Numerical simulation of geochemical compaction with discontinuous reactions

Abramo Agosti*, Luca Formaggia*, Bianca Giovanardi*, and Anna Scotti*

* Department of Mathematics,
Politecnico di Milano
P.za Leonardi da Vinci 32, 20133 Milano, Italy
e-mail: abramo.agosti@polimi.it, luca.formaggia@polimi.it, bianca.giovanardi@polimi.it, anna.scotti@polimi.it, web page: http://mox.polimi.it

ABSTRACT

The present work deals with the numerical simulation of porous media subject to the coupled effects of mechanical compaction and reactive flows that can significantly alter the porosity due to dissolution, precipitation or transformation of the solid matrix. This study is motivated by the occurrence of overpressures, i.e. pressures larger than hydrostatic, that are usually found in sedimentary basins. Their prediction is crucial for the safety of a number of energy related human activities. However, overpressures are not completely ascribable to mechanical compaction and seem to be correlated with temperature, thus, they are probably also related to temperature activated chemical reactions. In this work we first analyse the coupled problem of compaction, flow and geochemical reactions by means of a simplified one-dimensional model that is able to describe the deposition of different sedimentary layers, thus, to simulate the formation of a sedimentary basin [1]. We then focus our attention on two geochemical processes that can, combined with mechanical compaction, affect the porosity: oil generation, and mineral dissolution/precipitation. In the case of oil generation the solid organic matter, called kerogen, dissolves forming liquid or gaseous hydrocarbons that can be modelled as a fluid phase immiscible with water. In the case of mineral, for instance quartz, dissolution and precipitation are coupled with the passive transport of the solute in water. In both cases there is a strong coupling among fluid flow, mechanics and reaction: porosity changes affect the flow through the medium permeability, and fluid pressure can counteract mechanical compaction. At the same time, chemical reactions can cause dramatic changes in the porosity. We show that, in this framework, a naive iterative splitting can fail to converge for low permeabilities, while a full Newton approach is more robust but unpractical in most cases. Another relevant aspect of the problem is the presence of phenomena, such as retention in nanopores or mineral dissolution, which can be effectively modelled by ODEs with discontinuous right hand side, where the discontinuity depends on time and on the solution itself. Filippov theory can be applied to prove existence and to determine the solution behaviour at the discontinuities. From the numerical point of view, tailored numerical schemes are needed to guarantee positivity, mass conservation and accuracy. In particular, we rely on an event-driven approach such that, if the trajectory crosses a discontinuity, the transition point is exactly localized and integration is restarted accordingly [3]. This approach yields sharper results compared to the regularization of the right hand side, and does not introduce artificial stiffness in the system.

REFERENCES

[1] L. Formaggia, A. Guadagnini, I. Imperiali, V. Lever, G. Porta, M. Riva,A. Scotti, L. Tamellini, Global sensitivity analysis through polynomial chaos expansion of a basin-scale geochemical compaction model, Computational Geosciences 17 (2013), 25–42.

[2] K. Kumar, I.S. Pop, and F.A. Radu, Convergence analysis of mixed numerical schemes for reactive flow in a porous medium, SIAM Journal on Numerical Analysis 51 (2013), 2283–2308.

[3] L. Dieci and L. Lopez, Sliding motion in Filippov differential systems: theoretical results and a computational approach, SIAM Journal on Numerical Analysis 47 (2009), 2023–2051.