

Thermodynamic modelling of Butadiene Extractive Distillation Plant

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1.Summary

The aim of this study is thermodynamic modelling of butadiene unit. C₄ mixture are usually separated by extractive distillation. In the present work 1,3-butadiene is separated by N-methylpyrrolidone (NMP) as solvent to reach 98% purity. C₄ mixture produced in Ethylene unit as a byproduct of cracking process. Separation of 1,3- butadiene from the C₄ cut is not possible by conventional distillation due to several azeotrope mixtures and very close boiling point of the components. In this study modelling of vapour-liquid equilibria of the system have been performed by equation of state and activity models such as NRTL, WILSON and UNIQUAC. It was found that activity model is more accurate for prediction of the liquid behaviour of hydrocarbon and NMP system. The binary interaction coefficient of the components (hydrocarbon – NMP system and water – hydrocarbon system) are tuned by different methods using VLE data. It was found that NRTL equation is able to predict the experimental data with the minimum error. Simulation of extractive distillation columns of the unit have been performed by optimized NRTL model.

Keywords: Extractive Distillation, Vapour-Liquid Equilibrium, NMP, Butadiene, Binary Interaction Coefficient.

2.Extended Abstract

In this study, modelling of vapour-liquid equilibria of the system have been performed by activity models such as NRTL, WILSON and UNIQUAC for liquid phase. Vapour phase assumed ideal. The pressure of this system is about 6 bara and it is not so high that ideal gas equation can be a reasonable assumption. However after modelling, this assumption was checked and it was found that ideal gas can predict the equilibria behaviour of vapour phase of this plant. For liquid phase the binary interaction coefficients of the components (hydrocarbon – NMP system and water – hydrocarbon system) are tuned by different methods, using binary VLE data and equilibrium points of the plant. VLE data is available just for 1,3Butadiene-NMP, iso-Butene - NMP, H₂O-NMP. So for these systems, binary interactions were calculated by data regression method. For other systems binary interactions were calculated by using bubble points and dew points data of different points in the plant. The results were compared to experimental data.

Method 1. Equilibrium temperature for all points was calculated with existing binary interactions. For the systems that binary interaction was not available, it was assumed zero.

Method 2. Equilibrium temperature for all points was calculated with existing binary interaction. For the systems that binary interaction was not available, it was predicted with VLE UNIFAC method.

Method 3. Equilibrium temperature for all points was calculated with existing binary interaction. For the systems that VLE data was available, calculated interaction coefficients were assumed valid. For the systems that binary interactions didn't exist, it was assumed zero.

Method 4. Equilibrium temperature for all points was calculated with existing binary interaction. For the systems that VLE data was available, calculated interaction coefficients were assumed valid. For the systems that binary interactions were not available, they were predicted with VLE UNIFAC method.

The following different methods were utilized and the results were compared to the experimental data. The evaluation of this comparison is illustrated in the following figures:

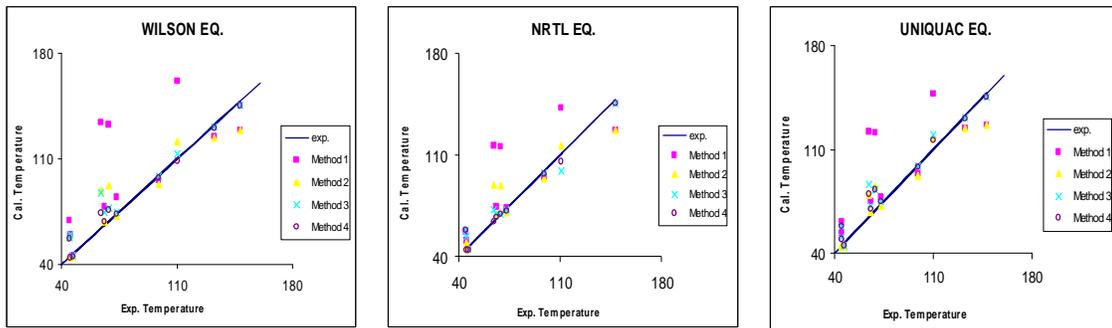


Fig 1. Comparison of Calculated equilibrium temperatures for WILSON, NRTL, UNIQUAC equations with mentioned methods versus experimental temperature

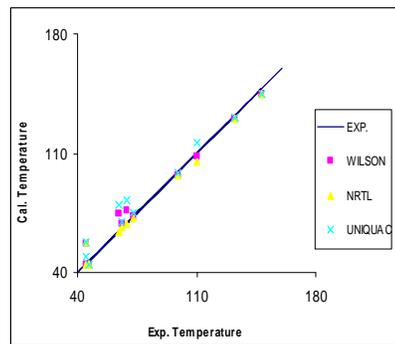


Fig 2. Calculated equilibrium temperature for all activity equations with fourth method versus experimental temperature

Consequently it was found that NRTL equation is able to predict the experimental data with the minimum deviation. Simulation of extractive distillation columns of this unit has been performed by using optimized NRTL model. Simulation of the plant showed water mol fraction distribution on the different trays is not suitable and an undesired two phase mixture (aqueous and organic) was formed on the various trays. This phenomena indicates thermodynamic model is not able to predict aqueous and organic properties correctly in spite of hydrocarbon-hydrocarbon system. So, binary interactions for hydrocarbons – water systems were corrected by using UNIFAC and Immiscible methods. The results showed UNIFAC method has the minimum error and it was selected as the optimum method for prediction of these systems behaviour in this plant.

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