0  rand  25.2  #
```

Keywords controlling the reporting of results

The remaining keywords are all optional. The default parameters are those given as example in each section, unless otherwise specified.

TITLE

All output files are prefixed by the indicated title (e.g. *title*_draincycle_1.out). If this keyword is omitted the title is taken to be the same as the name of the input data file.

```
TITLE
default
#
```

RES_FORMAT

There is a choice between three formats ('excel', 'matlab' or 'std') for the results files containing capillary pressure, relative permeability etc. The excel format will create files with extension .csv, the matlab format will create files with extension .m and the standard format will create files with extension .out.

```
RES_FORMAT
std
#
```

WRITE_NET

Using this keyword it is possible to write the network that was used for the simulation to file. Omitting this keyword will result in no network files being written.

- 1. Should the files be written in binary format (true 'T' or false 'F')?
- 2. The filename along with the relative path to be used. The extensions, _node1.dat, node.bin etc., will be automatically added to the filename.

```
WRITE_NET
T ../data/sandstone_s8
#
```

OUTPUT

Using this keyword it is possible to create output files containing the properties of individual network elements in terms of radii, volumes, connection numbers etc. (title_pores.out and title_throats.out) and files containing the distribution of saturations in the network at every reporting interval (title_pores_Sw.out and title_throats_Sw.out). Both sets of files can become very space consuming. The file format used is the same as that used by the geostatistical package GSLIB [Deutsch and Journel, 1998]. The data are stored in columns. The first row is some arbitrary file header, followed by the number of data columns and the titles of each column.

- 1. Create files with the properties of individual network elements (true 'T' or false 'F')?
- 2. Create files with the water saturation of all pores and throats at every reporting interval (true 'T' or false 'F')?

```
OUTPUT
F F
#
```

FILLING LIST

Output files indicating the sequence that pores and throats got filled during the simulation can be created. The resulting files are formatted for easy entry into matlab for post-processing, with the filenames being *poreLocation.m*, *throatConnection.m*, *fill_draincycle_1.m* and *fill_imbcycle_2.m*.

1. Create filling list for oil flooding cycles (true 'T' or false 'F')?

- 2. Create filling list for water flooding cycles (true 'T' or false 'F')?
- 3. Create files with pore location and throat connection data (true 'T' or false 'F')?

```
FILLING_LIST
F F F
#
```

Convergence related keywords

SOLVER_TUNE

The pressure solver used for relative permeability calculations is an algebraic multigrid solver [*Ruge and Stueben*, 1987].

- 1. The performance of the solver can be tuned by varying the solution tolerance. A lower tolerance will result in an increased number of required solver iterations.
- 2. Memory allocation for the solver can be adjusted by the memory scaling factor. For large models it might be necessary to increase the factor above the default value.
- 3. Performance related information about the solver is written to the file *fort.11*. A value of 0 produces minimal information whereas a value of 3 will produce substantial information about tolerance, memory requirements etc.
- 4. Setting this flag to true ('T') will output solver information to screen rather than to file.
- 5. In some cases it might be necessary to discard conductances below a certain threshold to ensure solver convergence. This option should be used with great care and only when problems are observed (typically when solving for the oil pressure in cycles greater than the secondary).

```
SOLVER_TUNE
1.0E-15 5 0 F 0.0E-30
#
```

SAT_COVERGENCE

This keyword controls the accuracy at which the incremental water saturation target is reached. It is generally not feasible to calculate water saturation after each filling event, as that would be computationally very expensive. When starting a new saturation step, an approximate number of required filling events is estimated. This estimate is however quite uncertain as the water saturation does not vary linearly with the number of filling events. The actual number of filling events performed before recalculating water saturation should

therefore be a relatively small fraction of the initial estimate. Subsequently an updated estimate of the required number of filling events is made, using information from the previous step. Still, only a fraction of the estimated filling events should be performed before recalculating water saturation, as the estimate remains fairly uncertain.

- 1. Minimum number of filling events between calculating water saturation.
- 2. Fraction applied to the initial estimate of required number of filling events.
- 3. Fraction applied to subsequent estimates of required number of filling events.
- 4. Maximum increase factor in required number of filling events estimates.
- 5. Only solve for relative permeability when a stable capillary configuration is reached (true 'T' or false 'F')?

