PREDICTION OF PHASE EQUILIBRIA IN THE TERNARY SYSTEM
CARBON DIOXIDE + 1-HEPTANOL + PENTADECANE

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INTRODUCTION

Investigation of fluid multiphase behavior is of considerable interest to experimental and theoretical applications. In this work high-pressure phase equilibria of binary and ternary mixtures containing carbon dioxide, 1-heptanol, and pentadecane have been investigated. The binary and ternary systems were modeled with the SRK-EOS coupled with the Huron-Vidal infinite dilution (HVID) mixing rules.
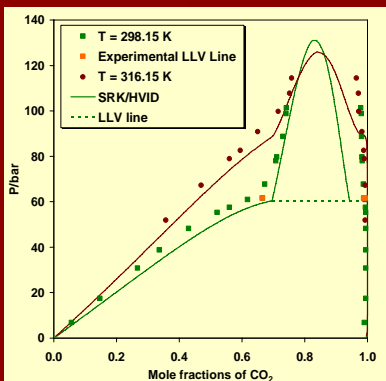
EXPERIMENTAL WORK

Phase equilibria measurements were made in a high-pressure visual cell with variable volume based on the static-analytical method. A detailed description of the apparatus and experimental procedure was presented in a previous paper [1]. Isothermal vapor-liquid equilibria measurements for binary and ternary mixtures containing carbon dioxide, 1-heptanol, and pentadecane at the temperatures of 298.15 and 316.15 K were done.

MODELLING

The phase equilibrium in the binary systems was correlated with the Soave-Redlich-Kwong (SRK) equation of state coupled with the Huron-Vidal infinite dilution (HVID) mixing rules. The binary parameters obtained by correlations were used for the prediction of phase equilibria in the ternary system carbon dioxide + 1-heptanol + pentadecane. Details on the model, the procedure of binary data correlation and ternary phase equilibria calculations were presented in previous papers [2-4].
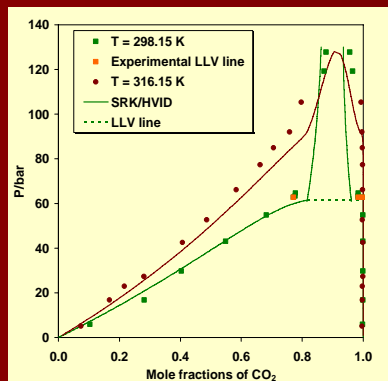
RESULTS

Some experimental results are shown in the figures below. The SRK/HVID parameter values are also presented. The correlations for binary systems and the predictions in the ternary system are included.

Comparison of experimental phase equilibrium data with calculated results by the HVID model for the carbon dioxide + 1-heptanol system at 298.15 and 316.15 K

Comparison of experimental phase equilibrium data with calculated results by the HVID model for the carbon dioxide + pentadecane system at 298.15 and 316.15 K
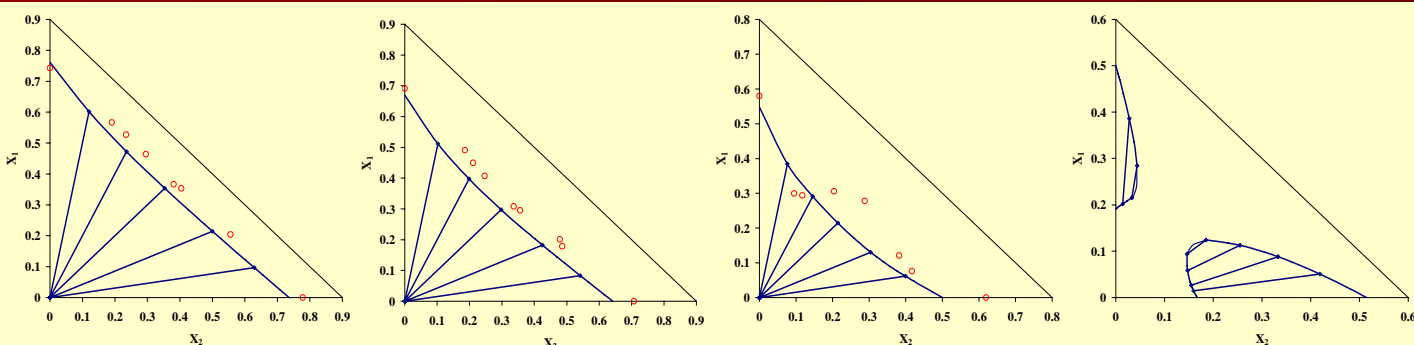
SRK/HVID binary interaction parameters at 298.15 and 316.15 K

