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Infinite-Dilution Partial Molar Properties of Naphthalene and Biphenyl in Carbon Dioxide from Supercritical Fluid Chromatography: Composition Effects in the Stationary Phase

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The temperature and pressure effects on retention of naphthalene and biphenyl in supercritical fluid chromatography are investigated within 35−70 °C and 75−150 bar. The retention factors are used to derive the infinite-dilution partial molar volumes of the two solutes in supercritical carbon dioxide, and the infinite-dilution molar enthalpies of transfer of the two solutes from the stationary phase to supercritical CO_2. The partial molar volumes are converted to quantities characterizing short-range interactions between CO_2 and the aromatic hydrocarbon. The resultant partial molar properties are corrected for the pressure- and temperature-dependent dissolution of CO_2 in the stationary polymer (poly(dimethylsiloxane)). The corrections for composition changes in the stationary phase include a composition derivative of the solute chemical potential that can only be obtained from a suitable theoretical model. Therefore, it is difficult to give a conclusive account of the performance of the corrections as these reflect the features of the model employed; here, the Scatchard−Hildebrand−Flory−Huggins theory or the Panayiotou−Vera lattice-fluid model are used for the purpose. However, comparison of the resultant partial molar volumes of naphthalene with literature data from high-precision, vibrating-tube densitometry indicates that the composition corrections improve the agreement between chromatographic and densitometric results.

Introduction

In addition to presenting a powerful technique for analytical and/or preparative separations, supercritical fluid chromatography (SFC) is a useful tool for acquiring thermodynamic information related to the transfer of solutes between the stationary and the mobile phases. In thermodynamic measurements by SFC, the low hydrodynamic resistance of open-tubular capillary columns makes them preferable to packed columns. Variations in the solute retention factor with pressure or temperature can be employed to obtain the difference between the partial molar volumes[1−9] or the difference between the partial molar enthalpies[3−5] of the solute in both phases, respectively. The resultant partial molar properties should be corrected for the pressure- and temperature-dependent shifts in the equilibrium proportion of the mobile-phase fluid in the stationary phase. In a preceding study[10] we evaluated the effect of composition corrections on the infinite-dilution partial molar properties of azulene and acenaphthylene in supercritical carbon dioxide. Application of the corrections made the partial molar volumes more negative. Because of the lack of independent data on the partial molar properties for the two solutes, however, it was not possible to evaluate the outcome of the corrections in comparing the chromatographic results with those obtained by other methods.

The present paper extends our previous study to naphthalene and biphenyl as solutes. There have been several previous chromatographic determinations of the partial molar volumes of naphthalene in supercritical CO_2.[2,4,5,7] Our primary purpose here is to evaluate the effect of the corrections for composition changes in the stationary phase by comparing the partial molar volumes of naphthalene in CO_2 with the literature values obtained by vibrating-tube densitometry.[11] We also illustrate the benefits of using relative retention of two solutes from a single injection to obtain the partial molar volumes, with one solute serving as a reference.

Experimental Section

The experimental equipment and procedure used in the retention measurements were described before.[10] Both solutes were purchased from Aldrich (Seoul, Republic of Korea), and used as received. The injection solution was prepared by dissolving naphthalene and biphenyl (1.2 mg of each) in 10 mL of methylene chloride. The mobile phase holdup time was marked by injections of methane. Retention factors of both solutes were measured along five isotherms within 35−70 °C. At least five injections were performed at any particular temperature and pressure. The resultant retention factors ranged between 0.18 and 4.6 in naphthalene and between 0.27 and 7.1 in biphenyl. The difference between the column inlet pressure and the mean pressure in the column, calculated as described before[12] using the viscosity of CO_2 from the wide range correlation by Vesovic et al.,[13] ranged from 0.3 bar at the lowest pressure to 1.5 bar at the highest pressure.

Data Analysis

The procedure for converting retention data to infinite-dilution partial molar volumes of the solutes in CO_2 ($\bar{v}_{1m}^{\infty}$) and to infinite-dilution molar enthalpies of transfer of the solutes from the stationary phase to CO_2 ($\bar{h}_{1m}^{\infty} - \bar{h}_{1s}^{\infty}$) was the same as

