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History matching of large-scale reactive transport problem based on deterministic and stochastic approaches

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Optimization of subsurface applications often constitutes large parameter estimation problem, i.e. inverse problem which can be solved by deterministic and stochastic approaches. Gradient-based algorithms are widely used to estimate parameters. However, the cost of numerically approximated gradient increases linearly with the number of adjusted parameters, making it intractable for large-scale problems. The adjoint-state method is a well-known approach to overcome this issue and is widely applied in hydrology for example. Still, the reactive problem consists of numerous partial differential and nonlinear algebraic equations of transport and chemistry that can be coupled in different ways, making the derivation and the implementation of the adjoint operator challenging.

This work presents an efficient and elegant approach based on the adjoint state to compute the gradient of the loss function. This approach is implemented in a reactive transport code HYTEC [1], which is based on a sequential iterative approach (SIA). By construction, solving the adjoint problem requires a corresponding SIA structure. Both spatial and time discretization methods should be considered. The discrete adjoint-state derivation accurately represents the gradient showing more consistent results than the continuous derivation. The developed approach is illustrated on a large-scale saturated reactive transport problem with heads and concentrations used as observations. This approach allows to estimate various parameters (porosity, diffusion, dispersion, permeability, mobile and immobile concentrations etc). Several benchmark studies were performed to compare a performance of the adjoint-based method, geostatistical and stochastic approaches.

[1] van der Lee, de Windt, Lagneau, and Goblet (2003), Computers & Geosciences 29, 3 (2003), 265–275.