

# Solvent Diffusion in Amorphous Polymers: Polyvinyl Acetate–Toluene System

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**ABSTRACT:** In a previous publication (Tihminlioglu et al., *J Polym Sci Part B: Polym Phys* 1997, 35, 1279), we presented an extensive analysis of the polyvinyl acetate–toluene system. The inverse gas chromatography (IGC) technique was used to measure phase equilibria and diffusion coefficients above and near the glass-transition temperature of a polymer. At temperatures above the glass transition, the capillary column model developed by Pawlisch et al. (*Macromolecules* 1987, 20, 1564) was used. For the finite concentration region, the modified model of Tihminlioglu and Danner (*J Chromatogr A* 1999, 845, 93) was applied. Data obtained with the IGC method were in agreement with data measured with the gravimetric and piezoelectric sorption techniques. In this work, we revisit the partition coefficient issue and provide some new data at lower temperatures. At temperatures near the glass-transition temperature, the modification of the capillary column model proposed by Vrentas et al. (*Macromolecules* 1993, 26, 6670) was used for the infinite dilution region. The diffusion data correlated well with the Vrentas–Duda free-volume model. © 2000 John Wiley & Sons, Inc. *J Polym Sci B: Polym Phys* 38: 2429–2435, 2000

**Keywords:** polyvinyl acetate; toluene; solvent diffusion; inverse gas chromatography; polymer; free-volume theory

## INTRODUCTION

As previously shown,<sup>1,2</sup> the inverse gas chromatography (IGC) method can be used to accurately and efficiently measure solubility and diffusivity in polymer–solvent systems in both the infinite and finite concentration ranges.

Capillary columns have a number of significant advantages over packed columns in the IGC method. They have a simple geometry with a thin and uniform coating, there is much less gas-phase dispersion, and there is no significant pressure drop. The method for analyzing the response from

a capillary column for an infinitely dilute input pulse was presented by Pawlisch et al.<sup>3,4</sup> and Arnould and Laurence.<sup>5</sup> This model fails, however, for low diffusion coefficients.<sup>6</sup> Vrentas et al.<sup>7</sup> showed that for low values of the diffusion coefficients, the capillary column IGC model (CCIGC) can be solved analytically for the outlet concentration profile. In this case, the diffusion in the gas phase is fast compared with the diffusion in the polymer phase; therefore, the diffusion resistance in the gas phase can be neglected. When these equations are applicable (at low values of the diffusion coefficients), one can solve for the product of the diffusion and phase equilibria terms. If one of the parameters is independently known, the other can be calculated. Frequently, the partition coefficient,  $K_p$ ,

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can be estimated by extrapolation from data at higher temperatures.

As shown in previous publications,<sup>1,2</sup> at the exit of the column the dimensionless equation for the response peak in the Laplace domain is

$$\frac{CL}{C_o u} = \exp\left(\frac{1}{2\Gamma}\right) \exp\left[-\left(\frac{1}{4\Gamma^2} + \frac{S}{\Gamma} + \frac{2\sqrt{S}}{\alpha\beta\Gamma} \tanh(\beta\sqrt{S})\right)^{1/2}\right] \quad (1)$$

$$\Gamma = \frac{D_g}{uL}; \quad \alpha = \frac{R}{K(1-\psi)\tau}; \quad \beta^2 = \frac{\tau^2}{D_p t_c} \quad (2)$$

where  $\tau$  is the thickness of the polymer film,  $K$  is equal to  $dC'/dC$  (which, for the infinitely dilute case, is equal to  $C'/C$ , the partition coefficient,  $K_p$ ),  $S$  is the Laplace operator, and  $D_g$  and  $D_p$  are the gas-phase and polymer-phase diffusion coefficients, respectively. The elution profile is a function of the three dimensionless parameters,  $\alpha$ ,  $\beta$ , and  $\Gamma$ .  $\alpha$  is inversely related to the partition coefficient,  $\beta^2$  is similarly related to the polymer diffusion coefficient, and  $\Gamma$  varies proportionately with the gas-phase diffusion coefficient. In other words, the parameter  $\alpha$  is a thermodynamic parameter, whereas  $\beta$  and  $\Gamma$  represent the polymer-phase and gas-phase transport properties, respectively. Surana et al.<sup>6</sup> suggested that  $\beta$  should have a value between 0.03 and 5.0 to obtain a good fit of the elution profile.  $\psi$  is the true molar fraction obtained by correction for the gas-phase nonideality and for compressibility effects due to the pressure gradient in the column.<sup>8</sup>

