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Abstract
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In deep geological disposal of radioactive waste, anaerobic metal corrosion, radioactive decay of the waste, radiolysis of organic materials and water, and other reactions lead to the formation of gaseous components, in particular hydrogen (H_2) which is highly compressible (and explosive). The accumulated gas with pressure increase could develop dilatant pathways for gas migration, which can have adverse effects on the host rock confinement properties and the long-term stability of engineered barriers. Pore pressure build-up due to gas production, fluid flow and the stresses evolution around the canister in the EDZ and sealings are investigated in a wide range of studies around the world. But inconsistencies in the gas pressure estimation of H_2 production models (corrosion model, gas source term, pathways in the engineered system) can lead to a misunderstanding of the physical phenomena and to incorrect modeling hypotheses for flow and Hydro-Mechanical (HM) coupling. Even if dilatancy of fluids and host rock has been previously studied (*Xu et al. 2020, Tunnelling and Underground Space Technology*), there is a need for enhancing the modeling of single-phase gas flow (as a special case of two-phase water-gas flow) by considering gas compressibility, in order to make reliable predictions of the gas pressure build-up because hydrogen is a highly compressible gas. So, despite the substantial physics incorporated into these tools, their results are sometimes restricted by the incompressible fluids hypothesis. The iTOUGH2 code (*Finsterle 2007: iTOUGH2 User's Guide. LBNL-40040*) includes some built-in constitutive relationships for the compressibility of the fluid and also the porous media (pore compressibility). In this work, the Equation-of-State module EOS5 of iTOUGH2 is applied to simulate a single-phase gas flow of hydrogen in a 1D configuration with Dirichlet boundary conditions (fixed gas pressures upstream and downstream). The mass conservation equation for the compressible H_2 gas is expressed using the law of perfect gases, and an analytical solution is developed at steady state. Pressure profiles obtained by iTOUGH2 from this gas “permeameter” simulation were fitted to the analytical solution to estimate a key parameter in compressible gas flows (the gas compressibility coefficient) using a least squares optimization method, with reasonably good results. This test may help assess by the numerical model the gas pressure build-up phenomena in a radioactive waste repository. We expect to account for real gas law and to design similar numerical experiments to identify mechanical and hydro-mechanical coefficients.