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EDEFIash - COMPUTER PROGRAM FOR THERMODYNAMIC MODELLING OF MULTICOMPONENT SYSTEMS

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The knowledge of vapor-liquid equilibrium data is of fundamental importance for the design of multistage gas extraction process. High-pressure vapor-liquid equilibrium data can be determined experimentally, or predicted using thermodynamic models, using equations of state, for instance. The correlation of experimental vapor-liquid equilibrium data using equations of state is of special importance, as it provides not only a general view of the phase behavior of the system, but makes possible to diminish the number of experiments.

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EDEFlash – COMPUTER PROGRAM FOR THERMODYNAMIC MODELLING OF MULTICOMPONENT SYSTEMS

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1 – INTRODUCTION

The knowledge of vapor-liquid equilibrium data is of fundamental importance for the design of multistage gas extraction process. High-pressure vapor-liquid equilibrium data can be determined experimentally, or predicted using thermodynamic models, using equations of state, for instance. The correlation of experimental vapor-liquid equilibrium data using equations of state is of special importance, as it provides not only a general view of the phase behavior of the system, but makes possible to diminish the number of experiments. To help in this task, the EDEflash program was developed (Araújo, 1997; Araújo and Meireles, 2000; Araújo et al, 2001).

2 – EDEflash PROGRAM

The EDEflash program was developed using Delphi 2.0 with the programming language Pascal guided to objects and offer routines to correlate vapor-liquid equilibrium data and to estimate phase equilibrium of multicomponent systems using cubic equation of state. The pure component data (critical temperature and pressure and acentric factor) are stored in a folder called OPTIONS (Figure 1).

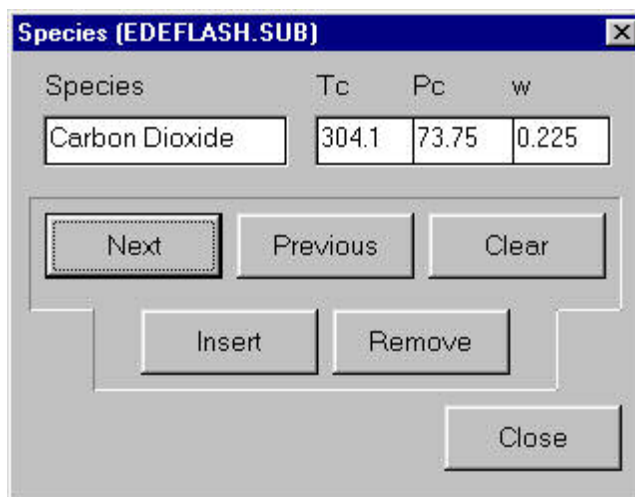


Figure 1 - EDEflash folder to store thermophysical pure component properties.

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2.1 - Equations of State and Mixing Rules

The EDEFflash program offers the option to use six different cubic equations of state Van der Waals, Redlich-Kwong, Soave-Redlich-Kwong, Peng-Robinson, Peng-Robinson modified and Soave-Redlich-Kwong modified. Van der Waals mixing rules with the combining rules with two binary interaction parameters and three binary interaction parameters proposed by Kwak and Mansoori (1986) and Park et al (1987) can be used.

2.2 - Binary Interaction Parameters Estimation

The EDEFflash program offers a routine (FITTING folder) to determine the binary interaction parameters computed by fitting experimental binary vapor-liquid equilibrium data. The binary interaction parameters are obtained using a P-T flash algorithm and the modified Simplex method of Nelder Mead (1965) (Figure 2). Depending on the available experimental data, the objective function can be chosen as:

(i) for vapor-liquid equilibrium experimental data:

$$OF = \sum_{j=1}^n \sum_{i=1}^2 \left[\left(\frac{x^c(i) - x^e(i)}{x^e(i)} \right)^2 + \left(\frac{y^c(i) - y^e(i)}{y^e(i)} \right)^2 \right] \quad (1)$$

(1)

(ii) for vapor phase experimental data:

$$OF = \sum_{j=1}^n \sum_{i=1}^2 \left[\left(\frac{y^c(i) - y^e(i)}{y^e(i)} \right)^2 \right] \quad (2)$$

(2)

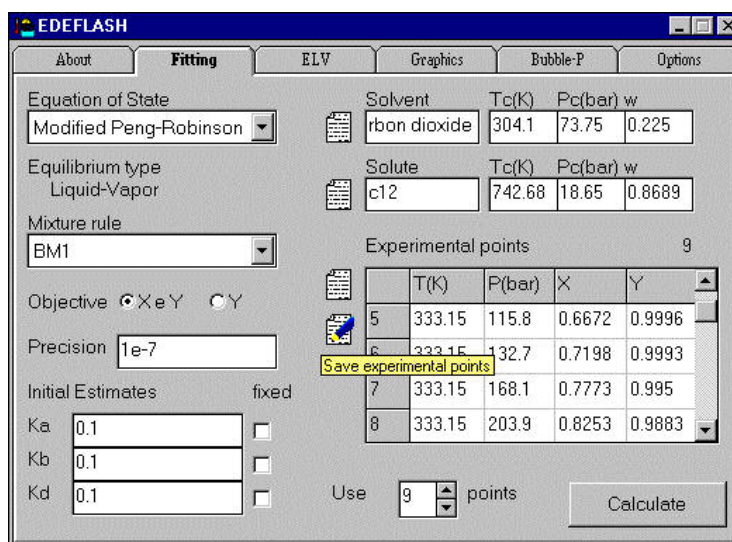


Figure 2 - EDEFflash folder to obtain the binary interaction parameters

2.3- Vapor-Liquid Equilibrium Calculation

The EDEFflash program offers routines to calculate phase equilibrium of binary or multicomponent

systems (ELV folder). Thermodynamic modeling of vapor-liquid equilibrium in the form of P-T flash requires as input data the pure component thermophysical properties and the binary interaction parameters obtained. Besides this, for modeling phase equilibrium of multicomponent systems the EDEFflash program requires the molar composition of the multicomponent mixture in solvent free basis. In order to enable the users to insert the binary interaction parameters obtained, for the multicomponent vapor-liquid equilibrium calculation the EDEFflash program generate a symmetrical matrix that depends on the number of components in the mixture (Figure 3).

