Goldschmidt 2023 Abstract
https://doi.org/10.7185/gold2023.19889

Multiphase multicomponent reactive transport and flow with HYTEC for gas storage applications

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Efforts have been done to deal with multiphase and multicomponent in our homemade reactive transport and flow simulator HYTEC since 10 years mainly around underground CO2 storage applications [1-4]. These improvements (i.e. a proper Peng-Robinson Equation Of State for the gas phase and an adapted numerical coupling scheme using operator splitting approach, among others), allow to consider:

- multi-components non-ideal gas mixtures and their interactions with water and highly concentrated brines,
- the potential reactivity of dissolved gas compounds (with minerals, bacteria...),
- the complex physical behavior of multiphase fluids including their interaction overcoming the induced coupling and numerical stability problems.

We verified our developments step by step using:

- solubility and reactivity batch experiments [1,5-8],
- some benchmark exercises [3-8],
- and field cases of CO2 and impurities co-injection [3-4].

These last simulations, even though numerically demanding, show the ability of our approach to model highly coupled physical processes related to complex phase composition such as density driven flow and chromatographic partitioning. HYTEC is now able to simulate realistic scenarios of not only CO2, but also compressed air [9], biomethane and H2 underground storage in various environments (e.g. saline aquifers, salt caverns, basalts...).

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