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Applying Thermodynamic Framework to Analyze Transport Self-Organization Due to Dissolution/Precipitation Reaction in Porous Medium at Varying Peclet Number: Entropy, Enthalpy, Heterogeneity

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Dissolution/precipitation processes in reactive transport in porous media are ubiquitous in a multitude of contexts within the field of Earth sciences, such as geological hydrogen and carbon storage, reactive contaminant transport and acid injection in petroleum reservoirs. In particular, the dynamic feedback between the reactive process and solute transport, capable of giving rise to the phenomenon of preferential flow paths, is critical to a variety of Earth science scenarios, as these paths are responsible for the alteration of transport properties of the porous medium; still, the approaches to its characterization remain disputed. It has been argued that the emergence of preferential flow paths in porous media can be considered a manifestation of transport self-organization, as they introduce spatial gradients that distance the system from the state of perfect mixing.

To investigate the dynamic feedback between the reactive and transport processes and its influence on transport self-organization, we consider a 2D Darcy-scale reactive transport setup, where dissolution and precipitation of the porous medium are driven by the injection of an acid compound, establishing local equilibrium with the resident fluid and the porous medium, composed of a calcite mineral. The coupled reactive process is simulated in a series of computational analyses employing the Lagrangian particle tracking approach, capable of capturing the subtleties of the multiscale heterogeneity phenomena. We employ the thermodynamic framework to investigate the emergence of the preferential flow paths as the manifestation of transport self-organization; in particular, we are interested in the relationship between the Shannon entropy, used to quantify self-organization and the enthalpy.

We find that, for an initially homogeneous medium, transport self-organization increases with the evolution of the reactive process, along with the emergence of heterogeneity in the medium due to feedback between the reaction and transport. We identify the reciprocal of the Peclet number as the driving force for transport self-organization, as the stochastic nature of diffusion leads to inhomogeneity of reaction, resulting in the emergence of heterogeneity in the medium; this causes re-distribution of the transport, thus increasing its self-organization, as signified by a decrease in Shannon entropy. The decreasing entropy is accompanied by an increase in enthalpy due to an enhanced global reaction rate. The self-organization of the breakthrough curve exhibits the opposite tendencies, explained from the thermodynamic perspective. The energy, required to maintain self-organization within the thermodynamic framework, is supplied by the hydraulic power under the applied hydraulic head drop boundary condition; this power increases with the heterogeneity.

To conclude, our findings suggest that Peclet number of the transport has a crucial impact on the interaction between the reactive and transport processes in porous medium, as expressed in terms of transport self-organization within the thermodynamic framework; this has important implications for both hydrogen and carbon geological storage due to reactive processes that take place in the storage medium, caused by the altered pH level.

Participation

In-Person

References

[1] Zehe, Erwin, Ralf Loritz, Yaniv Edery, and Brian Berkowitz (2021). "Preferential Pathways for Fluid and Solutes in Heterogeneous Groundwater Systems: Self-Organization, Entropy, Work". In: Hydrol. Earth Syst. Sci. 25, pp. 5337–5353. DOI: https://doi.org/10.5194/hess-25-5337-2021.

[2] Edery, Yaniv, Martin Stolar, Giovanni Porta, and Alberto Guadagnini (2021). "Feedback mechanisms between precipitation and dissolution reactions across randomly heterogeneous conductivity fields". In: Hydrol. Earth Syst. Sci. 25, pp. 5905–5915. DOI: https://doi.org/10.5194/ hess-25-5905-2021.

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