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Precipitation of Pure Solids in Fluid Mixtures: A Calculation Procedure Based on Gibbs Energy Minimization

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The possibility of phase equilibria involving solid phases is often ignored in the popular commercial phase-equilibrium calculation tools for the design and simulation of chemical processes. One possible way of accounting for the potential presence of solid phases is to assume that solids precipitate as pure compounds. Using this assumption, multicomponent systems may contain a number of pure solid phases equal to the number of components. Predicting the correct number of coexisting solid and fluid phases then becomes a challenge.

The objective of this study is to apply the minimization approach of molar Gibbs energy to calculate stable phase equilibria in non-reacting systems involving potentially fluid and solid phases. More specifically, we will focus on the calculation of the vapor-solid(s), liquid-solid(s) and multi-fluid-solid(s) equilibria when solid phases are assumed to contain pure species only.

The effectiveness of the proposed approach is demonstrated by applications to several examples. A Python code illustrating the proposed approach will be briefly introduced.

Reference:

[1] X. Xu, Jean-Noël Jaubert, G. de Combarieu, R. Privat (2023): **Precipitation of pure solids in fluid mixtures: A calculation procedure based on Gibbs energy minimization**, *Chemical Engineering Science*, 269, 118484.

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