numSCAL: Manual of Use

10th July 2017

numSCAL is a pore-scale numerical simulator that has been implemented using C++ and Qt technologies. The software is cross-platform and can be used on Windows, MacOS and Linux machines. Moreover, a Graphical User Interface (GUI) has been coded to allow fast access to the features provided by *numSCAL* (Figure 1) (although a console version is also available if the simulations are intended to run on a Linux supercomputer).

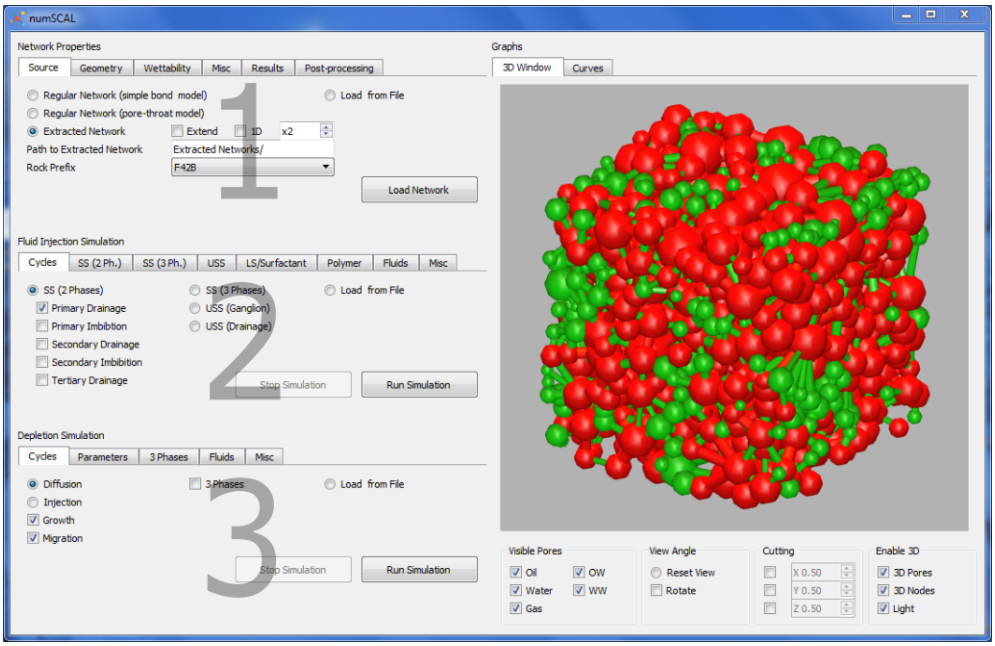

Figure 1: A screenshot of *numSCAL* software. (1) tabular section for loading the network (2) tabular section for running fluid injection simulations (3) tabular section for running depletion simulations.

A typical simulation workflow consists in two major parts: (1) generating the network (Figure 1 - 1) and (2) running a flow simulation on the network. The latter involves two subsets of simulations: (i) fluid injection (Figure 1 - 2) and (ii) depletion (Figure 1 - 3). We explain the main inputs required for each section in the following paragraphs.

1 Loading the Network

The first tabular section of *numSCAL* simulator is used to set the main inputs required to generate a pore network. We go through each tab separately.

Source (Figure 2)

This indicates the type of network we want to create.

- Regular Network (simple bond model): a network consisting of interconnected simple bonds elements.
- Regular Network (pore-throat model): a network consisting of nodes connected by throats.
- Extracted network: a network generated using microCT network files. These files need to be located in the "Path to extracted Network" folder. The rock prefix refers to the type of rock represented by the microCT files. By default, the simulator has access to numerous rock analogues downloaded from the Imperial College database
- Load from File: loads the last loaded network.

