Modeling of Liquid-Liquid Phase behavior for DES-containing Systems Using COSMO-SAC model

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Deep eutectic solvent (DES) is a new class of solvents typically formed by mixing choline chloride with hydrogen bond donors such as amines, acids, and alcohols. DES have been paid great attention to replace current harsh organic solvents and have been applied to many chemical processing such as extraction and synthesis.
However, most researches about DES have been focused on experiment. In this work, therefore, the theoretical modeling work on liquid-liquid equilibrium (LLE) is carried out by using COSMO-SAC model. The predicted results showed a similar work with experimental data.