Geophysical Research Abstracts
Vol. 17, EGU2015-12984-1, 2015
EGU General Assembly 2015

Interactive Visual Analytics Approch for Exploration of Geochemical Model Simulations with Different Parameter Sets

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Many geoscience applications can benefit from testing many combinations of input parameters for geochemical simulation models. It is, however, a challenge to screen the input and output data from the model to identify the significant relationships between input parameters and output variables. For addressing this problem we propose a Visual Analytics approach that has been developed in an ongoing collaboration between computer science and geoscience researchers.

Our Visual Analytics approach uses visualization methods of hierarchical horizontal axis, multi-factor stacked bar charts and interactive semi-automated filtering for input and output data together with automatic sensitivity analysis. This guides the users towards significant relationships. We implement our approach as an interactive data exploration tool. It is designed with flexibility in mind, so that a diverse set of tasks such as inverse modeling, sensitivity analysis and model parameter refinement can be supported. Here we demonstrate the capabilities of our approach by two examples for gas storage applications.

For the first example our Visual Analytics approach enabled the analyst to observe how the element concentrations change around previously established baselines in response to thousands of different combinations of mineral phases. This supported combinatorial inverse modeling for interpreting observations about the chemical composition of the formation fluids at the Ketzin pilot site for CO_2 storage. The results indicate that, within the experimental error range, the formation fluid cannot be considered at local thermodynamical equilibrium with the mineral assemblage of the reservoir rock. This is a valuable insight from the predictive geochemical modeling for the Ketzin site.

For the second example our approach supports sensitivity analysis for a reaction involving the reductive dissolution of pyrite with formation of pyrrothite in presence of gaseous hydrogen. We determine that this reaction is thermodynamically favorable under a broad range of conditions. This includes low temperatures and absence of microbial catalysators.

Our approach has potential for use in other applications that involve exploration of relationships in geochemical simulation model data.