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March 1988

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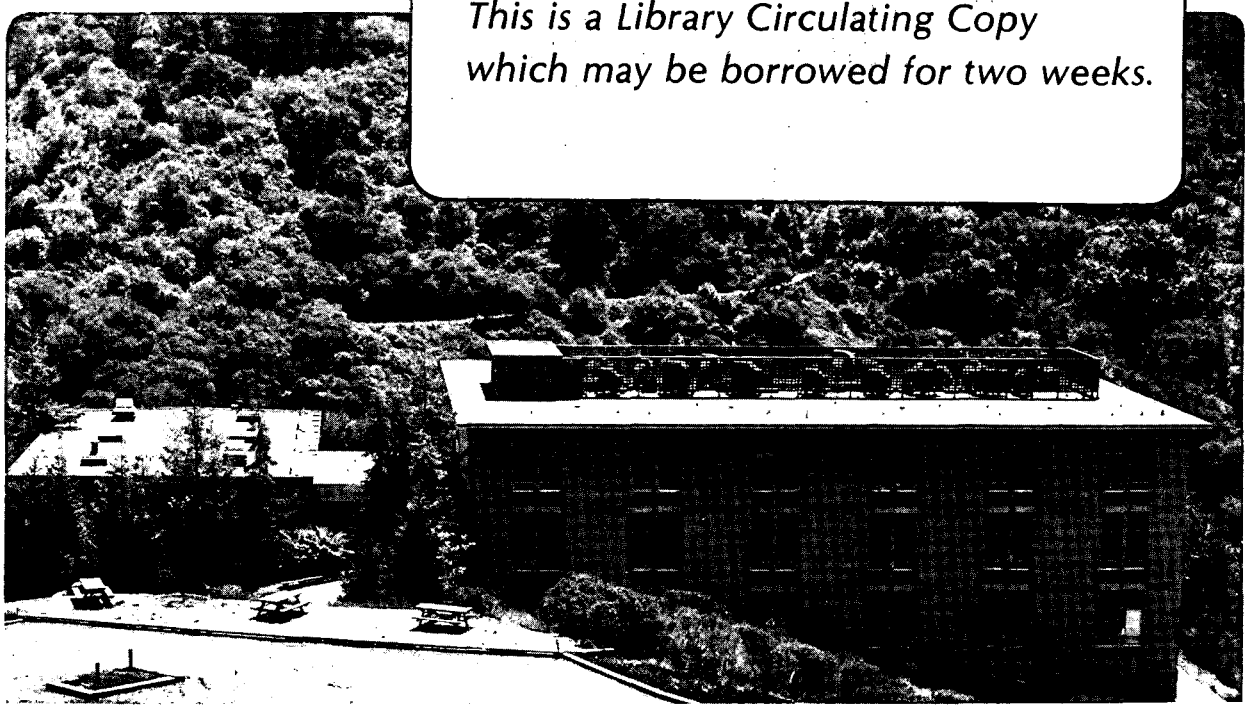

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Correlation of Liquid-Liquid Equilibria for Some Water/Organic Liquid Systems in the Region 20-250°C

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ABSTRACT

A group-contribution model of the UNIFAC type is used to correlate liquid-liquid equilibria for water/organic liquid systems over a wide temperature range. Good agreement with experiment is obtained when water-organic interaction parameters are temperature-dependent. This correlation may be useful for engineering design for processing of fossil fuels.

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Introduction

Mutual solubilities of hydrocarbons and water are of interest in the petroleum and related industries. Hydrocarbon-water systems are sometimes encountered at high temperatures; these systems may also contain a large number of hydrocarbon derivatives such as phenolics. For chemical process design, the compositions of coexisting water and hydrocarbon phases must be known or estimated.

Liquid-liquid equilibria (LLE) may be calculated from an equation-of-state or from an excess-Gibbs-energy model. In recent years, equations-of-state have been used to represent binary water-hydrocarbon equilibria (Tsonopoulos and Wilson, 1983; Kabadi and Danner, 1985; Lüdecke and Prausnitz, 1985). However, only limited success was achieved when the same equation-of-state was used to represent the compositions of both liquid phases over a wide range of temperatures.

Group-contribution models are often used for correlating and estimating fluid-phase equilibria; the best-known of these is UNIFAC (Fredenslund et al, 1975). In the original UNIFAC correlation, interaction parameters were fitted primarily to vapor-liquid equilibria (VLE); as a result, predictions of LLE were generally not quantitative. Magnussen and coworkers (1981) later published a set of UNIFAC interaction parameters fitted mostly to LLE data which gave significantly improved predictions of LLE. Further modifications to the UNIFAC model have focused on the combinatorial contribution to the excess Gibbs energy, and on the temperature dependence of the group-interaction parameters (for a review, see e.g., Fredenslund and Rasmussen, 1985; Gmehling, 1986). The most comprehensive and generally applicable group-contribution model currently available is the Modified UNIFAC model of Larsen et al (1987) intended primarily for predicting VLE and heats of mixing.

UNIFAC predictions are necessarily most reliable for those thermodynamic data for which the interaction parameters are optimized (e.g., VLE, LLE, heats of mixing) and for the temperature range over which the parameters are correlated. Further, since the UNIFAC model, in principle, applies to a large variety of mixtures, it is often not highly accurate for a limited class of mixtures.

This paper presents a UNIFAC model suitable for LLE of systems containing water and hydrocarbons (and some hydrocarbon derivatives) over a wide range of

temperatures. Interaction parameters between water and organic groups are temperature-dependent, while interactions not involving water are temperature independent. The combinatorial expression of original UNIFAC is replaced with that of Modified UNIFAC (Larson et al., 1987). Interaction parameters are presented for water and seven common organic groups.

UNIFAC Model

In UNIFAC, the activity coefficient is given as a sum of combinatorial and residual contributions:

$$\ln\gamma_i = \ln\gamma_i^C + \ln\gamma_i^R \tag{1}$$

Originally, the Staverman-Guggenheim combinatorial expression (Staverman, 1950) was used. Alternative combinatorial expressions are used in several variations of UNIFAC as reviewed by Gmehling (1986).

For this work we choose the combinatorial expression used by Larson and coworkers (1987) in their Modified UNIFAC model. Their expression is identical to that of Flory-Huggins, with the volume fractions replaced by surface fractions as suggested by Kikic et al. (1980). The modified Flory-Huggins combinatorial was shown to represent VLE of alkane mixtures significantly better than the Staverman-Guggenheim combinatorial (Larson et al., 1987).

For component i, we have

$$\ln\gamma_i^C = ln(\frac{\Phi_i}{x_i}) + 1 - (\frac{\Phi_i}{x_i}) \tag{2}$$

where the modified volume fraction (in effect, surface fraction) is

$$\Phi_i = \frac{x_i r_i^{2/3}}{\sum_j x_j r_j^{2/3}} \tag{3}$$

Molecular volume parameter r_i is calculated by summing over (Bondi) group volumes as in UNIFAC.

