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Modelling of diffusion-convection of reactive species - Application to dissolution and precipitation within porous materials

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Subject :
The study of the mass transport phenomena in porous media is of major interest in several domains, among them civil engineering, mechanics and geomechanics, hydrogeology and nuclear industry. In all these domains, the knowledge of mass transfer properties at the macro-scale (the scale of the structure), taking into account the multi-physics coupling involved at the micro scale, is fundamental to dispose of accurate predictive models for engineers.
Materials used in civil engineering (as concrete, geotechnical barriers) are often subjected to external chemical aggression as chloride penetration or leachate percolation for example. In this context, changes of solid phase volume inside pores due to reactive species can induce mechanical stress on the solid phase which can have impact at the macroscopic scale as fractures development. This subject can also be extended to chemical engineering and process engineering.
The interaction between the transported species and the solid matrix can lead to porosity modification, which in turn leads to the change in mechanical and/or transport properties as permeability and diffusivity. This porosity evolution is caused principally in this study by dissolution and/or precipitation of solid phases. The main objective of this work is to investigate porous media microstructure characteristics that govern species migration in porous space. This will be realized through a coupled study of fluid flow and convection-diffusion of solute species.
This PhD will be focused on the numerical modelling of multispecies transport in saturated porous media. More specifically, this work will be limited to the modelling of dissolution/ precipitation reactions and their consequences on solid matrix. The scientific challenge in this work is to develop numerical tool allowing the follow-up of the microstructure evolution under external severe solicitations and to characterize its consequences at the macro-scale in terms of transport properties. To succeed, a part of this work will be devoted to the development of numerical code of transport coupled to chemical reaction. In parallel homogenization procedure will be developed to upscaling the coupled reactive transport in the aim to determine the macroscopic behaviour of porous media. Finally, comparison with experimental results developed in our laboratory will be conducted.

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This PhD work follows the study carried out by Jianhua FAN (CSC 2014) and it will be supervised by M. Hellou (Prof.), M.-K. Bourbatache (assistant Prof.) and F. Lominé (assistant Prof.)

Keywords:
Porous media; Geochemistry; Diffusion/convection; Fluid flow; Lattice Boltzmann Method (LBM); Homogenization technique; Permeability; Diffusivity; Dissolution/ Precipitation.

Scientific skills :

- Civil engineering
- Fluid mechanics.
- Transport in porous media
- Convection, diffusion, reaction
- Upscaling methods (homogenization, volume averaging,...)
- Numerical method without meshing Lattice Boltzmann Method
- Competences in computer programming (C, C++, matlab, etc) would be necessary

Expected collaborations :

- LASIE University of La Rochelle, France
- OSUR, Geosciences, Rennes, France
- IRSTEA, Rennes, France
- LAMPA, Angers, France

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