A New Group Contribution Method For The Estimation Of The Surface Tension Of Non-Electrolyte Organic Compounds

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Abstract

Surface tension is an important property in the design of some unit operations such as extraction and distillation. Surface tension affects liquid-liquid phase separation, interfacial surface and mass transfer and the wetting of the column packing/walls strongly influencing tray/packing efficiency which ultimately determines the height of the column. Current estimation and correlation methods (Macleod 1923; Brock and Bird 1955; Zuo and Stenby 1997) require critical property data, molar volumes or experimental data to regress the model parameters which makes them less generally applicable. It is for this reason that the objective of this work is to develop a model whose parameters can be estimated from molecular structure (via group contributions) or are simple to acquire via measurement or estimation.

In group contribution methods the molecule is fragmented into functional groups. Each of these functional groups contributes to the value of the property being calculated e.g. surface tension. The Thermodynamics Research Unit and the Industrial Chemistry Group has developed several successful group contribution methods for the normal boiling point (Cordes and Rarey 2002; Nannoolal *et al*. 2004), critical properties (Nannoolal *et al*. 2007), vapour pressure (Moller *et al*. 2008; Nannoolal *et al* 2008) and liquid viscosity (Nannoolal *et al*. 2009) as part of an ongoing collaboration between the University of KwaZulu-Natal and the Carl von Ossietzky University.

The model development in this work will follow a route similar to that of the previously developed methods, and will be based on data from the Dortmund Data Bank (Gmehling *et al.* 2008) which contains about 22600 surface tension data points for over 2200 compounds. A critical examination of other available methods will be performed, and the performance of the new model will be compared to existing models.

Keywords: Surface Tension, Group Contribution.

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