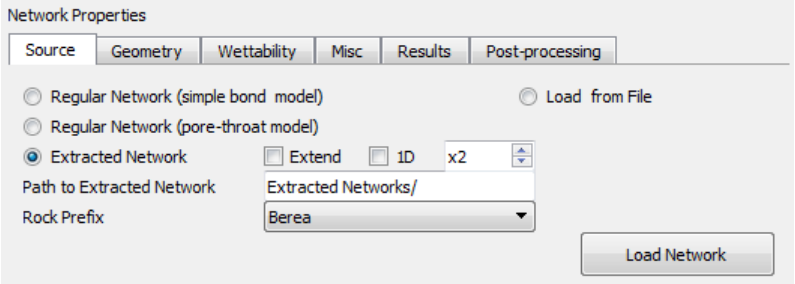

Figure 2: Network properties - Source.

Geometry (Figure 3)

- Nx, Ny, Nz: the number of nodes in each direction
- Seed: the seed number used when generating the radii of the capillaries.
- Min Radius, Max Radius (in μm): minimum and maximum values for the radii assigned to bonds (or throats). The assignment is performed according to various possible statistical distributions: Uniform, Rayleigh, Triangular, and Weibull.
- Vol. Cons. Vol. Cons, Cond. Cons. Cond. Exp.: these are the volume and conductivity constants and exponents used in the "3Rs" approach.
- Z: coordination number.
- Distort.: distortion factor.
- A. Ratio.: aspect ratio α. This parameter is used for regular networks with throats and nodes. Each node is assigned a radius r_n based on the following expression:

$$r_n = max(\alpha \frac{\sum_i^{nc} r_i}{n_c}, max(r_i)) \tag{1}$$

where i denotes the indices of the n_c neighbouring throats with corresponding radii r_i.

- Length (in μm): the average length of a bond (or throat) - only valid for regular networks.

Wettability (Figure 4)

- Wettability type: the user can select from various wettability configurations: water-wet, oil-wet, fractional-wet, mixed-wet small and mixed-wet large.
- Contact angles (deg): these are assigned by generating a random value between a minimum and a maximum value. For water-wet (oil-wet) elements, the contact angles must be between 0 and 90 (90 and 180).

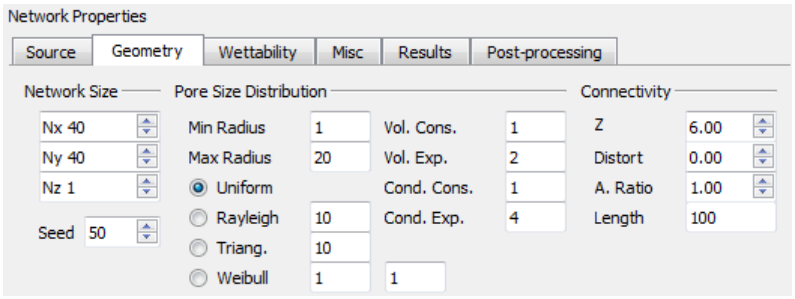

Figure 3: Network properties - Geometry.

- OW pores fraction: the fraction of oil-wet pores when a fractional-wet, mixed-wet small or mixed-wet large configuration is selected.
- Shape factor: the shape factor associated to the cross section of capillaries (only for regular networks). The default value corresponds to a circular cross section.

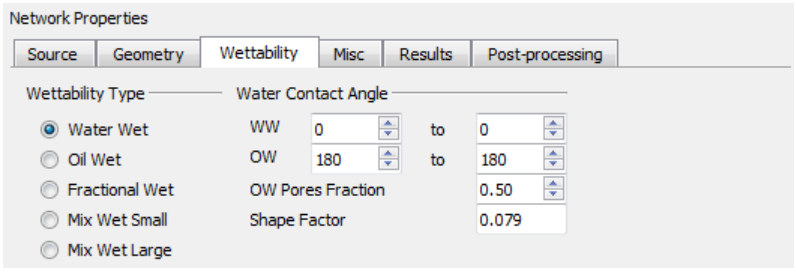

Figure 4: Network properties - Wettability.

