Geophysical Research Abstracts
Vol. 19, EGU2017-10568, 2017
EGU General Assembly 2017

Geochemical simulation of fluid rock interactions to predict flowback water compostions during hydraulic fracturing

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Black shales are a heterogeneous mixture of minerals, organic matter and formation water and little is actually known about the fluid-rock interactions during hydraulic fracturing and their effects on composition of flowback and produced water. Geochemical simulations have been performed based on the analyses of "real" flowback water samples and artificial stimulation fluids from lab experiments with the aim to set up a chemical process model for shale gas reservoirs.
Prediction of flowback water compositions for potential or already chosen sites requires validated and parameterized geochemical models. For the software "Geochemist's Workbench" (GWB) data bases are adapted and amended based on a literature review. Evaluation of the system has been performed in comparison with the results from laboratory experiments. Parameterization was done in regard to field data provided. Finally, reaction path models are applied for quantitative information about the mobility of compounds in specific settings.
Our work leads to quantitative estimates of reservoir compounds in the flowback based on calibrations by laboratory experiments. Such information is crucial for the assessment of environmental impacts as well as to estimate human- and ecotoxicological effects of the flowback waters from a variety of natural gas shales. With a comprehensive knowledge about potential composition and mobility of flowback water, selection of water treatment techniques will become easier.