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Type: **Oral Presentation**

Sorption in heterogenous porous media: a numerical study of the effects of spatial heterogeneity of pore structure

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We present a computational model to simulate both adsorption and desorption processes interactions with hydrodynamics. Flow and mass transport equations and various sorption kinetic equations are solved with Lattice Boltzmann method. The computational developments are used for direct numerical simulation of flow and transport in three-dimensional digitized soil samples and are supported and validated by experimentally measured data. The model allows to include the details of contact surface between adsorbate and adsorbent for computation of sorption rates within porous media. This modelling approach not only enables an important mechanism to be simulated for real-life applications, but also provides an enabling computational framework within which the fundamentals of sorption can be studied. The simulation data are used to drive mathematical formulations that predict macro-scale sorption rates based on tortuosity of fluid paths, pore velocity distribution and Peclet number.

Participation

In-Person

References

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Session Classification: MS08

Track Classification: (MS08) Mixing, dispersion and reaction processes across scales in heterogeneous and fractured media