CHAPTER VI

RESULTS AND DISCUSSION

6.1 Density of Benzene, Cyclohexane and n-Heptane System.

The experimental values of density of pure compounds at various states are presented in Table 6.1. It is found that densities of benzene are greater than densities of cyclohexane and n-heptane. In addition, pure liquid densities are sensitive to temperature and rarely are sensitive to pressure. The densities decrease as temperature increases at constant pressure and slightly decrease as pressure increases at constant temperature.

Table 6.1 Experimental density of pure components.

T (K)	P (bar)	Density (g/cm^3)		
		Benzene	Cyclohexane	n-Heptane
308.15	1.01325	0.86648	0.76955	0.67445
	2	0.86960	0.77203	0.67665
	5	0.87204	0.77381	0.67813
	10	0.88220	0.78276	0.68588
313.15	1.01325	0.86138	0.76468	0.66862
	2	0.86436	0.76687	0.67056
	5	0.86654	0.76808	0.67161
	10	0.87759	0.77775	0.68066
323.15	1.01325	0.85101	0.75303	0.66002
	2	0.85381	0.75593	0.66232
	5	0.85554	0.75734	0.66386
	10	0.86823	0.76807	0.67345
333.15	1.01325	0.84045	0.74479	0.65369
	2	0.84318	0.74738	0.65607
	5	0.84454	0.74880	0.65705
	10	0.85867	0.76141	0.66763

Table 6.2 shows comparison between experimental and literature density values of the pure components at 1.01325 bar. The results of this work are higher than those from the literatures by about 0.38-0.73 %.

Table 6.2   Comparison between experimental and literature density values of the pure components at 1.01325 bar.

Compounds	T (K)	Density (g/cm^3)	
		Experimental values	Literature values
Benzene	313.15	0.86138	0.85810 (Beg et al., 1993; Emmerling et al., 1998)
	323.15	0.85101	0.85010 (Emmerling et al., 1998)
Cyclohexane	308.15	0.76955	0.76420 (Aminabhavi et al., 1996)
			0.76400 (Aminabhavi and Banerjee, 1998)
	313.15	0.76468	0.75950 (Beg et al., 1993)
	333.15	0.74479	0.74040 (Beg et al., 1993)
n-Heptane	308.15	0.67445	0.67070 (Aminabhavi et al., 1996)

Moreover, density of mixtures varied with not only temperature and pressure but also composition. For benzene and cyclohexane system, since density of benzene is higher than that of cyclohexane, the densities increase with the mole fraction of benzene component (x_1) at all states as shown in Figure 6.1. It can be observed that as the pressure increases the density of the binary increases at constant temperature and composition. In addition, the results at low pressure were very closed together. It can be explained that generally, at low pressure slightly effect liquid density because nonpolar molecules of mixture attract with van der waals force, which is intermolecular interaction, when the molecules were compressed at low pressure, the small pressure could not compressed the molecules in mixture. And, as the temperature increases, the density of the binary decrease at constant pressure and
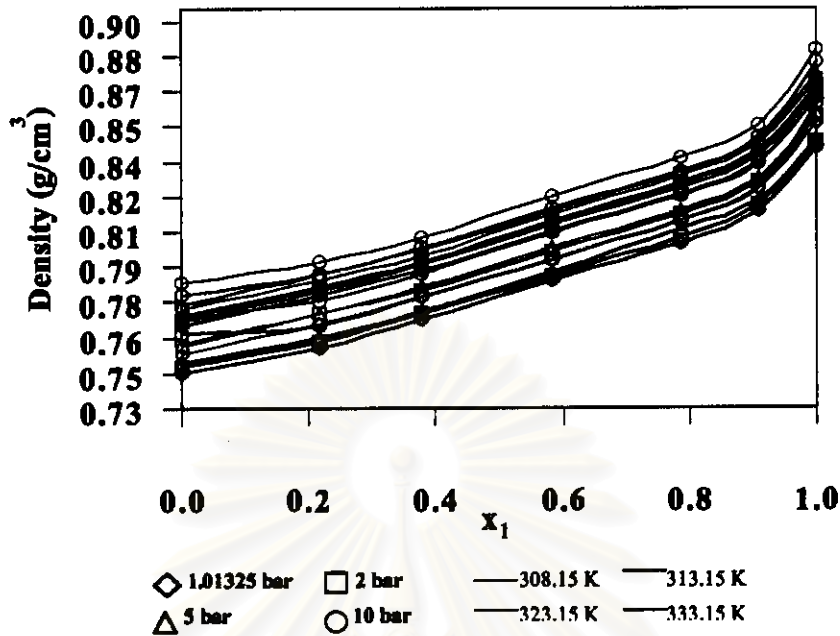
Figure 6.1 Density of benzene (1) and cyclohexane (2) system.

composition. It was observed that when temperature increase, the molecules of mixture vibrate more and were far between each molecule that is the molecules attract loosely with van der waals force, and thus the density of the mixture decrease.

