Flash calculation of chemical equilibria in multiphase reactive mixtures: Unified formulation and efficient computation

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The problem I will address in this talk can be formulated In a simple way: given a certain quantity of different atoms, what configuration in terms of chemical species is the most favorable from an energetic perspective, and thus the most likely to occur. From a mathematical perspective, it amounts to minimize a 1-homogeneous convex functional under linear constraints encoding the conservation of the atoms, and positivity constraints for the concentrations. The study of this question is of course not new, but still, the practical computation of such chemical equilibria requires most of the computational effort for the simulation of CO2 storage scenarios. The situation is particularly delicate as the model allows for the (dis)appearance of (solid, gaseous, liquid) phases. We propose then a new formulation allowing to treat such phase disappearance by the mean of persistent variables, and then propose an efficient Newton based algorithm that shows to outperform the state of the art approaches in terms of robustness and convergence speed. This is a joint work with Ibtihel Ben Gharbia, Thibault Faney, Maxime Jonval and Quang Huy Tran.