Contribution ID: **388** Type: **Poster Presentation**

Space-time upscaling of reactive transport in porous media

Monday, May 30, 2022 3:10 PM (1h 10m)

Reactive transport in saturated/unsaturated porous media is numerically upscaled to the space-time scale of a hypothetical measurement through coarse grained space-time (CGST) averages. The one-dimensional reactive transport is modeled at the fine-grained Darcy scale by the actual number of molecules involved in reactions which undergo advective and diffusive movements described by global random walk (GRW) simulations. The CGST averages verify identities similar to a local scale balance equation which allow us to derive expressions for the flow velocity and the intrinsic diffusion coefficient in terms of averaged microscopic quantities. The latter are further used to verify the CGST-GRW numerical approach. The upscaling approach is applied to biodegradation processes in saturated aquifers and variably saturated soils and the CGST averages are compared to classical volume averages. One finds that if the process is characterized by slow variations in time, as in homogeneous systems or in case of observations of reactive transport in heterogeneous aquifers made at large times or far away from the contaminant source, the differences between the two averages are negligible. Instead, the differences are significant if the averages are computed close to the source at early times, in case of aquifer simulations, and can be extremely large in simulations of biodegradation in soils. In the latter case, the volume average is totally inappropriate as model for experimental measurements, leading for instance to overestimations by 100% of the CGST average.

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

Deutschland

References

Time Block Preference

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

Participation

Online

Authors: Dr SUCIU, Nicolae (Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy); RADU, Florin Adrian (University of Bergen, Norway); POP, Iuliu Sorin (Hasselt University)

Presenter: Dr SUCIU, Nicolae (Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy)

Session Classification: Poster

Track Classification: (MS07) Mathematical and numerical methods for multi-scale multi-physics, nonlinear coupled processes