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Optimal formulation for visco-elasto-plastic hydro-thermomechanical models with mass transfer: C-component approach

Taras Gerya
DERDW-ETH, Zurich, Switzerland

Hydro-thermomechanical (HTM) modelling is an important branch of geodynamic modelling, which investigates evolution of coupled fluid/melt-solid systems under conditions of slow geodynamic deformation rates. One important point to discuss is how fluid-solid coupling could be implemented self-consistently into existing visco-elasto-plastic thermomechanical (TM) geodynamic codes thereby making them capable to model hydro-thermomechanical processes. From this point of view, an optimal self-consistent visco-elasto-plastic formulation has recently been developed by Yarushina and Podladchikov (2015), who derived their system of mass and momentum conservation equations based on principles of irreversible thermodynamics formulated for a two-phase fluid-solid system. This formulation is also consistent with Biot's poroelasticity theory (Biot, 1941). Based on this formulation, we develop a simple generic treatment of complex solid-fluid mass transfer processes (i.e. resulting from several simultaneously operating multi-component chemical reactions) based on considering a single chemically complex pseudo-component C. We characterize the reactive mass transfer simply by considering a net mass transfer (ΔM) from the solid to the fluid during a time increment Δt: positive ΔM values corresponds to the mass transfer from the solid to the fluid (dehydration, melting, dissolution, etc.), whereas negative ΔM values imply the mass transfer from the fluid to the solid (hydration, solidification, precipitation, etc.). The transferred mass is formally described as a single chemically complex pseudo-component of the solid and fluid (we call it C-component, Gerya, 2019) that has different density in its solid and fluid state, which can also differ from the bulk density of the solid and fluid. The advantage of this approach is that the form of the discretized conservation equations becomes independent of the actual chemistry, thermodynamics and kinetics of mass transfer, which can be computed separately during HTM-iteration. In this case, all mass transfer terms can be formulated locally as a function of six independent quantities: porosity and density of the solid and fluid before (i.e. for the beginning of the time step Δt) and after (for the end of the time step Δt) multi-component chemical reactions at given pressure, temperature and composition of the system. We present examples of using C-component approach for multi-component toy thermodynamic models of mantle melting and subducting slab dehydration.

References

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