# Using the Solubility Parameter Method MOSCED to Predict Phase Behavior and Gain Molecular-Level Insight

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Separation processes are expensive, non-spontaneous processes. It stands that even a minute improvement of existing separation process technologies could lead to significant cost savings. Central to the design and understanding of a separation process is the phase equilibrium thermodynamics of the system. Complementary, and perhaps even more important, is an understanding of the underlying molecular-level details of the system. After all, it is these molecular-level interactions upon which the entire process is built.

For these reasons, solubility parameter-based methods, which can both make quantitative predictions and offer insight in terms of the molecular-level interactions, have long been a valuable design tool. Here we draw attention to the solubility parameter-based method MOSCED (modified separation of cohesive energy density) [1-3]. The major advancement of MOSCED is in its treatment of association. We will demonstrate how this feature allows MOSCED to make a range of accurate quantitative phase-equilibrium predictions, including vapor/liquid equilibrium. Further, we will demonstrate cases where the molecular-level insight offered by MOSCED can be used to gain insight and design processes to separate azeotropic mixtures, and how MOSCED can be used to explain the phenomenon of solubility enhancement and design of co-solvent systems.

However, a major shortcoming of MOSCED has been its limitation of parameters. We will highlight our efforts to expand MOSCED to ionic liquids and to develop methods to predict MOSCED parameters. In particular we will highlight our work to map Abraham solute model descriptors [4] to MOSCED parameters. This has allowed us to expand the MOSCED parameter database to cover over 7000 molecules.

References

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