

Modeling Liquids with Varying Tendency for Ionicity

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The liquid phase is by far the most complicated to model with a closed Gibbs energy expression, even if one excludes fluids and aqueous solutions. The two main reasons for this are:

1. almost all elements are stable as liquids whereas they often have very different crystalline phases,
2. the liquid is often stable across the whole system whereas crystalline phases often have very limited solubilities.

As the elements are very different it means that the liquid phase may drastically change its properties with composition which can be difficult to model. While we are waiting for the ultimate model that can describe the gas, liquid and amorphous phase with a single Helmholtz energy function we will have to do with more or less crude approximations. To describe drastic changes at a particular composition all thermodynamic models assumes that the liquid at that composition consists of a single constituent. There are several frequently used models capable of this like the associated solution model, the modified quasichemical model and the partially ionic two-sublattice liquid model. Each of these models has its advantages and limitations and some of these will be discussed, in particular the aspect of extrapolations into multicomponent systems. Some examples from liquid phase modeled in existing thermodynamic databases will be discussed as well as recent applications in biomaterials.

[1] M Hillert, B Jansson, B Sundman and J Ågren, *Met. Trans. A*, **16A** (1985) 261-266