A geochemical database for integrated subsurface-wells-surface applications

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Subsurface storage of CO_2 is a potential technology to reduce carbon footprint and mitigate global warming. Regulations require geochemical assessment of the impact of CO_2 injection for specific target sites to ensure long-term integrity and containment of CO_2. In the storage complex a substantial amount of injected supercritical CO_2 partitions into the formation brine. This subsequently causes a lower pH and further geochemical alteration of the reservoir fluids and rock. Reactive transport modelling (RTM) couples gas and fluid flow with geochemical reactions, and is thereby able to predict reservoir rock alterations to assess reservoir integrity The in-house Shell reservoir simulator was recently coupled with open source geochemical software *PHREEQC*, enabling development and deployment of RTM for various applications. The software was successfully benchmarked with *TOUGHREACT*, which is important for confidence in simulation results. However, it is known that various geochemical databases lead to quantitatively different results even using the same simulator. At the same time geochemical data is used across many disciplines straddling the entire workflow (i.e. subsurface/wells/surface), involving different engineers. The aim of this work is to provide end users in our integrated projects with one consistent geochemical database.

We obtained geochemical input data from *SUPCRT92*. We compared these data with laboratory measurements and data from the commercial software *OLI Stream Analyzer*, which is frequently used for our well/surface applications. The Helgeson-Kirkham-Flowers (HKF) model was built into *MATLAB* and equilibrium constants (K) for relevant reactions were computed as a function of temperature. The data were then fitted according to a polynomial model used by *PHREEQC*, while pressure dependency parameters were mapped directly. The default activity model parameters from *PHREEQC* were used.

The constructed geochemical database was tested using our in-house RTM simulator and speciation results were compared with those from *OLI Stream Analyzer*. The database was then applied to simulation of a relevant CO_2 storage case study. Future RTM applications will not be limited to such cases, but will be further deployed in other developments in the oil and gas industry, such as H_2S storage and enhanced oil recovery.