Our residual expression is the same as that in original UNIFAC; however, interaction parameters between water and hydrocarbon groups are now temperature

dependent. For every pair of groups in a mixture, there are two binary interaction parameters

$$a_{ij} = \frac{u_{ij} - u_{jj}}{R} \tag{4a}$$

and

$$a_{ji} = \frac{u_{ji} - u_{ii}}{R} \tag{4b}$$

where u_{ij} characterizes the energy of interaction between group i and group j. When interaction parameters a_{ij} are obtained from water-hydrocarbon LLE data at several temperatures, we find that whenever i or j is water, a_{ij} shows a large temperature dependence. However, whenever i and j refer to organic groups, there is little temperature dependence.

The form of the temperature dependence for water-organic group interactions is determined empirically. Let 1 represent water and 2 represent an organic group. Interaction parameters a_{12} and a_{21} were adjusted independently over a wide range of temperatures for several hydrocarbon groups. The parameters behave regularly for different hydrocarbon classes; however the temperature dependence of a_{12} is different from that of a_{21}. For the region 20 - 250°C, the interaction parameters are given by

$$a_{12} = a_{12}^{(0)} + a_{12}^{(1)}T + a_{12}^{(2)}T^2 \tag{5a}$$

$$a_{21} = a_{21}^{(0)} + a_{21}^{(1)}T \tag{5b}$$

where T is in Kelvin.

Data Reduction

One goal of this work is to develop a UNIFAC correlation suitable for multicomponent water-hydrocarbon LLE at low and high temperatures. Very few high-temperature data are available for aqueous systems containing more than one hydrocarbon. Group-interaction parameters in the UNIFAC model were determined using binary data alone, and ternary data were used to test model predictions.

Mutual solubility data and water-pyridine VLE data were used to determine interaction parameters a_{12} and a_{21} where 1 stands for water. Parameters for organic-organic group interactions were determined primarily from VLE data. Table 1 gives sources of experimental LLE and VLE data.

The Redlich-Kwong equation-of-state was used for calculating vapor-phase fugacities. For non-polar components, pure-component parameters in the equation-of-state were evaluated from critical properties (Chueh and Prausnitz, 1967). For water, the pure-component energetic parameter was correlated as a function of temperature. Cross parameters were determined according to the combining rules of deSantis et al (1974).

All parameters were fit by minimizing the sums of the squared differences between experimental and calculated VLE and LLE K-factors. UNIFAC structural parameters R_k and Q_k are those from the original work of Fredenslund (1975).

Table 2 presents coefficients for determining temperature-dependent interaction parameters a_{12} and a_{21} for water with seven organic groups according to Equations 5a and 5b. Figure 1 shows the temperature dependence of parameters a_{12} and a_{21} for three representative organic groups with water. Table 3 gives temperature-independent parameters for organic-organic group interactions.

Table 1

Experimental data used for determining group-interaction parameters

Interaction	Binary	Data Type	No. of points	Min. T (Kelvin)	Max. T (Kelvin)
H2O-CH2	water-octane	LL	5	273	303
	water-octane	LL	6	310	553
	water-hexane	LL	3	373	473
	water-pentane	LL	3	311	423
H2O-ACH	water-benzene	LL	15	273	343
	water-benzene	LL	4	313	473
	water-benzene	LL	8	374	476
H2O-ACCH2	water-toluene	LL	4	273	298
	water-toluene	LL	6	372	473
	water-m-xylene	LL	5	273	333
	water-m-xylene	LL	6	373	473
	water-1-methylnaphthalene	LL	1	298	
	water-1-methylnaphthalene	LL	7	310	550
	water-ethylbenzene	LL	4	368	536
H2O-ACOH	water-m-cresol	LL	2	293	298
	water-m-cresol	LL	4	313	413
	water-p-cresol	LL	2	298	313
	water-p-cresol	LL	4	333	393
	water-phenol	LL	8	273	333
H2O-AN	water-quinoline	LL	11	293	493
	water-pyridine	VL	11	343	
	water-pyridine	VL	17	363	
H2O-AS	water-thiophene	LL	4	398	473
	water-thianaphthene	LL	9	332	490
H2O-ACNH2	water-aniline	LL	8	293	413
CH2-ACH	hexane-benzene	VL	7	342	351
	octane-benzene	VL	6	355	388
CH2-ACCH2	heptane-toluene	VL	6	371	383
	octane-p-xylene	VL	6	399	409
	octane-ethylbenzene	VL	5	384	392
CH2-ACOH	octane-phenol	VL	6	383	
	octane-phenol	VL	8	399	477
	octane-phenol	VL	5	383	
	octane-phenol	LL	6	293	318
CH2-AN	octane-pyridine	VL	13	353	

	octane-pyridine	VL	17	381		394
	nonane-pyridine	VL	13	386		415
CH2-AS	heptane-thiophene	VL	23		328	
CH2-ACNH2	hexane-aniline	LL	5	298		333
	heptane-aniline	LL	4	298		323
ACH-ACCH2	benzene-toluene	VL	5	357		379
	benzene-m-xylene	VL	6	359		402
ACH-ACOH	benzene-phenol	VL	12		343	
	benzene-phenol	VL	28		353	
ACH-AN	benzene-pyridine	VL	7		298	
	benzene-pyridine	VL	6	355		380
ACH-AS	benzene-thiophene	VL	10		328	
ACH-ACNH2	benzene-aniline	VL	11		343	
	benzene-aniline	VL	21	355		453
ACCH2-ACOH	toluene-phenol	VL	9	384		445
ACCH2-AN	toluene-pyridine	VL	6	383		386
	m-xylene-pyridine	VL	8	389		410
ACCH2-AS	toluene-thiophene	VL	7	359		378
	toluene-thiophene	VL	7	359		378
ACCH2-ACNH2	toluene-aniline	VL	10		353	
	toluene-aniline	VL	16		363	
	toluene-aniline	VL	12		373	
ACOH-AN	phenol-pyridine	VL	12	391		455
	phenol-4-methylpyridine	VL	11	376		420
	phenol-4-methylpyridine	VL	10	397		422
	phenol-4-methylpyridine	VL	11	411		455
	phenol-4-methylpyridine	VL	11	419		463
ACOH-AS	phenol-thiophene	VL	10		357	
ACOH-ACNH2	3-methylphenol-2-methylaniline	VL	8	475		477
	3-methylphenol-3-methylaniline	VL	7	476		477
AN-AS	pyridine-thiophene	VL	14	357		387
AN-ACNH2	pyridine-aniline	VL	9	390		446