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TABLE 1: Infinite-Dilution Partial Molar Volumes of Naphthalene in CO_2, Calculated with and without the Composition Correction in the Stationary Phase

t/°C	ρ_m/mol L^{-1}	$\bar{v}_{1m}^{\infty}$/L mol^{-1} composition correction		
		yes, PV[a]	yes, SHFH[b]	no
35	6	−3.01	−2.71	−2.42
	7	−4.13	−3.84	−3.53
	8	−5.79	−5.51	−5.20
	9	−7.35	−7.07	−6.76
	10	−7.59	−7.32	−7.01
	11	−6.46	−6.19	−5.88
	12	−4.60	−4.35	−4.04
	13	−2.57	−2.42	−2.24
	14	−1.19	−1.13	−1.06
	15	−0.573	−0.523	−0.461
	16	−0.275	−0.234	−0.181
	17	−0.122	−0.090	−0.046
40	5	−1.66	−1.42	−1.17
	6	−1.95	−1.71	−1.45
	7	−2.34	−2.12	−1.85
	8	−2.75	−2.54	−2.28
	9	−2.94	−2.75	−2.49
	10	−2.76	−2.59	−2.35
	11	−2.24	−2.11	−1.94
	12	−1.58	−1.50	−1.40
	13	−1.02	−0.956	−0.871
	14	−0.587	−0.537	−0.464
	15	−0.314	−0.272	−0.209
	16	−0.154	−0.120	−0.067
	17	−0.060	−0.033	0.011
50	5	−1.29	−1.13	−0.915
	6	−1.38	−1.22	−1.01
50	7	−1.47	−1.33	−1.12
	8	−1.51	−1.38	−1.19
	9	−1.44	−1.34	−1.16
	10	−1.26	−1.18	−1.03
	11	−1.01	−0.949	−0.832
	12	−0.755	−0.704	−0.605
	13	−0.519	−0.476	−0.391
	14	−0.327	−0.292	−0.218
	15	−0.187	−0.158	−0.094
	16	−0.092	−0.068	−0.014
60	5	−1.03	−0.912	−0.725
	6	−1.04	−0.931	−0.743
	7	−1.04	−0.942	−0.762
	8	−1.00	−0.921	−0.754
	9	−0.091	−0.849	−0.700
	10	−0.782	−0.728	−0.599
	11	−0.625	−0.582	−0.471
	12	−0.468	−0.432	−0.335
	13	−0.326	−0.296	−0.211
70	5	−0.831	−0.742	−0.570
	6	−0.802	−0.724	−0.554
	7	−0.767	−0.701	−0.539
	8	−0.713	−0.659	−0.508
	9	−0.633	−0.589	−0.452
	10	−0.532	−0.496	−0.374
	11	−0.421	−0.393	−0.284

[a] $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ calculated from the PV model. [b] $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ calculated from the SHFH theory.

before.[10] The properties of pure CO_2 were computed from a Jacobsen−Stewart type modification of the Benedict−Webb−Rubin equation of state (EOS).[14] The pressure and temperature derivatives of the equilibrium mass fraction of CO_2 in the stationary phase, $(\partial w_{3s}/\partial P)_{T,\sigma}$ and $(\partial w_{3s}/\partial T)_{P,\sigma}$, respectively, were calculated from the Panayiotou−Vera (PV) mean-field lattice model[15] with the parameters specified before.[16] For both solutes, the isothermal, isobaric derivative of the solute chemical potential in the stationary phase with respect to the mass fraction of CO_2 in the stationary phase, $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$, was evaluated from the Scatchard−Hildebrand−Flory−Huggins (SHFH) theory. The solubility parameters of subcooled liquid solutes were estimated as described by Prausnitz et al.,[17] using the molar volumes of subcooled liquid solutes obtained from the modified Rackett equation.[18] The cohesive energies of subcooled liquids were calculated from vapor pressures of the solid[19] and the liquid[20] naphthalene and the solid[21] and the liquid[22] biphenyl. Within 308−353 K, the resultant solubility parameter of subcooled liquid naphthalene may be fitted by a quadratic polynomial in absolute temperature, T, as

$$\delta_1 = 30.132 - 3.905 \times 10^{-2}T + 2.3381 \times 10^{-5}T^2 \quad (1)$$

while the following relationship applies to subcooled liquid biphenyl,

$$\delta_1 = 29.014 - 3.905 \times 10^{-2}T + 1.4902 \times 10^{-5}T^2 \quad (2)$$

In naphthalene, the derivative $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ was also evaluated alternatively from the PV model with the parameters specified before.[16]

