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NRTL-NRF NRTL

NRTL-NRF

Key Words: Solubility, Carbon Dioxide, Organic Solvent, Modeling, Low Temperature

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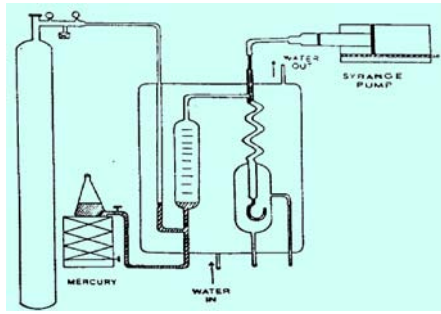
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NRTL-NRF NRTL

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$$\frac{PV_g}{RT} = 1 + \frac{B}{V_g} \quad (1)$$

$$PV_g^2 - CV_g - BC = 0 \quad (2)$$

$$V_g = 0.5C + 0.5(C^2 + 4BC)^{0.5} \quad (3)$$

$$n_g = \frac{v}{V_g} \quad (4)$$

$$n_s = \frac{f.t.d}{MW} \quad (5)$$

$$X_g^e = \frac{n_g}{n_g + n_s} \quad (6)$$

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	P	T	$\frac{\quad}{x_g^e}$	$\frac{\quad}{x_g^e}$	ER.
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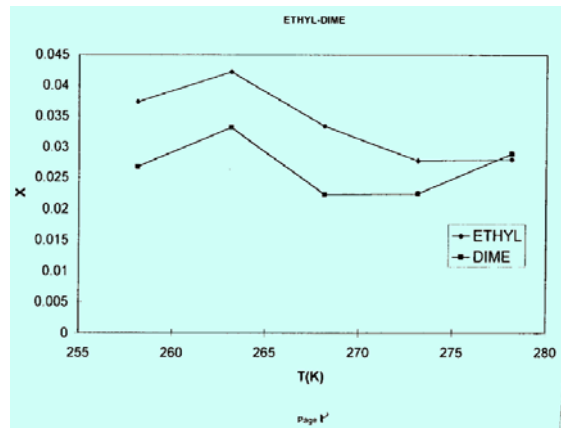
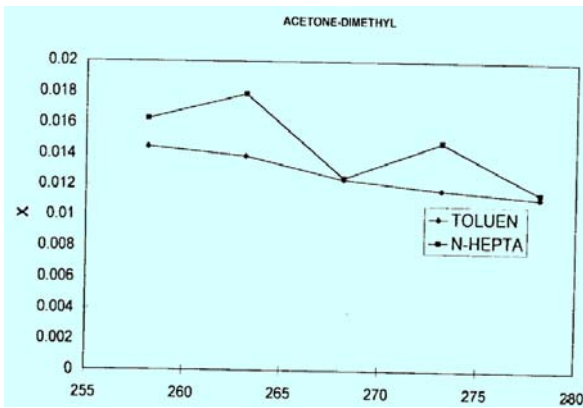
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$$P_g = P - P_s^s \left[1 - x_g^e \right] = H x_g^e \quad (1)$$

$$\ln H_{CO_2}^R = aT^3 + bT^2 + cT + d \quad (2)$$

	a	B	c	d	R
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	- /	- /	/	- /	/
		/	- /	/	/

$$Y_{1p} = X_{1p}^s \gamma_1 \quad (3)$$

$$Y_2 p = X_2 p_2^s \gamma_2 \quad ()$$

$$: \quad X_1 + X_2 = 1 \quad Y_1 + Y_2 = 1$$

$$X_2 = \frac{P - \gamma_1 P_1^s}{\gamma_2 P_{21}^s - \gamma_1 P_1^s} \quad ()$$

$$\text{RMSD} = \sqrt{\frac{1}{N} \sum_i \left| \frac{x_i^e - x_i^c}{x_i^c} \right|^2} \quad ()$$

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Input data

Select model of activity coefficient

Initial guess for binary parameter

Solubility calculation for binary system

$$\text{RMSD} = \sqrt{\frac{1}{N} \sum_i \left| \frac{x_i^e - x_i^c}{x_i^c} \right|^2}$$

Optimization

RMSD < ε

Print result

NRTL-

NRTL - NRF , NRTL

NRTL-NRF [] NRF

$$\left(\frac{g^E}{RT} \right)_{\text{NRTL-NRF}} = X_1 X_2 \left[\frac{\tau_{21} G_{21}}{X_1 + X_2 G_{21}} + \frac{\tau_{12} G_{12}}{X_2 + X_1 G_{12}} - [\tau_{12} - \tau_{21}] \right] \quad ()$$

$\ln \gamma_2 \quad \ln \gamma_1 \quad () \quad \tau_{21} \quad \tau_{12}$

$$\text{Ln}\gamma_1 = X_2^2 \left[\tau_{21} \left(\frac{G_{21}}{X_1 + X_2 G_{21}} \right)^2 + \frac{\tau_{12} G_{12}}{(X_1 + X_1 G_{12})} - (\tau_{12} + \tau_{21}) \right] \quad ()$$