The ratio  $C'/C$  is then the partition coefficient obtained from the CCIGC model. In our previous article on this system,<sup>1</sup> the partition coefficient was defined as the slope of the isotherm  $dC'/dC$  rather than the ratio of the concentrations. The more useful quantity is the ratio of concentrations, which we define as  $K_p$ , the true partition coefficient. The concentration in the polymer phase is obtained by integration of the  $dC'/dC$  values from zero concentration to the concentration of interest. The resulting ratio,  $C'/C$ , is the partition coefficient obtained from the CCIGC model.

An alternate method of obtaining the partition coefficient is through the theoretical relationships developed by Conder and Young<sup>9</sup> and Price and Guillet.<sup>10</sup> In this case, the net retention volume,  $V_N$ , is expressed as

$$V_N = V_s(1 - \psi) \frac{d'C}{dC} \quad (3)$$

where  $V_s$  is the volume of the stationary phase. By integrating eq 3 and introducing the weight of the polymer used,  $w$ , we can find the concentration of the solvent in the polymer phase,  $Q$ :

$$Q = \frac{j}{w} \int_0^c \frac{V_N}{(1 - \psi)} dC \quad (4)$$

where  $j$  is the pressure-drop correction factor.<sup>9</sup> To determine an isotherm, retention volumes were measured for a series of solute concentrations. Evaluation of the integral was done by the fitting of a polynomial to the data and integration. The partition coefficients determined in this way are called *retention theory values*.

The IGC experimental procedure is described in the previous article.<sup>1</sup> For the data reported here, the capillary column was 15 m long with an 0.53-mm inner diameter. The thickness of the polymer coating was 5.0  $\mu\text{m}$ . The toluene was reagent-grade (>99.0% purity) and was obtained from Aldrich Chemical; it was injected as a liquid. The polyvinyl acetate (PVAC) was obtained from Scientific Polymer Products, Inc. It had a density of 1.18 g/cm<sup>3</sup>, a molecular weight of approximately 100,000, and a glass-transition temperature of 33 °C.

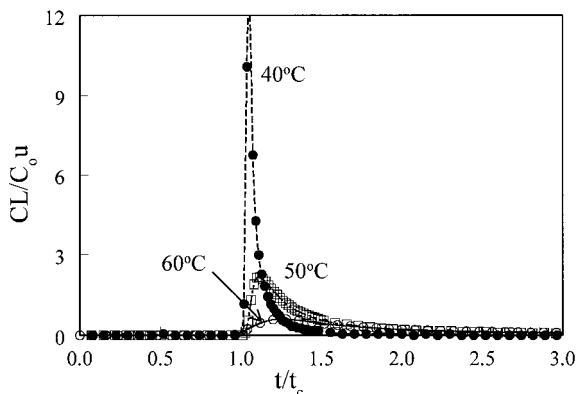
## RESULTS AND DISCUSSION

### Infinitely Dilute Region

Infinitely dilute data were obtained at 40, 50, and 70 °C (Table I) to supplement the high-temperature data reported by Tihminlioglu et al.<sup>1</sup> Between 80 and 110 °C, the model fits the experimental elution profiles very well. The values of  $\beta$  in this temperature range varied from 0.186 at

**Table I.** Partition and Diffusion Coefficients for the PVAC–Toluene System at Infinite Dilution Determined by the IGC Technique

$T$ (°C)	$K_p$	$D_p$ (cm <sup>2</sup> /s)
70	199	$2.23 \times 10^{-10}$
50	400	$3.92 \times 10^{-12}$
40	586	$8.29 \times 10^{-13}$



**Figure 1.** Elution profiles of the PVAC–toluene system at three different temperatures.

110 °C to 1.39 at 80 °C. Figure 1 shows the elution curves obtained for three different temperatures near the glass-transition temperature of the polymer. Because most of the solvent does not enter the polymer at these temperatures, the elution profiles show sharp fronts and long tails. The peak height increases with a decrease in temperature. Difficulties were encountered in obtaining good regression results at temperatures lower than 80 °C. This is because the value of  $\beta$  exceeded its allowable range as the diffusion coefficients decreased below  $10^{-11}$  to  $10^{-13}$  cm<sup>2</sup>/s.