```
SAT_COVERGENCE
10 0.1 0.8 2.0 F
#
```

SAT_COMPRESS

This keyword will change the target saturation interval, specified by entry 3 in SAT_TARGET, once relative permeability of the defending fluid drops below a specified threshold. If this keyword is omitted, the originally specified interval target will be used.

- 1. Relative permeability threshold.
- 2. New target saturation interval between the reporting of results.
- 3. Apply to oil flooding cycle (true 'T' of false 'F')?
- 4. Apply to water flooding cycle (true 'T' of false 'F')?

```
SAT_COMPRESS
0.1 0.005 T F
#
```

RELPERM DEF

- 1. Use flow rate at residual saturation ('residual') to calculate relative permeability, rather than that at single phase conditions ('single')? Using residual saturations will normalize all relative permeabilities between 0 and 1.
- 2. Maintain the conditions for trapping as defined in keyword TRAPPING (true 'T' or false 'F')? If set to false, the defending fluid only has to be connected to one face to be considered as not trapped, even when injecting from a single face of the network.

```
RELPERM_DEF
single T
#
```

Keywords specifying fluid and rock properties

INIT_CON_ANG

The initial receding contact angles θ_r , used in elements that have never been invaded by oil, are distributed either uniformly or according to a truncated weibull distribution.

- 1. Minimum initial receding contact angle (degrees).
- 2. Maximum initial receding contact angle (degrees).
- 3. δ exponent (set to a negative number for a uniform distribution).
- 4. γ exponent (set to a negative number for a uniform distribution).

```
INIT_CON_ANG
0.0 0.0 0.2 3.0
#
```

FRAC_CON_ANG

Not all oil invaded elements need necessarily attain oil-wet characteristics in mixed-wet systems. This effect can be modelled by defining two separate distributions of intrinsic contact angles. This wettability alteration will be applied after primary oil-flooding and will replace the contact angles defined by EQUIL_CON_ANG in those elements selected to belong to this second distribution. Only a single distribution, as defined by EQUIL_CON_ANG, will exist if this keyword is omitted. The first line of data defines the second distribution.

- 1. The fraction of oil invaded elements following primary oil flooding whose contact angles should be altered.
- 2. Should the fraction be pore volume based ('T') or a quantitative split between pores ('F').
- 3. Minimum intrinsic contact angle (degrees).
- 4. Maximum intrinsic contact angle (degrees).
- 5. δ exponent (set to a negative number for a uniform distribution).
- 6. γ exponent (set to a negative number for a uniform distribution).

The second line defines how this second distribution is distributed on the pore-scale. Four approaches are possible. The first approach assumes that the second distribution is spatially correlated. This approach is selected by the keyword 'corr' followed by the diameter (in terms of pores) of the correlated regions. One can also select to make the largest ('rMax') or smallest ('rMin') pores belong to the second distribution. The final approach is randomly selecting the pores ('rand'). In the last three approaches the connecting throats will be assigned the same contact angle as the pore with a probability equal to the altered fraction (as defined by the first entry in line 1).

- 1. How should the second distribution be distributed on the pore-scale ('corr', 'rMax', 'rMin' or 'rand')?
- 2. Correlation diameter when using the spatially correlated approach.

```
FRAC_CON_ANG
0.7 T 100.0 130.0 -1.0 -1.0
corr 7
#
```

FLUID

The fluid description is very simple with no pressure dependent properties.

- 1. Interfacial tension (mN·m⁻¹)
- 2. Water viscosity (cp)
- 3. Oil viscosity (cp)
- 4. Water resistivity (Ohm·m)
- 5. Oil resistivity (Ohm·m)
- 6. Water gravity (kg·m⁻³)
- 7. Oil gravity (kg·m⁻³)

```
FLUID
30.0 1.0 1.2 1000.0 1000.0 1000.0
#
```

GRAV CONST

Define the gravitational constant g(z = 0) is at the bottom of the model).

- 1. Gravitational component in the x direction (m/s^2) .
- 2. Component in y direction.

3. Component in *z* direction.