For cyclohexane and n-heptane system, it can be observed that the density were more sensitive to temperature than pressure. As the pressure increases the density of the binary slightly increase at constant temperature and composition and as the temperature increases the density of the mixture decrease at constant temperature and composition as shown in Figure 6.2. Also, the density increase with the mole fraction of cyclohexane component (x_1) at all states because density of cyclohexane is higher than the density of n-heptane. Comparison between experimental and literature (Aminabhavi et al., 1996) density values are shown in Figure 6.3. It was found that experimental values agreed with
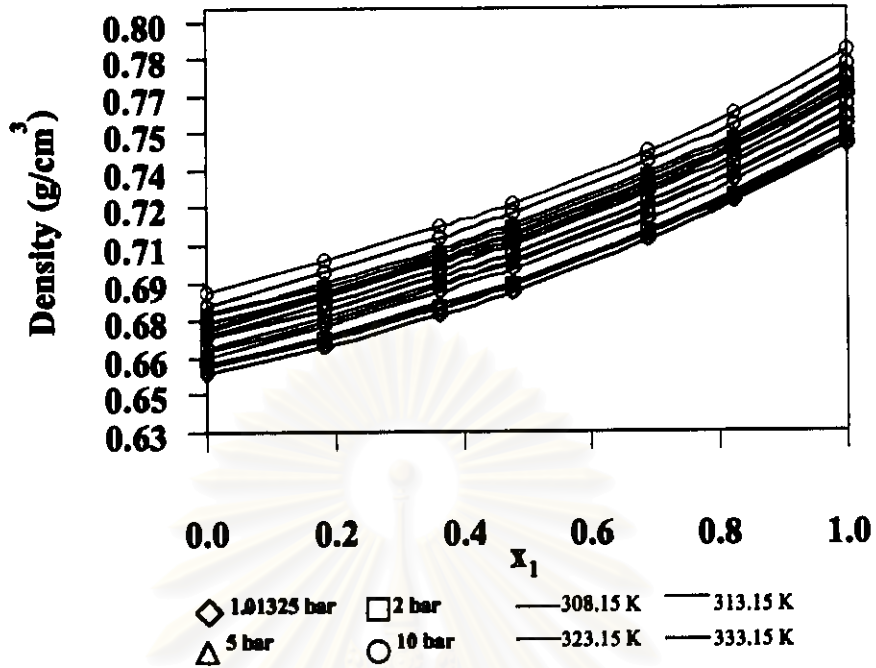
Figure 6.2 Density of cyclohexane (1) and n-heptane (2) system.
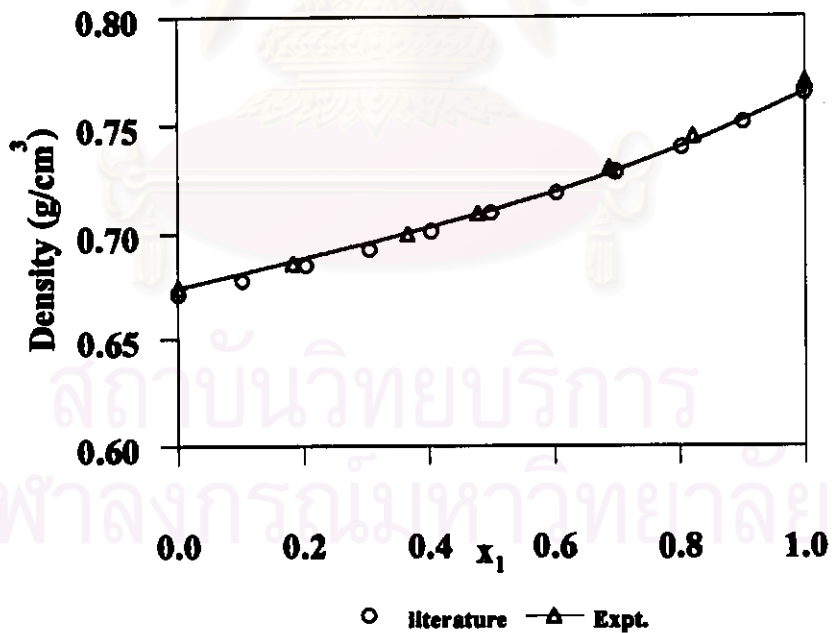

Figure 6.3 Comparison of density data between this work and literature

(Aminabhavi et al., 1996) of cyclohexane and n-heptane system

at 308.15 K.

literature values. Consequently, DMA 512P densitometer could accurately measure density values efficiently. Moreover, the results of the literature indicated that the density was a function of temperature and composition. As the temperature increased the density of the mixture decreased at atmosphere pressure and the same composition.

For benzene and n-heptane system, it indicated that density varied with temperature, pressure and composition as illustrated in Figure 6.4. When pressure increase at constant temperature and composition, the density rarely increase because low pressure rarely effects density in liquid phase. The density decrease, when temperature increase at constant pressure
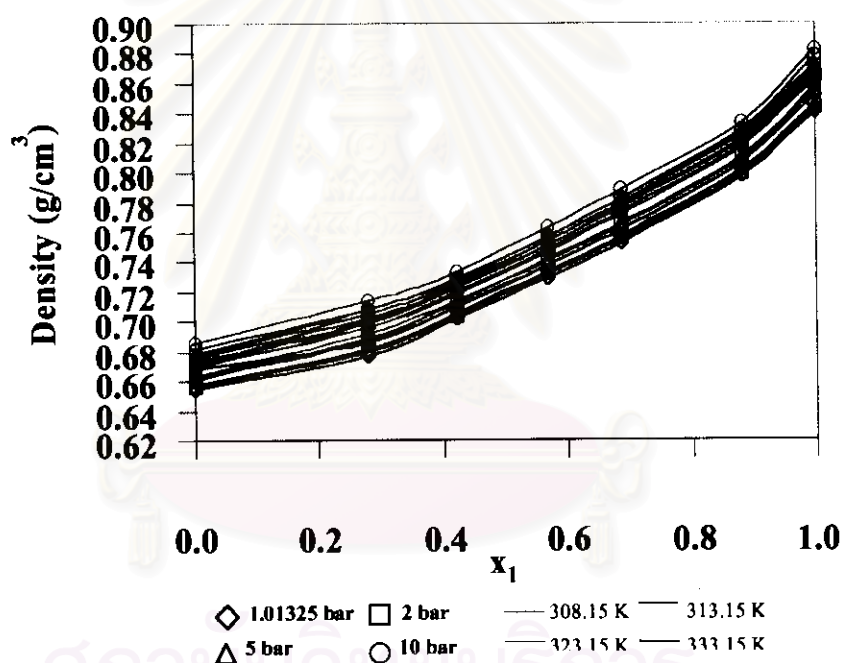

Figure 6.4 Density of benzene (1) and n-heptane (2) system.

and composition. It was found that when temperature increase, molecules in the mixture vibrate more and were far between each molecule that is the molecules attract loosely with van der waals force, thus the volume of the mixture expand or the density decreases.

The density data for ternary system of benzene, cyclohexane and n-heptane are given in Table 6.3. It was found that density varied with temperature, pressure and composition. That is the results slightly increase when pressure increase at constant temperature and composition and when temperature increase at constant pressure and composition.

