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A Method for Incorporating Chemical Reactions into Multiphase Flow Models for CO_2 Injection

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CO_2 injection in deep saline aquifers involves many different processes, including multiphase flow, heat and mass transport, rock deformation and minerals precipitation and dissolution. All these processes are coupled. Therefore, their modeling is difficult and requires complex computer codes to describe and assess them numerically. We developed a method for incorporating chemical reactions into multiphase flow codes. It is limited to chemical systems that can be calculated as a function of the state variables of the multiphase flow model (e.g. liquid pressure, gas pressure, temperature). It consists of calculating the chemical composition of this system as a function of these state variables by means of chemical speciation codes and redefining the components of the multiphase flow code (e.g., water, CO_2). We applied this method to incorporate chemical reactions of a H_2O–CO_2–NaCl–$CaCO_3$ system into CodeBright, a code that can handle multiphase flow, heat transport, mass transport and deformation. We used this code to model CO_2 injection into a saline aquifer containing calcite. The model could simulate well the interaction between the development of the CO_2 bubble, dissolution of CO_2 into the brine, calcite dissolution and density dependent flow.