

Computer-Aided Pure Component Property Prediction for Isomers

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In product/process design, reliable and predictive property models are necessary. Many biological, medical, pharmaceutical, agricultural, and food products and processes involve stereo-isomers. Their chemical, medicinal, organoleptic, and biological properties can differ significantly. Knowledge of how their thermodynamic properties differ is necessary to model such systems.

Numerous property prediction methods, based on concepts such as group contributions (GC), graphical descriptors, molecular mechanics, quantum mechanics etc., exist. Great efforts have been made to develop simple, reliable, and predictive methods. Additional rewards result if the method has a form that can be used in molecular (product) design algorithms.

The objective of this work is to develop a new class of GC models. This work addresses the limitations of the current GC models, so that chemical product/process synthesis and design problems can be solved reliably and efficiently with model-based approaches. Currently, a cis/trans isomer distinction can not be made with group models, because these models do not describe different spatial conformations. To overcome this, the relationships between structural properties and thermodynamic properties for cis/trans isomers have been explored. Using a large database, a preliminary model correlating the structural properties with the thermodynamic properties, such as boiling points, has been developed. Using this knowledge, we are developing additional correction terms to add to the existing GC method, to take into account the structural properties of cis/trans isomers.

The methodology includes the: (1) generation of a new database for cis/trans isomers including atomic interactions, steric properties, and intermolecular forces (generated through atomic level calculations) related with specific properties of interest; (2) generation of a new term that takes into account structural terms; and (3) implementation of this term into a GC method.

In this way, a distinction between cis/trans isomer properties is made with good accuracy using easy-to-use software. The method is available for process and/or product design.