Table 6.3 Experimental liquid densities of benzene (1), cyclohexane (2) and n- heptane (3).

x_1	x_2	Density (g/cm^3)			
		P = 1.01325 bar	P = 2 bar	P = 5 bar	P = 10 bar
T = 308.15 K					
1.0000	0.0000	0.86648	0.86960	0.87204	0.88220
0.0000	1.0000	0.76955	0.77203	0.77381	0.78276
0.0000	0.0000	0.67445	0.67665	0.67813	0.68588
0.2368	0.1774	0.71583	0.71887	0.72050	0.72590
0.2073	0.3413	0.72696	0.72973	0.73157	0.73702
0.2024	0.5063	0.74331	0.74614	0.74809	0.75355
0.1979	0.6526	0.75966	0.76239	0.76466	0.77030
0.3787	0.1792	0.73796	0.74085	0.74294	0.74798
0.3655	0.3361	0.75419	0.75690	0.75862	0.76418
0.3823	0.4742	0.77359	0.77645	0.77806	0.78391
0.5363	0.1391	0.76226	0.76569	0.76776	0.77331
0.5613	0.2956	0.78822	0.79102	0.79312	0.79890
0.6458	0.1980	0.79469	0.79811	0.80003	0.80557

Table 6.3 Experimental liquid densities of benzene (1), cyclohexane (2) and n-heptane (3), (continued).

x_1	x_2	Density (g/cm^3)			
		P = 1.03125 bar	P = 2 bar	P = 5 bar	P = 10 bar
T = 313.15 K					
1.0000	0.0000	0.86138	0.86436	0.86654	0.87759
0.0000	1.0000	0.76468	0.76687	0.76808	0.77775
0.0000	0.0000	0.66862	0.67056	0.67161	0.68066
0.2368	0.1774	0.71239	0.71451	0.71548	0.72046
0.2073	0.3413	0.72344	0.72565	0.72697	0.73218
0.2024	0.5063	0.73976	0.74200	0.74381	0.74872
0.1979	0.6526	0.75570	0.75828	0.75947	0.76478
0.3787	0.1792	0.73385	0.73669	0.73771	0.74291
0.3655	0.3361	0.75180	0.75227	0.75353	0.75849
0.3823	0.4742	0.76819	0.77176	0.77320	0.77852
0.5363	0.1391	0.75871	0.76111	0.76225	0.76802
0.5613	0.2956	0.78440	0.78677	0.78810	0.79352
0.6458	0.1980	0.79092	0.79334	0.79443	0.79980
T = 323.15 K					
1.0000	0.0000	0.85101	0.85381	0.85554	0.86823
0.0000	1.0000	0.75303	0.75593	0.75734	0.76807
0.0000	0.0000	0.66002	0.66232	0.66386	0.67345
0.2368	0.1774	0.70221	0.70504	0.70645	0.71137
0.2073	0.3413	0.71356	0.71612	0.71764	0.72237
0.2024	0.5063	0.72944	0.73190	0.73376	0.73896
0.1979	0.6526	0.74478	0.74763	0.74951	0.75461
0.3787	0.1792	0.72388	0.72654	0.72791	0.73346
0.3655	0.3361	0.73935	0.74195	0.74355	0.74885
0.3823	0.4742	0.75862	0.76137	0.76276	0.76810
0.5363	0.1391	0.74791	0.75068	0.75216	0.75736
0.5613	0.2956	0.77378	0.77636	0.77792	0.78294
0.6458	0.1980	0.77934	0.78242	0.78404	0.78948

Table 6.3 Experimental liquid densities of benzene (1), cyclohexane (2) and n-heptane (3), (continued).

x_1	x_2	Density (g/cm^3)			
		P = 1.03125 bar	P = 2 bar	P = 5 bar	P = 10 bar
T = 333.15 K					
1.0000	0.0000	0.84045	0.84318	0.84454	0.85867
0.0000	1.0000	0.74479	0.74738	0.74880	0.76141
0.0000	0.0000	0.65369	0.65607	0.65705	0.66763
0.2368	0.1774	0.69407	0.69632	0.69761	0.70232
0.2073	0.3413	0.70482	0.70711	0.70869	0.71328
0.2024	0.5063	0.72069	0.72331	0.72454	0.72954
0.1979	0.6526	0.73594	0.73878	0.74027	0.74597
0.3787	0.1792	0.71535	0.71780	0.71929	0.72433
0.3655	0.3361	0.72991	0.73277	0.73495	0.73956
0.3823	0.4742	0.74911	0.75196	0.75313	0.75850
0.5363	0.1391	0.73738	0.74074	0.74259	0.74787
0.5613	0.2956	0.76222	0.76600	0.76753	0.77288
0.6458	0.1980	0.76973	0.77301	0.77437	0.77965

6.2 Excess Molar Volumes for Binary systems and Ternary System.

From relation between density and volume, equation (3.1), the molar volume of the mixtures was calculated as

$$V_{mix} = \sum_{i}^{c} \frac{x_i MW_i}{\rho} \qquad (6.1)$$

where x_i is the mole fraction of component 'i' in the mixtures, MW_i, its molecular mass and ρ, the measured density of the mixtures.

The molar volumes of the ternary system and their binary systems are functions of mole fraction at various states. The results indicate that, with increase in temperature or decrease in pressure, the molar volumes increase.

Excess molar volumes (V^E) were calculated from molar density or molar volume. The calculated V^E results of benzene and cyclohexane, cyclohexane and n-heptane and, benzene and n-heptane systems are presented in Figure 6.5-6.28. For three binary systems, excess molar volumes were calculated by using the equation as follow:

$$V^E = V_{mix} - (x_1 V_1 - x_2 V_2) \qquad (6.2)$$

where V_{mix} is the molar volume of binary mixture and V_1 and V_2 are the molar volume of the first and the second pure component respectively. The excess molar volumes of the binary mixtures versus mole fraction are positive over the whole composition range. In addition, the results indicated that the three binary systems behaved as nonideal solution.

Figure 6.29-6.34 presented excess molar volumes of previous literatures. Studying of previous literatures, it appears that the V^E of Chevalier et al., 1990; Dimitri et al., 1991; Aminabhavi et al., 1996; Anwel et al., 1992 (for benzene and n-heptane system) and Thomas et al., 1989 are positive over the whole composition range except V^E of Anwel et al., 1992 for benzene and cyclohexane system and of Stefanos et al., 1989 for benzene and n-heptane system are both negative and positive as shown in Figure 6.30 and 6.32 respectively. In Figure 6.34, the V^E results of cyclohexane and n-heptane system at 308.15 K and 1.01325

