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MODELING VLE OF BIOALCOHOL WITH HYDROCARBON SYSTEMS USING EQUATIONS OF STATE.

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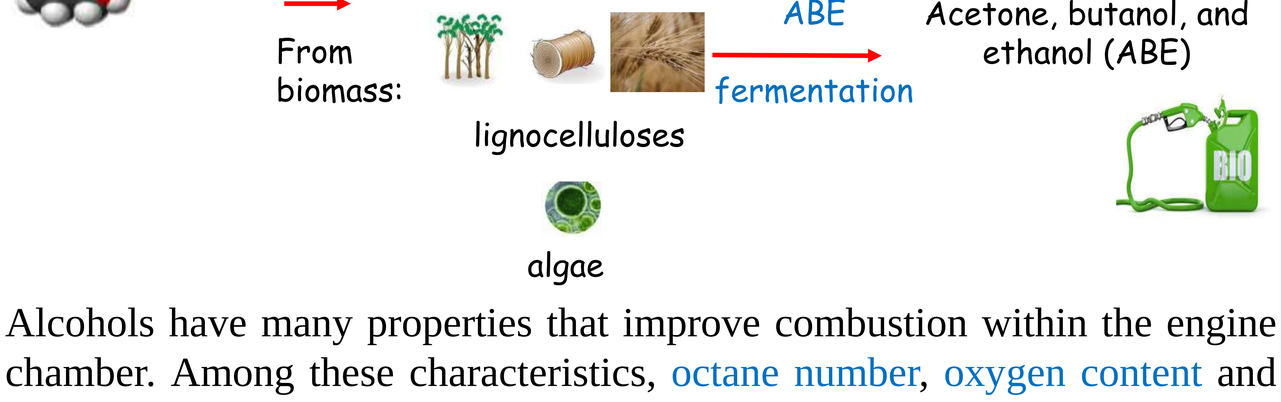
1. INTRODUCTION

- ✓ Traditional fuels are widely used in transport, domestic, agriculture, commercial, and industrial sectors [1] which lead to increasing emission of greenhouse gases (GHG) and depletion of natural resources and petroleum products so the world is facing gradually climate change problem. ⇒ It is important to identify and produce alternative fuels with sufficiently high energy content [2].
- ✓ Biofuels are synthetic fuels derived from biomass and waste streams that can be directly upgraded into transportation fuels such as gasoline [3].
- ✓ Nowadays, alcohols are mixed with traditional fuels [4] which can be obtained by anaerobic fermentation of ligno-cellulosic biomass (agricultural waste and forestry biomass).

Example:



- ✓ Alcohols have many properties that improve combustion within the engine chamber. Among these characteristics, octane number, oxygen content and flame speed that helps to raise the efficiency and quality of the combustion and thus reduce the emission of pollutants [5].
- ✓The accuracy of a process simulation depends strongly on the thermodynamic models used to describe the physical behavior of the involved components.
- ✓In this paper, Cubic-Plus-Association (CPA), Perturbed Chain Statistical Association Fluid Theory (PC-SAFT) equations state are used to calculate the phase equilibrium for these mixtures.
- ✓The purpose of this paper is to investigate the VLE of these mixtures and to verify the capability of CPA, PC-SAFT equations of state.

2. THERMODYNAMIC MODELS : EQS

2.1. Cubic-Plus-Association CPA equation of state [6].

- The CPA EoS combines the SRK equation of state term and the contribution of the association term is given by the following expressions in term of pressure as:

$$P^{CPA} = P^{SRK} + P^{Assoc} \quad (1)$$

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m - b)} + \frac{1}{2}\frac{RT}{V_m}\left(1 + \rho\frac{\delta \ln g}{\delta \rho}\right)\sum_i x_i \sum_{A_i}(1 - X_{Ai}) \quad (2)$$

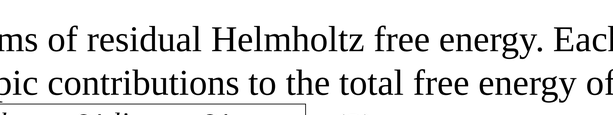
- The CPA EoS has five parameters: a, c_1 parameters in the energy term, the co-volume b, ε^{AiBj} and β^{AiBj} the association energy and volume parameters respectively.

