Vapor-liquid phase equilibria behavior prediction of water/organic-organic binary mixture using machine learning

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Abstract

Basic thermodynamic data plays an important role in chemical applications. However, the traditional acquisition of thermodynamic data through experiments is laborious. Thermodynamic data prediction is considered as an alternative to the experiments, especially when qualitative analysis is needed prior to experimental studies. In this work, we report a successful machine-learning based approach to predict the fundamental thermodynamics characteristics of vapor-liquid equilibrium (VLE) process. A new dataset of the VLE experimental data of 210 kinds of binary mixture with screened descriptors were constructed. The obtained results show that the VLE characteristics of the target system can be fully revealed for a pre-analysis by ML methods and the RF model has more excellent predictive ability on the VLE behavior than the ANN model. This work pioneers the development of the generalized model on the prediction of the VLE data and provide useful information for mechanistic study on the VLE phenomenon.

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