bar of this work are compared with literature of Aminabhavi et al., 1996. The experimental curve is in excellent agreement with that of literature. However, excess molar volumes of this work are slightly greater than these of the literature; but determination of percent deviation with respect to molar volume of the mixture of this work was about 0.34 %.
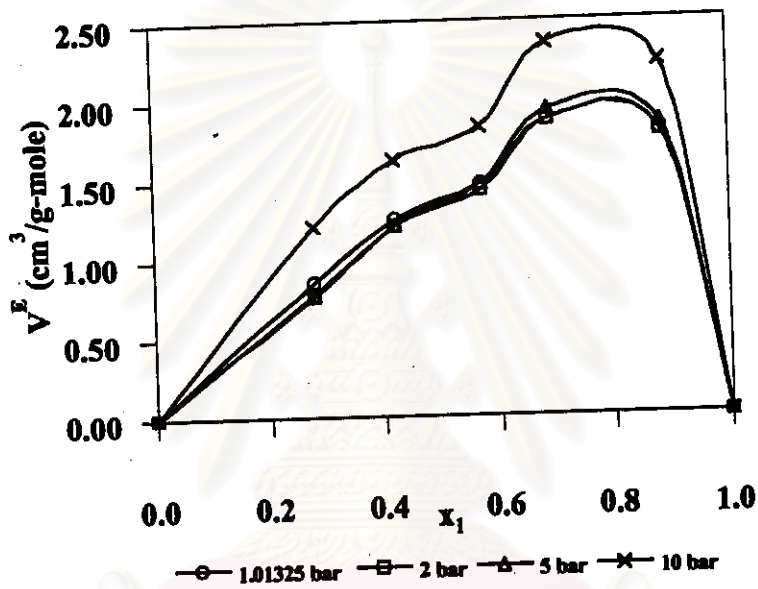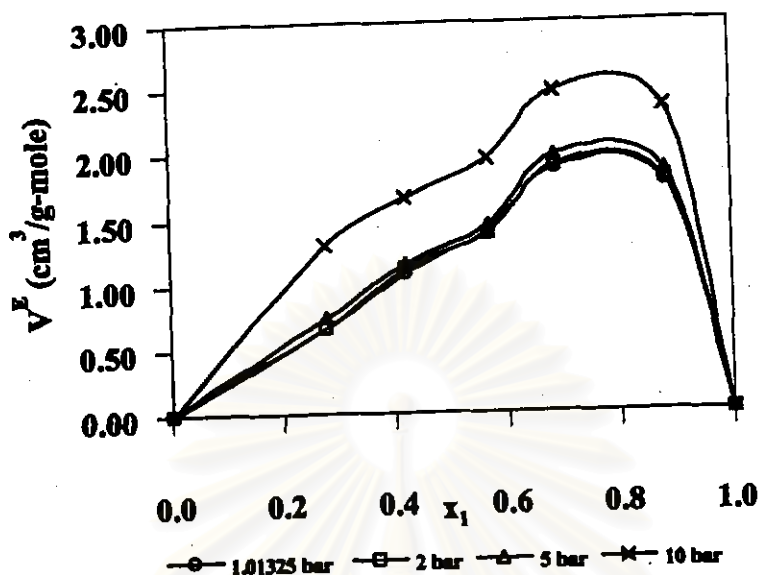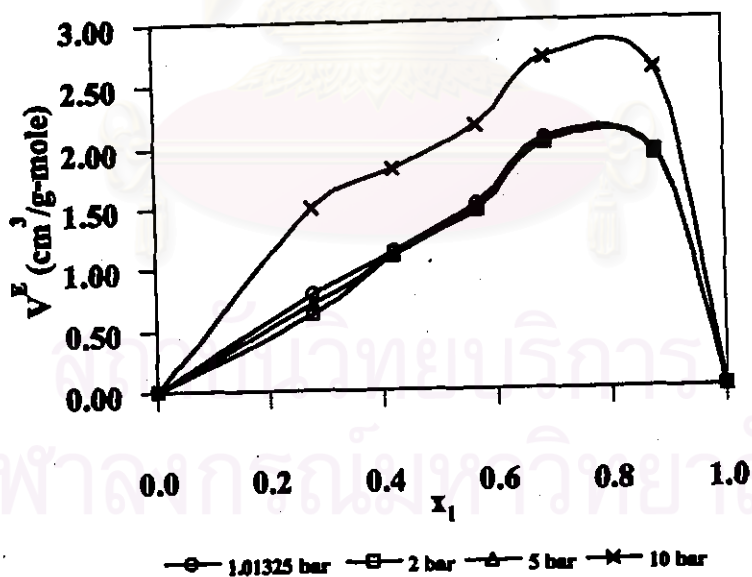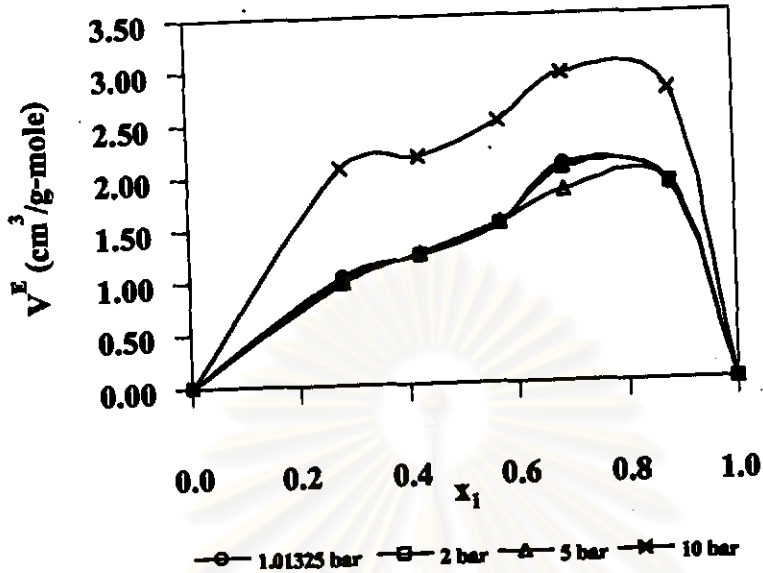

Figure 6.5 Excess molar volumes of benzene (1) and cyclohexane (2) system at 308.15 K.

Figure 6.6 Excess molar volumes of benzene (1) and cyclohexane (2) system at 313.15 K.

Figure 6.7 Excess molar volumes of benzene (1) and cyclohexane (2) system at 323.15 K.

