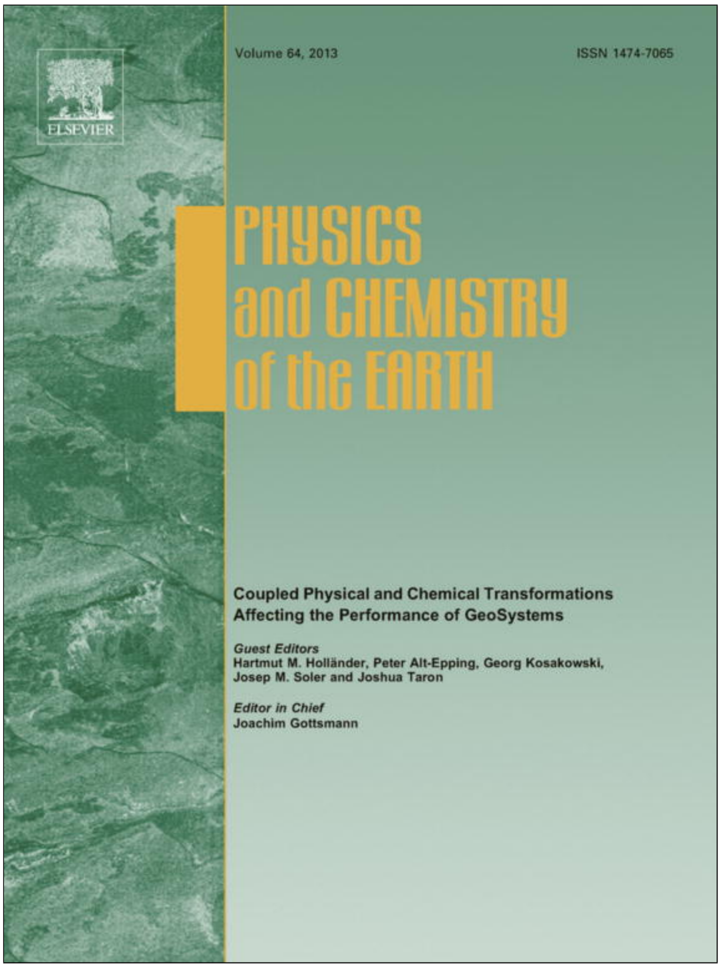
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Modeling the influence of $MgSO_4$ invariant points on multiphase reactive transport process during saline soil evaporation

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ABSTRACT

In the present work, we modeled a laboratory experiment where a sand column saturated with a $MgSO_4$ solution is subject to evaporation. We used a compositional formulation capable of representing the effect of geochemistry on flow and transport for concentrated solutions under extreme dry conditions. The model accounts for the water sink/sources terms due to hydrated mineral dissolution/precipitation and the occurrence of invariant points, which prescribe the water activity. Results show that the occurrence of the invariant points at the top of the domain could affect the vapor flux at the column top and salt precipitation along the column. In fact, the invariant points occurrence could explain the spatial fluctuation on the salt precipitates formation. Results also suggest that the complex hydrochemical interactions occurring during soil salinization, including osmotic effects, are crucial not only to understand the salt precipitation, but also the evaporation rate.

1. Introduction

Evaporation in soils is an important component of the hydrological cycle because it exerts a significant influence on soil water budget. Evaporation triggers a series of complex processes, like liquid and gaseous mass flow, energy flow, solute reactive transport and eventually salt precipitation. Numerical modeling of these processes, in combination with field and laboratory experiments, provides the means for testing conceptual models and for evaluating complex interactions of processes in soils and other porous media (Steefel et al., 2005). Models allow obtaining quantitative approximations of processes and variables that are difficult or impossible to measure directly in field or laboratory.

Unsaturated liquid water flow was the first process modeled in soil evaporation codes (Remson et al., 1971). Since then, more complex processes have been added to soil evaporation models including vapor flux (Fayer et al., 1986), interaction between water and heat flow (Milly, 1980), and salinity effects on evaporation (Nassar and Horton, 1989). More recently, the modeling of soil salinization, biological nutrient degradation and evolution of mine tailings have led to the inclusion of reactive transport in soil evaporation modeling (Zee, 1990). Wissmeier and Barry (2008) compiled several examples in agricultural and environmental engineering, including water irrigation efficiency (Wenninger et al., 2010), water management practices and irrigation techniques in arid and semiarid areas (Cortes-Jimenez et al., 2007; Xu and Shao 2002), reclamation strategies for sodic soils (Bauer et al., 2006; Qadir et al., 2000), evaluation of the suitability of irrigation waters (Ghassemi et al., 1991), and acid mine drainage and rehabilitation of residue disposal sites (Acero et al., 2009; Bea et al., 2010b, Lefebvre et al., 2001; Mayer et al., 2006). Numerical modeling has also been used for designing and analyzing evaporation experiments and has helped to improve the understanding of salt and efflorecense precipitation and evaporation at the macro and pore scales in homogeneous and heterogeneous porous media (Bechtold et al., 2011; Guglielmini et al., 2008; Nachshon et al., 2011; Rad and Shokri, 2012).

One aspect that has not been considered, even in the most advanced codes, is the effect of geochemical reactions on water content and thus on flow (Wissmeier and Barry, 2008). This reflects the fact that geochemical effects on water balance can be neglected in most cases. However, in arid or semiarid climates soils may reach extremely dry conditions, so that hydrated mineral dissolution/precipitation may generate water sinks/source terms comparable to the remaining processes. Another potentially relevant often ignored aspect in saline and dry conditions, is the occurrence of invariant points. In such cases, mineral paragenesis (typically, simultaneous presence of several minerals with similar stoichiometry but different levels of hydration) prescribes water activity (Bea et al., 2010a; Gamazo et al., 2011; Risacher and Clement, 2001).

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