Influence of NRTL Parameters on the Separation of Water + Alcohol Systems

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The dehydration of low molecular mass alcohols is an important separation process applicable to the production of biofuels and other anhydrous alcohols, as well as the processing of Fischer-Tropsch reaction water. These alcohols can be dehydrated using a combination of distillation and advanced separation techniques, the latter being required for ethanol and higher alcohols due to the presence of an azeotrope. To design these processes a reliable thermodynamic model is required that can describe the relationship between temperature, pressure and composition. The NRTL model has the ability to describe water + alcohol systems well due to its ability to capture the effect of the molecular interactions present in the system. The literature is abundant with reliable data on water + alcohol systems but each of these data sets results in different model parameters. The aim of this paper is to investigate how different data sets influence the model parameters of water + alcohol systems and the prediction of the separation that can be achieved in a simple distillation column. This study is limited to fully miscible binary aqueous-alcoholic systems i.e. water + (methanol, ethanol, 1-propanol or 2-propanol) for data at pressures below 0.5 MPa. Vapour-liquid equilibrium (VLE) data available in the NIST TDE were collected and data not fulfilling the L-W thermodynamic consistency test omitted. For each data set, temperature dependent model parameters were fitted through minimization of the SSE. The various fitted parameter sets were used to predict the water + alcohol separation with a distillation column in Aspen Plus® V11.1. The results show small differences in the degree of separation that can be achieved, irrespective of the parameter sets used, and are similar to that predicted with the default Aspen Plus parameters for these systems. The study provides an outcome of the expected variation in the separation prediction of water + alcohol systems when using different parameter sets.