Figure 6.8 Excess molar volumes of benzene (1) and cyclohexane (2) system at 333.15 K.
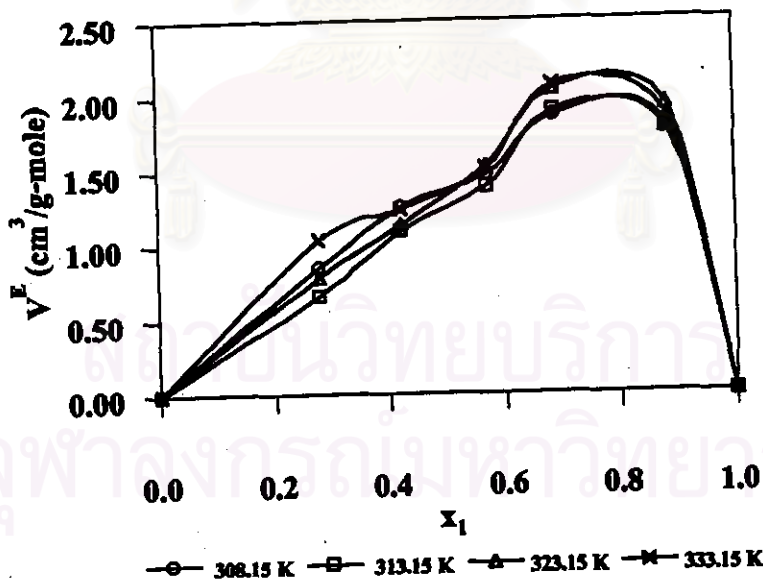

Figure 6.9 Excess molar volumes of benzene(1) and cyclohexane(2) system at 1.01325 bar.
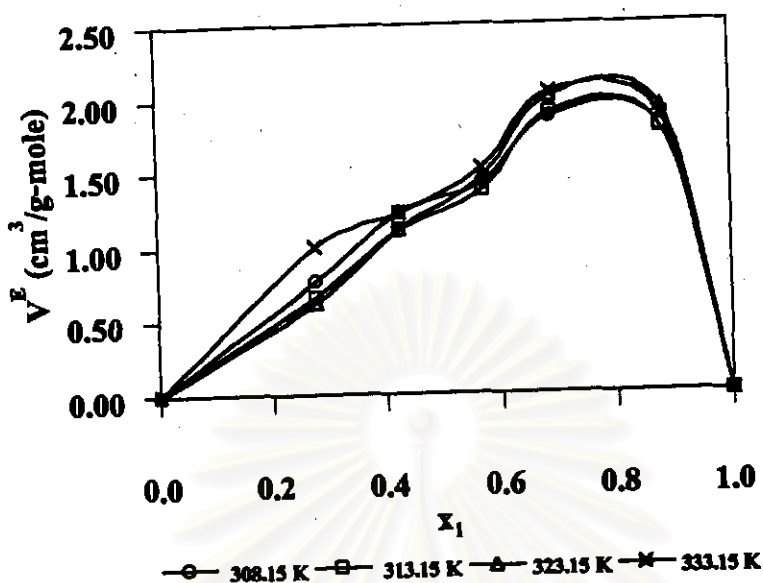
Figure 6.10 Excess molar volumes of benzene (1) and cyclohexane (2) system at 2 bar.
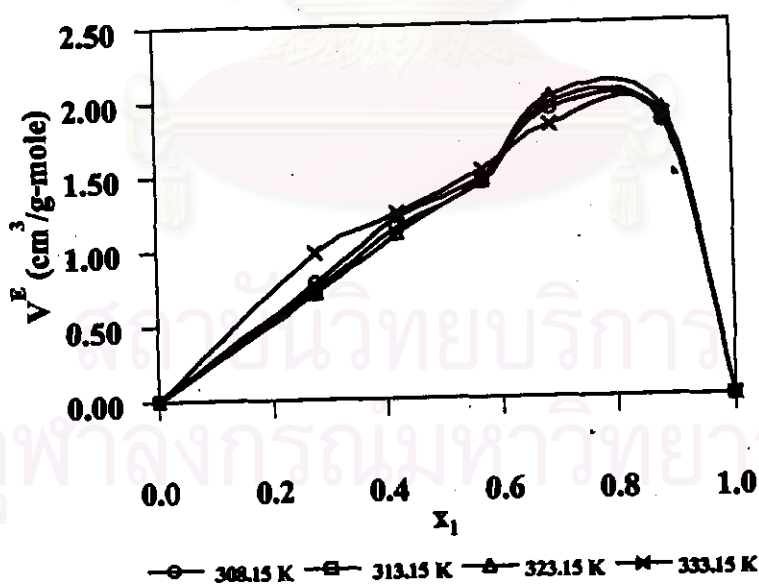

Figure 6.11 Excess molar volumes of benzene (1) and cyclohexane (2) system at 5 bar.
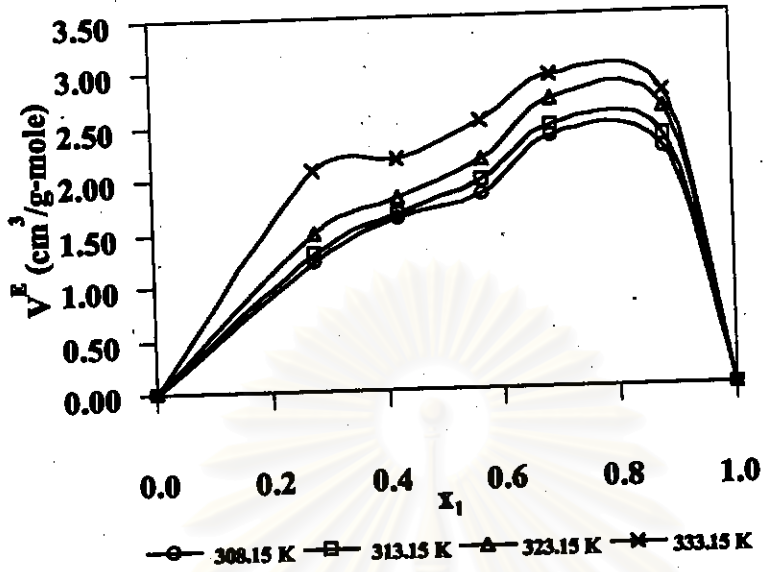
Figure 6.12 Excess molar volumes of benzene (1) and cyclohexane (2) system at 10 bar.
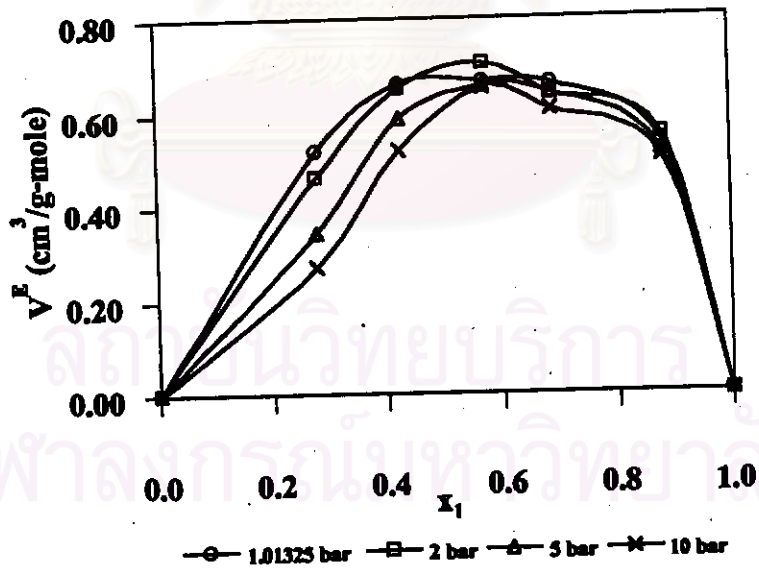