Therefore, the modification of Vrentas et al.<sup>7</sup> was used. They showed that for low diffusivities, the CCIGC model can be solved analytically to describe the outlet concentration profile. The first step was to extrapolate the higher temperature (80–100 °C)  $K_p$  values obtained from the standard CCIGC model to the lower temperature range. The solid points in Figure 2 ( $\ln K_p$  versus  $1/T$ ) were extrapolated linearly to the lower temperatures.

The solubility behavior of the toluene in PVAC is shown in Figure 3. This plot shows that the solvent volume fraction at a given activity is essentially independent of the temperature. With the well-known theory of Flory and Huggins, the relation between the Flory–Huggins interaction parameter ( $\chi$ ), the activity ( $a_i$ ), and the weight fraction ( $w_i$ ) is

$$\chi = \ln\left(\frac{a_i}{w_i}\right) - \left(1 - \frac{1}{r}\right) + \ln\left(\frac{\rho_1}{\rho_2}\right) \quad (5)$$

An average  $\chi$  value of 0.70 adequately represents these data, as shown in Figure 3. Values for the solvent density,  $\rho_1$ , were obtained from Daubert

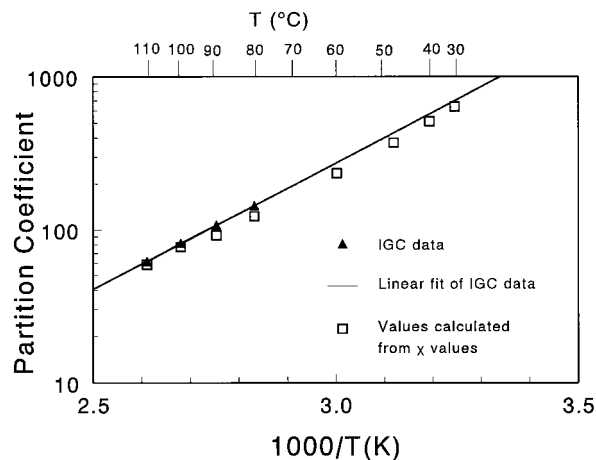
and Danner,<sup>11</sup> whereas the polymer density,  $\rho_2$ , was obtained from *Polymer Handbook*.<sup>12</sup>

Vrentas et al.<sup>13</sup> collected literature data for the toluene–PVAC system and correlated them via the Flory–Huggins method. They determined  $\chi$  at each temperature for which they had data. The partition coefficient can be calculated from  $\chi$  as follows:

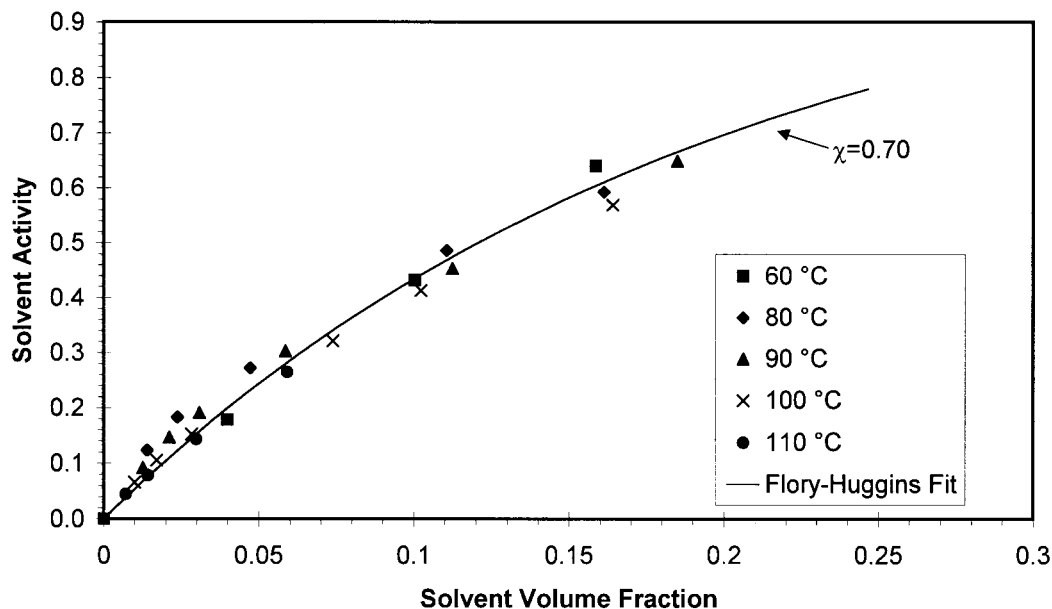
$$K = \frac{R_g T}{P_1^0 \hat{V}_1 \exp(1 + \chi)} \quad (6)$$

