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A coupled discrete-continuum approach to simulating CO₂ migration and dissolution in porous media

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Carbon capture and storage (CCS) has emerged as a principal emissions reduction technology for the energy transition. Its effectiveness hinges largely on the security of the storage reservoir, which may be susceptible to leakage through permeable pathways such as abandoned wells and faults. Storage failure presents risks of environmental impacts, increases in atmospheric carbon emissions, reduces both the value of carbon credits and public confidence in CCS as a viable technology for the energy transition. Given the importance of storage security, our understanding of CO₂ leakage and its fate and transport in overburden must be improved to help in the prediction, detection and assessment of leaks. Shallow groundwater monitoring for dissolved gases can be complicated by multicomponent mass transfer dynamics in the subsurface. As CO₂ migrates through the subsurface, much of the mass will partition from the gaseous to the aqueous phase, and conversely background dissolved gases present in groundwater such as N₂ and O₂ may partition to the gaseous phase, impacting both the evolution of dissolved gas concentrations and the persistence of free-phase gas in the subsurface. This process may also impact the performance of noble gas tracers in groundwater monitoring techniques. There is therefore a need for numerical models capable of accurately predicting the fate and transport of CO₂ in the subsurface. However, traditional multiphase flow models struggle to describe the buoyant unstable gas flow regime expected at leak sites, dominated by gravity and capillary forces.

Unstable gas flow is characterized by discontinuous gas clusters and sharp variations in gas saturations in space, in contrast with the smooth variation in gas saturation predicted by continuum multiphase flow models. Discrete approaches such as macroscopic invasion percolation (MIP) are better equipped to model unstable gas flow, however they are limited by assumptions of instantaneous gas movement. ET-MIP (Electro-thermal MIP) is a general purpose model which couples continuum-based electrical, thermal, groundwater and chemical species modules with a discrete MIP gas flow module. This coupled approach allows for accurate simulation of slow gas displacement characteristic of shallow subsurface gas releases while simultaneously predicting the dissolution of CO₂. ET-MIP has been validated against bench scale experiments and shown to accurately predict gas generation, multiphase transport and capillary trapping – all mechanisms which govern the fate of CO₂ in the subsurface. This talk will present comparison of ET-MIP with a bench-scale CO₂ injection and dissolution experiment and a

sensitivity study showing the effects of key model parameters on CO₂ migration. Findings highlight the benefits of using a discrete-continuum coupled approach for simulating CO₂ migration in porous media, and the importance of considering background dissolved gases in the subsurface.