Computer simulation of subsurface drip irrigation using coalbed methane produced waters

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Development of coalbed methane (CBM) as an energy resource typically requires extraction of large volumes of water from underground coal seams. In the semiarid Powder River Basin of Wyoming and Montana, some of the CBM water is put to beneficial use through use for irrigation. Careful management is necessary due to high conductivites (2-3 mS cm^{-1}), high sodium adsorption ratios (SAR = 20-50) and sodium-bicarbonate composition of the water. One management strategy is deep subsurface drip irrigation (SDI), where drip tapes are placed ~92 cm below the surface in conjunction with a deep-rooted crop like alfalfa. CBM water is acidified to reduce alkalinity prior to application and is applied to fields year-round.

We are using computer simulations to help understand and predict effects of chemical and physical processes as native and introduced salts mix in soils of SDI fields. Spatial and temporal distributions of water and solutes in the soil are being simulated by using the computer program VS2DT. Geochemical modeling with the program PHREEQC suggests dissolution of native gypsum (0 to 4 wt. %) provides a short-term source of Ca to mitigate adverse effects of Na in soil solution. Detrital and pedogenic carbonate minerals (1 to 6 wt. %) should provide longer-term sources of Ca and Mg. Soil pCO$_2$ influences the concentration of Ca via calcite solubility and will influence the SAR of soil solution and resulting soil structure. Model predictions are being evaluated using field data from moisture and conductivity sensor arrays and soil pCO2 measurements, as well as laboratory data on soil chemistry, mineralogy, and texture. Computer simulations can help predict the long-term fate of introduced solutes and the functioning of similar SDI systems in other settings or climates.

Multiscale study of gas shale properties and thermal evolution

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Gas shales will greatly expand worldwide energy supply. These geological formations of economic significance constitute unconventional self-contained source-reservoir systems of gas accumulation. Generated gas can be stored as free gas in porosity and fractures, adsorbed onto kerogen and clay particles or dissolved in kerogen and bitumen [1]. Currently, worldwide exploration activities of potential shale gas are drastically increasing. However, the chemical and structural variability of gas shales at the submicrometer scale is still poorly documented. Consequently, hydrocarbon generation and retention processes occurring within such unconventional systems are still poorly constrained.

As part of the European GASH project (GAs SHales) coordinated by the GFZ-Potsdam, organic-rich calcareous mudstone samples from Northern Germany at varying stages of thermal maturation have been characterized using an original combination of compositional organic geochemistry and spectromicroscopy techniques, including synchrotron-based STXM (scanning transmission X-ray microscopy) [2]. STXM is currently the only available method that allows *in situ* imaging of organic-rich samples with a chemical-based contrast at a 30-nm spatial resolution while providing spatially-resolved information of organic constituent speciation.

Within the selected gas shale samples, we document multi-scale chemical and mineralogical heterogeneities, from the millimeter down to the nanometer scale. Different types of bitumen, genetically derived from thermally degraded organic precursors, have been detected in close association with authigenic minerals. These observations provide key constraints on the thermal history of this gas shale formation and shed new light on the influence of the organic precursor chemistry on the thermal generation of the various organic moieties which can be encountered in gas shales. Overall, we show that the multi-scale and multi-technique methodology used in this study, including STXM, may help to better constrain the factors controlling gaseous hydrocarbon production within such complex systems.

[1] Jarvie *et al*. (2007) *AAPG*. **91**, 475–499. [2] Bernard *et al*. *Chemie der Erde - Geochemistry*, submitted.