Table 2

Coefficients for temperature-dependent water(1)/organic-group(2) interaction parameters a_{12} and a_{21}

	j						
	CH2	ACH	ACCH3	ACOH	AN	AS	ACNH2
$a_{1j}^{(0)}$	-40.72	-39.04	-50.19	-39.10	-31.85	-60.08	-29.31
$a_{1j}^{(1)}$	3.826	3.928	3.673	2.694	4.579	6.309	1.081
$100a_{1j}^{(2)}$	-4.110	-4.370	-5.061	-4.377	-3.565	-6.724	-3.286
$a_{j1}^{(0)}$	3060.6	2026.5	2143.9	-199.25	-211.03	3005.4	-1553.4
$a_{j1}^{(1)}$	-5.374	-3.267	-3.076	-0.5287	-2.515	-5.630	6.178

Table 3

Temperature-independent interaction parameters a_{ij} and a_{ji} for organic groups

	j						
i	CH2	ACH	ACCH3	ACOH	AN	AS	ACNH2
CH2	0.0	131.3	-1.613	8143.8	6831.9	271.46	4472.8
ACH	-71.4	0.0	-27.67	1208.5	2905.8	108.48	763.60
ACCH3	15.27	47.31	0.0	816.21	7665.2	892.62	599.2
ACOH	7094.0	2717.3	7857.3	0.0	-350.53	14518.0	4563.4
AN	6778.2	1936.2	21531.0	-1748.2	0.0	-534.30	-1320.3
AS	4633.5	1707.7	3424.7	828.80	2229.2	0.0	*
ACNH2	5620.2	9859.0	5277.0	-486.49	1831.2	*	0.0

*no data available for fitting AS-ACNH2 interaction

Correlation of Binary Mutual Solubilities

We compare predictions of binary water-hydrocarbon mutual solubilities with experimental data. Because all binary solubility data spanning a wide temperature range were included in the parameter optimization, we cannot directly test the predictive capabilities of the model with binary data. However, we can determine the ability of the model to correlate simultaneously mutual solubilities for many hydrocarbons over a wide range of temperatures.

In addition to comparison with experimental data, we also compare with predictions from Magnussen et al (1981) and from Larson et al (1987). Magnussen established a UNIFAC parameter set for LLE using the original UNIFAC model with temperature-independent parameters. Larson and coworkers established a Modified UNIFAC model in which temperature-dependent interaction parameters were correlated using 6 adjustable coefficients per pair of groups. Larson's parameters were fit primarily to VLE and heat-of-mixing data, although some mutual-solubility data were used to fit water-organic interactions for which other data were not available. Predictions from these earlier correlations are used only as a benchmark; both were developed for a much wider range of systems than that considered here and therefore a direct comparison is not appropriate.

As a first example, we consider the mutual solubilities of benzene and water in the range 0-200°C. Figure 2 presents experimental data and predictions based on the three models. Magnussen's parameters accurately predict mutual solubilities of benzene and water at 25°C (the temperature at which the parameters were optimized) but extrapolations away from room temperature are poor. Predictions based on Modified UNIFAC are reasonably accurate between 0 and 100°C, but errors as large as 100% are observed at higher temperatures. The model presented in this work gives reasonable predictions over the entire temperature range for which data are available. None of the models predicts the observed minimun in hydrocarbon solubility at room temperature.

We next consider mutual solubilities of water and phenol; water is highly soluble in phenol at room temperature, and the two liquids are completely miscible above 65°C. Figure 3 presents experimental data and model predictions. Again, solubility predictions based on Magnussen's parameters are accurate at room temperature but give large errors at higher (and lower) temperatures. An erroneous lower consolute point is predicted in this case. Modified UNIFAC predicts solubilities which are too low and are relatively temperature insensitive; the predicted upper consolute temperature is well above 200°C. As expected from any classical model for the excess Gibbs energy, predictions of this work overshoot the upper critical solution temperature but give reasonble predictions well below that temperature.

Magnussen's work is successful in its intended purpose of predicting LLE at near-ambient temperatures; it is, however, of little use at temperatures remote from ambient. Modified UNIFAC appears useful in cases where interaction parameters were fit to LLE data (e.g., H_2O-ACH interactions in the water-benzene binary), but less useful for cases where VLE data were used in data reduction (e.g., $H_2O-ACOH$ interactions in water-phenol systems).

Figures 4 and 5 present experimental data and predictions of this work for some additional binary aqueous systems. Figure 4 shows solubilities of organic liquids in water, while Figure 5 presents the solubility of water in organic liquids. The solubility of water in unsubstituted aliphatic and aromatic hydrocarbons does not vary substantially for different hydrocarbons. Thus, for clarity, solubility data for water in toluene are omitted from Figure 5.

The results presented here indicate that binary water-hydrocarbon mutual solubilities are correlated well with our UNIFAC model. Reasonable agreement with experimental data is obtained over a wide temperature range and for liquids exhibiting a wide range of mutual solubilities with water. Predictions are least accurate for systems near a liquid-liquid critical point. For the critical region, it is necessary to apply a non-classical correction as discussed by dePablo and Prausnitz (1988).

Prediction of Ternary Mutual Solubilities

Very few ternary data are available for water-hydrocarbon mixtures at temperatures exceeding 100°C. Because only binary data were used in determining the UNIFAC parameters, we can use the limited ternary data to test model predictions. We again refer to the correlations of Magnussen et al and Larson et al, although we recognize that these are not intended for high-temperature water-hydrocarbon LLE.

Figure 6 presents measured and predicted mutual solubilities for the system water/toluene/phenol at 200°C. As expected, predictions based on Magnussen's temperature-independent parameters are poor at this elevated temperature. Modified UNIFAC incorrectly predicts an immiscibility region for the water/phenol binary, and overestimates the solubility of water in toluene by a factor of two. The predicted two-phase region is thus in poor agreement with experiment. Predictions

of this work correctly match the binary water/toluene boundary and give semi-quantitative agreement with experiment along the binodal curve.

Figure 7 shows results for the water-rich region of the water/toluene/phenol ternary at 200°C. The UNIFAC model presented here predicts the binodal curve almost within experimental error.

As a final example, Figures 8 presents measured and predicted LLE at 150°C for the system water/thiophene/pyridine. Predictions are again in semi-quantitative agreement with experiment.

Conclusions

This work presents a UNIFAC correlation for LLE in water-hydrocarbon systems for the temperature region 20-250°C. This correlation may be useful for engineering design for petroleum, coal-gasification or coal-liquification processes.

Acknowledgement

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract Number DE-AC03-76SF00098. One of us, S.M., gratefully acknowledges the Henrich-Hertz-Foundation (West Germany) for the grant of a fellowship.