where  $P_1^0$  is the vapor pressure of the solvent and  $\hat{V}_1$  is the partial molar volume of the solvent, which has necessarily been assumed to be the pure component molar liquid volume. Vrentas et al. found that the  $\chi$  values ranged approximately from 0.53 to 0.75 over the temperature range 60–110 °C. In Figure 2, the results of this procedure are plotted as open squares. The  $K$  values extrapolated from the IGC data with a constant  $\chi$  value of 0.70 are in good agreement with those calculated from the  $\chi$  values of Vrentas et al. This indicates that the relation is not very sensitive to the  $\chi$  value.

The standard CCIGC model was used to calculate the diffusion coefficients for temperatures of 80 °C and higher. For the lower temperatures, the values of  $K_p$  from extrapolation were used with equations given in Vrentas et al.<sup>7</sup> to calculate the diffusion coefficients in the polymer. All these values, of course, are for infinitely dilute solvent. Table I lists the partition and diffusion coefficients at infinite dilution.



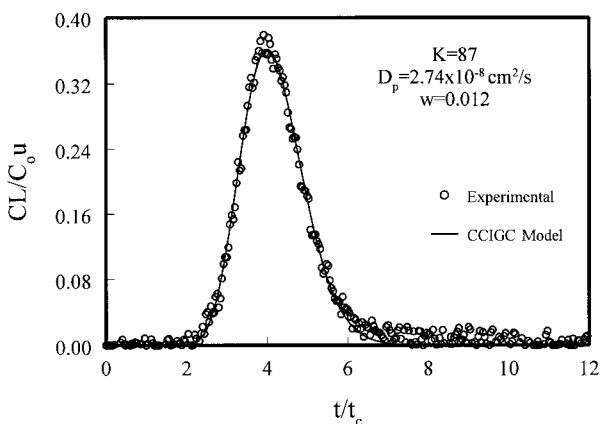
**Figure 2.** Comparison of the partition coefficients determined in three different ways.



**Figure 3.** Solubility of toluene in PVAC correlated with the Flory–Huggins interaction parameter,  $\chi$ .

### Finite Concentration Region

Data were previously reported for the PVAC–toluene system over a temperature range of 60–110 °C at finite concentrations up to about 14 wt % toluene in the polymer. A typical elution profile observed in the finite concentration cases is shown for a solvent weight fraction of 0.012 at 100 °C in Figure 4. The scatter in the experimental data, which is significantly greater than in the infinitely dilute case, is the result of slight variations in the saturator flow and temperature. Nev-

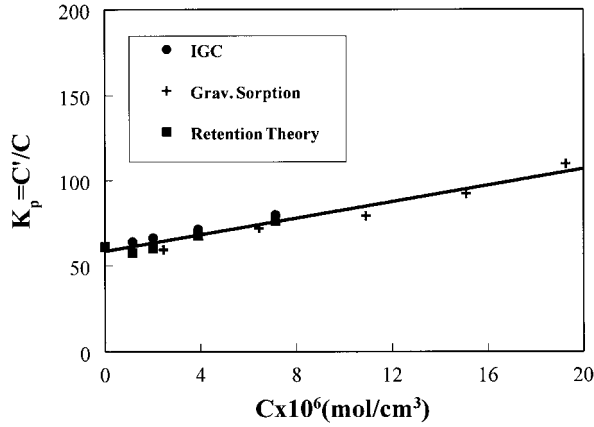


**Figure 4.** Comparison of the experimental elution profile and CCIGC model for the PVAC–toluene system.

ertheless, the model reproduces the experimental curve quite well.

For the infinite dilution case, retention volume is equal to the product of the stationary phase volume and partition coefficient ( $V_N = V_s K_p$ ). The partition coefficient is the ratio of the solvent concentration in the polymer phase to the solvent concentration in the gas phase ( $K_p = C'/C$ ). Retention volume at a given concentration, however, is not in terms of  $C'$  but in terms of  $dC'/dC$ , which is the slope of the tangent to the absorption isotherm. At concentrations approaching infinite dilution, the tangent and the absorption isotherm coincide, giving rise to a simple linear relationship between the solvent concentrations in the polymer and gas phases. At higher concentrations, however, the absorption isotherm is no longer linear, and the slopes of the tangent may vary a lot, depending on the temperature and concentration of the polymer–solvent system. A number of measurements in small steps in the concentration of the gas phase were made to accurately calculate the integral and, thus, the final concentration of the solvent in the polymer.