System	SRK/HVID T = 298.15 K		SRK/HVID T = 316.15 K	
	$\Delta u_{12}/R$ [K]	$\Delta u_{21}/R$ [K]	$\Delta u_{12}/R$ [K]	$\Delta u_{21}/R$ [K]
CO2 + n-Pentadecane	290.8	32.1	303.9	5.7
CO2 + 1-Heptanol	136.6	88.0	115.6	94.0
n-Pentadecane + 1-Heptanol (Data generated by UNIFAC 93 model)	303.2	-193.8	303.2	-193.8

Comparison of the experimental data with predicted results by the SRK/HVID model for the pentadecane (1) + 1-heptanol (2) + carbon dioxide (3) system (liquid phase) at 298.15 K and 48, 56, and 61 bar, and predicted results at 298.15 K and 72 bar (mass fractions).
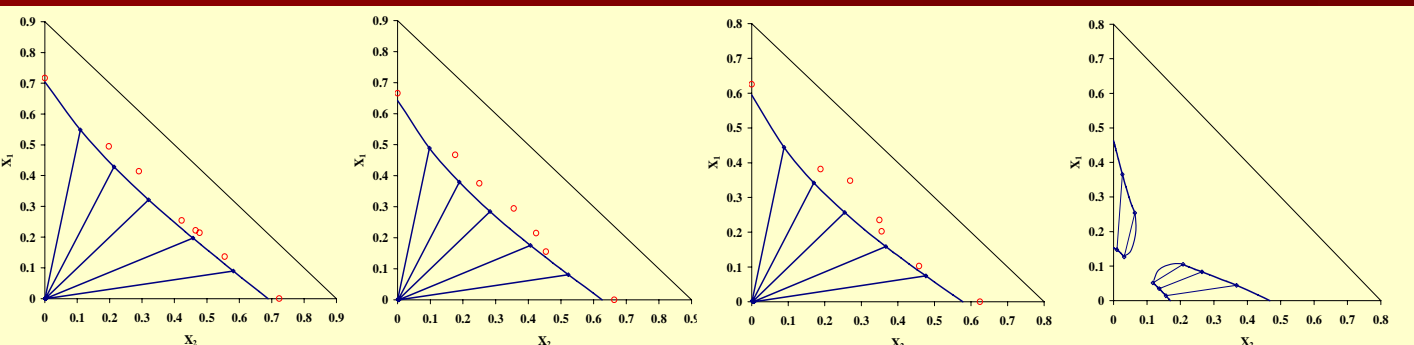
Comparison of the experimental data with predicted results by the SRK/HVID model for the pentadecane (1) + 1-heptanol (2) + carbon dioxide (3) system (liquid phase) at 316.15 K and 72, 80, and 85 bar, and predicted results at 316.15 K and 105 bar (mass fractions).

CONCLUSIONS

New VLE and LLE experimental data for the binary systems carbon dioxide + 1-heptanol and carbon dioxide + n-pentadecane were measured at 298.15 and 316.15 K. Isothermal VLE data for the pentadecane + 1-heptanol + carbon dioxide ternary system were obtained at 298.15 and 316.15 K and pressures ranging from 48 to 85 bar. The behavior of the pentadecane + 1-heptanol + carbon dioxide system is highly complicated, because at pressures above the VLLE line the cosolvency effect occurs. For the first time, calculated results are presented illustrating such complex phenomena. The HVID model is capable of satisfactory predictions.

REFERENCES

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