Geochemical consistency between subsurface-wells-surface applications

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Reactive transport modelling (RTM) is becoming more recognized as a tool in the oil and gas industry. This is mainly due to increasing importance of subsurface projects involving production and injection of more reactive fluids and gases, for example storage of CO_2 and H_2S, enhanced oil recovery (EOR), and water flooding. Several years ago, the in-house Shell reservoir simulator MoReS was coupled to *PHREEQC*. This enhances development and deployment of RTM at elevated pressure (*P*) and temperature (*T*) conditions encountered in subsurface reservoirs. *OLI Stream Analyzer* (OLI) is currently the standard tool in Shell for computing chemical reactions and phase partitioning of solids, fluids, and gases in wells and downstream applications (production chemistry). The aim of this work is to develop a *PHREEQC* geochemical database, consistent with OLI, to enable consistent integrated modelling.

We used OLI to compute the equilibrium constant (*K*) as a function of temperature (*P*=1 bar) for approximately 500 geochemical reactions. The results were fitted to a polynomial expression that *PHREEQC* uses to compute the *T*-dependence of *K*. The results were validated by computing *K* using the Helgeson-Kirkham-Flowers (HKF) model. Parameters for *P*-dependency were directly mapped. The activity model is part of the Mixed Solvent Electrolyte (MSE) framework in OLI, based on long-range, mid-range, and short-range interactions. Activity model parameters were directly mapped and the source code of *PHREEQC* was modified accordingly. Simulations with *PHREEQC* were run using the converted geochemical database. All operations described above were carried out using a *MATLAB* script.

Saturation indices (SIs) and molar amounts of various species were computed using OLI and *PHREEQC* in a wide *P*,*T*, and salinity range. The results demonstrate that the geochemical database conversion was carried out properly. The developed workflow enables implementation of new experimental results into the *PHREEQC* geochemical database. This will enhance deployment of RTM technology in the oil and gas industry.