The amount absorbed was determined with both the CCIGC model and the retention theory. Figure 5 shows the partition coefficients for this system as a function of solvent concentration in the gas phase at 110 °C. The solid circles show the partition coefficients obtained from the finite con-



**Figure 5.** Partition coefficients for toluene in PVAC at 110 °C.

centration CIGC model, and the solid squares show the partition coefficients obtained from the retention volume expression (eq 4). The values given by the plus symbols were obtained by gravimetric sorption in our laboratory. There is good agreement between all three sets of data. Similar results were obtained at other temperatures. The curve is a linear fit of all the experimental data. Table II lists the experimental values of the partition and diffusion coefficients in the finite concentration region. The previous article<sup>1</sup> listed the  $dC'/dC$  values. The  $K_p$  values given in Table II are of more interest. The diffusion coefficients are as given in the previous article.

The free-volume theory of Vrentas and Duda<sup>14,15</sup> was used to correlate the diffusivity results. The self diffusion coefficient,  $D_1$ , is obtained as follows:

$$D_1 = D_0 \exp\left(-\frac{E}{R_g T}\right) \exp\left[-\frac{\gamma(\omega_1 \hat{V}_1^* + \omega_2 \hat{V}_2^* \xi)}{\hat{V}_{FH}}\right] \quad (7)$$

where  $D_0$  is a constant pre-exponential factor,  $E$  is the activation energy per mole that a molecule needs to overcome attractive forces holding it to its neighbors,  $\hat{V}_i^*$  is the specific critical hole free volume required for a diffusive jump of the component  $i$ , and  $\gamma$  is an overlap factor that accounts for shared free volume. The quantity  $\xi$  is defined as the ratio of the critical volume of the solvent per mole to that of the polymer:

$$\xi = \frac{\hat{V}_1^* M_{j1}}{\hat{V}_2^* M_{j2}} \quad (8)$$

where  $M_{ji}$  is the molecular weight of a jumping unit of component  $i$ .  $\hat{V}_{FH}$  is the specific hole free volume of the polymer–solvent mixture given by

$$\hat{V}_{FH} = \omega_1 K_{11}(K_{21} + T - T_{g1}) + \omega_2 K_{12}(K_{22} + T - T_{g2}) \quad (9)$$

where  $K_{ki}$  is a free-volume parameter and  $T_{gi}$  is the glass-transition temperature of component  $i$ .

If the thermodynamic theory of Flory–Huggins is invoked, the mutual diffusion coefficient,  $D_p$ , is calculated from

$$D_p = D_1(1 - \phi_1)^2(1 - 2\phi_1\chi) \quad (10)$$

where  $\phi_i$  is the volume fraction of component  $i$ . The experimental data were regressed to obtain three parameters: the ratio of the jumping units,

