Non-iterative description of CO2-brine equilibria for efficient numerical CCS-modelling

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We introduce the development of a numerical model, suitable for simulating geological storage applications of carbon dioxide. The governing equations cover twophase flow of immiscible fluids, strongly coupled with heat transport and solid deformation.

Although immiscible, component-based phase transitions between the fluids are considered, governed by thermodynamic relations. This choice of processes allows the description of CO2 propagation in the reservoir, reservoir temperature evolution, the safety assessment of rock integrity, and the quantification of structural, residual and solubility trapping mechanisms in geological CCS applications.

For the description of the vapour-liquid and solution equilibria, a non-iterative method was developed, following well-known and established thermodynamic relations and empirical models. By avoiding iterative computations, this method is very efficient and thus well-suited for simulations exhibiting many degrees of freedom.