A Thermochemical Approach to Thermophysical Properties - Modelling Surface and Interfacial Tension of Liquids

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Abstract

A method has been developed for calculation of surface tension in multi-component mixtures using ChemSheet. The method is based on the widely used monolayer model, where the surface effects are attributed to the atomic or molecular layer closest to the surface. In addition to this, strongly segregating species can be included as a separate adsorption layer.

Required input data consists of the normal thermodynamic (Gibbs energy) data of the mixture system, molar surface areas of each component together with pure component surface tension values, and the relevant adsorption energies.

In the model, new system components are defined for the surface area and adsorption areas; the chemical potential of the surface area component becoming proportional to the surface tension.

Additionally, a model extension to several interacting surface layers is discussed; layer-layer interaction requiring the use of user-defined model feature of ChemApp. When applied to an interface between two condensed phases, the extended model leads to predictions on interfacial energy based on the bulk thermodynamic excess properties.

The example cases discussed will be mostly on the area of metal alloys.