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Introducing microbiological reactions in a modular multiphase code : coupling Openfoam and Phreeqc

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The field of underground hydrogen injection is developing rapidly. However, classical multiphase codes often contain too simple reaction formulations. The proposed coupling aims at using all the developments made with Phreeqc in the field of biotic reactions in the presence of hydrogen. Phreeqc is coupled to OpenFoam which allows to manage parallel simulations on unstructured meshes and efficient advective schemes for multiphase equations, with solute and gas species transport. The flexibility of OpenFoam allows to reformulate the equations according to the needs (variation of parameters according to the temperature...). The proposed coupling allows to simulate conditions where the perfect gas law is no longer valid (Peng-Robinson formulation) and to manage gas formation or consumption. The code is freely available and problems can be set and visualized in a performing free graphical user interface. The presentation will focus on a simulation close to a real case and will aim to determine the capabilities and limits of this type of model, both in terms of computational capacity but also according to the type of equations involved.

Hydrogen consumption kinetics can vary according to the context, include several intermediates such as acetate or formate and present possible competition with other kinetics such as sulfate reduction or methanogenesis. The links between these different reaction pathways will be discussed. Furthermore, the link between reaction kinetics, fluid movement and phase exchange will be detailed by varying key parameters. Different domains will be identified according to the spatial and temporal scales of the experiments.