



The interplay of flow, chemistry and compaction in sedimentary basins

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ABSTRACT

The present work deals with the numerical simulation of the processes that occur, at geologic time scales, in sedimentary layers subject to compaction and in the presence of reactive flows that can significantly alter the porosity due to dissolution, precipitation or transformation of the solid matrix. We focus our attention on two geochemical processes: 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 minerals, 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. The numerical challenges in the simulation of these processes are several-fold, [1]. First of all, the model is described by a coupled non-linear system that should be solved with a suitable iterative method. It can be shown that not all methods guarantee stability. Moreover, mass conservation should be preserved up to some desired tolerance. Another issue is that we are dealing with evolving domains due to the compaction of the medium, the formation/dissolution of the solid matrix, and the deposition/erosion of sedimentary layers. Finally, we model phenomena such as retention in nanopores or mineral dissolution, which can be effectively modelled by ODEs with discontinuous right hand side. 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. 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] B. GIOVANARDI, A. SCOTTI, L. FORMAGGIA, P. RUFFO, A general framework for the simulation of geochemical compaction *Computational Geosciences*

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