```
GRAV_CONST
0.0 0.0 -9.81
#
```

PRS DIFF

It is possible to include gravity effects when solving the pressure field. How much influence it will have depends on both the fluid density and the pressure difference imposed across the model.

- 1. Inlet pressure (Pa).
- 2. Outlet pressure (Pa).
- 3. Should gravity effects be included when solving the pressure field (true 'T' or false 'F')?

```
PRS_DIFF
1.0 0.0 F
#
```

Keywords for various network modelling options

RAND_SEED

This is the seed to the random number generator, which should be a large positive integer. If the keyword is omitted the computer clock will be used as seed.

```
RAND_SEED
54356457
#
```

CALC_BOX

Most of the elements close to the injection faces will be filled by the injecting fluid, resulting in most of the pressure loss occurring in this region when solving the pressure field for the displaced fluid. To avoid these boundary effects it is normal to only use a fraction of the network (away from the injecting faces) when calculating saturation and relative permeabilities.

- 1. Dimensionless location for lower boundary.
- 2. Dimensionless location for higher boundary.

```
CALC_BOX
0.50 1.00
#
```

PRS BDRS

To avoid boundary effects only a section of the network is used for calculating relative permeability and water saturation, as defined by the CALC_BOX keyword. When computing relative permeability it is possible to solve the pressure field in the entire network, using the average pressure at the section boundaries for relative permeability,

$$k_{rp} = \frac{q_{tmp} \, \Delta P_{sp}}{q_{tsp} \, \Delta P_{mp}},\tag{2}$$

where ΔP_{sp} and ΔP_{mp} are the single and multiphase pressure drops for phase p across the selected section. Alternatively the pressure field can be solved only within the selected section by applying constant pressures at the section boundaries, with relative permeability given by

$$k_{rp} = \frac{q_{\text{tmp}}}{q_{tsp}} \,. \tag{3}$$

- 1. Solve the pressure field in the entire network (true 'T' or false 'F')?
- 2. Record the average pressure at cross-sectional planes within the selected section of the network (true 'T' or false 'F')? This is just for reporting purposes and the pressures will be written to the results files.
- 3. The number of cross-sectional pressure planes where the average pressure is to be recorded.

```
PRS_BDRS
F F 0
#
```

TRAPPING

This keyword controls some aspects of the trapping routine. If fluid is injected from only one face of the model, the defending fluid must be connected to both the inlet and outlet to be considered as not trapped. If injecting from both faces, the defending fluid only has to be connected to one face to be considered as not trapped.

- 1. Inject fluid from inlet face?
- 2. Inject fluid from outlet face?
- 3. Allow drainage of dangling ends (pores with only one connecting throat) through wetting layers.

4. The water conductance (m⁴·Pa⁻¹·s⁻¹) of circular elements completely filled with oil.

```
TRAPPING
T F T 0.0E-30
#
```

POINT SOURCE

Rather than inject fluid from the face of the network, it is possible to inject from any interior pore. If this keyword is included it will take precedence over the TRAPPING keyword, and no fluid will be injected from any network face.

1. Pore index to inject from. This will have to be greater than 0 and less than the total number of pores.

