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Equation of State for thermodynamic equilibrium of gas mixtures and brines to allow simulation of the effects of impurities in CO_2 storage

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Comprehensive understanding and prediction of chemical, reactive processes during and following injection of CO_2 in depleted gas reservoirs and saline aquifers is important for the assessment of the performance and impacts of planned and existing Carbon Capture and Storage (CCS) projects. Over the last decade significant improvements have been made in numerical modelling of the complex, coupled processes involved. Among the many remaining issues where progress is still called for, is the consistent simulation of impacts of gas mixtures. In particular the presence of 'impurities' or 'co-contaminants' in the injected CO_2 stream that are retained from the original flue-gases, such as H2S, SO_2, have the potential, upon dissolution in the pore water, to alter aqueous and water-mineral reactions. Moreover, presence of these and other injected or in-situ (CH4) gases affect CO_2 solubility and thermodynamic properties of the fluid and gas phases, which, in turn, impact transport processes.
To be able to evaluate the impact of gas mixtures on these processes, a new non-iterative Equation of State (EOS) has been developed which allows accurate and efficient modelling of thermodynamic equilibrium of gas mixtures and brines over a large range of pressure, temperature and salinity conditions. Presently the model includes CO_2, SO_2, H2S, CH4 and N2. This model is based on equating the chemical potentials in the system, using the modified Redlich–Kwong EOS to calculate the fugacity of the gas phase. Preliminary analysis shows, for instance, that CO_2 solubility is most sensitive to CH4 admixture and least sensitive to the presence of SO_2 in the injected gas mixture. The model design/approach will be outlined. Furthermore, the model performance will be illustrated with respect to experimental data from literature and other EOS's. In further work we aim to use this EOS in coupled flow and chemical reactive-transport simulations to investigate the impact of gas mixtures for CO_2 storage.