2.2. Pertubed Chain-Statistical Associating Fluid Theory PC-SAFT equation of state [7].

PC-SAFT equation are usually written in terms of residual Helmholtz free energy. Each term in the equation represents different microscopic contributions to the total free energy of the fluid. The equation writes:

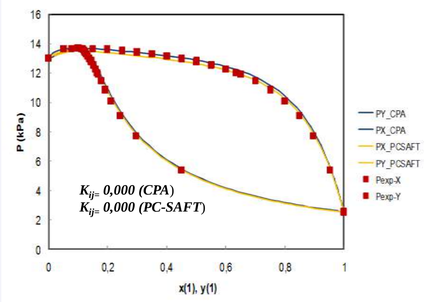
$$\tilde{a}^{res} = \tilde{a}^{hc} + \tilde{a}^{disp} + \tilde{a}^{assoc} \quad (3)$$

- The segment number m_i,
- The segment energy ε_i/k
- The segment diameter σ_i,
- The association energy $\varepsilon^{AiBi/k}$,
- The association volume k^{AiBi}

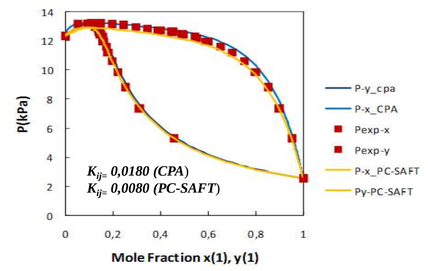


3. RESULTS AND DISCUSSION

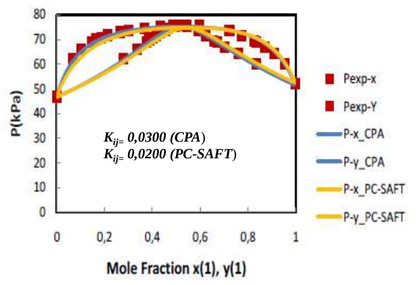
Figures 1 to 8: VLE of the binary system : Comparison between the experimental points and the results with CPA and PC-SAFT equations of state.



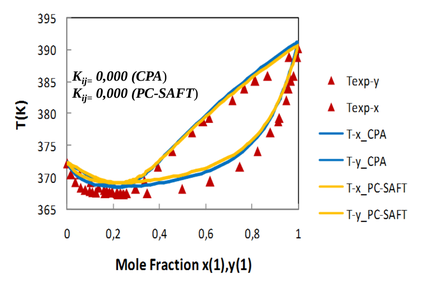
Figures 1: 1- butanol (1) + 2,2,4-trimethylpentane (2) at T=313,15 K



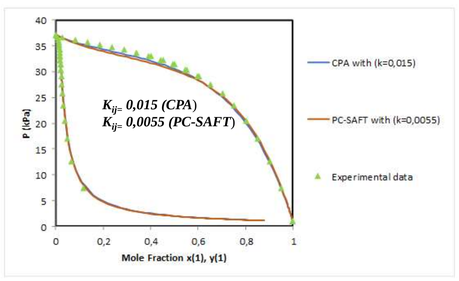
Figures 2: 1-butanol (1) + heptane (2) at T=313,15 K



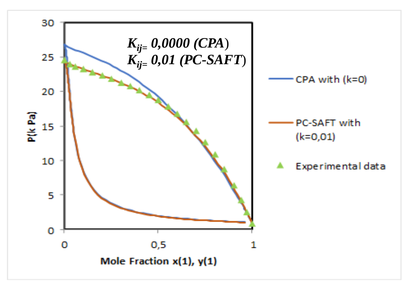
Figures 3: 1-butanol (1) + octane (2) at T=373,15 K



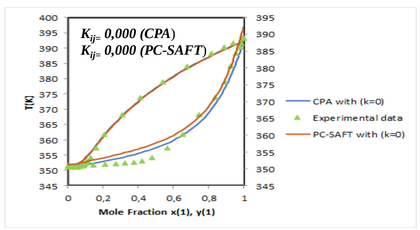
Figures 4: 1-butanol (1) + 2,2,4-triméthylpentane (2) at P=101,3kPa



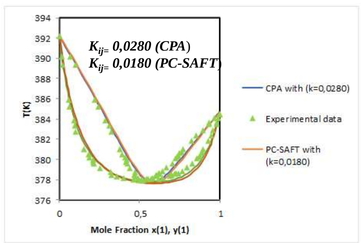
Figures 5: 1-pentanol (1) + hexane (2) at T=313,15 K



Figures 6: 1- pentanol (1) + benzene (2) at T=313,15 K



Figures 7: 1-pentanol (1) + 1-heptane (2) at P=53,3kPa



Figures 8 1-pentanol (1) + nonane (2) at P=40,0kPa

4. CONCLUSION

- ➢It can be seen in figures (1to 8) that accurate results are obtained using CPA, PC-SAFT equations of state.
- ➢ Generally, the results show that CPA and PC-SAFT models are capable of accurately modeling the vapor liquid equilibria.

of the studied systems (alcohol + hydrocarbon).

- ➢ In somes cases the modeling requires a binary interaction parameter. The values of binary interaction parameters are lower and they improve the prediction of phase equilibria.

5. REFERENCES

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