## Using Molecular Simulations for Predicting the Binary Interaction Parameters of the Non-Random Two-Liquid (NRTL) Model

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Predicting the phase equilibria of liquid mixtures is vital for designing chemical processes. For this purpose, activity coefficient based thermodynamic models such as non-random two-liquid (NRTL) and UNIQUAC are often employed in industry. To accurately predict the phase equilibrium properties, these models require an input parameter known as the binary interaction parameter. The binary interaction parameters quantify the nature of molecular interactions between different components in the mixture. These parameters are usually calculated by fitting experimental data to the thermodynamic models. A drawback of this procedure is that many experimental data sets with low uncertainties are required to determine the binary interaction parameters. In this work, we develop an approach combining theory and molecular simulations to predict the binary interaction parameters of the NRTL model. The methodology we propose here is completely predictive and requires no knowledge of experimental data. We show that the binary interaction parameters depend on the molecular size and the interaction strength, each of which can be directly calculated from simulations. The following binary mixtures are used as model systems to validate the proposed approach: water + methanol, methanol + methyl acrylate, and water + methyl acrylate. In each case we show that there is a reasonable agreement between the NRTL parameters calculated from molecular simulations and those obtained from data regression. The phase equilibrium properties predicted using the binary interaction parameters obtained from both the approaches (molecular simulations and data regression) are also in good agreement.