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THE POTENTIAL OF GROUP CONTRIBUTION METHODS IN PREDICTING PHASE EQUILIBRIUM OF VOCs IN WATER, GLYCOLS AND BIODIESEL AS A TOOL IN PROCESS SIMUALTION, DESIGN AND FEASIBILITY STUDIES

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Abstract

Group contribution methods such as the UNIFAC are of major interest to researchers and engineers involved synthesis, feasibility studies, design and optimization of separation processes as well as other applications of industrial use. They can be applied successfully to predict phase equilibrium and excess properties especially in the development of chemical processes. Reliable knowledge of the phase equilibrium behavior of pure compounds, their mixtures in the whole composition, wide temperature and pressure range is crucial for the prediction of the fate of the chemical in the environment and other applications. The objective of this study was to predict the solubility of selected volatile organic compounds (VOCs) in water, glycol polymers (PEG 300, 350, 400) and biodiesel. The biodiesel used here is a methanol transesterificated product of rape seed oil. Measurements can be expensive and time consuming, hence the need for thermodynamic models which allow the calculation of the phase equilibrium behavior using a limited number of experimental data. Predictive methods especially those based on group contribution methods can replace measurements if they are giving precise and reliable estimations. The results obtained in this study for the infinite dilution activity coefficients compare very well those published in literature obtained through measurements. Therefore it is suggested in this work that in preliminary design or feasibility studies of absorption systems for the abatement of volatile organic compounds, prediction procedures