```
POINT_SOURCE
5050
#
```

PORE_FILL_ALG

During spontaneous invasion, the capillary entry pressure for pore bodies will depend on the number n of adjacent oil filled throats (cooperative pore body filling). Several different models have been proposed in the literature. The default model ('blunt2') is the one proposed by Blunt [1998],

$$P_c = \frac{2\sigma\cos\theta_a}{r} - \sigma \sum_{i=1}^n A_i x_i , \qquad (4)$$

where A_i are arbitrary numbers and x_i are random numbers between zero and one. Another model proposed by Blunt [1997] is given by ('blunt1')

$$P_c = \frac{2\sigma\cos\theta_a}{r + \sum_{i=1}^{n} A_i x_i}.$$
 (5)

Also implemented is the model proposed by Øren et al. [1998], given by ('oren1')

$$P_c = \frac{2\sigma\cos\theta_a}{r + \sum_{i=1}^{n} A_i r_i x_i},$$
(6)

where r_i is the radius of connecting throat i. A similar model correcting for non-circular pore shapes is given by ('oren2')

$$P_c = \frac{(1+2\sqrt{\pi G})\sigma\cos\theta_a}{r+\sum_{i=1}^n A_i r_i x_i}$$
 (7)

Model to be used for cooperative pore body filling ('blunt1', 'blunt2', 'oren1' or 'oren2').

```
PORE_FILL_ALG
blunt2
#
```

PORE_FILL_WGT

The weights A_i , used in the models for pore body filling, will clearly have an impact on the filling sequence during spontaneous invasion. These are specific to the chosen model, specified by the keyword PORE_FILL_ALG. Typical values for $A_I - A_6$ for the models proposed by Øren *et al.* [1998] are 0.0, 0.5, 1.0, 2.0, 5.0 and 10.0. In the default model ('blunt2') by Blunt [1998] A_i have dimensions of m⁻¹, hence we chose to relate it to permeability,

$$A_2 - A_n = \frac{0.03}{\sqrt{K}} \,, \tag{8}$$

where the permeability K is measured in m^2 . This approximately reproduces the results by Blunt [1998]. When only one connecting throat contains oil (I_I event) the process is similar to piston-like displacement and hence $A_I = 0.0 \, \mu m^{-1}$. This is also the most favoured event.

- 1. Weight for an I_1 event, A_1 .
- 2. Weight for an I_2 event, A_2 .
- 3. Weight for an I_3 event, A_3 .
- 4. Weight for an I_4 event, A_4 .
- 5. Weight for an I_5 event, A_5 .
- 6. Weight for an I_6 event, A_6 , and up.

```
PORE_FILL_WGT
0 15000 15000 15000 15000
#
```

Keywords for tuning the network properties

If any of the keywords in this section are omitted, the original properties of the network will be retained.

MODIFY_PORO

All pore and throat volumes can be adjusted by a constant factor such that the target porosity is reached. We assume that the total porosity, $\phi_t = \phi_n + \phi_c$, is made up of the net porosity ϕ_n and the micro and clay bound porosity ϕ_c .

- 1. Target net porosity, ϕ_n .
- 2. Target micro and clay bound porosity, ϕ_c .