**Table II.** Experimental Finite Concentration Data for the PVAC–Toluene System

$T$ (°C)	$\omega_1$	$P_1^o$ (bar)	$K_p$	$D_p$ (cm <sup>2</sup> /s)
60	0	—	281	$5.05 \times 10^{-11}$
	0.029	$3.25 \times 10^{-2}$	276	$3.62 \times 10^{-10}$
	0.074	$7.88 \times 10^{-2}$	312	$2.81 \times 10^{-9}$
	0.119	$1.17 \times 10^{-1}$	348	$4.45 \times 10^{-8}$
80	0	—	149	$1.48 \times 10^{-9}$
	0.010	$4.71 \times 10^{-2}$	158	$5.67 \times 10^{-9}$
	0.017	$6.99 \times 10^{-2}$	163	$9.45 \times 10^{-9}$
	0.034	$1.04 \times 10^{-1}$	178	$2.12 \times 10^{-8}$
	0.081	$1.86 \times 10^{-1}$	223	$1.05 \times 10^{-7}$
90	0	—	270	$3.82 \times 10^{-7}$
	0.009	$4.90 \times 10^{-2}$	108	$4.10 \times 10^{-9}$
	0.015	$7.85 \times 10^{-2}$	111	$7.89 \times 10^{-9}$
	0.022	$1.02 \times 10^{-1}$	114	$1.59 \times 10^{-8}$
	0.042	$1.62 \times 10^{-1}$	117	$2.95 \times 10^{-8}$
	0.082	$2.42 \times 10^{-1}$	124	$5.75 \times 10^{-8}$
100	0	—	133	$3.42 \times 10^{-7}$
	0.0138	$3.47 \times 10^{-1}$	165	$1.00 \times 10^{-6}$
	0	—	82	$1.35 \times 10^{-8}$
	0.007	$4.82 \times 10^{-2}$	84	$2.05 \times 10^{-8}$
	0.012	$7.71 \times 10^{-2}$	87	$2.74 \times 10^{-8}$
	0.02	$1.11 \times 10^{-1}$	91	$4.49 \times 10^{-8}$
	0.053	$2.35 \times 10^{-1}$	105	$7.68 \times 10^{-8}$
110	0	—	113	$1.80 \times 10^{-7}$
	0.074	$3.02 \times 10^{-1}$	127	$8.59 \times 10^{-7}$
	0.121	$4.16 \times 10^{-1}$	127	$8.59 \times 10^{-7}$
	0	—	61	$2.93 \times 10^{-8}$
	0.005	$4.39 \times 10^{-2}$	64	$4.19 \times 10^{-8}$
	0.010	$7.64 \times 10^{-2}$	66	$6.32 \times 10^{-8}$
	0.021	$1.40 \times 10^{-1}$	71	$9.59 \times 10^{-8}$
	0.042	$2.59 \times 10^{-1}$	80	$1.66 \times 10^{-7}$
0.112	$4.17 \times 10^{-1}$	94	$8.46 \times 10^{-7}$	



**Table III.** Free-Volume Parameters

Parameters	PVAC-Toluene
$\hat{V}_1^*$ (cm <sup>3</sup> /g)	0.917
$\hat{V}_2^*$ (cm <sup>3</sup> /g)	0.728
$K_{11}$ (cm <sup>3</sup> /gK)	$1.45 \times 10^{-3}$
$K_{12}$ (cm <sup>3</sup> /gK)	$4.33 \times 10^{-4}$
$K_{21} - T_{g1}$ (K)	-86.32
$K_{22} - T_{g2}$ (K)	-258.2
$\xi$	0.709
$\chi$	0.70
$D_0$ (cm <sup>2</sup> /s)	0.0975
$E$ (cal/mol)	3923

1 = toluene; 2 = PVAC.

$\xi$ ; the pre-exponential factor,  $D_0$ ; and the activation energy,  $E$ . All other free-volume parameters were taken from Zielinski and Duda.<sup>16</sup> The average value of the Flory-Huggins interaction parameter,  $\chi = 0.70$ , was used at all temperatures. The parameters are given in Table III. Figure 6 shows the correlation obtained for the mutual diffusion coefficient at various temperatures. Except for the deviation at 60 °C, the fit is quite good. The suspected cause of this deviation is error in the data because of the difficulty in determining accurate results for very small diffusivities.

## CONCLUSION

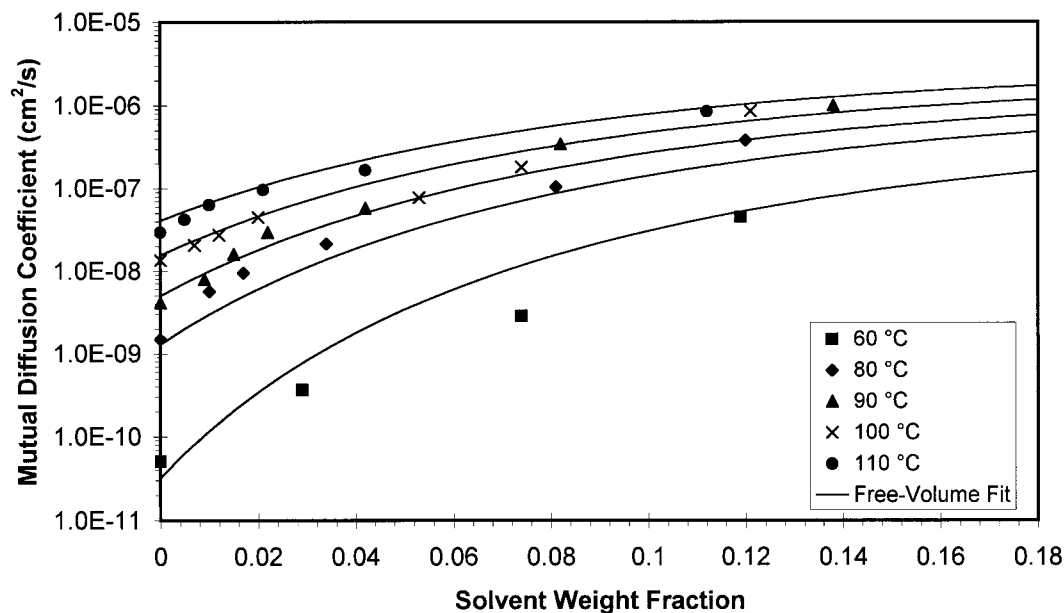
The CCIGC technique has been demonstrated to be a good method to measure partition and diffu-

