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นางสาว เขมิกา สุวจีจารัณ

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ACTIVITY COEFFICIENTS BASED ON HEAT OF MIXING DATA AND VAPOR-LIQUID EQUILIBRIA DATA

Miss Khemmika Suwacheecharan

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By	Miss Khemmika Suwacheecharan
Department	Chemical Engineering
Thesis Advisor	Associate Professor Kroekchai Sukanjanajtee, Ph.D.

Accepted by the Faculty of Engineering, Chulalongkorn University in Partial Fulfillment of the Requirements for the Master's Degree

..... Dean of Faculty of Engineering

(Professor Somsak Panyakeow, Dr. Eng.)

Thesis Committee

..... Chairman

(Associate Professor Chirakarn Muangnapoh, Dr. Ing.)

..... Thesis Advisor

(Associate Professor Kroekchai Sukanjanajtee, Ph.D.)

..... Member

(Seeroong Prechanont. Ph. D.)

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ศึกษาค่าสัมประสิทธิ์แอกทิวิตีที่ได้จากข้อมูลของความร้อนของการผสมและข้อมูลสมดุลไอ-ของเหลว เทียบเคียงข้อมูลที่ได้รับการตีพิมพ์ของระบบสองสารจำนวน 13 ระบบโดยใช้สมการวิลสันและยูนิควอเพื่อคำนวณหาพารามิเตอร์ของแรงที่กระทำระหว่างโมเลกุลของทั้งสองสมการ

จากข้อมูลสมดุลไอ-ของเหลว ทั้งสองสมการให้ผลการทำนายความดันที่ดีสำหรับทุกระบบที่ศึกษา เนื่องจากค่าเบี่ยงเบนเฉลี่ยสูงสุดคิดเป็นร้อยละ 2.26 ทั้งสองสมการให้ผลการทำนายค่าสมบัติส่วนเกินของเอนทัลปีโดยใช้พารามิเตอร์ได้ไม่ดีในทุกกรณี สมการวิลสันให้การทำนายที่ดีที่สุดที่ความเบี่ยงเบนเฉลี่ยร้อยละ 11.6 สำหรับระบบ 1,2-ไดคลอโรอีเทน กับ ไดบิวทิลอีเธอร์ ที่อุณหภูมิ 288.15 เคลวิน

จากข้อมูลของความร้อนของการผสม การทำนายค่าสมบัติส่วนเกินของเอนทัลปีสำหรับระบบสองสารด้วยสมการยูนิควอให้ผลดีกว่าสมการวิลสันยกเว้นระบบ 1,2-ไดคลอโรอีเทน + ไดบิวทิลอีเธอร์, 1,1,1-ไตรคลอโรอีเทน + ไดบิวทิล- อีเธอร์ และ เอทิลฟอร์เมต + เบนซีน การทำนายความดันจากพารา-มิเตอร์ที่ได้จากสมการยูนิควอ เหมาะสมมากกว่าสมการวิลสัน ยกเว้นระบบ 1,2-อีพอกซีบิวเทน + แอลกอฮอล์, เอทิลฟอร์เมต + เบนซีน, เอทิลฟอร์เมต + ไซโคลเฮกเซน, และ บิวเทนไนติล + 2-บิวทานอล สมการยูนิควอให้ผลการทำนายที่ดีที่สุดสำหรับ 1-คลอโรเพนเทน และ ไดเอทิลอีเธอร์ ที่อุณหภูมิ 323.15 เคลวิน

พารามิเตอร์เหล่านี้ไวต่อข้อมูลของความร้อนและไม่ค่อยไวต่อข้อมูลสมดุลไอ-ของเหลว

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สาขาวิชา	วิศวกรรมเคมี	ลายมือชื่ออาจารย์ที่ปรึกษา.....K. Sukanyajanta.....
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Activity coefficients based on heat of mixing data and vapor-liquid equilibrium (VLE) data were studied. Published data of thirteen binary systems were correlated using the Wilson and UNIQUAC equations in order to investigate interaction parameters of these models.

Based on VLE data, both models gave a good prediction of pressures for the thirteen binary systems since the maximum percent absolute average deviation between the predicted and experimental pressures is 2.26%. With these parameters both equations gave poor prediction of H^E in all cases. The Wilson gave the best prediction of 11.01 %AAD for the 1,2-dichloroethane with di-n-butyl ether system at 288.15 K.

Based on H^E data, prediction of H^E for the binary systems with the UNIQUAC equation is better than the Wilson model except for the 1,2-dichloroethane + di-n-butyl ether, 1,1,1-trichloroethane + di-n-ethyl ether, and ethyl formate + benzene systems. Prediction of pressure based on these parameters obtained by the UNIQUAC is more suitable than the Wilson except for the 1,2-epoxybutane + alkanols, ethyl formate + benzene, ethyl formate + cyclohexane, and butanenitrile + 2-butanol systems. The UNIQUAC gave the best prediction for the 1-chloropentane and di-n-butyl ether system at 323.15 K.

Finally, these parameters are sensitive on H^E data and rarely sensitive on VLE data.

ภาควิชา	วิศวกรรมเคมี	ลายมือชื่อนิสิต.....
สาขาวิชา	วิศวกรรมเคมี	ลายมือชื่ออาจารย์ที่ปรึกษา.....
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NOMENCLATURES

A	Helmholtz free energy
A,B	initial parameters
$\hat{a}$	activity
a_{ij}	adjustable binary energy parameter in UNIQUAC model
∂, d	partial, total derivative symbols
G	Gibbs free energy
H	enthalpy
M	molar property
MW	molecular weight, [g/g-mole]
$\overline{M}_i$	partial molar property
n	number of experimental data points
P	pressure [Pa]
q_i	surface area parameter for species i.
R	gas constant [Joule /mole]
r_i	volume parameter for species i.
S	entropy
T	temperature [K]
U	internal energy
V	molar volume [cm^3/mole]
x_i	liquid mole fraction of species i
x_{ij}	local composition in Eq. 2.8
y_i	vapor-phase mole fraction of species i
z	co-ordination number in UNIQUAC model
z_i	local volume fraction of species i in Eq. 2.9, 2.11

Subscripts

cal	calculated value
con	configurational term in UNIQUAC model
exp	experimental value
i	i th component

j	j th component
mix	mixing or mixture
res	residual term in UNIQUAC model
t	total

Superscripts

E	excess property on mixing
id	ideal property
L	liquid phase
V	vapor phase

Greek letter

Δ	finite change
γ	activity coefficient
μ	chemical potential
λ	energy of interaction of the Wilson model
Λ	the Wilson parameter in Eq. 2.10, 2.12
ϕ	pure substance parameter of UNIQUAC model in Eq. 2.22
θ	pure substance parameter of UNIQUAC model in Eq. 2.22
τ	parameter of UNIQUAC model in Eq. 2.23