
Contribution ID: **332** Type: **Oral 20 Minutes**

# New trends in Vortex Methods for reactive flows

*Wednesday 16 May 2018 09:50 (15 minutes)*

This talk will focus on the numerical aspects of reactive flows and pore-scale modeling, and how involving vortex-like methods can substantially improve computational efficiency, that is to say optimize the use of computing resources (computational time and memory storage). After briefly describing the numerical approach, a few numerical simulations of calcite dissolution will be presented.

Vortex Methods are Lagrangian methods -also called particle methods- well fitted to the study of complex transport phenomena[5]. We will first exhibit this feature on bead stacks and their related permeability estimations, and on heterogeneous Xanthan injection in real rock geometries obtained by MicroCT scans[6]. Their hybrid formulation uses high order interpolations between grids and particles, such that adequate numerical schemes are performed either on grids or on particles. The goal is then to compute transport on particles and to use as much as possible fast solvers on grids, in order to minimize the computational time. The penalization method can be included in such schemes[4], making possible to consider arbitrarily shaped body and their dissolution. Consequently, the millimeter scale flow is modeled by the non-linear Stokes-Brinkman equation[3] whose Brinkman term is evolving with a coupling to transport[1] of acid and chemical product.

Concerning reactive flows, three time scales are involved: a hydrodynamic time scale (under the second) in which the flow is able to cross the domain at the pore-scale; a time scale allowing to reach a quasi-stationary reactive state of reaction rate; a dissolution time scale for which the solid body evolves. We will consider the case of a calcite core dissolution at pH=2, in the context of a collaborative study with S. Molins, S. Soulaine and N. Prasianakis. For this configuration, these three time scales are about 1s, 10s and 1h, respectively.

The numerical method is built specifically with a time-splitting algorithm such that velocity computing and interpolations are performed meaningfully in order to avoid useless computations. In practice we will show that a good strategy is to compute chemistry, diffusion of species and transport on particles, while penalization, velocity computation and viscous diffusion are performed on grids. This strategy decreases the number of interpolations thus improving the computational time. In this spirit, chemistry and hydrodynamics can be considered at different resolutions, and require only a down-scaling of solid concentration. This fits very well to GPU or hybrid CPU-GPU computing, which is currently one of our main developments.

Beyond the multi-scale aspects in time and space, two key points can be mentioned. On the one hand, we will show that time step adaptation can be performed, based on the chemistry evolution (or lack thereof). On the other hand, introducing vorticity unlocks the necessity to make the penalization implicit (usually, explicit penalization has stability issues), which allows the use of fast grid solvers based on Fast Fourier Transforms (FFT), in the spirit of [2]. Finally, several simulations will illustrate how far it is possible to go in terms of resolution and physical time simulated, for Reynolds numbers from 0.24 to 240.

## References

[1] R. Chatelin, D. Sanchez and P. Poncet, Analysis of penalized variable viscosity 3D Stokes equations coupled with transport and diffusion, ESAIM: Math. Model. Numer. Anal. 50:2, 565-591 (2016).

[2] R. Chatelin and P. Poncet, Hybrid grid–particle methods and Penalization: A Sherman–Morrison–Woodbury approach to compute 3D viscous flows using FFT, J. Comput. Phys. 269, 314-328 (2014).

[3] R. Chatelin and P. Poncet, A hybrid grid-particle method for moving bodies in 3D Stokes flow with variable viscosity, SIAM J. Sci. Comp. 35(4), B925-B949 (2013).

[4] M. El Ossmani and P. Poncet, Efficiency of multiscale hybrid grid-particle vortex methods, SIAM MMS 8(5), 1671-1690 (2010).

[5] G-H. Cottet and P. Poncet, Advances in Direct Numerical Simulations of three-dimensional wall-bounded flows by Particle in Cell methods. J. Comput. Phys., 193, 136-158 (2003).

[6] D. Sanchez, L. Hume, R. Chatelin and P. Poncet, Analysis of 3D generalized Stokes problem coupled to transport-diffusion for miscible shear-thinning heterogeneous microscale flows: Applications to digital rock physics and mucociliary clearance, Submitted.

## Acceptance of Terms and Conditions

Click here to agree

**Author:** Prof. PONCET, Philippe (University Pau & Pays Adour, France)

**Co-authors:** HUME, Laurene (University Pau & Pays Adour, France); ETANCELIN, Jean-Matthieu (University Pau & Pays Adour, France)

**Presenter:** Prof. PONCET, Philippe (University Pau & Pays Adour, France)

**Session Classification:** Parallel 6-F

**Track Classification:** MS 4.22: Evolving porous media and coupled chemical and physical processes