Invited Lecture IL 05

Improvements on the Predictive COSMO-SAC Model and its Applications in Process and Produce Design

Authors and affiliation

Shiang-Tai Lin*,[1], Cheih-Ming Hsieh[2], Chang-Che Tsai[1], and Chen-Hsuan Huang[1]

[1]Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan

[2]Department of Chemical and Materials Engineering, National Central University, Taoyuan 32001, Taiwan

*E-mail: stlin@ntu.edu.tw

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Abstract (less than 300 words)

Thermodynamic properties and fluid phase equilibria are crucial for the design and development of a chemical process. However, such data may not always be available, particularly for fine and specialty chemicals. Furthermore, in order to design new chemical products with desired functionalities, it is important to estimate their properties based on chemical structures. It is therefore desirable to have a reliable predictive method for the estimation of the thermodynamic properties. In this presentation, we will demonstrate how we develop accurate and reliable predictive models for thermophysical properties and fluid phase equilibria. In particular, we will introduce the COSMO-SAC model[1] for liquid activity coefficient, and its extension, the PR+COSMOSAC EOS[2], for fugacity of any fluid and fluid mixtures.

Equally important is to integrate the predictive methods with process simulators, such as AspenPlus, so that any chemical engineers can perform the routine design without the hassle of conducting the detailed property predictions. To this end, we have developed a new platform, T.E.A.M, that provides all the necessary thermodynamic information needed in a chemical process design in the format of AspenPlus file. The T.E.A.M has a web-based front-end, where the user can specify the chemicals involved in the process submit the request for determination of the all the variables needed for AspenPlus. If any of the needed properties are not available in the AspenPlus database, TEAM performs the needed calculations based on COSMO-SAC and PR+COSMOSAC equation of state. We will illustrate the use of T.E.A.M for the design of a process for converting CO2 to high value chemicals[3]. This process involves 10 chemicals but about 20% of pure fluid properties and 85% of mixture properties are not available in AspenPlus. With the help of T.E.A.M we successfully developed a carbon-neutral and economically profitable process for utilization of CO_2.

Reference

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