

Calculation of the Gibbs Adsorption Isotherm of Binary Systems: An Alternative Approach using Liquid Bulk and Vapor-Liquid Interface Concentrations

L.F. Ramírez-Verduzco

Programa de Crudo Maya-Reducción de Azufre en Diesel, Instituto Mexicano del Petróleo, México D. F., Mexico

A. Romero-Martínez^S

Programa de Ingeniería Molecular - Área de Investigación en Termofísica, Instituto Mexicano del Petróleo, México D. F., Mexico

A. Trejo^C

Competencia de Ciencias Básicas, Instituto Mexicano del Petróleo, México D. F., Mexico

In this work, the calculation of the Gibbs adsorption isotherm for binary systems is carried out employing two different schemes. The first one is that traditionally performed using surface tension experimental data as a function of concentration of one of the components in the liquid phase and/or the activity of the same component; the second one utilizes only the concentrations of the bulk liquid phase and that of the vapor-liquid interface together with values for the molar surface area of each component. Values of the concentration of the vapor-liquid interface used in the second scheme were derived during the prediction of mixture surface tension values using a thermodynamic model for both the liquid bulk phase and the vapor-liquid interface together with the activity coefficient model UNIFAC. Details about this prediction were included in a work presented in a previous event of this symposium.[1]. It has to be stressed that using the second scheme, there is no need for information of surface tension values as a function of liquid concentration. The calculation of the Gibbs adsorption isotherm was carried out for 31 binary systems, with different chemical nature, at different temperatures, covering the entire concentration range. As an example of the type of results obtained, in this work comparisons are included, using the two different calculation schemes, for the following binaries: n-decanol/isobutanol, butanenitrile/n-heptane, n-hexadecane/cyclohexane, and nitrobenzene/1,4-dioxane, at different temperatures. The calculation results obtained using both schemes are comparable and consistent with what is expected with respect to the functionality of the preferential adsorption as a function of the liquid concentration.

[1] L. Ramírez-Verduzco, A. Romero-Martínez, and A. Trejo. Work presented at the Fourteenth Symposium on Thermophysical Properties. NIST-University of Colorado. Boulder, CO, USA, June (2000).