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A general approach for reactive transport simulations in stiff geochemical/biogeochemical systems

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The integration of reaction transport models (RTMs) with detailed geochemical/biogeochemical reaction mechanisms has largely improved the prediction accuracy of RTMs. However, the reaction mechanism in most of the geochemical/biogeochemical systems is very complex and is characterized by a wide range of timescales, which creates stiffness to the models. Since the stiffness would significantly enhance the numerical oscillations in the solving process, the stiff geochemical/biogeochemical RTMs are especially difficult for simulation and require extra approach to reach accurate numerical solutions in reasonable computational time. The correct and efficient simulation of such stiff models is fundamental to better understands numerous natural geochemical/biogeochemical processes and designs environmental remediation plans. Currently, there is still a lack of research on overcoming this dilemma.

In this study, we have developed a new general approach to simulate the stiff geochemical/biogeochemical RTMs based on the computational singular perturbation. This approach can reformulate the geochemical/biogeochemical reaction mechanisms by decoupling fast and slow reactions regardless of reactions type and complexity. All decoupled fast reactions were assumed to be in the quasi-steady. With the reformulation of reaction terms, the stiffness was reduced and computational costs were also cut down to a reasonable range. The new approach was implemented in a validated RTM for describing hydrogen peroxide production in riparian aquifers. Compared to the previous simulation, the computational efficiency had been increased by about 40 times while maintaining accuracy.

This new approach is universal and the mathematical rigor of that has been proven. The computer program of this approach was coded by Python, and it can be employed by many existing geochemical/biogeochemical simulation software. This approach significantly facilitated the integration of RTMs and reaction mechanisms and expanded the application scenarios of reactive transport models in earth sciences.