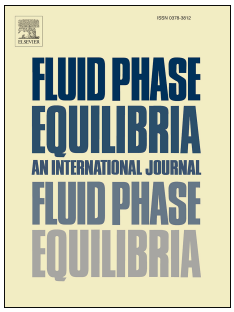
Accepted Manuscript



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PII: S0378-3812(18)30250-4

DOI: 10.1016/j.fluid.2018.06.014

Reference: FLUID 11869

To appear in: *Fluid Phase Equilibria*

Received Date: 16 April 2018

Revised Date: 19 June 2018

Accepted Date: 23 June 2018

Please cite this article as: M. Jaber, W. Babe, E. Sauer, J. Gross, R. Lugo, J.C. de Hemptinne, An improved group contribution method for PC-SAFT applied to branched alkanes: Data analysis and parameterization, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2018.06.014.

An improved group contribution method for PC-SAFT applied to branched alkanes: Data Analysis and parameterization

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Abstract

In this work, the heterosegmented GC-PC-SAFT model is parameterized for branched alkanes. Branched alkanes can be regarded as the skeleton of more complex molecules. Analyzing experimental data of branched alkanes in comparison to the linear analogous gives rationale to decisions about what substances require a more refined or individualized parameterization.
A neighborhood-correction of the segment-number parameter is then proposed for branched alkanes as function of the distance between the functional groups. This correction leads to better agreement with experimental data in the prediction of vapor pressure (27 % AAD compared to 39 %) and allows distinguishing isomers.

1. Introduction

It is desirable in process engineering to replace measurements of some properties by predictive methods. This is specially the case for the first steps of process design, when the feasibility of the process has to be evaluated with the data available in literature and without willingness to conduct additional experiments. Increasingly complex molecules, i.e. substances with multiple functional groups and branched structures are targeted in process design, which necessitates predictive methods with strong physical basis. Before analyzing complex multifunctional molecules and mixtures, it is essential that pure and less complex compounds such as branched alkanes are adequately modeled. To this end, many approaches exist [1], but the most well-known ones are based on group contributions.

In group-contribution (GC) methods, the molecular structure is decomposed into building blocks referring to functional groups and any property of a considered molecule is estimated as a function of the contributions of these building blocks. The assumption is that the electron structure of a functional group is not (much) altered by neighboring groups. As a consequence, the parameter value of any group is considered to have the same contribution to the property of a considered species, irrespective of the other groups present in that molecule. GC methods are thus predictive by definition.

GC-methods can be used to estimate pure component properties. For example, such methods have been developed to determine critical properties of pure components in a predictive