Figure 6.13 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 308.15 K.
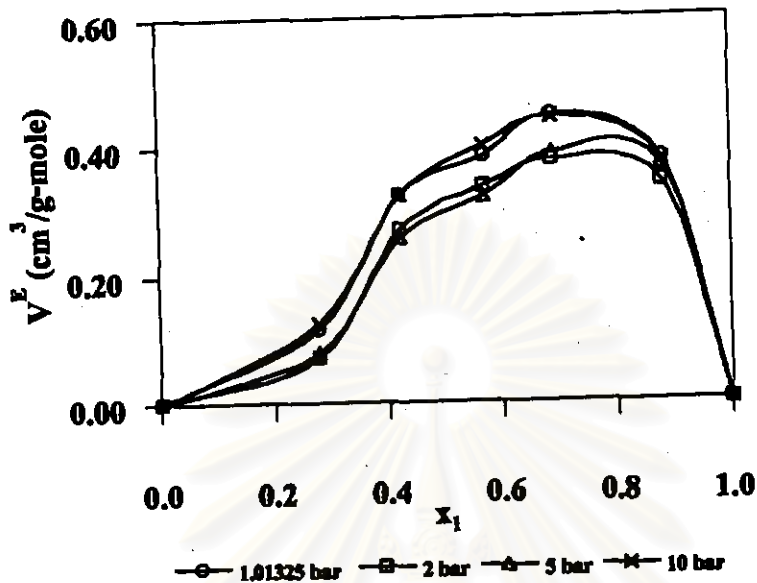
Figure 6.14 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 313.15 K.
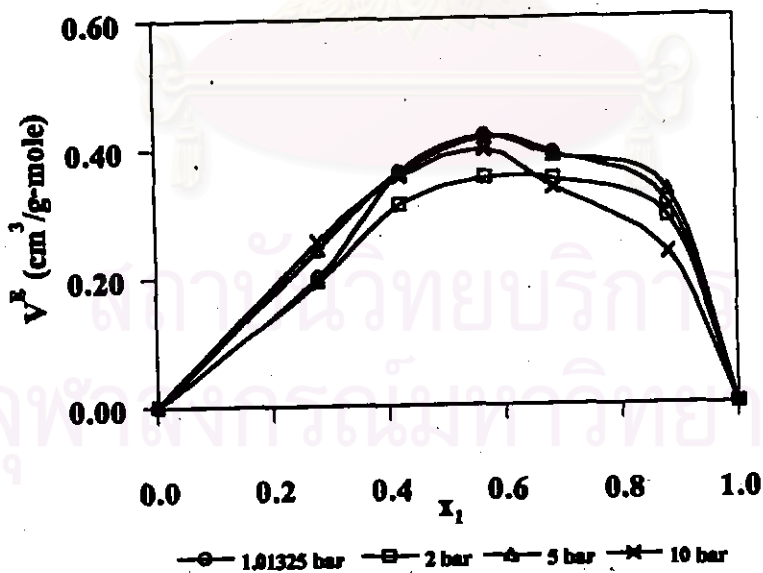

Figure 6.15 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 323.15 K.
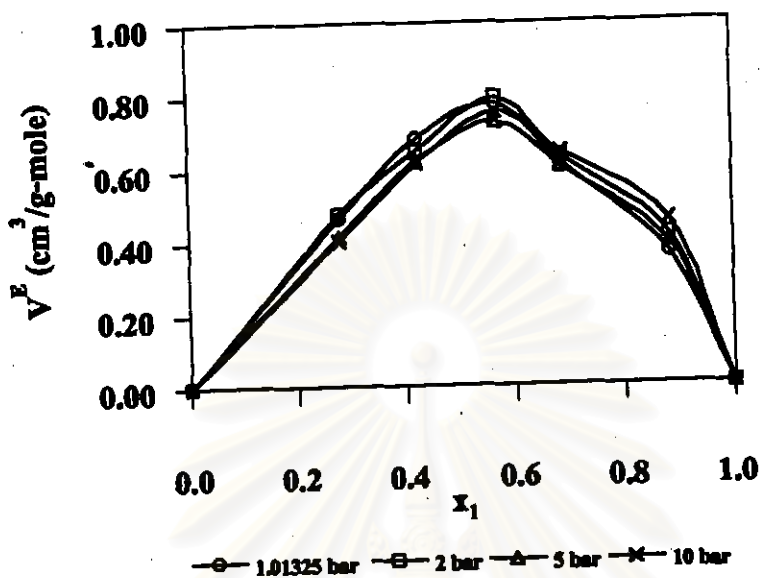
Figure 6.16 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 333.15 K.

Figure 6.17 Excess molar volumes of cyclohexane (1) and n-heptane (2) system
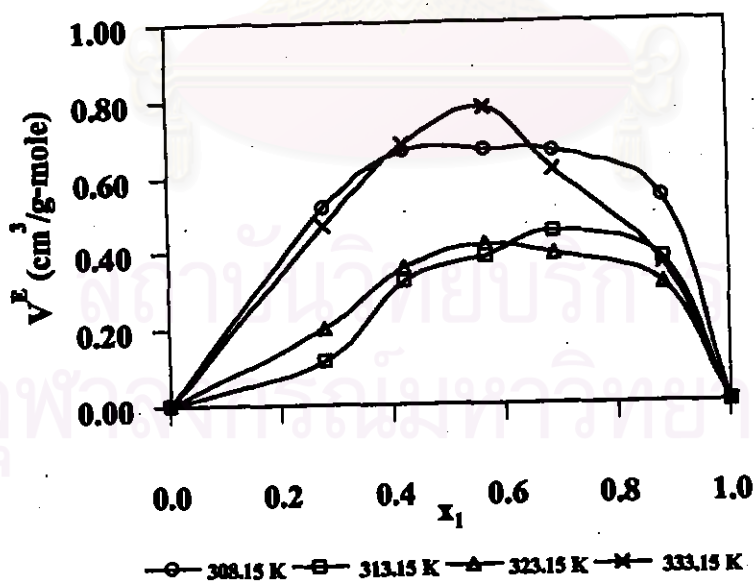
at 1.01325 bar.

