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COMPUTATION OF LIQUID-LIQUID-VAPOR EQUILIBRIUM USING EQUATIONS OF STATE

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พิมพ์ต้นฉบับบทคัดย่อวิทยานิพนธ์ภายในกรอบสีเขียวนี้เพียงแผ่นเดียว

เจตน์ รัตนมาลากร : การคำนวณสมดุลระหว่างวัฏภาคของเหลว-ของเหลว-ไอโดยใช้สมการสภาวะ(COMPUTATION OF LIQUID-LIQUID-VAPOR EQUILIBRIUM USING EQUATIONS OF STATE) อ.ปรึกษา : รศ.ดร.เกริกชัย สุกาญจนัจที,168 หน้า.ISBN 974-578-333-1

สมการสภาวะจำนวน 4 สมการคือ Soave-Redlich-Kwong(SRK), Harmens & Knapp(HK),Peng & Robinson(P&R)และ modified Soave-Redlich-Kwong(Graboski & Daubert)(G&D) นำมาใช้ทำนายปริมาตรโมลาร์ของของเหลว,ปริมาตรโมลาร์ของไอ และเศษส่วนโมลขององค์ประกอบของระบบ 3 วัฏภาค ของเหลว-ของเหลว-ไอ ของของผสม มีเธน-อีเธน-นอร์แมลโดโคเซน(Methane-Ethane-n-Docosane)ที่อุณหภูมิเท่ากับ 298.15 K และ 303.15 K และของผสม คาร์บอนไดออกไซด์-ไนโตรเจน-นอร์แมลโนนาดีเคนที่อุณหภูมิ 294.15 K,297.15 K และ 301.15 K

สำหรับในวัฏภาคไอนั้นการคำนวนปริมาตรโมลาร์ของไอและเศษส่วนโมลโดยใช้สมการสภาวะทั้ง 4 พบว่าส่วนใหญ่ทำนายได้ดีโดยที่สมการของ P&R สามารถทำนายปริมาตรโมลาร์ของไอได้ดีที่สุดคือให้ค่าความคลาดเคลื่อนเฉลี่ยสัมบรณ์ (absolute error deviation)เท่ากับ 2.1490% ในขณะที่ H&K ให้ผลการคำนวนเศษส่วนโมลของอีเธนได้ดีมากคือให้ค่าความคลาดเคลื่อนเฉลี่ยสัมบูรณ์เพียง 0.2284% เท่านั้นที่อุณหภูมิเท่ากับ 298.15 K สำหรับระบบของผสม คาร์บอนไดออกไซด์-ไนโตรเจน-นอร์แมลโนนาดีเคนที่อุณหภูมิเท่ากับ 297.15 K สมการ P&R สามารถทำนายปริมาตรโมลาร์ของไอโดยให้ค่าความคลาดเคลื่อนเฉลี่ยสัมบูรณ์เพียง 0.6817% เท่านั้น

ส่วนในวัฏภาคของเหลวนั้นพบว่าทุกสมการมีความสามารถในทำนายน้อยกว่าในวัฏภาคไอโดยที่ H&K สามารถทำนายปริมาตรโมลาร์ของของเหลวในระบบคาร์บอนไดออกไซด์-ไนโตรเจน-นอร์แมลโนนาดีเคนและมีเธน-อีเธน-นอร์แมลโดโคเซนได้ดีกว่าสมการของ SRK,P&R และ G&D โดยให้ความคลาดเคลื่อนเฉลี่ยสัมบูรณ์ในวัฏภาคของเหลวที่ 1 และ 2 น้อยกว่า 12% และ 5% ตามลำดับ นอกจากนี้ยังพบว่าทุกสมการสภาวะใช้ทำนายเศษส่วนโมลในวัฏภาคของเหลวของระบบคาร์บอนไดออกไซด์-ไนโตรเจน-นอร์แมลโนนาดีเคนไม่ดีนักอย่างไรก็ตามสมการของ H&K ให้ความคลาดเคลื่อนเฉลี่ยสัมบูรณ์ของ ไนโตรเจน น้อยกว่า 15% สำหรับระบบที่ประกอบด้วย มีเธน-อีเธน-นอร์แมลโดโคเซน พบว่า H&K ให้ความคลาดเคลื่อนเฉลี่ยสัมบูรณ์ของ อีเธน ในวัฏภาคของเหลวที่ 1 และ 2 น้อยกว่า 6% และ 2% ตามลำดับ

ภาควิชา วิศวกรรมศาสตร

สาขาวิชา วิศวกรรมเคมี

ปีการศึกษา 2533

ลายมือชื่อนิสิต ....

