Geophysical Research Abstracts
Vol. 19, EGU2017-19053, 2017
EGU General Assembly 2017


# Modelling of clay diagenesis using a combined approach of crystalchemistry and thermochemistry: a case study in the smectite illitization.

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Diagenetic transformations occurring in clayey and arenaceous sediments is investigated in a number of hydrocarbon reservoirs with an integrated approach that combines mineralogical analysis, crystalchemistry, estimation of thermochemical parameters of clay minerals, and geochemical modelling.
Because of the extremely variable crystalchemistry of clays, especially in the smectite – illite compositional range, the estimation of thermochemical parameters of site-specific clay-rich rocks is crucial to investigate water-rock equilibria and to predict mineralogical evolutionary patterns at the clay-sandstone interface. The task of estimating the thermochemical properties of clay minerals and predicting diagenetic reactions in natural reservoirs is accomplished through the implementation of an informatized, procedure (IP) that consists of:
(i) laboratory analysis of smectite, illite and mixed layers (I/S) for the determination of their textural characteristics and chemical composition; (ii) estimation of the thermodynamic and structural parameters (enthalpy, entropy, and free energy of formation, thermal capacity, molar volume, molar weight) with a MS Excel tool (XLS) specifically developed at the French Bureau of Geological and Mining Researches (BRGM); (iii) usage of the SUPCRT (Johnson et al., 1992) software package (thereinafter, SSP) to derive log K values to be incorporated in thermodynamic databases of the standard geochemical codes; (iv) check of the consistency of the stability domains calculated with these log K values with relevant predominance diagrams; (v) final application of geochemical and reactive transport models to investigate the reactive mechanisms under different thermal conditions (40-150°C). All the simulations consider pore waters having roughly the same chemical composition of reservoir pore waters, and are performed with The Geochemist Workbench (Bethke and Yeakel, 2015), PHREEQC (Parkhurst, 1999) and TOUGHREACT (Xu, 2006).

The overall procedure benefits from: (i) (minor) improvements of the I/O structure of the SSP; (ii) the development of a suite of python scripts to automate the steps needed to augment the thermodynamic database by integrating the external information provided by potential users with the XLS tool and the SSP; (iii) the creation of specific outputs to allow for more convenient handling and inspection of computed parameters of the thermodynamic database.

A case study focused on non-isothermal smectite–illite transformation is presented to show the capability of our numerical models to account for clay compaction under 1D geometry conditions. This model considers fluid flow driven by the compaction of a clay layer, and chemistry-fluid flow mutual feedback with the underlying sandstone during the advancement of the diagenesis. Due to this complex interaction, as a result of the smectite-illite transformation in the clays, significant quartz cementation affects the sandstone adjacent to the compacting clay.