Figure 6.18 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 2 bar.

Figure 6.19 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 5 bar.

Figure 6.20 Excess molar volumes of cyclohexane (1) and n-heptane (2) system at 10 bar.
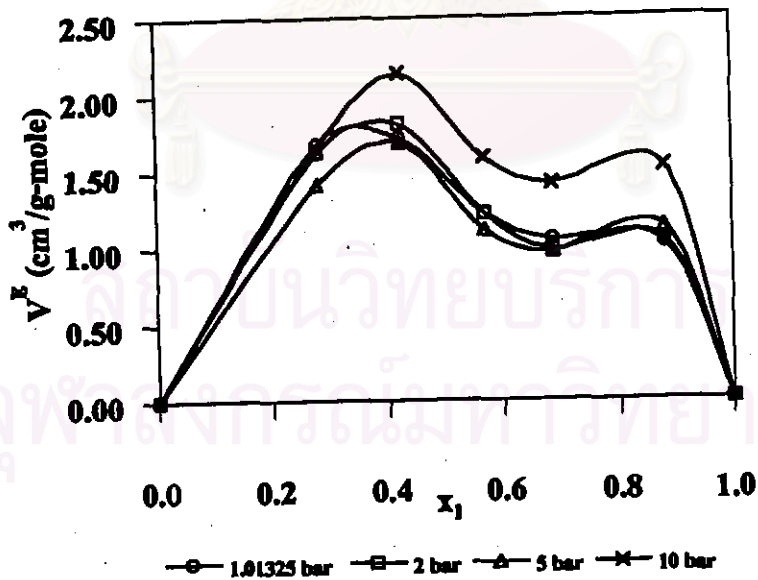
Figure 6.21 Excess molar volumes of benzene (1) and n-heptane (2) system at 308.15 K.
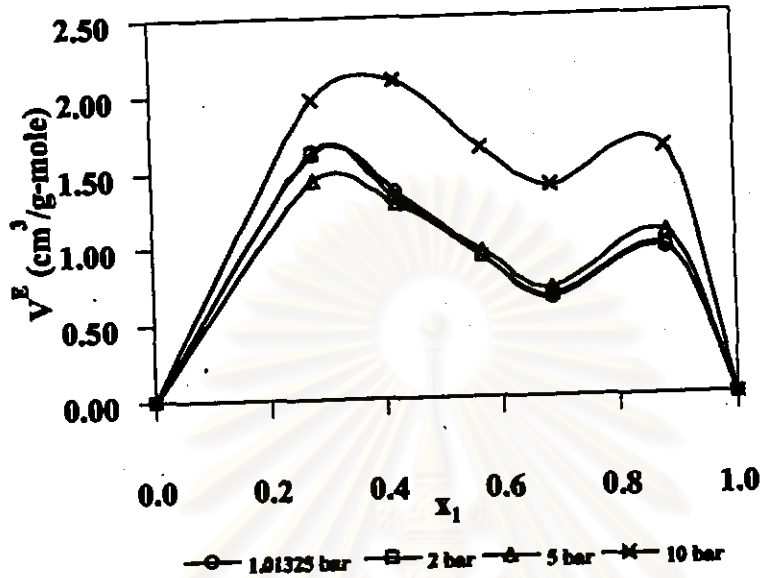
Figure 6.22 Excess molar volumes of benzene (1) and n-heptane (2) system at 313.15 K.
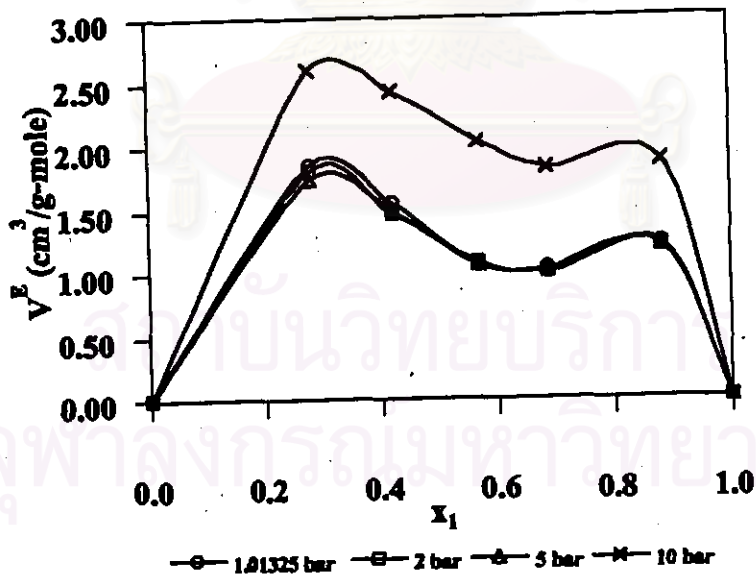
Figure 6.23 Excess molar volumes of benzene (1) and n-heptane (2) system at 323.15 K.
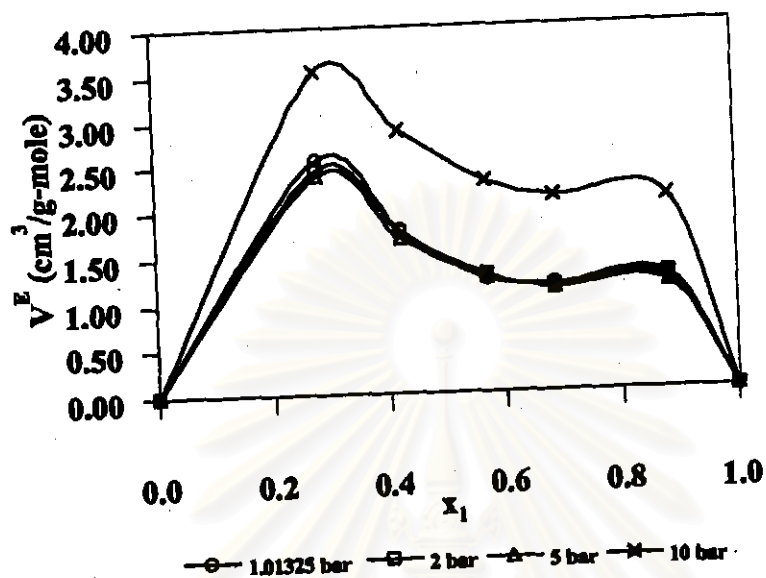
Figure 6.24 Excess molar volumes of benzene (1) and n-heptane (2) system at 333.15 K.
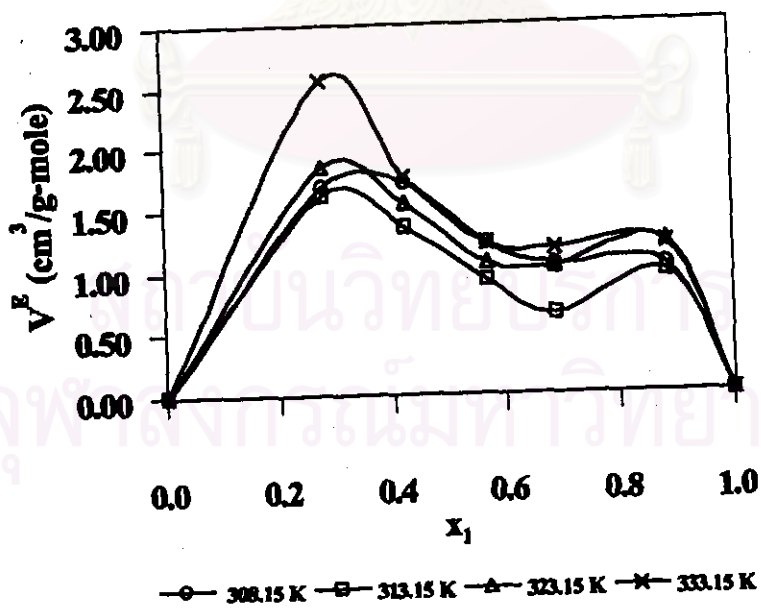
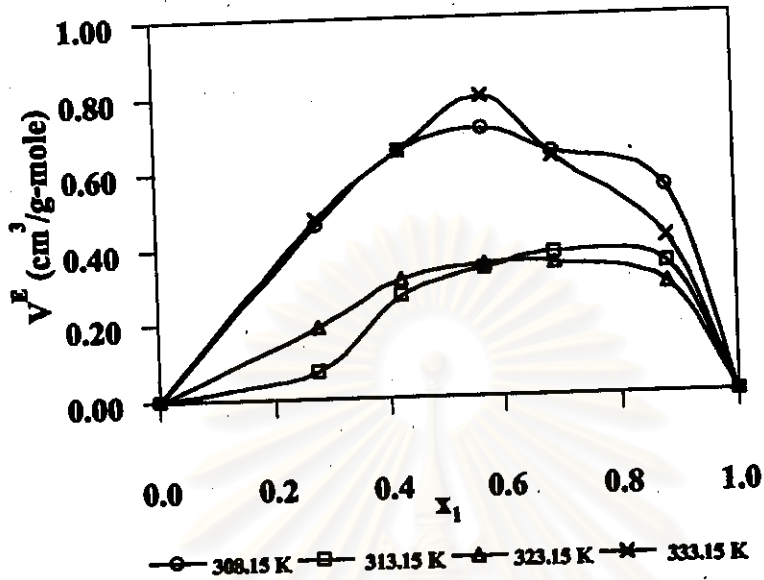Figure 6.25 Excess molar volumes of benzene (1) and n-heptane (2) system at 1.01325 bar.
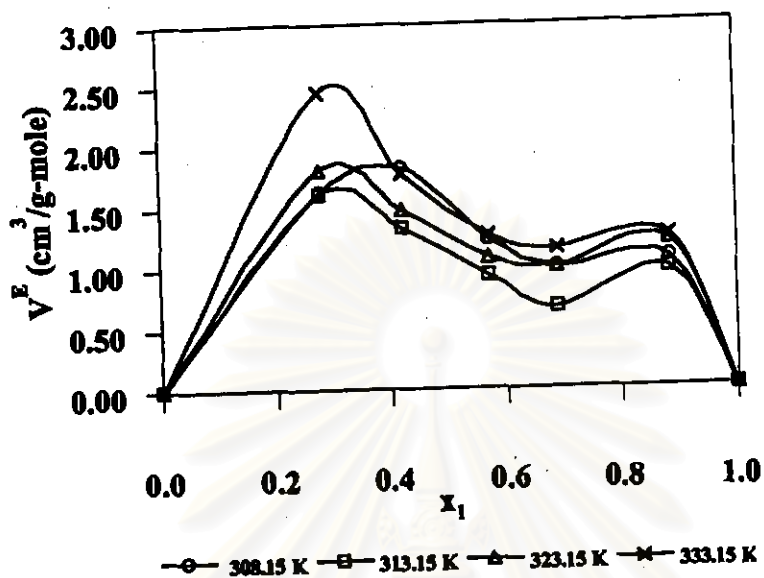
Figure 6.26 Excess molar volumes of benzene (1) and n-heptane (2) system at 2 bar.

