14. Studio ScaleChem Chemistry

Aqueous Chemistry

The Studio ScaleChem chemistry uses the OLI Aqueous Model as well as the MSE model to predict the distribution of species. The OLI Aqueous Model is unique because it can predicatively model the speciation of a wide range of chemicals in water. Like other process simulation software, the OLI Aqueous and MSE Model consider the vapor-liquid equilibrium (VLE) of a given chemistry for the molecular species.

ScaleChem Standard Chemistry

ScaleChem Standard was developed with a specifically defined chemistry set. It is known as the Standard Chemistry Model.

As ScaleChem Standard use grew, users requested additional chemistry. From this development work, an Expanded Chemistry Model was created.

The Standard Chemistry Model

As originally developed, the Standard Chemistry model contained a vapor phase, an aqueous phase and a limited number of solid phases.

Standard Chemistry: Aqueous phase

Na^{+}, K^{+}, Ca^{+2}, Mg^{+2}, Fe^{+2}, Ba^{+2}, Sr^{+2}
Cl^{-}, SO_4^{-2}, HCO_3^{-}, HS^{-}, $B(OH)4^{-}$, $CH3COO^{-}$
H_2S^{o}, CO_2^{o}, SiO2, B(OH)3, CH_4^{o}

Standard Chemistry: Vapor phase

H_2O, H_2S, CO_2, CH_4

Standard Chemistry: Solid phases

anhydrite	$CaSO_4$	barite	$BaSO_4$
calcite	$CaCO_3$	gypsum	$CaSO_4.2H2O$
siderite	$FeCO_3$	pyrrhotite	FeS
halite	NaCl	celestite	$SrSO_4$

Disordered Dolomite ($CaMg(CO_3)_2$), or simply dolomite is not the Standard Chemistry but is represented as an inflow only species in the expanded chemistry.

Dolomite is not considered to be a possible scaling solid under most oil field operations.

The Expanded Chemistry Model

Expanded Chemistry: Aqueous phase

This includes the Standard model plus:
Cations: H^+, Cs^+, Zn^{+2} Pb^{+2}, Ni^{+2}, Cu^+, Cu^{+2}, NH_4^+, Fe^{+3}, Al^{+3},
Anions: OH^-, F^-, Br^-, $H_2SiO_4^-$, $H_3SiO_4^-$, SO_3^{-2}, S^{-2}, CO_3^{-2}, NO_3^-, NO_2^-, $COOH^-$, $C_3H_7COO^-$ $C_4H_9COO^-$ $C_5H_{11}COO^-$
Organic acids: formic, acetic, propanoic, butanoic, pentanoic
Alcohols: methanol, ethanol, ethylene glycol,
Mineral Acids: HF, HCl, H2SO4, HBr, HNO3, H2SO4,
Hydrocarbons: methane, ethane, and propane
Other: NH3, N2, CO2

Expanded Chemistry: Vapor phase

This includes the Standard Model plus:
Ethane, propane, butane, isobutane, pentane, isopentane, hexane, cyclohexane, heptanes, octane, isooctane, nonane, and decane

Expanded Chemistry: Solid phases

The Expanded Solids phases include fifty-nine solids that are practical to oilfield operations. This allows solids analysis from the new cations and anions which have been added.

Expanded solids is automatically accessed when using the expanded chemistry. It can also be accessed for the standard chemistry by using the radio buttons on the Precipitates Page, in any Scaling request.

Scaling tendencies for every solid with a scaling tendency > 1.0E-05 are reported for a calculation using expanded solids.

Hydrocarbon Petroleum Fractions

Frequently a hydrocarbon analysis is the only data available for entry into the software. This analysis is usually a distillation curve where the volume distilled as a function of temperature of a petroleum fraction has been analyzed. This information must be turned into a vapor, organic and aqueous component for use in the simulator.

ASTM D86

Used for light and medium crudes, and is carried out at atmospheric pressure. The results are converted internally in the OLI model generator to a TBP (True Boiling Point) Curve. This curve is fit to a spline to smooth the curve. The cuts are taken from the spline.

ASTM D1160

Used for heavier crudes, and is carried out under vacuums as low as 1 mm Hg. The results are converted internally in the OLI model generator to a TBP Curve. This curve is fit to a spline. The cuts are taken from the spline.

ASTM D2887

Uses gas chromatography to produce the distillation curve and is applicable to a wide range of petroleum products. The results are reported on a volume percent basis. The results are converted internally in the OLI model generator to a TBP Curve. This curve is fit to a spline. The cuts are taken from the spline

TBP

This is the true boiling point curve. These curves, in practice, are difficult to obtain. The other methods are usually used instead.

Density

The density units for the average bulk density are:

Specific Gravity

Unitless

Degrees API (°API)

This is calculated via the following equation:

$$°API(60F) = \left(\frac{141.5}{s.g.(60F)}\right) - 131.5$$

where, SG is the specific gravity at 60 °F.

Watson K

The Watson K has no units but is calculated via:

$$K = \left(\frac{NBP^{1/3}}{SG}\right)$$

where NBP is the normal Boiling point.

Thermodynamic Methods (pseudo-components and petroleum fractions)

API Uses the specific gravity to estimate the critical parameters. The specific gravity, if not entered, can be estimated from the API gravity or the Watson K. The boiling points are taken from the assay data.

Cavett This method uses the API gravity method to determine the critical properties. The API gravity, if not entered can be estimated from the actual specific gravity or the Watson K. The boiling points for the pseudo-components are taken from the assay.

Lee-Kesler This method uses the Watson K and the specific gravity (which can be estimated via the Watson K) to determine the critical parameters.

Summary

The use of a full speciation model allows for more accurate calculations. Using just a simple vapor-liquid equilibrium approach is not valid for aqueous systems.