```
MODIFY_PORO
0.24 0.03
#
```

MODIFY_RAD_DIST

This keyword is used for modifying the pore size distribution, useful when tuning a network to become representative of a given type of porous medium. The first line of data refers to throats and the second to pores. The various options for pores are identical to those for throats.

1. There are 6 approaches available for how the pore/throat size distribution should be modified. Setting the index to '-1' will bundle the throats together with the pores or vice versa. So if the first line of data is set to '-1' the second line will apply to pores and throats, rather than just pores. Setting the index to '0' will result in nothing being done. The pore/throat size distribution can be read from file by setting the index to '1'. Setting the index to '2' will result in the pore/throat radius being determined by the radii of connecting pores or throats. When setting the index to '3', each pore/throat radius will be multiplied by a constant factor. The shape of the pore/throat size distribution can also be stretched or compressed by setting the index to '4'. Finally, by setting the index to '5' the radii are randomly distributed, either uniformly or according to a truncated weibull distribution. For options 1 to 5 additional parameters are needed.

READ FROM FILE (OPTION '1')

2. The file containing the target distribution. The file should contain two columns. The first column is the pore/throat diameter in micrometers. This should be monotonically

decreasing. The second column should be the corresponding fraction of pore/throat space occupied, going from 0 to 1.

- 3. If the target distribution is derived from mercury injection data it might be necessary to apply a lower cut-off to exclude effects from mercury entering the micro porosity. Micro porosity (and clays) should be accounted for with the MODIFY_PORO keyword. No cut-off will be applied if a negative value is specified.
- 4. It might also be necessary to apply a higher cut-off.

ASPECT RATIO (OPTION '2')

The average connecting radius will be multiplied by a user defined aspect ratio, α , distributed uniformly or according to a truncated weibull distribution. The radius of a pore body is then given by

$$r_p = \max\left(\alpha \frac{\sum_{i=1}^n r_i}{n}, \max(r_i)\right), \tag{9}$$

while the throat radius is given by

$$r_t = \min\left(\frac{\sum_{i=1}^n r_i}{\alpha \frac{1}{n}}, \min(r_i)\right). \tag{10}$$

Minimum aspect ratio. If minimum and maximum aspect ratios are set to a negative number the original ratios of the network will be used.

- 2. Maximum aspect ratio.
- 3. δ exponent (set to a negative number for a uniform distribution).
- 4. γ exponent (set to a negative number for a uniform distribution).

MULTIPLICATION FACTOR (OPTION '3')

2. Multiplication factor.

STRETCH OR COMPRESS DISTRIBUTION (OPTION '4')

The original pore/throat size distribution will be either stretched or compressed along the size axis according to the function

$$r = \frac{r_o^{\text{a}}}{\bar{r}_o^{\text{a-1}}},\tag{11}$$

where r_o is the original radius and $\bar{r_o}$ is the pore volume based average radius.

- 2. The exponent a determines if the distribution is stretched (a > 1) or compressed (a < 1).
- 3. Should the function be applied to pores or throats with radii greater than the volume based average (true 'T' or false 'F')?
- 4. Should the function be applied to pores or throats with radii less than the volume based average (true 'T' or false 'F')?

NEW RANDOM DISTRIBUTION (OPTION '5')

- 2. Minimum radius.
- 3. Maximum radius.
- 4. δ exponent (set to a negative number for a uniform distribution).
- 5. γ exponent (set to a negative number for a uniform distribution).

The third line of data contains some additional parameters.

- 1. Should the average throat length to radius ratio be maintained from the original network? If this is set to true ('T') all throat lengths will be scaled along with pore locations and absolute model size.
- 2. Should the new pore and throat size distributions be written to file (true 'T' or false 'F')? The files will be named *RadDist pores.csv* and *RadDist throats.csv*.
- 3. How many data points should there be in the distributions written to file?

```
MODIFY_RAD_DIST

1    ./hg_final.txt    -1.0    -1.0

2    -1.0    -3.0    0.2    3.0

T    T    50
#
```

MODIFY_G_DIST

In the same way that pore and throat size distributions can be modified, so can the various shape factors. Again, the first line of data refers to throats and the second to pores, and the various options for pores are identical to those for throats. Square (G = 1/16) and circular $(G = 1/4\pi)$ elements will not be modified. For triangular elements the maximum shape factor is $\sqrt{3}/36$ which represents an equilateral triangle.

1. There are 5 approaches available for how the shape factor distribution should be modified. Setting the index to '-1' will bundle the throats together with the pores or vice versa. So if the first line of data is set to '-1' the second line will apply to pores and throats, rather than just pores. Setting the index to '0' will result in nothing being done. The shape factor distribution can be read from file by setting the index to '1'. When setting the index to '3', each pore or throat shape factor will be multiplied by a constant factor. The shape of the shape factor distribution can also be stretched or compressed by setting the index to '4'. Finally, by setting the index to '5' the shape factors are randomly distributed, either uniformly or according to a truncated weibull distribution. For options 1 to 5 additional parameters are needed, but these are identical to those described for MODIFY_RAD_DIST and will not be repeated here. When applying (Error! Reference source not found.) to shape factors, \$\overline{G}_o\$ refers to the median rather than the volume based average. If the distributions are read from file, the second column refers to the quantitative fraction of pores or throats.

The third line contains some additional parameters.

- 1. Should the new pore and throat shape factor distributions be written to file (true 'T' or false 'F')? The files will be named *ShapeFactDist_pores.csv* and *ShapeFactDist_throats.csv*.
- 2. How many data points should there be in the distributions written to file?

