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Chapter 1 : CiteSeerX Citation Query Prediction of Vapor-Liquid Equilibria by the ASOG

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The activity coefficients obtained from the experimental data were correlated by using different thermodynamic mathematical models. All the binary systems show a positive consistency when subjected to the point-to-point test of Van Ness. This system has also been reported at isobaric conditions by Perelygin and Volkov and Nishi see Gmehling and Onken, and by Ortega et al. The experimental data of this paper at 0. All data included in this work have passed the consistency test according to the Fredenslund criteria Fredenslund et al. The purity and the experimental values of density, refractive index and normal boiling point of these products are shown in Table 1. The normal boiling point at 0. The measures of the pure substance properties are compared with literature values. VLE Equipment and Procedure A still ebulliometer developed and built in copper, with all its different pieces assembled with silver-weldings is presented in Figure 1. The still has a configuration similar to the apparatus made of glass by de Afonso et al. The equipment has a double-walled inverted vessel where a boiling mixture of liquid and vapor is generated by an electric heater. This boiling mixture rises in a tube that works like a Cottrell pump. The Cottrell tube is connected to a vessel that acts like an equilibrium chamber. The liquid and vapor phases are carried out on separate paths from this equilibrium chamber. A tube connected to a funnel collects and circulates the liquid phase in the equipment. This tube has a lateral path that ends in a valve. The vapor phase is carried out to the cooler. The cooler has a coaxial tube that returns the condensate to the still and it has a lateral path with a finishing valve. Therefore, both phases are refluxed. The equilibrium equipment has been designed to work at moderate pressures. Therefore, slight modifications were made to this copper still in order to ease sampling of both phases at the working pressures see Figure 1. Some airtight outer vessels must be used. In addition, it was necessary to prepare J-type thermocouples with a ring silver-soldered to both its cover and the ebulliometer. Thermocouples of Thermocoax range K with 0. The working pressure was measured with a NuovaFima manometer with a range from 0 to 1. The copper still described in this paper showed good agreement with the ebulliometer previously used, the operation procedure also being similar de Afonso et al. The procedure differs in the residence time of the mixture inside the ebulliometer and the sampling method. The ebulliometer has a cm³ mixture capacity, the reason why a 90 min recirculation time is necessary for the mixture. This was evaluated by a previous test of operation time vs. Samples of the liquid and vapor phases were removed from the airtight vessels with syringes and the compositions of the equilibrium phases were obtained by densimetry at Also included in Table 2 are the activity coefficients of the liquid phase for each system, calculated by using the following equation: The fugacity coefficients were calculated by using the virial state equation truncated at the second term, and from the following equation: The liquid molar volumes of the pure compounds were estimated by the equation of Yen and Woods VLE experimental data in this paper were verified by using the thermodynamic consistency test of Van Ness et al. The proposed computer program of Fredenslund et al. To calculate the constants of each model, a non-linear regression procedure was employed Nelder and Mead, , considering a minimization of the objective function OF Holmes and Winkle, ; Postigo et al. The results of the correlations with thermodynamic mathematical models are presented in Table 3. The models give good fit to the experimental data and show acceptable mean deviations for the prediction of the vapor phase composition. In addition, as in previous papers Ortega et al. Results of the experimental data treatment with the different FF, using the Nelder and Mead procedure to minimize the summation of the square of the deviations, are shown in Table 4. A mathematical treatment similar to literature data Ortega et al. The fits of the experimental data of this paper Table 4 are plotted in Figure 2 and 3 , respectively. The examination of the equilibrium data obtained in this work shows a good variation with pressure see Figure 2 and an appreciable relation can be

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also observed between our systems at 0. In Figure 2 , some differences are seen between data from this study at 0. The above mentioned relationship between the data from this work and literature data at 0. On the other hand, the differences observed in Figure 3 between data from this paper at 0. The experimental data from this paper at 0. This result does not differ significantly with the literature data Gmehling et al. On the other hand, for 0. A representation of the experimental azeotropic data of this paper and the bibliografic data Gmehling et al. Azeotropic data at 0. Results are presented in Table 5. However, all models generally return a higher average error in the prediction of the activity coefficient when applied to the systems studied at 0. A new determination of the parameters of the different models will probably be required. On the other hand, the group contribution models Table 5 yield acceptable predictions at 0. Nevertheless, at higher pressures, several models present significant discrepancy. The experimental data passed positively the consistency test of Van Ness and showed satisfactory agreement with literature data. This binary system forms an azeotrope at 0. It has been also verified that the azeotropic data expressed as ester mole fraction decreases with a pressure increase. The new isobaric data obtained at moderate pressures have been used to verify the predictive behavior of several group contribution models. The predictions achieved using the UNIFAC and ASOG models were verified by the determination of the mean deviations in the vapor phase mole fraction and the mean error in the estimation of the liquid phase activity coefficient. Results show that the predictions are good for the VLE at atmospheric pressure, while higher deviations were obtained with the pressure increase. When the UNIFAC and ASOG models were used for the azeotropic data prediction, the calculated values did not show a good agreement with the experimental data from this work at moderate pressures.