Calculation of Surface Tension by Direct Gibbs Energy Minimization

R. Pajarre$^{C, S}$ and T. Tanaka
Technical Research Centre of Finland, VTT, Finland
Risto.Pajarre@vtt.fi

P. Koukkari
VTT Process Chemistry, FI, Finland

A thermodynamic model for calculating surface tension by direct Gibbs energy minimization has been constructed. Surface is modeled as a monolayer phase, and surface tension values and the composition of the surface layer are obtained from the model in a single equilibrium calculation [1]. In the model surface area is considered a component of the system and the corresponding calculated chemical potential is directly proportional to the surface tension of the mixture. The results are equivalent with those of the Butler model [2]. The model can handle mixtures of multiple components and any available non-ideal mixture phase data compatible with data format of the used software (ChemApp/ChemSage; implementation in other environments is in principle also possible), while the thermodynamic excess energy equations for the surface phase can be adjusted in the model based on theoretical and empirical considerations for the surface phase interactions. Example cases of metal alloys and salt melts will be discussed.

[1] R. Pajarre, P. Koukkari, T. Tanaka, J. Lee, *Calphad*, accepted for publication.
[2] J. A. V. Butler, *Proc. Roy. Soc. A*, **135,** 348 (1932).