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GPSFLOW: A Novel Simulator for Modelling Underground Hydrogen, CO₂ and Gas Mixture Storage

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Underground hydrogen storage can store grid-scale energy for balancing both short-term and long-term inter-seasonal supply and demand. However, there is no numerical simulator which is dedicated to the design and optimisation of such energy storage technology at grid scale. This study develops novel simulation capabilities for GPSFLOW (**G**eneral **P**urpose **S**ubsurface **F**low Simulator) for modelling grid-scale hydrogen and gas mixture (e.g., H₂-CO₂-CH₄-N₂) storage in cavern, deep saline aquifers and depleted gas fields.

The accuracy of GPSFLOW is verified by comparisons against the National Institute of Standard and Technology (NIST) online thermophysical database and reported lab experiments, over a range of temperatures from 20-200 °C and pressure up to 1000 bar. The simulator is benchmarked against an existing model for modelling pure H₂ storage in a synthetic aquifer. Several underground hydrogen storage scenarios including H₂ storage in a synthetic salt cavern, H₂ injection into a CH₄-saturated aquifer experiment, and hydrogen storage in a depleted gas field using CO₂ as a cushion gas are used to test the GPSFLOW's modelling capability. The results show that GPSFLOW offers a robust numerical tool to model underground hydrogen storage and gas mixture at grid scale on multiple parallel computing platforms.