Results and Discussion

Table 1 shows the resultant infinite-dilution partial molar volume of naphthalene as a function of temperature and density of CO_2, and the results for biphenyl are given in Table 2. In Tables 1 and 2, the values of $\bar{v}_{1m}^{\infty}$ calculated without the corrections for composition effects in the stationary phase are compared with the composition-corrected values ensuing from the use of the SHFH theory to express the derivative $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$. In addition, Table 1 also lists the composition-corrected values of $\bar{v}_{1m}^{\infty}$ for naphthalene that result when the PV model is employed to express $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$. Ap-

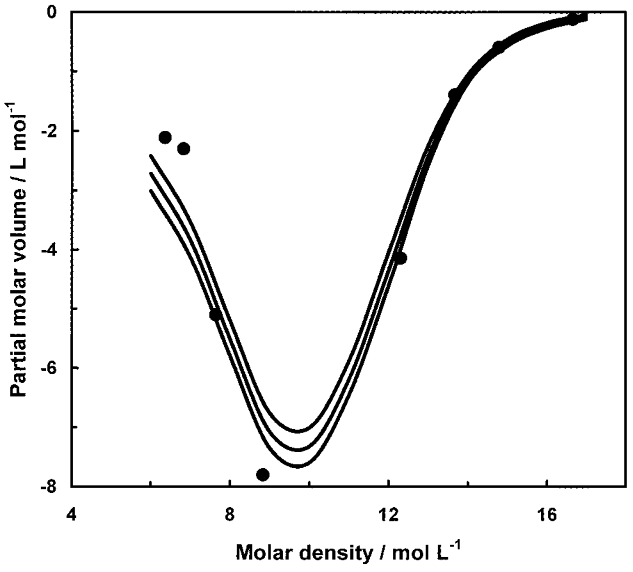

Figure 1. Infinite-dilution partial molar volume of naphthalene in CO_2 at 35 °C as a function of molar density of CO_2. Lines from above: SFC, uncorrected data; SFC, $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ from the SHFH theory; SFC, $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ from the PV model. Points: vibrating-tube densitometry[11] at 35.23 °C.

TABLE 2: Infinite-Dilution Partial Molar Volumes of Biphenyl in CO_2, Calculated with and without the Composition Correction in the Stationary Phase

		$\bar{v}_{1m}^{\infty}$/L mol^{-1} composition correction	
t/°C	ρ_m/mol L^{-1}	yes[a]	no
35	6	−2.80	−2.48
	7	−3.96	−3.63
	8	−5.69	−5.36
	9	−7.30	−6.97
	10	−7.56	−7.22
	11	−6.39	−6.06
	12	−4.48	−4.16
	13	−2.48	−2.29
	14	−1.15	−1.07
	15	−0.521	−0.455
	16	−0.222	−0.166
	17	−0.072	−0.026
40	5	−1.68	−1.41
	6	−2.03	−1.75
	7	−2.51	−2.23
	8	−3.02	−2.74
	9	−3.28	−3.01
	10	−3.09	−2.84
	11	−2.52	−2.34
	12	−1.80	−1.69
	13	−1.14	−1.05
	14	−0.636	−0.559
	15	−0.319	−0.252
	16	−0.137	−0.081
	17	−0.034	0.013
50	5	−1.34	−1.11
	6	−1.45	−1.22
	7	−1.58	−1.35
	8	−1.65	−1.44
	9	−1.60	−1.41
	10	−1.41	−1.25
	11	−1.13	−1.01
	12	−0.839	−0.734
	13	−0.566	−0.475
	14	−0.343	−0.265
	15	−0.183	−0.115
	16	−0.076	−0.018
60	5	−1.10	−0.895
	6	−1.12	−0.917
	7	−1.14	−0.940
	8	−1.11	−0.931
	9	−1.02	−0.864
	10	−0.879	−0.741
	11	−0.702	−0.582
	12	−0.520	−0.416
	13	−0.355	−0.263
70	5	−0.946	−0.760
	6	−0.923	−0.739
	7	−0.894	−0.718
	8	−0.841	−0.678
	9	−0.753	−0.605
	10	−0.635	−0.504
	11	−0.502	−0.385

[a] $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ calculated from the SHFH model.