	Carbon D	C-12	C-14	C16:0	C-18:0	C-18:1	C-18:2	C18:3
Carbon D	0	0	0	0	0	0	0	0
C-12	0	0	0	0	0	0	0	0
C-14	0	0	0	0	0	0	0	0
C16:0	0	0	0	0	0	0	0	0
C-18:0	0	0	0	0	0	0	0	0
C-18:1	0	0	0	0	0	0	0	0
C-18:2	0	0	0	0	0	0	0	0
C18:3	0	0	0	0	0	0	0	0

Figure 3 - EDEFflash folder to insert the binary interaction parameters for the multicomponent phase equilibrium calculation

Figure 4 presents the EDEFflash folder to calculate phase equilibrium of binary or multicomponent systems (ELV folder). Figure 5 presents the experimental and predicted phase equilibria using EDEFflash for the system CO₂ with lauric acid (C-12) at 333.15 K. The Peng-Robinson equation of state with van der Waals mixing rules with two binary interaction parameters and three binary interaction parameters combining rules proposed by Kwak and Mansoori (1986) and Park et al (1987) were applied.

Name	Tc(K)	Pc(bar)	w	Xa
1 C-12	742.68	18.65	0.8689	0.1
2 C-14	762.11	16.42	0.9432	0.1
3 C-16	780.38	14.67	1.0104	0.4
4 C-18:1	796.34	12.42	0.9245	0.28
5 C-18:2	796.03	12.4	0.7767	0.1
6 C18:3	795.72	12.38	0.6295	0.02

Figure 4 - EDEFflash folder for modeling phase equilibria of multicomponent systems

The Peng-Robinson equation of state, with two parameters and van der Waals mixing rules was used to predict vapor-liquid equilibrium of the multicomponent mixture palm kernel oil/carbon dioxide to provide a data base for the separation analysis (Araújo et al, 1999) (Figure 6). Palm kernel oil was assumed to be constituted by a mixture of fatty acids. The binary interaction parameters were obtained from solubility and/or vapor-liquid equilibrium data available in the literature for the binary pairs of palm kernel compounds based on it's fatty acid composition. Therefore, equations of state model are useful tools for the prediction of multicomponent system phase equilibrium.

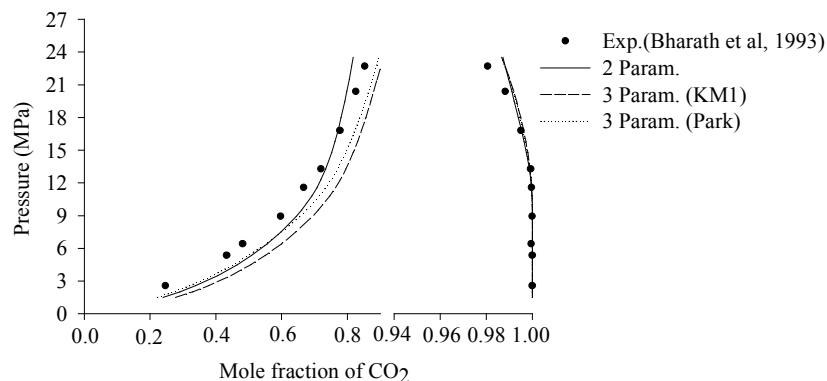


Figure 5 - Experimental and predicted phase equilibria for the system CO₂ with lauric acid at 333.15 K (Araújo and Meireles, 2000).

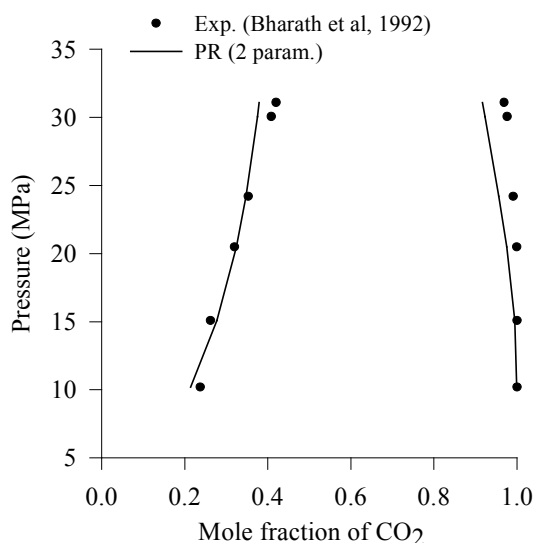


Figure 6 - Phase equilibria for the multicomponent system palm kernel oil/CO₂ at 353 K (Araújo et al, 1999).

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Nomenclature

K_a, K_b, K_d - binary interaction parameters

P - pressure (*bar*)

P_c - critical pressure (*bar*)

T - temperature (*K*)

T_c - critical temperature (*K*)

OF - objective function

Y - vapour phase molar fraction

X - liquid phase molar fraction

X_a - molar fraction of the component i in the mixture (in solvent free basis)

ω - acentric factor