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Evaluation of Predictive Subsurface Transport Models – How to compare?

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Subsurface transport models are valuable tools to predict the behavior of solutes in groundwater, e.g. after a spill event or of controlled tracer experiments. Solute movement does not only depend on the mean flow velocity, but its spreading is strongly influenced by the spatially variable distribution of hydraulic conductivity i.e. on heterogeneity. The prevailing lack of transport data at the given site usually prevents model calibration. Thus, there is a need for predictive models based on knowledge of the subsurface structure. A multitude of aquifer heterogeneity conceptualizations exist, from deterministic hydraulic conductivity structures to stochastic and geostatistical approaches such as Multi-Gaussian or multi-indicator models. These concepts have been applied to model tracer distribution patterns of controlled field-scale transport experiments at a few sites.

One of the critical questions is "How should transport models be compared to observed data?". There are multiple influencing factors and thus the method of comparing impinges on the outcome. We discuss significant aspects like:

- What are meaningful indicators for a quantitative comparison?
- What are pros and cons of a qualitative/visual comparison?
- What is the impact of data preparation with regard to the scale (linear/log) and mass recovery?
- What is the area of interest? Is the emphasis on predicting the mean, the peak concentration, the tail or the leading front?
- Is the evaluation in time (BTC) or in space (mass distribution) the preferred mode? Given the different aspects of relevance, we emphasize that there is no straight forward way of comparing and the evaluation of models depends on the goal-orientation.

To illustrate the issue we present examples from the MADE site. The aquifer is known to display a complex transport behavior which was monitored in detailed experiments. Multiple predictive transport models are available for the site with conductivity conceptualization ranging from deterministic to stochastic and geostatistical. The different concepts make use of the multitude of available data obtained by distinct methods like DPIL, litho-logs, pumping tests, or flowmeter logs. The comparison of predictive transport models for the MADE site provides valuable insights to merits and drawbacks of several hydraulic conductivity models given a specific goal-orientation.