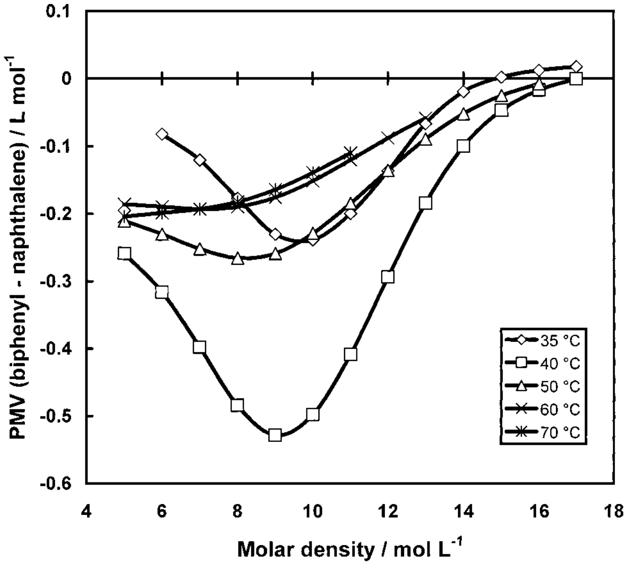

Figure 2. Difference between the infinite-dilution partial molar volumes of biphenyl and naphthalene in CO_2, calculated with the correction for composition changes in the stationary phase.

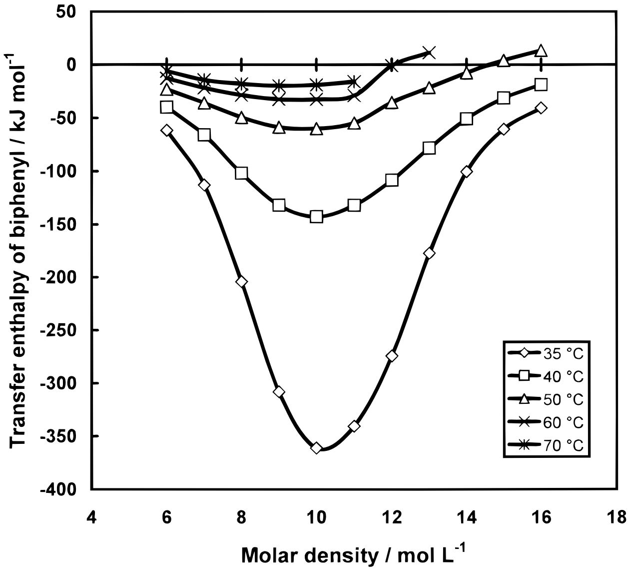

Figure 3. Infinite-dilution molar enthalpy of transfer of biphenyl from the CO_2-saturated poly(dimethylsiloxane) to pure CO_2, calculated with the correction for composition changes in the stationary phase.

plication of the correction for composition changes in the stationary phase makes the partial molar volumes of naphthalene and biphenyl algebraically lower (more negative), in the same way as noted before in azulene and acenaphthylene.[10] In naphthalene, the partial molar volumes obtained when $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ is expressed from the PV model are still more negative than the values resulting from the SHFH theory. This is because, in the naphthalene−poly(dimethylsiloxane)−CO_2 system, the values of $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ predicted from either treatment are negative, and those obtained from the PV model are 1.25−2 times larger in magnitude compared with the corresponding values from the SHFH theory.

Figure 1 shows a comparison of the chromatographic values of $\bar{v}_{1m}^{\infty}$ for naphthalene at 35 °C with the results obtained by Eckert et al.[11] from high-precision, vibrating-tube densitometry at 35.23 °C. Considering the temperature difference between densitometric and chromatographic results, it appears that the composition correction brings the partial molar volumes from SFC closer to the static results, at least in the density region at and above the minimum in $\bar{v}_{1m}^{\infty}$. Of course, it has to be admitted that the fair agreement shown in Figure 1 could be