Misc (Figure 5)

- Solver: the type of solver used for pressure calculation. The user can choose the Cholesky factorisation method (high precision, fast for 2D networks but can be slow for 3D ones) or BICSTAB (bi-conjugate gradient method - lower precision but fast for 3D networks).
- Extract data: when selected, the state of the network (the phase occupying each capillary element + tracer concentrations) is exported into text files in the folder "Results/Network_Status" at each time step.

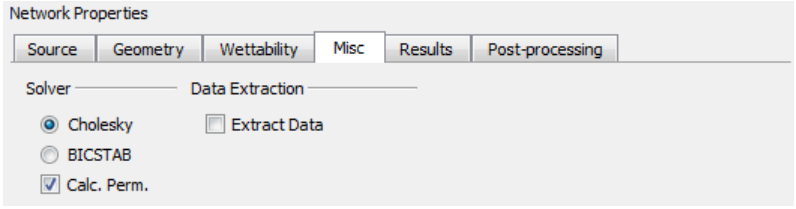

Figure 5: Network properties - Misc.

Results (Figure 6)

Once a network is loaded, some of its properties are displayed in this tab: absolute permeability (mDarcy), porosity, total number of pores (throats) and nodes.

- Save network image: this button allows to save a "png" image of the network displayed on the screen.

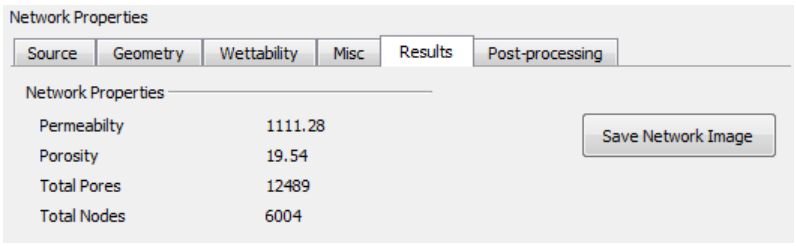

Figure 6: Network properties - Results.

Post-processing (Figure 7)

It is possible to recreate the network state after a simulation finishes. This proves to be useful when running the console version of *numSCAL* on Linux supercomputers.

- Render Network Status from Files: the user can recreate a single instant of the simulation by loading the corresponding data files (located in the folder "Results/Network_Status") into the simulator.
- Render a video from Files: the full simulation can be exported as an mp4 video by selecting this option.

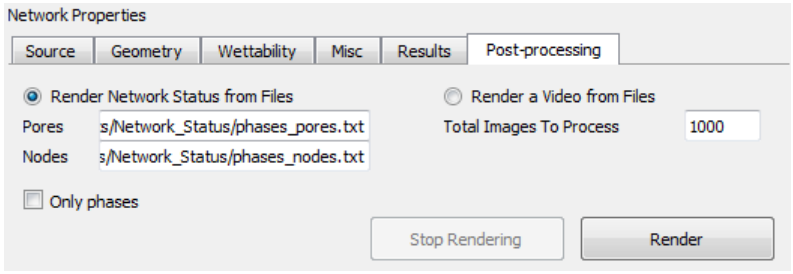

Figure 7: Network properties - Postprocessing.

2 Running a Fluid Injection Simulation

Once the network loaded, the user can run a wide variety of flow simulation.

Cycles (Figure 8)

This section lists the 4 processes that can be simulated:

- SS (2Phases): a steady-state simulation of alternate oil-water injection, where a full cycle of drainage and imbibition processes can be simulated.
- SS (3Phases): a steady-state simulation of three-phase flow. This includes WAG processes or a custom scenario defined in the "SS (3 Ph.)" tab.
- USS (Ganglion): simulation of unsteady state injection of water using the *numSCAL* ganglion module.
- USS (Fast): simulation of unsteady state injection of water using *the numSCAL* drainage module.