ลายมือชื่ออาจารย์ที่ปรึกษา K. Sukanjanajtee

ลายมือชื่ออาจารย์ที่ปรึกษาร่วม ....

พิมพ์ต้นฉบับบทคัดย่อวิทยานิพนธ์ภายในกรอบสีเขียวนี้เพียงแผ่นเดียว

CHET RATTANAMALAKORN : COMPUTATION OF LIQUID-LIQUID
-VAPOR EQUILIBRIUM USING EQUATIONS OF STATE.
THESIS ADVISER : ASSO. PROF. KROEKCHAI SUKANJANAJTEE,
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Four equations of state Soave-Redlich-Kwong(SRK), Harmens & Knapp(H&K),Peng & Robinson(P&R) and modified SRK (Graboski & Daubert)(G&D) are used to evaluate liquid molar volume,vapor molar volume and phase compositions of liquid-liquid-vapor system of Methane-Ethane-n-Docosane mixtures at T=298.15 K,303.15 K and CO_2-N_2-n-Nonadecane mixtures at T=294.15 K,297.15 K and 301.15 K.

For vapor phase,prediction of vapor molar volume and composition by all the equation of state are generally good. P&R equation could predict vapor molar volume best with an absolute deviation of 2.1490% .While H&K gave very good result in ethane mole fraction with an absolute deviation of 0.2284% at T=298.15 K .For CO_2-N_2-n-Nonadecane system at T=297.15 K,the P&R equation could predict the vapor molar volume with an absolute deviation of only 0.6819%.

For liquid phase,predictions are not as good as those of vapor phase. Regarding liquid molar volume prediction,H&K equation predicted liquid molar volumes of both methane-ethane-n-Docosane and CO_2-N_2-n-Nonadecane systems better than SRK,P&R and G&D equations. Absolute deviation of liquid molar volume in L^{I} and L^{II} phases evaluated by H&K equation is less than 12% and 5% respectively. For liquid phase mole fraction,all equation of state gave poor value of liquid mole fraction for the CO_2-N_2-n-Nonadecane. However, H&K equation gave N_2 mole fraction with an absolute deviation of less than 15%.For methan-ethane-n-Docosane,H&K equation gave absolute deviation of ethane mole fraction in L^{I} and L^{II} phases less than 6% and 2% respectively.

ภาควิชา วิศวกรรมศาสตร

สาขาวิชา วิศวกรรมเคมี

ปีการศึกษา 2533

ลายมือชื่อนิสิต

ลายมือชื่ออาจารย์ที่ปรึกษา

ลายมือชื่ออาจารย์ที่ปรึกษาร่วม

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NOTATION

A,B = Parameters in the equation of state

a,b = Parameters in the equation of state

D = Determinant of the Jacobian matrix,equation 12

F = Total moles of feed to the flash

f_i = Mole of component i in feed to flash

f_i = Fugacity of component i for mixture

f_i^o = Fugacity of component i for pure

G = Gibbs free energy

H = Enthalpy per mole

K = Vapor-liquid equilibrium ratio(K-value)

k_{ij} = Binary interaction parameter

L = Liquid flow rate

n_j = Moles of component j

P_c = Pure component critical pressure

P = Pressure

P_r = Reduce pressure = P/P_c

p = Partial pressure

p_1, p_2, P_3 = Functions defined by equation(3.21-3.23)

Q_1, Q_2 = Functions defined by eqaution(3.24,3.25)

Q = Heat transfer rate

R = Gas constant

S = Entropy

T = Absolute temperature

T_c = Pure component critical temperature

T_r = Reduced temperature = T/T_c

u_1, u_2 = Fraction of feed in liquid phase 1,2

($u_1 = L'/F, u_2 = L''/F$)

V = Vapor flow rate;volume

v = Molar volume

v = Partial molal volume

w = Pitzer's accentricity

x = Liquid mole fraction

y = Vapor mole fraction

z = Feed mole fraction

Z = Compressibility factor

Greek Letters

ϕ_i^o = Fugacity coefficient of pure component i

ϕ_i = Fugacity coefficient of component i of mixture

μ_i = Chemical potential of component i

γ_i = Activity coefficient of component i

Subscripts

v = Vapor phase

L = Liquid phase

F = Feed

i, j, k = Component number

superscripts

I, II = indexes for liquid phase