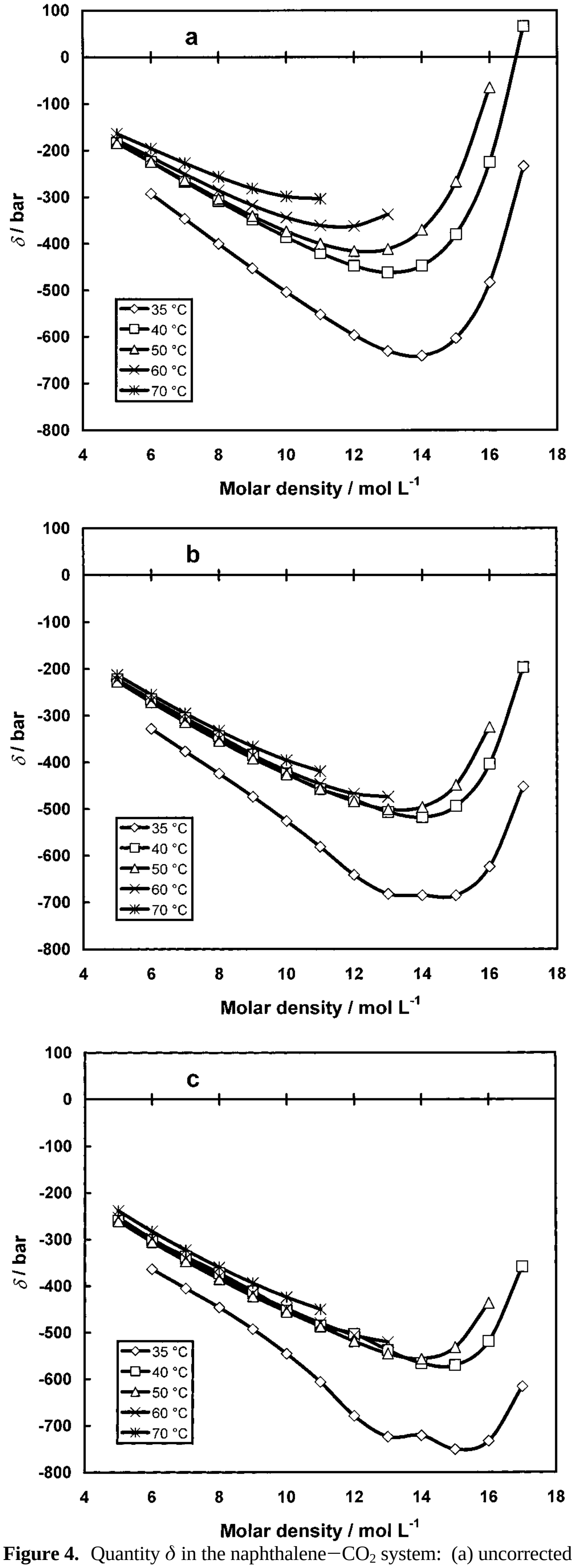

Figure 4. Quantity δ in the naphthalene$-$CO$_2$ system: (a) uncorrected data; (b) corrected results, $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ from the SHFH theory; (c) corrected results, $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ from the PV model.

partly fortuitous because, unlike the densitometric data on $\bar{v}_{1m}^{\infty}$, the chromatographic values depend on the particular choice of the EOS for CO$_2$ (through the calculated isothermal compressibility of CO$_2$). However, the correction-induced, negative shift in the chromatographic results occurs irrespective of the particular EOS employed. Further, in the density region below the minimum in $\bar{v}_{1m}^{\infty}$, the rate of the pressure change in $\bar{v}_{1m}^{\infty}$ suggested by the densitometric results seems much steeper than the chromatographic rates, whether corrected or not. There are several possible causes of the rate difference: the effect of pressure drop along the capillary column, the particular choice of the EOS for CO$_2$, or, most likely, underestimation of the derivative $(\partial w_{3s}/\partial P)_{T,\sigma}$ calculated from the PV model (in the composition-corrected chromatographic results).

If the chromatographic measurements comprise a simultaneous injection of two solutes, A and B, and if A and B separate well under the particular operating conditions, the pressure dependence of relative retention of the two solutes can be used to obtain the difference in their respective partial molar volumes in the mobile-phase fluid, $\bar{v}_{Am}^{\infty} - \bar{v}_{Bm}^{\infty}$. The use of relative retention makes the chromatographic determination of partial molar properties a comparative method because one of the two solutes may serve as a reference, with the respective property obtained from an independent source. As an example, Figure 2 presents such a difference between biphenyl and naphthalene. In this particular case, the effect of composition correction in the stationary phase is very small. Except in the low-temperature, high-density region, the partial molar volume of biphenyl is more negative than the respective value for naphthalene. The temperature course of the minimum in $\bar{v}_{Am}^{\infty} - \bar{v}_{Bm}^{\infty}$ is complicated. As the temperature decreases, the minimum shifts to more negative values but an unexpected reversal occurs between 40 and 35 °C. The reversal is not caused by the composition correction, and it also does not result from the pressure drop along the column. Mutual cosolvency effects between the two solutes also do not provide a plausible explanation because the two solutes separate well under the particular conditions. Therefore, the reversal does not appear to be an artifact of the chromatographic method.