- Load from File: run a simulation with last used settings.

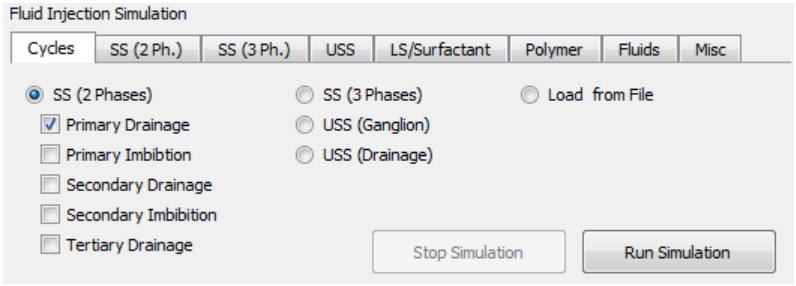

Figure 8: Injection simulation - Cycles.

Steady-State simulation (2 Phases) (Figure 9)

- Steps: the number of steps we use to discretise the drop (or increase) of capillary pressure in order to allow oil (or water) to displace all the accessible water (or oil) from the network.
- Ang. Inc. after Aging: the incremental value in contact angles (for Oil-Wet and Water-Wet capillaries) after primary drainage.
- Water/Oil films: a flag that signals whether fluids can escape from capillaries via film flow.

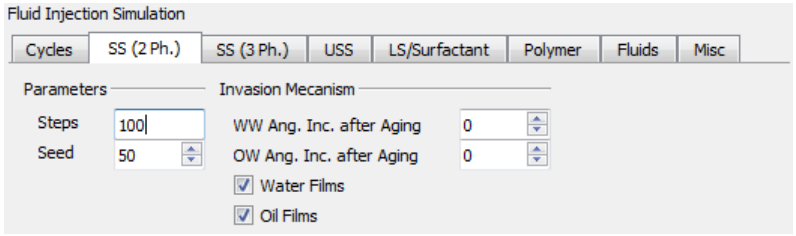

Figure 9: Injection simulation - Steady-State (2 phases).

Steady-State simulation (3 Phases) (Figure 10)

- 3 Phase experiments: the user can simulate a full WAG cycle or a custom scenario.
- No snap-off: this flag disables snap-off mechanism during the three-phase simulation.
- Stop at Breakthrough: this flag allows the simulation to stop when the invading phase reaches the outlet pores of the network.
- WAG cycle: each option denotes the process that occurs during the simulation. It is possible to repeat the full cycle for several times if the 'repeat' check box is selected.
- Custom: when a custom scenario is selected, the user can customise the initial defending phases (saturations can be specified in Fluids tab) and the invading phase.

Unsteady-state simulation (Figure 11)

- Flow rate (in $m^3 s^{-1}$): the volumetric rate of fluid flow through the entire network.
- Precision factor (between 0 and 1): the value denotes the critical test fraction used in the ganglion model.

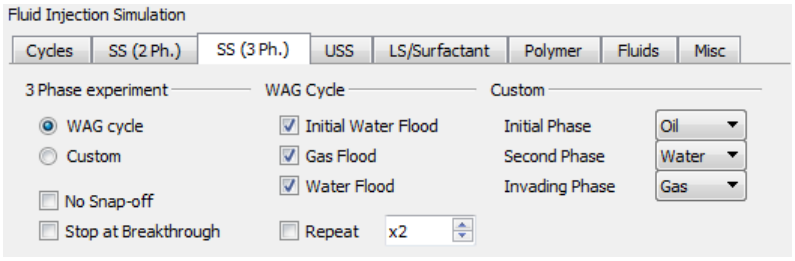

Figure 10: Injection simulation - Steady-State (3 phases).