```
MODIFY_G_DIST
-1
5 0.001 0.04811 -1.0 -1.0
F 50
#
```

MODIFY_CONN_NUM

The average coordination number of the network is very important for fluid connectivity and hence relative permeability. For a given network this can be reduced by removing throats.

- 1. Target coordination number. This should be less than the original (can be found from the .prt file).
- 2. Which throats should be removed? Four different options are available. Lowest volume ('volume'), smallest shape factor ('shape'), smallest radius ('radius') or selected at random ('rand').

```
MODIFY_CONN_NUM
4.0 radius
#
```

MODIFY_MOD_SIZE

By changing the absolute size of the network the absolute permeability will also change. All lengths will be scaled (pore positions, radii, volumes and lengths). In most cases it is however best to let the model size be scaled through the keyword MODIFY_RAD_DIST where the length to radius ratio is maintained from the original network.

1. Fractional change to the absolute size of the model.

```
MODIFY_MOD_SIZE
1.2
#
```

Examples of input data files

Water-wet Berea sandstone

```
SAT_TARGET
%finalSat maxPc maxDeltaSw maxDeltaPc calcKr calcI
        1.0E21
                            500000.0 T
500000.0 T
                 0.02
  0.00
                                                 F
  1.00 -1.0E21
                                                 F
                 0.02
INIT_CON_ANG
% min \max delta gamma 0.0 0.0 -0.2 -3.0
EQUIL_CON_ANG
% model min max delta gamma scheme m2_separation
  3 50.0 60.0 -1.0 -1.0 rand
                                      25.2
RES_FORMAT
 matlab
REL_PERM_DEF
% kr_def trpCond
 single F
SAT_COMPRESS
% kr_thres maxDeltaSw OilFlood WatFlood
   0.1 0.001 T
#
```

```
TRAPPING
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
               F
                                                    0.0E-30
        T
                                   Т
#
SOLVER_TUNE
% min memory scaling solver verbose conductance % tolerance factor output solver cut-off 1.0E-30 8 0 F 0.0
PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
                      F
PORE_FILL_ALG
 blunt2
PORE FILL WGT
0.0 18904 18904 18904 18904 18904
FLUID
% interfacial water oil water oil
                                                         water
\mbox{\tt \%} tension viscosity viscosity resist. resist. density density
% (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3) 30.0 1.05 1.39 1.2 1000.0 1000.0
CALC_BOX
0.5 1.0
NETWORK
% bin filename
 T ../Data/Berea
SAT COVERGENCE
% minNumFillings initStepSize nextStepSize maxIncr stable
                                          0.8 2.0 F
                         0.1
#
Water-wet sand pack
RAND SEED
 9512367
SAT_TARGET
%finalSat maxPc maxDeltaSw maxDeltaPc calcKr calcI
  0.00 16000.0 0.3 100000.0 F

1.00 -1.0E21 0.3 100000.0 F

0.00 16000.0 0.02 1000.0 T

1.00 -1.0E21 0.02 1000.0 T
                                                             F
                                                              F
                                                              F
                                                              F
#
```

