VLE, LLE AND VLLE DATA OF WATER-ETHANOL-HYDROCARBON SYSTEMS IN CHEMICAL PROCESS SIMULATION SOFTWARE

INTRODUCTION

Design and optimization of distillation columns for ethanol dehydration, using a hydrocarbon as entrainer, implies a good knowledge of vapor-liquid (VLE), liquid-liquid (LLE) and vapor-liquid-liquid equilibrium (VLLE). Chemical process simulation programs always require the use of a thermodynamic model that can properly reproduce those equilibria. NRTL, UNIQUAC and UNIFAC are the most applied models in the calculation of equilibrium data for the water-ethanol-hydrocarbon systems. These systems are highly non-ideals, with wide heterogeneous regions and some azeotropes: three binaries and one ternary. The equilibrium data for these systems are necessary to the study of ethanol dehydration columns with gasoline.

OBJECTIVES

To study the accuracy of the different methods, interaction parameters of the literature and models in the calculation of the VLE, LLE and VLLE of water + ethanol + hydrocarbon (hexane, heptane, cyclohexane and iso-octane) systems by means of:

1. Analysis of the contribution groups models
2. Use of bibliographic activity coefficient models parameters
3. Correlation of VLLE data using activity coefficient models
4. Correlation of only LLE data

CONCLUSIONS

All the studied models predict acceptably the VLE. However, the main error found in this study is that none of the models predict correctly the LLE, especially in the closeness of the plait point. The experimental non-isothermal binodal curve is markedly asymmetrical, contrary to the calculated one.

NOTE

All the studied systems present the same behaviour. For this reason only the system water - ethanol - cyclohexane have been shown.