sion coefficients over a wide temperature range for both infinite and finite concentrations. For infinitely dilute regions, at temperatures well above the glass-transition temperature of the polymer, the original CCIGC model can be used effectively. In general, this is limited to values of  $\beta$  between 0.03 and 5.0. For lower diffusion coefficients as encountered near the glass transition, the modification of Vrentas et al.<sup>7</sup> is recommended. In this way, diffusion coefficients as low as  $10^{-13}$  cm<sup>2</sup>/s can be measured.

Results obtained by IGC are in good agreement with the gravimetric sorption data. IGC is advantageous because it is a fast, reliable, and accurate technique. Although the data analysis is somewhat complex, once the procedure has been worked out, multiple data points can be obtained much more expediently than with standard sorption techniques. The diffusivity data have been successfully correlated by the Vrentas-Duda free-volume theory. This study shows that IGC can be effectively used to make both infinite and finite concentration measurements of diffusion coefficient measurements, thus increasing its applicability.

## NOMENCLATURE

- $a_i$  activity of component  $i$   
 $C$  solute concentration in the gas phase (mol/cm<sup>3</sup>)



**Figure 6.** Correlation of the diffusivity with the free-volume theory.

$C'$	solute concentration in the polymer phase (mol/cm <sup>3</sup> )	$\rho_i$	density of component $i$ (g/cm <sup>3</sup> )
$C_0$	strength of the inlet impulse (mol · s/cm <sup>3</sup> )	$\Phi_i$	volume fraction of component $i$
$D_1$	solvent self-diffusion coefficient (cm <sup>2</sup> /s)	$\chi$	Flory–Huggins polymer–solvent interaction parameter
$D_o$	pre-exponential factor (cm <sup>2</sup> /s)	$\omega_i$	mass fraction of component $i$
$D_g$	solvent diffusion coefficient in the mobile phase (cm <sup>2</sup> /s)		
$D_p$	solvent diffusion coefficient in the polymer phase (cm <sup>2</sup> /s)		
$E$	activation energy (J/mol)		
$j$	pressure-drop correction factor		
$K$	slope of the sorption isotherm ( $dC'/dC$ )		
$K_p$	equilibrium partition coefficient ( $C'/C$ )		
$K_{1i}$	free-volume parameter of component $i$ (cm <sup>3</sup> /g · K)		
$K_{2i}$	free-volume parameter of component $i$ (K)		
$L$	length of the column (cm)		
$M_{ji}$	molecular weight of a jumping unit of component $i$ (g/mol)		
$P_1^o$	vapor pressure of solvent in the saturator (bar)		
$Q$	solvent concentration in the polymer phase (mol/g polymer)		
$r$	number of polymer repeat units		
$R$	inner radius of the column (cm)		
$R_g$	gas constant (J/mol · K)		
$S$	Laplace operator		
$t_c$	residence time of the carrier gas (s)		
$T$	temperature (K)		
$T_g$	glass-transition temperature (K)		
$u$	mean velocity of the carrier gas (cm/s)		
$V_N$	net retention volume (cm <sup>3</sup> )		
$V_s$	volume of the stationary liquid phase (cm <sup>3</sup> )		
$\hat{V}_i$	partial molar volume of component $i$ (cm <sup>3</sup> /mol)		
$w$	mass of polymer (g)		
$\alpha$	dimensionless thermodynamic parameter		
$\beta$	dimensionless polymer-phase diffusion parameter		
$\gamma$	overlap factor that accounts for shared free volume		
$\Gamma$	dimensionless gas-phase diffusion parameter		
$\psi$	pressure-corrected molar fraction of vapor in carrier gas		

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