Nomenclature

a_{ij} = interaction parameter for i-j interaction

LLE = liquid-liquid equilibria

Q_k = surface area parameter for group k

R_k = volume parameter for group k

r_i = molecular volume parameter for component i

u_{ij} = interaction parameter for i-j interaction

VLE = vapor-liquid equilibria

T = temperature

x_i = mole fraction of component i in liquid

Greek Symbols

γ_i = activity coefficient for component i

γ_i^C = activity coefficient, combinatorial part

γ_i^R = activity coefficient, residual part

Φ_i = modified volume fraction of component i in mixture

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List of Figure Captions

Figure 1a: Temperature Dependence of Water(1)-Hydrocarbon(2) Group-Interaction Parameter a_{12}

Figure 1b: Temperature Dependence of Hydrocarbon(2)-Water(1) Group-Interaction Parameter a_{21}

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Figure 3: Experimental and Calculated Mutual Solubilities of Water and Phenol

Figure 4: Experimental and Calculated Solubilities of Some Hydrocarbons in Water

Figure 5: Experimental and Calculated Solublity of Water in Some Hydrocarbons

Figure 6: Liquid-Liquid Equilibria for the System Water/Toluene/Phenol at 200°C

Figure 7: Water-Rich Compositions for the System Water/Toluene/Phenol at 200°C

Figure 8: Liquid-Liquid Equilibria for the System Water/Thiophene/Pyridine at 150°C

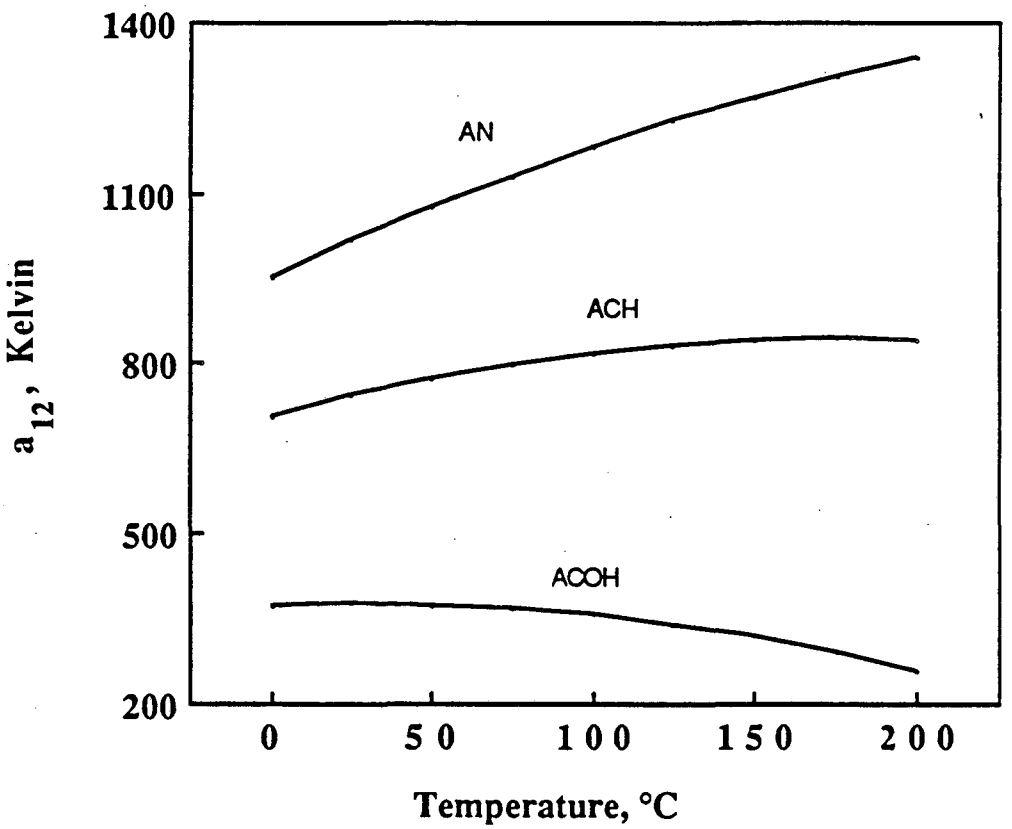


Figure 1a: Temperature dependence of water(1)-hydrocarbon(2) group interaction parameter a_{12}

