Vapor–Liquid equilibrium modeling of Fatty Acid Esters Systems using the CPA–EoS

Follegatti–Romero, L.A.[1]; Lanza, M.[3]; Batista,F.R.M.[1]; Batista, E.A.C.[1]; Oliveira, M.B.[2]; Coutinho, J.A.P.[2] ;Meirelles, A.J.A.[1]

1 - University of Campinas, Brazil, 2 - University of Aveiro, Portugal, 3 - Federal University of Santa Catarina, Brazil

Fatty acid esters are known from a long date as high–value fine chemicals used in the manufacturing of pharmaceuticals, cosmetics, detergents, surfactants, food packaging, etc. These compounds are currently produced in batch and continuous processes and are key products of the chemical process industry, involved not only in specialty chemicals but also in the production of biodiesel. Distillation has been used for partial separation of mixtures of fatty acid esters. The knowledge and description of the corresponding phase equilibrium is essential for optimizing the purification of these esters. In the present work, the Cubic–Plus–Association Equation of State (CPA–EoS) capability to model the phase vapor–liquid equilibria of binary systems composed of fatty acid esters was evaluated. Modeling results for several binary systems containing ethyl palmitate + ethyl stearate/oleate/linoleate at 5332.9 Pa and ethyl palmitate + ethyl oleate at 9332.6 Pa are presented. Other binary systems containing: methyl laurate + methyl myristate and methyl myristate + methyl palmitate at several pressures were also modeled. Excellent results for the vapor pressures and liquid densities were achieved, with global deviations below 2.5 % and 0.8 %, respectively. The very good predictive performance of the CPA EoS was achieved in the modeling of the vapor–liquid equilibria data of binary systems containing fatty acid esters, using only the CPA pure compound parameters. Hence, it can be applied to explore the operating conditions in the separation process during distillation of fatty acid esters.

Supported by FAPESP (08/56258–8), CNPq (304495/2010-7+480992/2009–6), CAPES and Fundação para a Ciência e a Tecnologia (SFRH/BD/29062/2006).