Figure 3 shows the infinite-dilution molar enthalpy of transfer of biphenyl from the CO$_2$-saturated poly(dimethylsiloxane) to pure CO$_2$, $\bar{h}_{1m}^{\infty} - \bar{h}_{1s}^{\infty}$. The values shown in Figure 3 are corrected for composition changes in the stationary phase with $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ expressed from the SHFH theory. Transfer enthalpies of naphthalene are more positive than those for biphenyl. At 35 °C and 10 mol L^{-1}, for example, the transfer enthalpy of naphthalene amounts to -325 kJ mol^{-1} compared to -360 kJ mol^{-1} for biphenyl. Application of the composition correction shifts the transfer enthalpies toward more negative values. With the derivative $(\partial w_{3s}/\partial P)_{T,\sigma}$ calculated from the PV model, the relative importance of the correction increases with decreasing magnitude of the transfer enthalpy. Near the critical temperature of CO$_2$, the transfer enthalpies of both naphthalene and biphenyl appear to be more negative (exothermic) than those of azulene;[10] the actual magnitudes of the transfer enthalpies of azulene are 10 times lower than shown mistakenly in Figure 3 of ref 10.

Short-range interactions between a solute and a supercritical solvent can be characterized, e.g., by the quantity δ introduced by Debenedetti and Mohamed[23] and defined by

$$\delta = \bar{v}_{1m}^{\infty}\rho_m/\beta_{mT} \tag{3}$$

where ρ_m is the molar density of the solvent and β_{mT} is the isothermal compressibility of the solvent,

$$\beta_{mT} = (1/\rho_m)(\partial\rho_m/\partial P)_T \tag{4}$$

Figure 4 presents the values of δ in the naphthalene−CO_2 system. The irregularities seen in the composition-corrected isotherms at 35 and 40 °C result from using the PV model to calculate the derivative $(\partial w_{3s}/\partial P)_{T,\sigma}$. The values of δ in the biphenyl−CO_2 system are more negative compared to those in the naphthalene−CO_2 system, except for the highest densities in the 35 and 40 °C isotherms (cf. Tables 1 and 2). Further, the minimum values of δ in the naphthalene−CO_2 system are more negative compared to what the minimum values of δ would be in the azulene−CO_2 system at the same temperature.[10] The short-range interactions between azulene and CO_2 therefore appear to be less attractive compared to those between naphthalene and CO_2. When going from the naphthalene−CO_2 to the azulene−CO_2 system, the decrease in the energy of solute−solvent dispersion interaction is not offset by polar interactions between the dipole in azulene and the quadrupole in CO_2. Apart from rendering the δ values more negative, especially in the high-density region, application of the composition correction tends to suppress the effect of temperature on the δ values in the low-density region.

The results described above support the conclusion that, in reducing SFC retention data to partial molar properties of solutes in supercritical mobile-phase fluid, the corrections for composition changes in the stationary phase are pertinent. The pressure and temperature derivatives of the equilibrium mass fraction of CO_2 in the stationary phase, $(\partial w_{3s}/\partial P)_{T,\sigma}$ and $(\partial w_{3s}/\partial T)_{P,\sigma}$, can in principle be obtained from experimental studies on sorption of the particular mobile-phase fluid in the particular stationary polymer. However, the isothermal, isobaric derivative of the solute chemical potential in the stationary phase with respect to the mass fraction of dissolved mobile-phase fluid, $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$, reflects the features of the molecular model employed. In general, therefore, the performance of composition corrections remains an open issue. In the particular case of the naphthalene−poly(dimethylsiloxane)−CO_2 system with the present parametrization, the PV model seems superior to the SHFH theory in modeling $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ as indicated by comparison of the resultant partial molar volumes of naphthalene in CO_2 with high-precision densitometric data.[11] Superiority of the PV model can partly result from the fact that the present parametrization[16] for this model includes unlike-interaction parameters between any two components of the naphthalene−poly(dimethylsiloxane)−CO_2 system. The SHFH theory, however, requires pure-component properties only, and Figure 1 suggests that the PV model with binary parameters brings relatively little refinement over the SHFH theory. In reducing retention data to partial molar properties of solutes in mobile-phase fluids, therefore, the derivative $(\partial\mu_{1s}^{\infty}/\partial w_{3s})_{T,P,n_{2s}}$ can conveniently be estimated from the SHFH theory and used together with the solute-independent quotients $(\partial w_{3s}/\partial P)_{T,\sigma}$ or $(\partial w_{3s}/\partial T)_{P,\sigma}$ obtained from studies of sorption of the particular fluid in the particular stationary polymer. With this procedure and the necessary instrumental equipment, capillary-column SFC can be a rapid and relatively reliable source of infinite-dilution partial molar property data of nonvolatile solutes in a number of supercritical fluids (e.g., in alternative refrigerants).

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