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Multi-component diffusion in a coupled free-flow porous-medium system

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A standard approach to model diffusion in porous media is the assumption of the validity of Fick's Law. Although widely used, that description can only be employed for binary mixtures or low concentrations of the components as it neglects molecular interactions of the different species.

When looking e.g. at gas migration of an organic component in soil where higher concentrations of components can occur, more complex laws need to be employed. In this work we present a multi-phase, multi-component model incorporating the Maxwell-Stefan's approach to diffusion which takes into account all interactions between the molecules of different species. Therefore it is possible that the diffusion behaviour is very different to the one seen in the standard continuum advection-diffusion description.

We present a coupled free-flow porous-medium model, where the Maxwell-Stefan diffusion approach is employed in both domains. Consistent coupling conditions for coupling the free-flow domain to the porous medium are presented as well.

The model is implemented in the numerical software framework DuMuX and can be used for various applications. The example application presented is a study on evaporation together with gas migration in the porous medium and across the porous-medium free-flow interface. Different concentrations of the gas components and their influence on evaporation rates and gas migration rates across the porous-medium free-flow interface are compared.

References

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Primary authors: HECK, Katharina (University Stuttgart); Prof. HELMIG, Rainer (University of Stuttgart)

Presenter: HECK, Katharina (University Stuttgart)

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