Contribution ID: **465** Type: **Oral Presentation**

Water confined in salt crusts: insights from molecular simulations

Thursday, 2 June 2022 09:10 (15 minutes)

The evaporation of water from a bare soil can be accompanied by the formation of a layer of crystallized salt. This salt crust forms an additional porous layer that affects the evaporation of water in a counter-intuitive way: depending on the conditions (i.e. depending on the pore size of the crust, soil-crust connection, external atmospheric conditions), the crust can hinder or enhance the net flow of water. To better understand the transport properties of water through porous salt crusts, we use molecular simulations and explore the behavior of water confined by three types of solid surfaces: NaCl, Na2SO4, and charged silica. We measure NMR relaxation times T1 and T2, extract their values for different degrees of confinement, relative humidity, and surface rugosity, and discuss their relation with the structure of water near solid interfaces. Then, using non-equilibrium molecular dynamics, we study the transport properties of water at the salt interface. Our results show that at low humidity, transport through salt crust is likely to be dominated by a thin layer of water of a few molecules at the salt wall.

Acceptance of the Terms & Conditions

Click here to agree

MDPI Energies Student Poster Award

No, do not submit my presenation for the student posters award.

Country

Germany

References

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Online

Primary author: GRAVELLE, Simon (Institute for Computational Physics)

Co-authors: HABER-POHLMEIER, Sabina (Institut für Wasser und Umweltsystemmodellierung); Prof. SCHLAICH, Alexander (Institute for Computational Physics); Prof. HOLM, Christian (Institute for Computational Physics)

Presenter: GRAVELLE, Simon (Institute for Computational Physics)

Session Classification: MS13

Track Classification: (MS13) Fluids in Nanoporous Media