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CompReact - Enhancing CO_2 Storage Simulation with Advanced Geochemical Modeling

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Carbon dioxide storage in geological formations is pivotal for mitigating greenhouse gas emissions due to its potential to reduce emissions from the hard-to-abate industries. However, this process triggers complex physical and chemical interactions underground, spanning various time and length scales. Accurate modeling is essential for estimating storage capacities, identifying operational risks, and ensuring long-term storage safety. The CompReact project aims to enhance CO_2 storage simulations through advanced geochemical modeling, with a focus on integrating a robust compositional algorithm into the open-source reservoir simulator GEOS developed by Stanford University, LLNL (Lawrence Livermore National Laboratory), and TotalEnergies.

The project comprises two main steps: the development of a novel compositional CO_2 storage module incorporating a newly developed multiphase geochemical algorithm, and the subsequent integration of the module into the GEOS. The first step lies in a novel RAND-based multiphase reaction algorithm that can treat phase and chemical equilibrium simultaneously, which is especially suited to CO_2 storage simulation involving many speciation and mineral precipitation reactions. The developed module will conduct simultaneous equilibrium calculations, thereby improving robustness and efficiency. The second step focuses on enhancing the compositional capabilities in GEOS. GEOS currently has limited compositional features and no geochemical calculation. By integrating the module into GEOS, the simulation and long-term prediction of compositional and geochemical effects during post-injection analysis will become feasible.

Accurate geochemical modeling is vital due to the complex chemical interactions during geological CO_2 storage, such as mineral dissolution and precipitation. These chemical processes are intertwined with species transport and fluid flow in porous media. Therefore, enhancing reactive transport modeling of these coupled processes would improve simulation accuracy.

Several challenges exist in integrating reactive transport and chemical processes. The complexity of the geochemical systems increases with multiphase flow and transport and the system non-ideality. Another challenge is the scale dependence of various processes, necessitating consideration of heterogeneity effects and effective reaction rates during upscaling from pore to field scale. Furthermore, achieving numerical stability and efficiency is always a challenge. These RAND-based multiphase reaction algorithms partly address these challenges through simultaneous treatment of chemical and phase equilibria. Additionally, the algorithms will be designed for GPU computation deployment, and GEOS with an integrated reactive transport module will allow for high-performance computing, leveraging parallel computing for large scale simulations.