- Simulation time (in s): the duration of the simulation process.
- Injected PVs: this option, when selected, override the simulation time option. The simulation stops when the number of specified pore volumes have been injected.
- Rate bump: when activated, the flow rate is multiplied by a selected factor (4 by default) after a specific duration of the simulation has elapsed (80% by default).

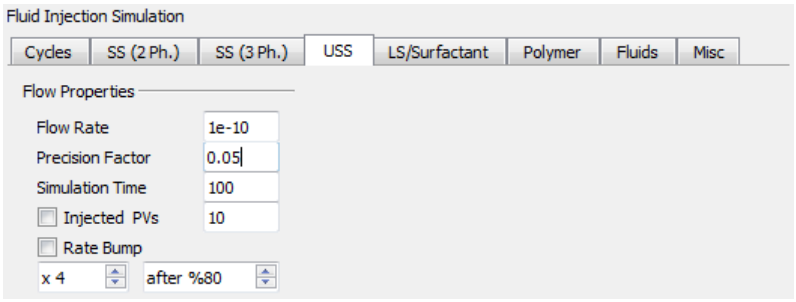

Figure 11: Injection simulation - Unsteady state.

Low Salinity (Figure 12)

- Secondary Injection: LS/Surfactant is injected in secondary mode.
- After Breakthrough: LS/Surfactant is injected in tertiary mode.
- After 1/2 Sim. Times. LS/Surfactant is injected after half of the simulation time has elapsed (or half of the chosen pore volumes have been injected).
- Remove after Breakthrough: LS/Surfactant water is replaced by HS water after breakthrough (only valid when LS is injected in secondary mode).
- Remove after 1/2 Sim. Time: LS/Surfactant water is replaced by HS water after half of the simulation time has elapsed.
- Angle change (in deg): the induced contact angle modification for a LS tracer concentration equal to 1 (salinity equal to 0).
- IFT change (in %): the induced IFT modification for a surfactant tracer concentration equal to 1.

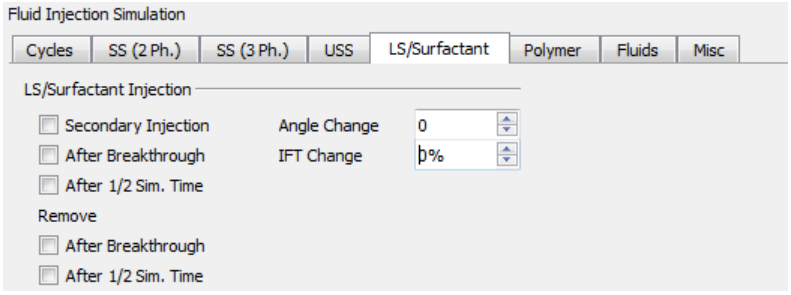

Figure 12: Injection simulation - Low salinity.

Polymer (Figure 13)

Most of the parameters here have similar functions to those described in the LS/Surfactant section. The parameters unique to polymer injection simulation are described below.

- Viscosity change (in cP): the induced water viscosity change for a polymer tracer concentration equal to 1.
- Microscopic diversion: capillaries with radii inferior to the value specified by "Crit. Radius" are shut when their polymer concentration reaches 1.

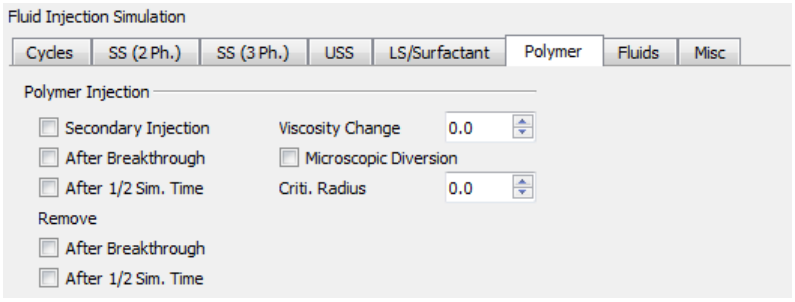

Figure 13: Injection simulation - Polymer.