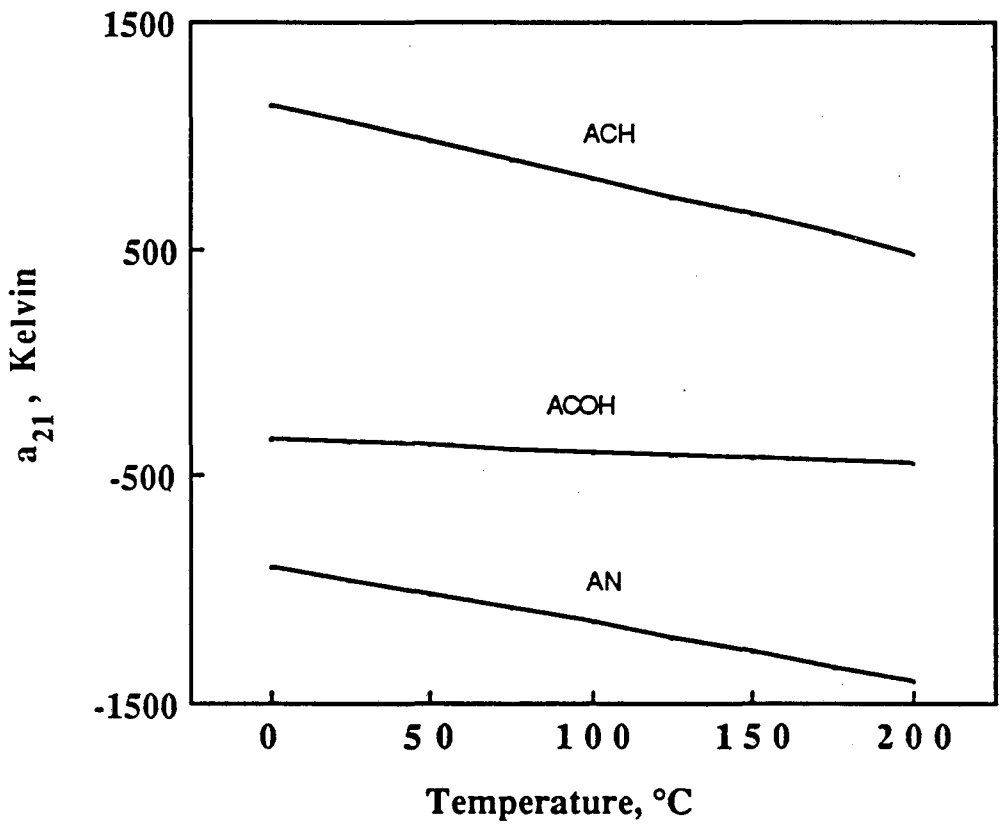
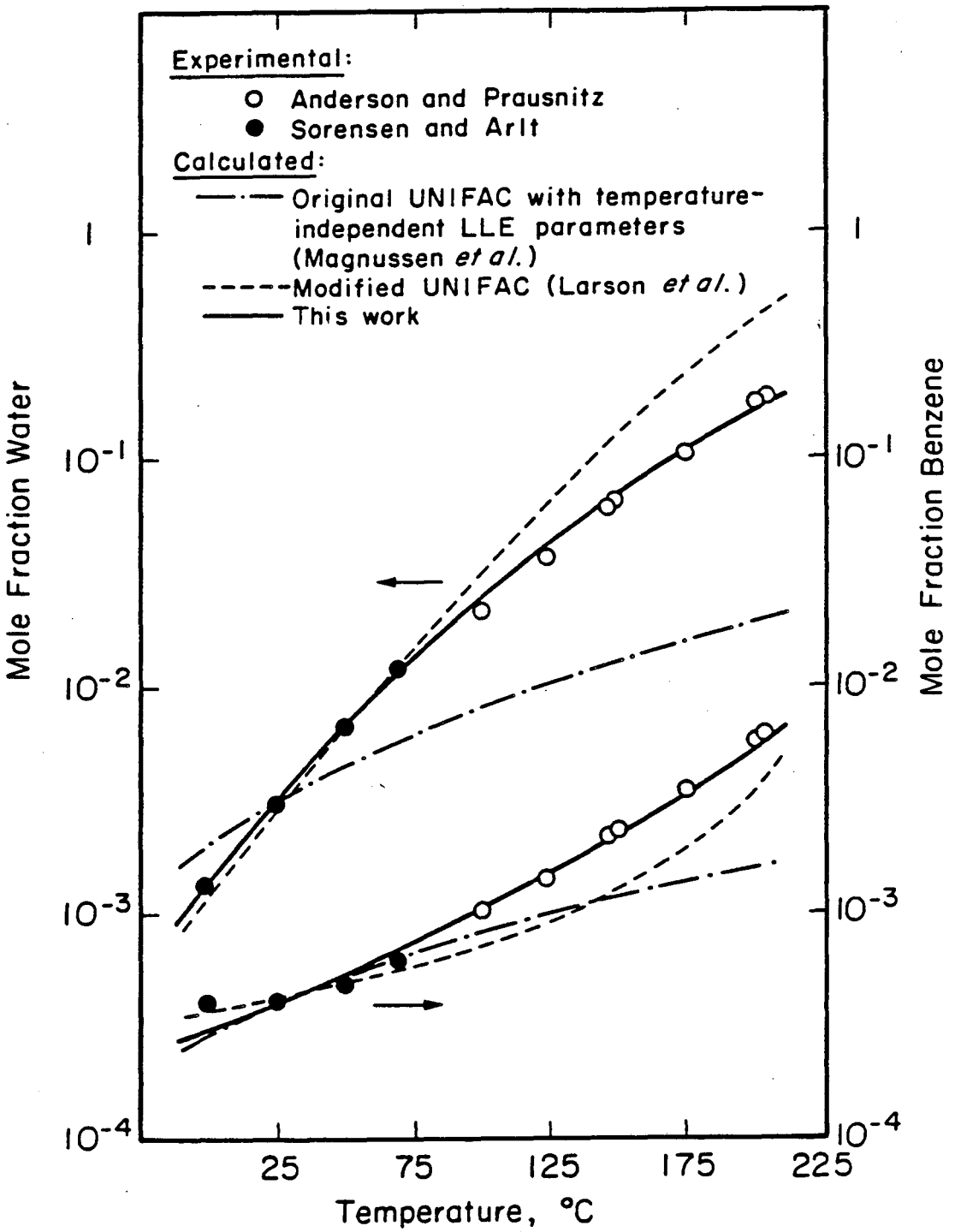
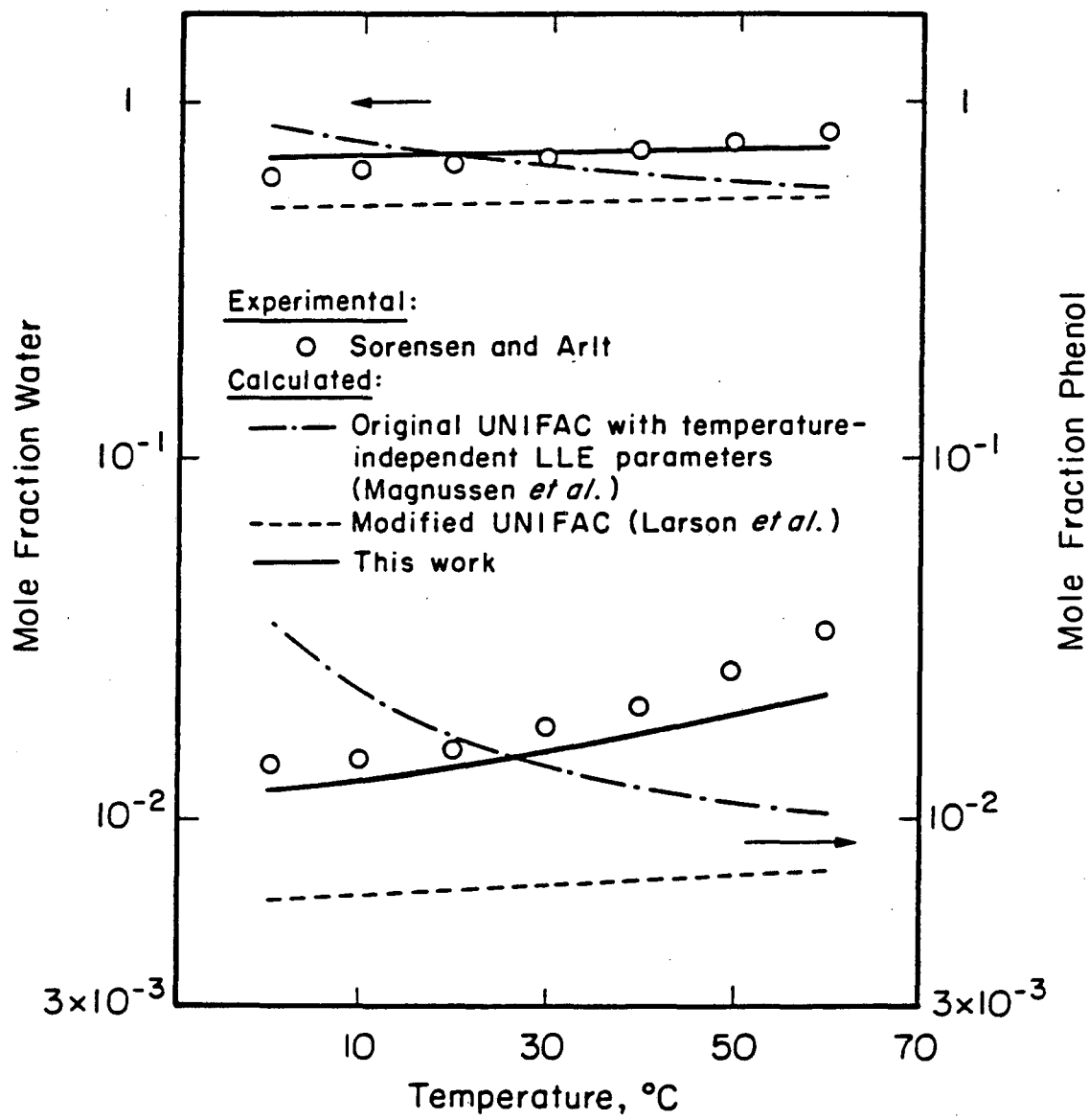