```
SAT_COMPRESS
% kr_thres maxDeltaSw OilFlood WatFlood
  0.1 0.005
                      F
INIT_CON_ANG
            delta gamma
% min max
      0.0 0.2 3.0
0.0
EQUIL_CON_ANG
% model min max delta gamma scheme m2_separation 3 30.0 40.0 -1.0 -1.0 rand 25.2
RES FORMAT
 matlab
TRAPPING
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
       T F
                                               0.0E-30
                               т
RELPERM_DEF
% kr_def trpCond
residual F
SOLVER_TUNE
% min memory scaling solver verbose conductance
% tolerance factor output solver cut-off
  1.0E-30 7
                                      F
                                                   0.0
                             0
PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
     F
                   F
                                 20
#
PORE_FILL_ALG
blunt2
#
PORE_FILL_WGT
0 7473 7473 7473 7473 7473
FLUID
% interfacial water oil water
% tension viscosity viscosity resist. resist. density density % (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3) 70.25 0.97 0.018 1.2 1000.0 1000.0 1.22
#
CALC_BOX
0.50 1.00
```

Mixed-wet Berea sandstone

This is the data file used for the variable wettability case and $S_{wi} = 0.24$.

```
RAND SEED
6844625
SAT TARGET
%finalSat maxPc maxDeltaSw maxDeltaPc calcKr
                                                                        calcI

      0.24
      1.0E21
      0.20
      500000.0

      0.90
      -1.0E21
      0.015
      500000.0

      0.14
      1.0E21
      0.015
      500000.0

      0.91
      -1.0E21
      0.015
      500000.0

                                                            F
                                                                          F
                                          500000.0
                                                               Т
                                                                          F
                                                             Т
                                                                         F
                                                              Т
                                                                         F
INIT_CON_ANG
% min \max delta gamma 0.00 0.00 0.2 3.0
EQUIL_CON_ANG
   model min max delta gamma scheme m2_separation 3 50.0 60.0 -1.0 -1.0 rand 25.2
% model min max
FRAC CON ANG
% fraction volBased min max delta gamma 0.94 T 90.0 112.0 -10.0 -1.0
                                                        gamma
% method
   rMax
RES FORMAT
 matlab
TRAPPING
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
          T F
                                                              0.0E-30
                                     Т
SOLVER_TUNE
% min memory scaling solver verbose conductance
% tolerance factor output solver cut-off
   1.0E-30 8
                                       0
                                                   F
                                                                0.0E-35
```

```
PRS_BDRS
% calc kr using record press num press
% avg press profiles
                               profiles
                   F
    F
                                 50
PORE_FILL_ALG
 blunt2
PORE_FILL_WGT
 0.0 18904
             18904 18904 18904 18904
FLUID
% interfacial water
                        oil
                                 water oil
                                                 water
% tension viscosity viscosity resist. resist. density density
  (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3)
12.3 0.991 5.23 1.2 1000.0 1044.0 845.0
#
CALC_BOX
 0.50 1.00
NETWORK
% bin
              filename
       ../../Data/Berea_76pc_clay
```

Mixed-wet carbonate

This is the data file used for sample 2 with a lower oil-wet fraction.

```
SAT_TARGET
%finalSat maxPc
              maxDeltaSw maxDeltaPc calcKr
                                             calcI
                         500000.0
              0.20
                                   F
 0.220 1.0E21
                                              F
                 0.02
 1.000 -1.0E21
                           500000.0
                                       Т
                                              F
 0.030 1.0E21
                  0.02
                           500000.0
                                      F
                                              F
INIT_CON_ANG
% min max delta gamma
 0.0 0.0 0.2 3.0
EQUIL_CON_ANG
% model min max delta gamma scheme m2_separation
   3 25.0 65.0 -1.0 -1.0 rand
                                   25.2
FRAC_CON_ANG
% fraction volBased min max delta gamma
         T 80.0 82.0 -1.0
  0.65
                                    -1.0
% method
  rmin
```

```
RES_FORMAT
matlab
TRAPPING
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
       T F
                                  т
                                                   0.0E-30
#
SOLVER_TUNE
\% min memory scaling solver verbose conductance \% tolerance factor output solver cut-off 1.0E{-}40 7 0 F 0.0E-40
PRS BDRS
% calc kr using record press num press
% avg press profiles profiles
                      F
PORE_FILL_ALG
blunt2
PORE_FILL_WGT
0 844113 844113 844113 844113 844113
FLUID
% interfacial water oil water oil water oil
% tension viscosity viscosity resist. resist. density density
% (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3)
29.9 0.927 6.17 1.2 1000.0 829.3 1094.6
PRS_DIFF
% prsIn prsOut gravity
 1.0 0.0 T
CALC BOX
0.50 1.00
NETWORK
        filename
% bin
T ../../Data/Shell_carb_24
```

Mixed-wet sandstone

This is the data file used when using spatially correlated mixed-wetting.

