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Thermo-chemo-mechanical coupling in Maxwell-Stefan multi-component diffusion

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Classical Fickian linear diffusion of inert or trace-like elements is restricted to ideal solution models of components with equal molar mass. Simultaneous diffusion of multiple concentrations is well-treated by the classical Maxwell-Stefan model. Quantitative predictions of concentrations evolution in real mixtures require careful replacement of concentration gradients by gradients of chemical potentials. Coupling of multi component diffusion to mechanics result in pressure gradients that contribute to Gibbs-Duhem relationship. We aim at developing of thermodynamically admissible multicomponent thermo-chemo-mechanical (TMC) model with ensured non-negative entropy production. We also ensure correct equilibrium limit with zero gradients of chemical potentials of individual components and satisfaction of classical Gibbs-Duhem and Maxwell relationships under pressure gradients. Following recent Tajčmanová et al. (2021) we consider both molar and mass formulations. We present optimal pseudo-transient numerical scheme for multi-diffusional fluxes coupled to visco-elastic bulk deformation.

Tajčmanová, L., Podladchikov, Y., Moulas, E. and L. Khakimova. The choice of a thermodynamic formulation dramatically affects modelled chemical zoning in minerals. Sci Rep 11, 18740 (2021).