Figure 1b: **Temperature dependence of hydrocarbon(2)-water(1) group interaction parameter a_{21}**



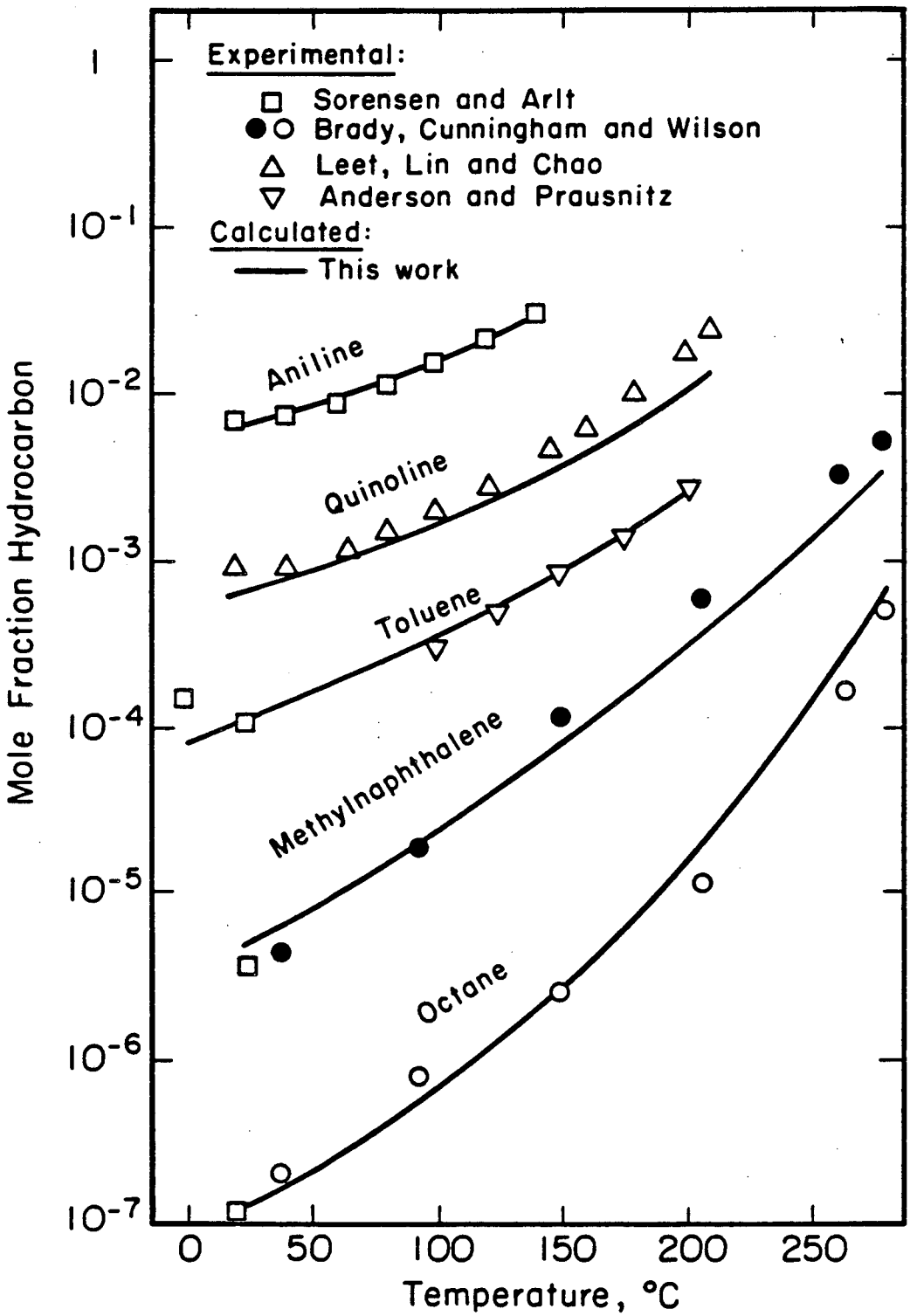
Experimental and Calculated Mutual Solubilities of Water and Benzene

Figure 2



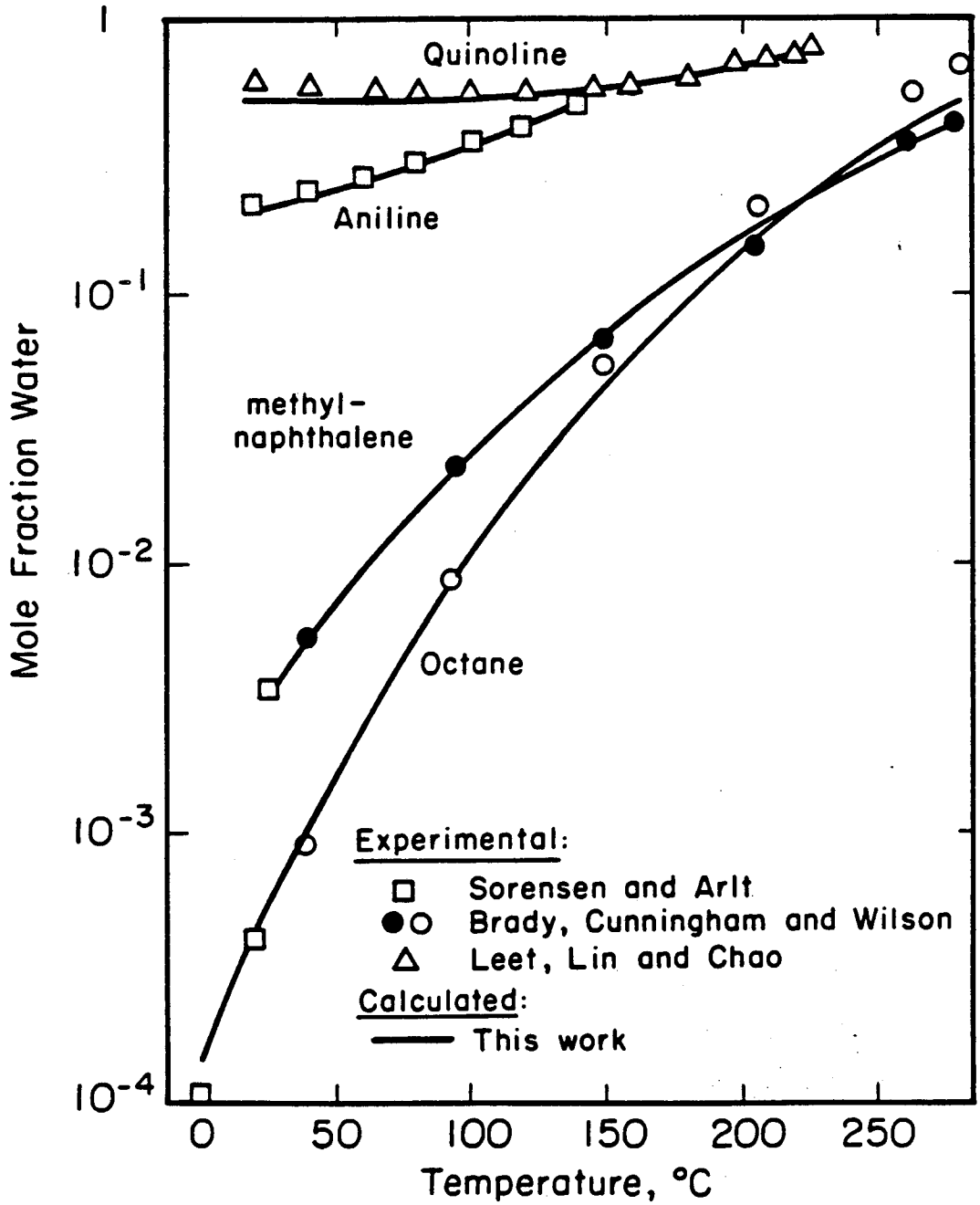
Experimental and Calculated Mutual Solubilities of Water and Phenol