Fluids (Figure 14)

This section includes the fluid properties used for all the simulations.

- Viscosities (in cP): for oil, water and gas.
- IFT (in dyn/cm): for oil-Water (OW), oil-gas (OG) and water-gas (WG).
- Sw: the initial water saturation. (For three-phase simulation - custom scenarios, this is the saturation of the second phase).
- Distribution of the Swi:
  - Random: the water occupies random capillaries.
  - Small: water occupies the smallest capillaries.
  - Large: water occupies the largest capillaries.
  - After PD: a primary drainage (oil invades a water-wet water-filled network) is simulated first until the specified Swi is reached.
- Aging: if this option is selected, capillaries filled with the initial water are assigned a water-wet angle (even when the network is oil-wet).

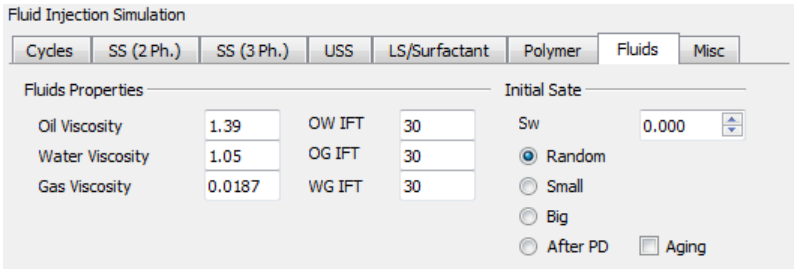

Figure 14: Injection simulation - Fluids.

Misc (Figure 15)

- Gravity ON: (experimental) a flag that let gravitational forces be included in the capillary entry pressure.
- Viscous Forces ON: (experimental) a pressure gradient is applied (P at inlet - P at outlet in Pa) across the network. The viscous drop across each capillary is included a a perturbation to the capillary entry pressure.
- R. Permeabilities: allows the calculation of relative permeabilities (this option is deactivated by default as it can slow down the steady-state simulations).
- Post-processing: the OpenGL screen is recorded in real time and the corresponding video is exported at the end of the simulation (located in Videos folder).

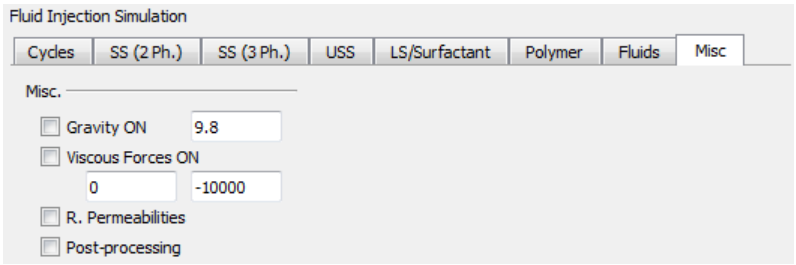

Figure 15: Injection simulation - Misc.

3 Running a Depletion Simulation

After loading the network, the user can also simulate a full depletion process by using the third tabular section of *numSCAL* software.

Cycles (Figure 16)

- Diffusion/Injection: the gas transfer mode into the nucleated bubbles.
- Growth: simulates bubble growth.
- Migration: simulates bubble migration. Only valid when gravity or viscous forces are activated.
- 3 Phases: needs to be selected for three-phase depletion processes - the three-phase module is called in that case.
- Load from File: run a simulation with last used settings.

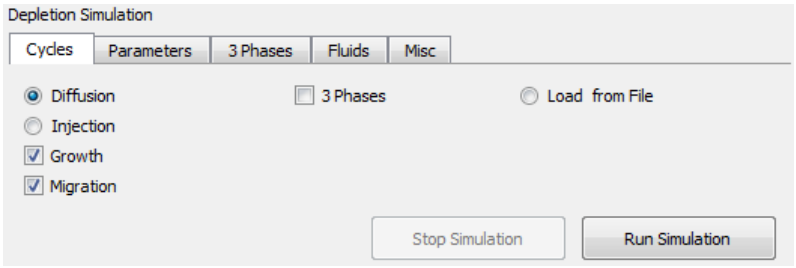

Figure 16: Depletion simulation - Cycles.

