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ลิขสิทธิ์ของจุฬาลงกรณ์มหาวิทยาลัย

**EQUATIONS OF STATE FOR N-HEPTANE, BENZENE AND
CYCLOHEXANE SYSTEM BASED ON DENSITY DATA**



Miss Chompoonut Bupasiri

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การทำนายปริมาตร โมลาร์ของระบบสามองค์ประกอบนี้ ด้วยสมการสถานะมอดิไฟด์ เรดลิช-กวง (modified Redlich-Kwong) ให้ผลดีกว่า สมการสถานะเพง-โรบินสัน (Peng-Robinson), สมการสถานะเพง-โรบินสัน-สไตรเจค-วีระ 2 (Peng-Robinson-Stryjek-Vera2) และสมการสถานะเพง-โรบินสัน-สไตรเจค-วีระ (Peng-Robinson-Stryjek-Vera) ในทุก ๆ อุณหภูมิและความดัน ค่าความหนาแน่นของระบบสององค์ประกอบพร้อมด้วยระบบสามองค์ประกอบวัดโดยใช้เครื่อง DMA512P densitometer รวมทั้งแสดง ปริมาตร โมลาร์ (Molar volume), ปริมาตร โมลาร์ส่วนเกิน (Excess molar volume) และปริมาตร โมลาร์ย่อย (Partial molar- volume) ที่ทำนายโดยสมการสถานะเพง-โรบินสัน สำหรับระบบสององค์ประกอบ

สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

ภาควิชา วิศวกรรมเคมี
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CHOMPOONUT BUPASIRI: EQUATIONS OF STATE FOR N-HEPTANE, BENZENE AND CYCLOHEXANE SYSTEM BASED ON DENSITY DATA. THESIS

ADVISOR: ASSOC. PROF. KROEKCHAI SUKANJANAJTEE, Ph.D. THESIS CO-

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Cubic equations of state were studied for the ternary system of n-heptane, benzene and cyclohexane based on density data at temperature of 308.15, 313.15, 323.15 and 333.15 K and pressure of 1.01325, 2, 5 and 10 bar.

Prediction of molar volume of the ternary system with a modified Redlich-Kwong (MRK) is better than Peng-Robinson (PR), Peng-Robinson-Stryjek-Vera (PRSV2), and Peng-Robinson-Stryjek-Vera (PRSV) equations of state at all temperatures and pressures. The density data of the binary systems as well as the ternary system were measured by DMA512P densitometer. Molar volume, excess molar volume and partial molar volume by PR equation of state for binary systems were presented.

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NOMENCLATURES

A	Helmholtz free energy
<i>a, b</i>	parameters of equation of state
∂, d	partial, total derivative symbols
G	Gibbs free energy
H	enthalpy
k_{ij}	binary interaction parameter
M	molar property
MW	molecular weight, [g/g-mole]
\bar{M}_i	partial molar property
N	number of experimental data points
n	number of moles, number of components
n_i	function of acentric factor, equations (3.32)
P	pressure [Pa]
P_c	critical pressure [Pa]
P_r	reduce pressure
R	gas constant [cm ³ Pa /mole K]
S	entropy
T	temperature [K]
T_c	critical temperature [K]
T_r	reduce temperature
U	internal energy
V	molar volume [cm ³ /mole]
v	specific volume
V_t	volume of mixture
$V_{t, \text{pure}}$	sum of pure components volumes
ΔV_{mix}	volume change on mixing [cm ³ /mole]

x_i	liquid mole fraction of species i
y_i	vapor-phase mole fraction of species i
Z	compressibility factor

Subscripts

cal	calculated value
c	critical property
expt	experimental value
i	i th component
j	j th component
l	liquid phase
mix	mixing or mixture
pure	pure component
r	reduced property
t	total
v	vapor phase

Superscripts

E	excess property on mixing
-----	---------------------------

Greek letter

ρ	density
ω	acentric factor
Δ	finite change
κ	thermal compressibility, function of reduced temperature and acentric factor, equation (3.39)
κ_0	function of acentric factor, equation (3.40) and (3.48)
κ_1	pure compound parameter, equation (3.39) and (3.47)
κ_r, κ_s	pure compound parameter, equation (3.47)
β	expansion coefficient, coefficient defined by equations (3.22)
α	coefficient defined by equations (3.20), (3.21), (3.31), (3.38) and (3.46)