Figure 3



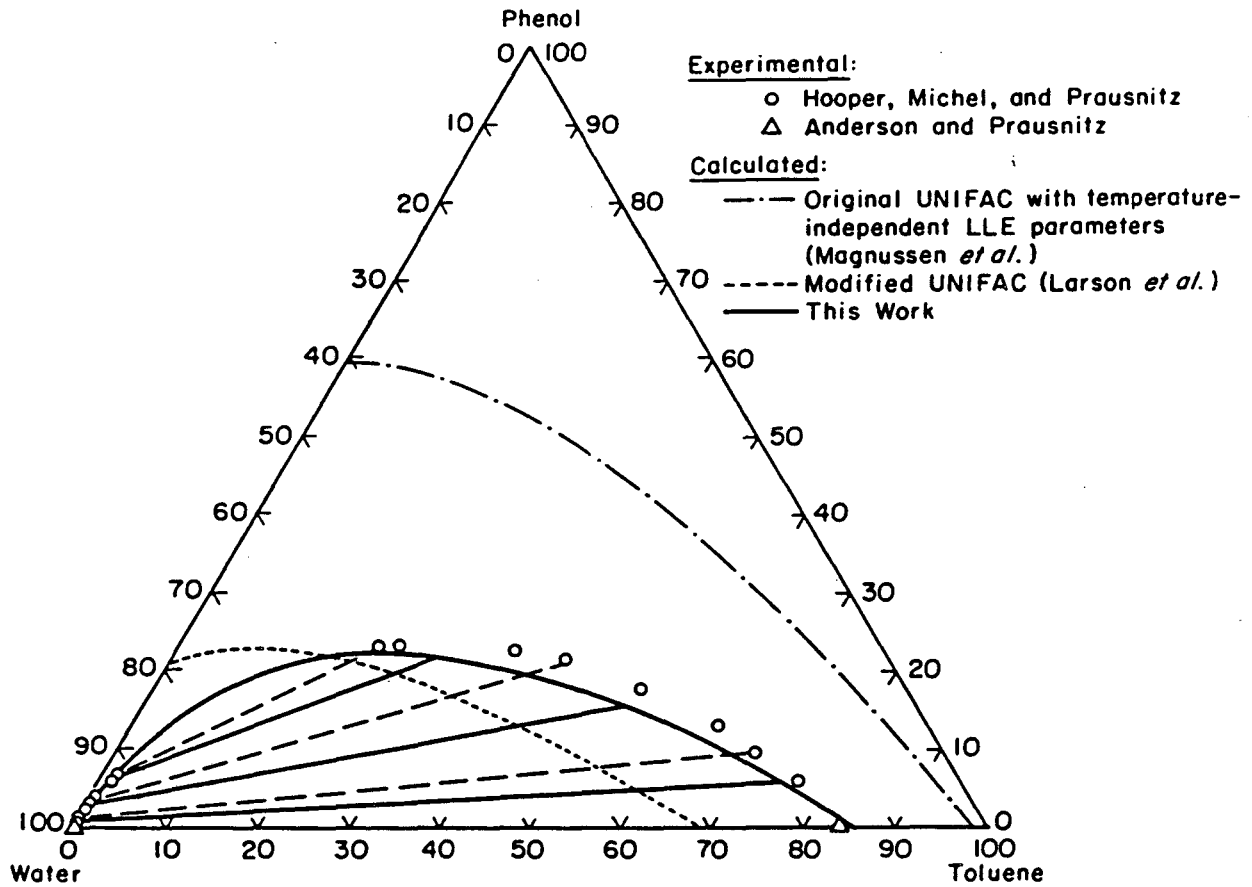
Experimental and Calculated Solubilities of Some Hydrocarbons in Water