Parameters (Figure 17)

- BP Pressure (in psi): bubble point pressure.
- Dep. Rate (in psi/day): depletion rate.
- Dep. Time (in days): depletion time.
- Dep. Steps: the number of steps we use to discretise the pressure drop.
- Optimal Step: when selected, the minimum number of steps that ensures mass conservation is applied (might slow down the simulation).
- Injection rate (in $\mu g/day$): the mass of gas injected in the bubbles when injection mode is selected.
- Nucleation parameters: the user can select between instantaneous (IN) or progressive (PN) nucleation.
- Bubble Number: the number of bubbles nucleated using IN module.
- Min/Max Cavity Radius: cavities are assigned radii uniformly sampled between these two values when PN nucleation module is selected.
- Cavity Density: the number of pores per one cavity.
- Growth Parameters: the user can select between the multi-filling module (where gas invades multiple pores simultaneously) or the invasion percolation approach (where the accessible capillaries are sequentially invaded from the largest to the smallest).

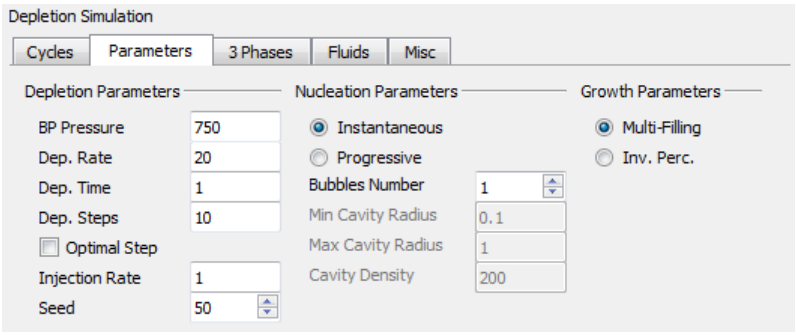

Figure 17: Depletion simulation - Parameters.

Fluids (Figure 18)

Most of the fluid options have similar functions to those described in the 'Fluid Injection' section. Those unique to depletion are described below.

- Oil Diff Coeff. (in $10^{-5}cm^2s^{-1}$): oil diffusion coefficient.
- Water Diff Coeff. (in $10^{-5}cm^2s^{-1}$): water diffusion coefficient.
- Data Folder: path to the folder that contains pressure-dependent data (viscosity, IFT, dissolved gas concentration, density, volume factor).
- Override with fixed values: when selected, pressure dependent data are overridden by the fixed values specified in this tab.

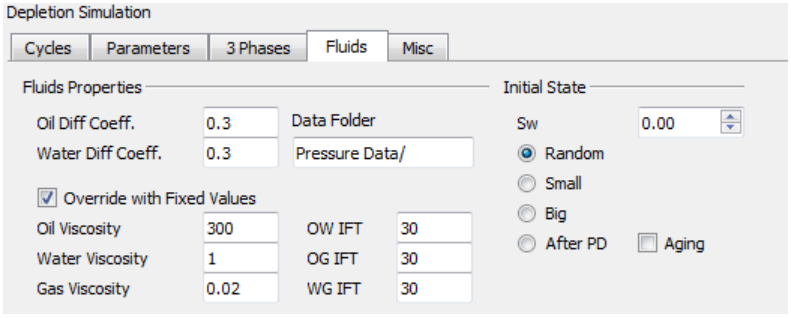

Figure 18: Depletion simulation - Fluids.

3 Phases (Figure 19)

These options have similar functions to those described in the 'Fluid Injection' section.