```
SAT_TARGET
%finalSat maxPc maxDeltaSw maxDeltaPc calcKr
                                                        calcI
  0.000 1.0E21 0.20 500000.0
1.000 -1.0E21 0.01 500000.0
                                              F
                   0.01 500000.0
0.20 500000.0
                                                Т
                                                        F
                                               F
   0.000 1.0E21
                                                         F
INIT_CON_ANG
% min max delta gamma
  0.0 0.0 0.2
                     3.0
EQUIL_CON_ANG
% model min max delta gamma scheme m2_separation
  3 0.0 60.0 -1.0 -1.0 rand 25.2
FRAC_CON_ANG
                                     delta gamma
% fraction volBased min
                             max
            T 100.0
                             160.0 -1.0
                                              -1.0
   0.43
% method corrDiam
   corr
#
RES FORMAT
 matlab
TRAPPING
  Inject fluid from allow drainage water cond in entry exit of dangling ends filled circ elem
              F
                                               0.0E-30
SOLVER_TUNE
% \hspace{1cm} \text{min} \hspace{1cm} \text{memory scaling} \hspace{1cm} \text{solver} \hspace{1cm} \text{verbose} \hspace{1cm} \text{conductance}
% tolerance factor output solver cut-off
   1.0E-40
                              0
                                        F
                                                  0.0E-40
PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
                                  20
                     F
PORE_FILL_ALG
 blunt2
PORE_FILL_WGT
 0 33472 33472 33472 33472 33472
```

```
FLUID
% interfacial water
                         oil
                                  water oil
                                                 water
% tension viscosity viscosity resist. resist. density density % (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3) 30.0 1.05 1.39 1.2 1000.0 1000.0 1000.0
#
PRS DIFF
% prsIn prsOut gravity
  10.0 0.0
CALC_BOX
 0.50 1.00
NETWORK
% bin
              filename
       ../../Data/Shell_sst
MODIFY_PORO
% phi_eff phi_clay
  0.18
          0.09
Oil-wet sandstone
SAT_TARGET
%finalSat maxPc maxDeltaSw maxDeltaPc calcKr calcI
 0.03 1.0E21 0.20 500000.0 F
                                                    F
         -1.0E21
                              500000.0
                                            Т
 1.00
                   0.01
                                                    F
                                         F
                              500000.0
 0.03 1.0E21
                   0.20
                                                    F
INIT_CON_ANG
% min max delta gamma
20.0 60.0 -0.2 -3.0
EQUIL_CON_ANG
% model min max delta gamma scheme m2_separation
  3 70.0 123.0 -1.0 -1.0 rand 25.2
RES_FORMAT
 matlab
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
             F
                             Т
                                            0.0E-30
SOLVER_TUNE
% min memory scaling solver verbose conductance
                                              cut-off
% tolerance factor
                           output solver
  1.0E-40
               8
                             0
                                      F
                                               0.0E-40
```

#

```
PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
                     F
   F
                                     20
PORE_FILL_ALG
blunt2
PORE_FILL_WGT
0 24837 24837 24837 24837 24837
FLUID
% interfacial water oil water oil water oil
% tension viscosity viscosity resist. resist. density density
% (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3)
30.0 1.0 0.289 1.2 1000.0 1000.0 800.0
#
PRS_DIFF
% prsIn prsOut gravity
10.0 0.0 T
#
CALC_BOX
0.5 1.0
NETWORK
% bin
               filename
 T ../../Data/Statoil_sst_40avg
MODIFY_PORO
% phi_eff phi_clay
 0.153 0.0
#
```

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