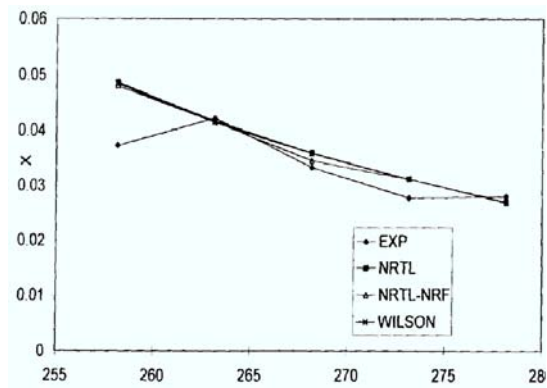
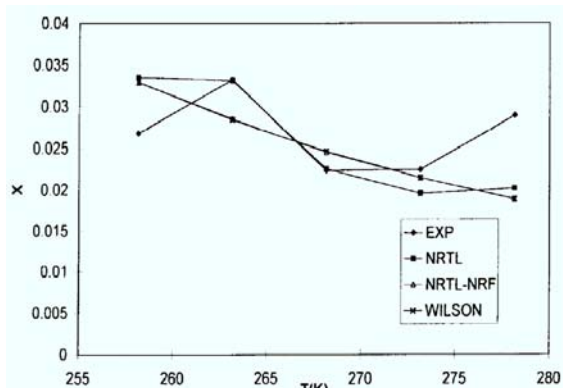
$$\text{Ln}\gamma_2 = X_1^2 \left[\tau_{12} \left(\frac{G_{12}}{X_2 + X_1 G_{12}} \right)^2 + \frac{\tau_{21} G_{21}}{(X_1 + X_2 G_{21})} - (\tau_{12} + \tau_{21}) \right] \quad ()$$

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$$\left(\frac{gE}{RT} \right)_{\text{NRTL-NRF}} = \left(\frac{gE}{RT} \right)_{\text{NRTL}} - X_i X_j (\tau_{ij} + \tau_{ji}) \quad ()$$

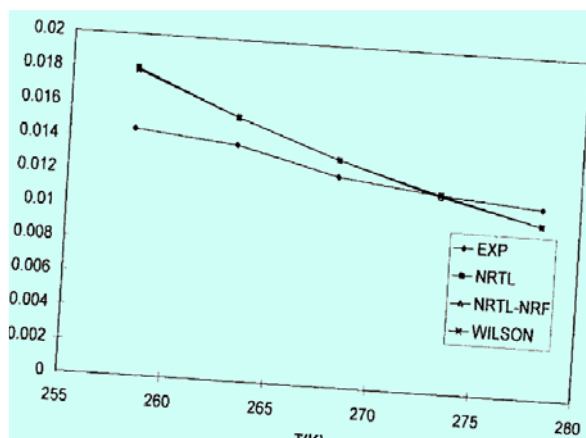
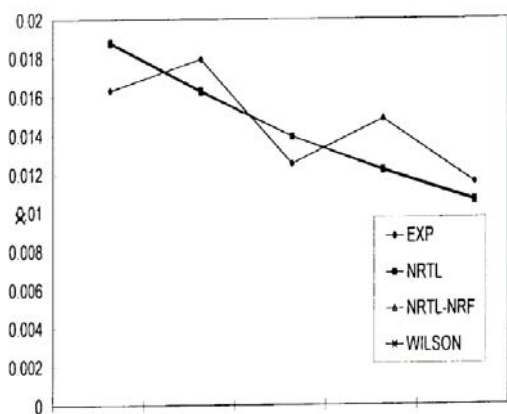
$$(\text{Ln}\gamma_i)_{\text{NRTL-NRF}} = (\text{Ln}\gamma_i)_{\text{NRTL}} - X_j^2 (\tau_{ij} + \tau_{ji}) \quad ()$$

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RMSD

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NRTL-NRF

NRTL-NRF NRTL

RMSD

	NRTL-NRF NRTL			RMSD		
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	$\lambda = - - /$	$\tau = - - /$	$\Lambda = /$	/	/	/
	$\lambda /$	$\tau = - - /$	$\Lambda = /$	/	/	/
	$\lambda = /$	$\tau = - - /$	$\Lambda = - - /$	/	/	/
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NRTL-NRF,NRTL

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NRTL

NRTL-NRF

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NRTL-NRF, NRTL

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NRTL-NRF

MW

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N

g

f

mole/min

s

gr/cm

P

atm

R

atm.cm³/mole.k

c

R²

e

RMSD

NF

NRTL-NRF

t

min

NR

NRTL

T

K

R

V

cm³

s

V_g

Cm³/mol

W

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X

Y

γ

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