Figure 4



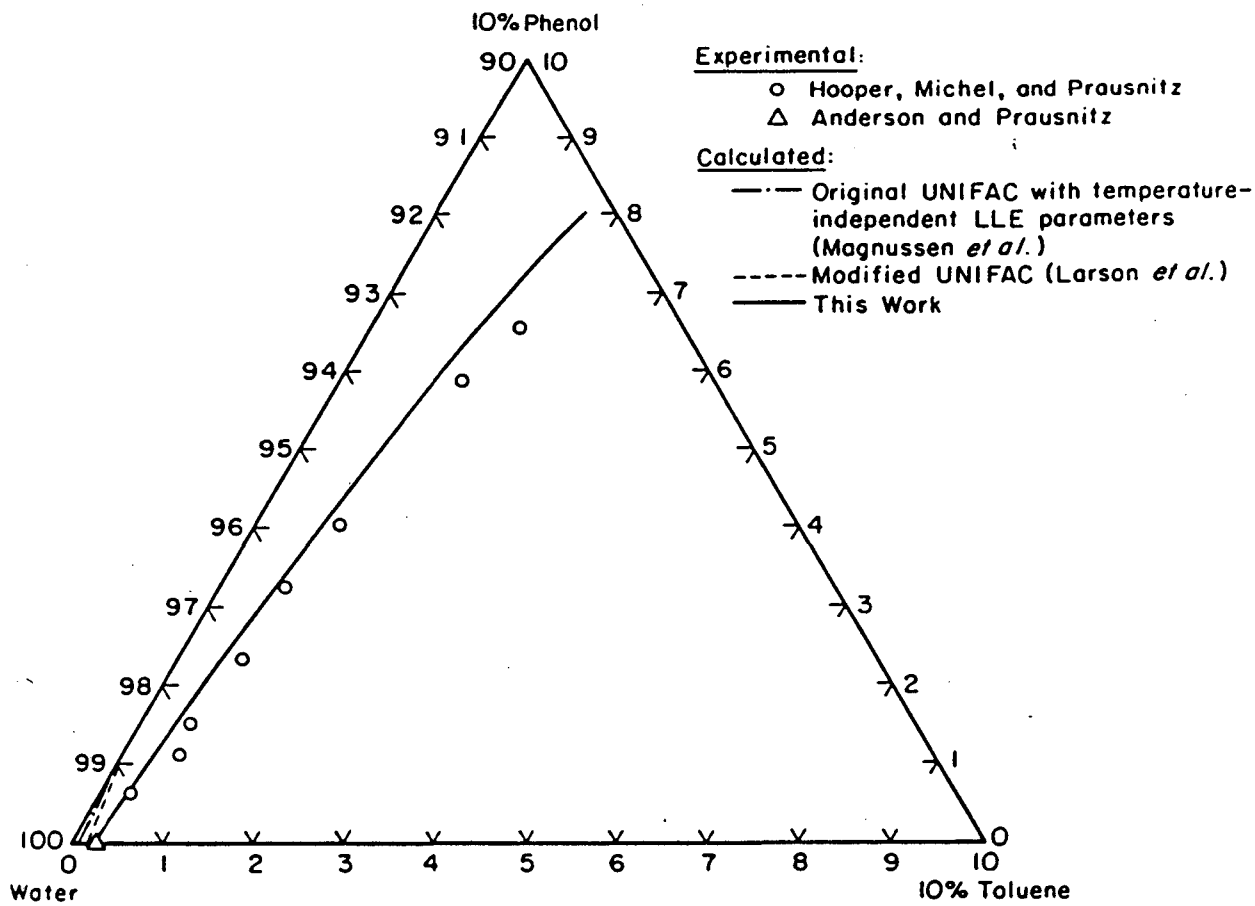
Experimental and Calculated Solubility of Water in Some Hydrocarbons

Figure 5



Liquid-Liquid Equilibria for the System Water/Toluene/Phenol at 200°C
(Compositions in mole percent)

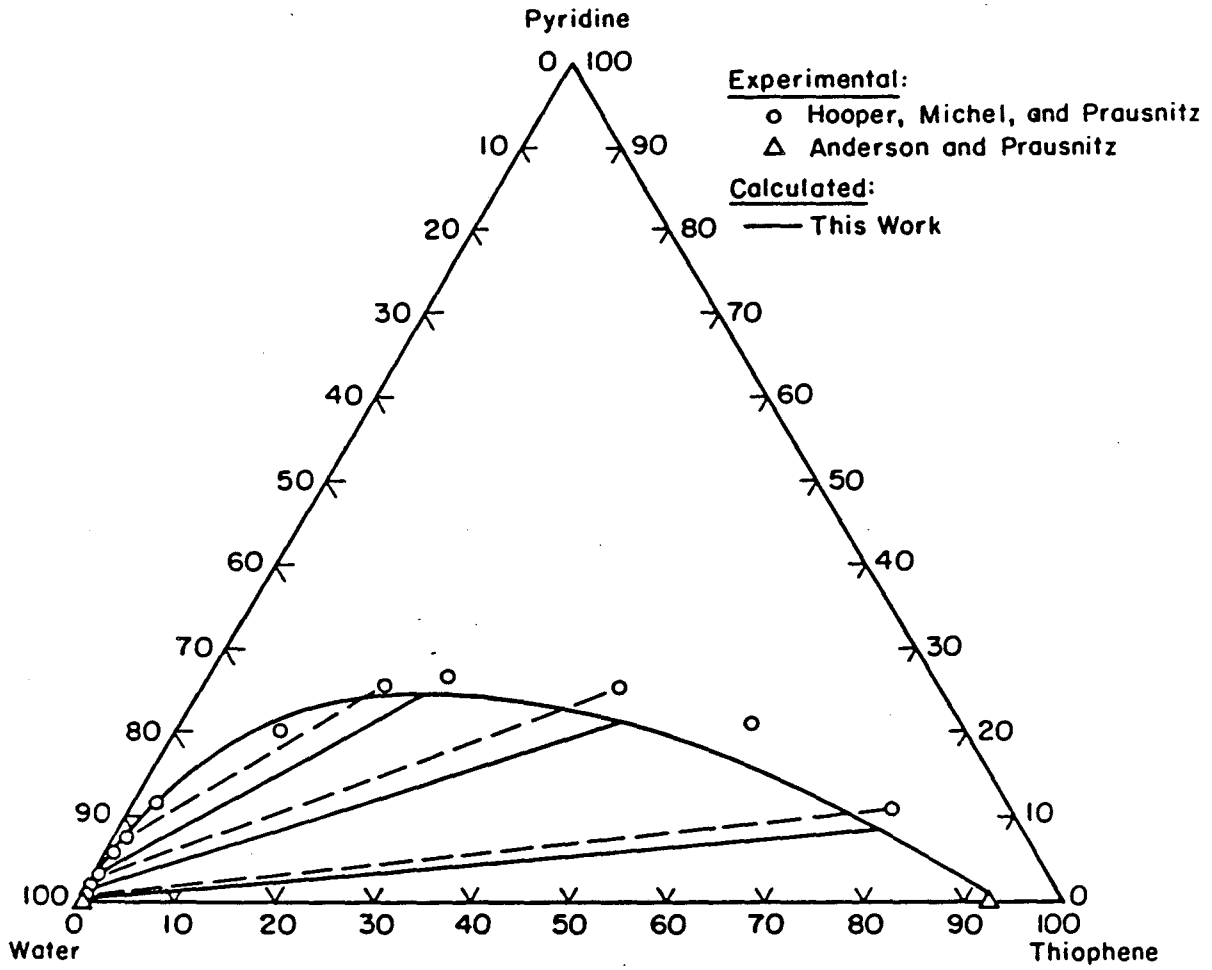
Figure 6



Water-Rich Compositions for the System Water/Toluene/Phenol at 200°C

(Compositions in mole percent)

Figure 7



Liquid-Liquid Equilibria for the System Water/Thiophene/Pyridine at 150°C
(Compositions in mole percent)

Figure 8

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