Prediction for the surface tension of binary liquid systems based on the multivariate statistical analysis method

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The empirical model to estimate and predict surface tension of binary liquid systems is proposed by using the partial least squares(PLS) based on the multivariate statistical analysis method. Surface tension is one of the most interesting thermophysical properties which has been most widely used to characterize surfaces of liquids in chemistry and chemical engineering area. PLS method for estimating and predicting of surface tension is composed by the thermophysical properties of pure substances such as activity coefficients and surface concentration, and experimental surface tension data. The data set for experimental surface tension of binary liquid systems is divided into a training set for estimating and test set for predicting. The results of estimating and predicting indicate that PLS method would be a useful tool for predicting surface tension of binary liquid systems.