Figure 19: Depletion simulation - three-Phase.

Misc (Figure 20)

These options have similar functions to those described in the 'Fluid Injection' section.

4 Interacting with the Graphical Engine

numSCAL provides an interactive OpenGL screen that enables the user to observe in real time the running simulation on the underlying network. Moreover, more options are provided to allow the visualisation of specific phases or capillaries with specific wettability (Figure 21 - Visible Pores). It is also possible to display partial slices of the network to observe obstructed elements (Figure 21 - Cutting). Although the network elements are displayed in 3D by default, these can replaced by simple lines (Figure 21 - 3D) which can improve performance for very large networks.

Figure 20: Depletion simulation - miscellaneous.

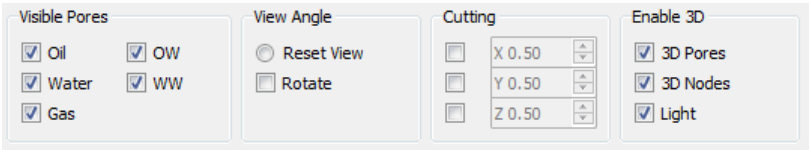

Figure 21: *numSCAL* Graphics Options.

numSCAL also provides a plotting window in order to minimise the interaction with third-party software. The user can readily display curves of the simulated data by pointing to the corresponding files and several options have been already included to customise the final figure (Figure 22).

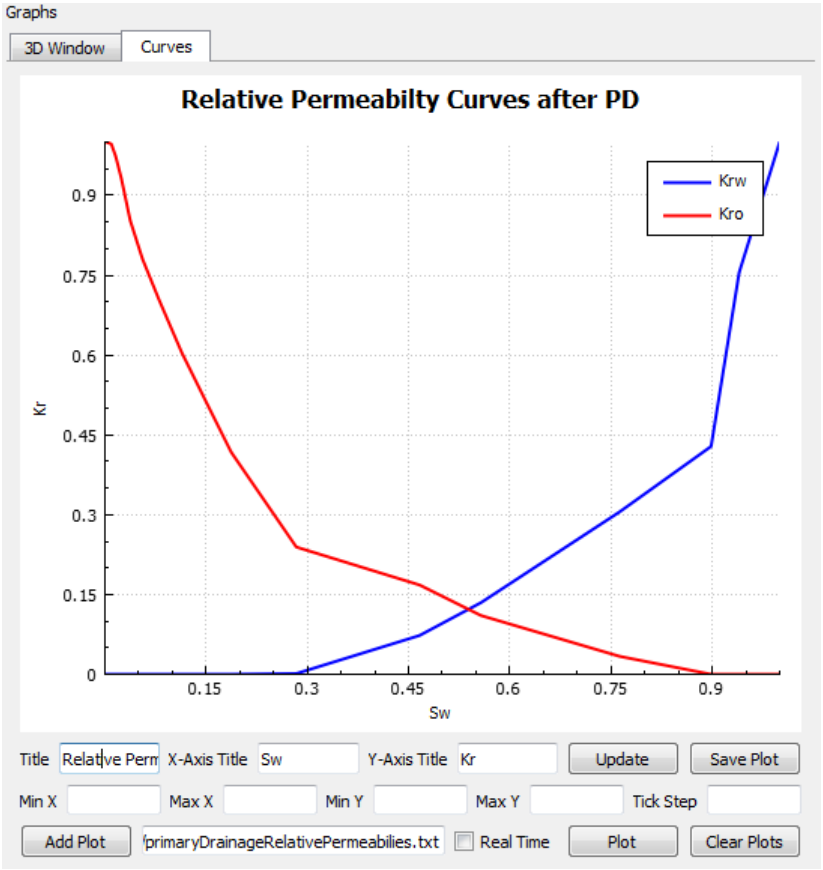

Figure 22: *numSCAL* Plotting Options.