

Non-isothermal multiphase and multicomponent reactive transport in coupled soil/atmosphere systems

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The subsurface and the atmosphere are two strongly coupled environmental compartments and the interchange of mass, momentum and energy across their interface controls the dynamics of fluid(s) flow, component transport and geochemical reactions in the subsurface. The migration of water vapor at the soil/atmosphere interface (i.e., soil water evaporation) is an important example of such exchange phenomena, which induce a non-isothermal fluid phase displacement in soils and thus control the spatiotemporal distribution of liquid and gaseous phases in the pore space. The correct description of the fluid phase distribution, resulting from the evaporation-induced drainage, is of great importance because it influences the migration behavior of important gas components that are essential for a wide range of biogeochemical reactions controlling pore water quality.

The objective of our study is to explore the propagation of gas components, like O₂ and CO₂, in porous media under different atmospheric forcing and to understand the external (e.g., temperature and wind flow) and internal (e.g., grain size) factors controlling their transport behavior in coupled soil/atmosphere systems. To this end, we performed a set of well-controlled laboratory experiments in different porous media and considering different conditions: (i) no evaporation, (ii) natural evaporation (i.e., room temperature), and (iii) enhanced evaporation (i.e., in presence of heat source). The experiments allowed us to study the evolution of temperature and conservative transport of oxygen in initially anoxic porous media and to compare the O₂ propagation behavior under single-phase and two-phase conditions [1]. Additionally, we developed and applied a non-isothermal compositional multiphase flow model to quantitatively interpret the experimental observations. The code explicitly resolves the phase change, phase displacement, heat propagation, component transport mechanisms within and across different phases in the porous media, and relies on a geochemical speciation code for simulation of chemical reactions (i.e., coupling with the PhreeqcRM module). The developed simulator allowed us to explore reactive scenarios involving gaseous transport in the presence of reactive minerals and under different atmospheric forcing in coupled soil/atmosphere systems [2].

References

[1] Ahmadi et al. (2022), Water Resour. Res 58, DOI: