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Modeling the influence of geochemical processes on multiphase fluid dynamics for concentrated solutions under dry conditions.

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Reactive Transport modeling may involve simulating flow of fluid phases, transport of species and energy, and reactions between species within the same or different phases. Most reactive transport codes decouple phase flow calculations from reactive transport. This approach has been successfully applied to a wide range of problems, but it may be unsuitable for problems like the chemical evolution of unsaturated tailings or the salinization of soils, where concentrated solutions or extremely dry conditions are reached. The amount of liquid water in these cases can be so small that both vapor and water in hydrated minerals become significant for the water balance. Under these extreme conditions gas transport becomes important and water activity, which controls vapor pressure, is affected by capillary and salinity effects. Moreover, certain mineral paragenesis (the ones that produce invariant points) fix water activity, causing the geochemistry to control vapor pressure, which is a key gas flow variable. Thus, a fully coupled solution of phase fluxes and reactive transport is required for these conditions.

In this work we present a compositional formulation capable of representing the effect of geochemistry on flow and transport for concentrated solutions under extreme dry conditions. The formulation is used to model a laboratory experiment where a sand column saturated with an MgSO4 solution is subject to evaporation. The interaction between multiphase fluid dynamics and geochemical processes on the model is analyzed. Model results shows that the occurrence of invariant points on the top of the domain can have an appreciable effect on the outlet of vapor from the column and on the distribution of salt precipitates along the column. In fact, invariant points explain spatial fluctuation of salt precipitates.