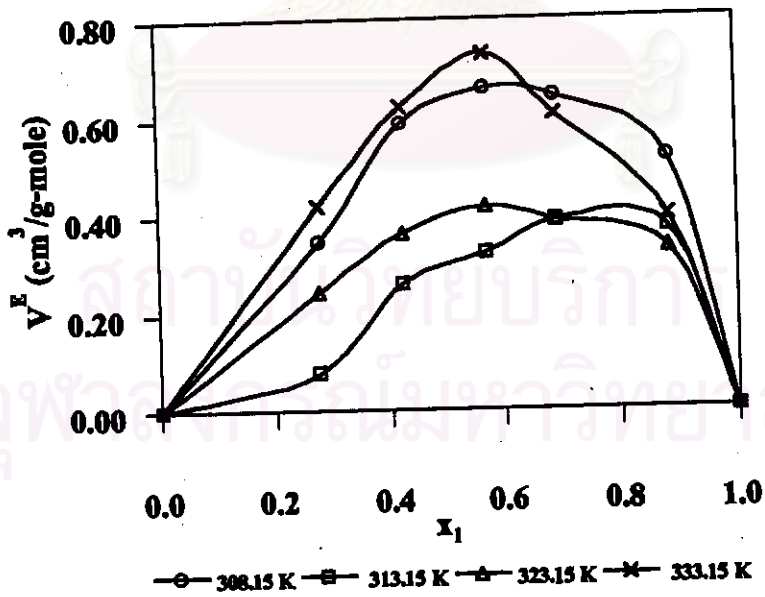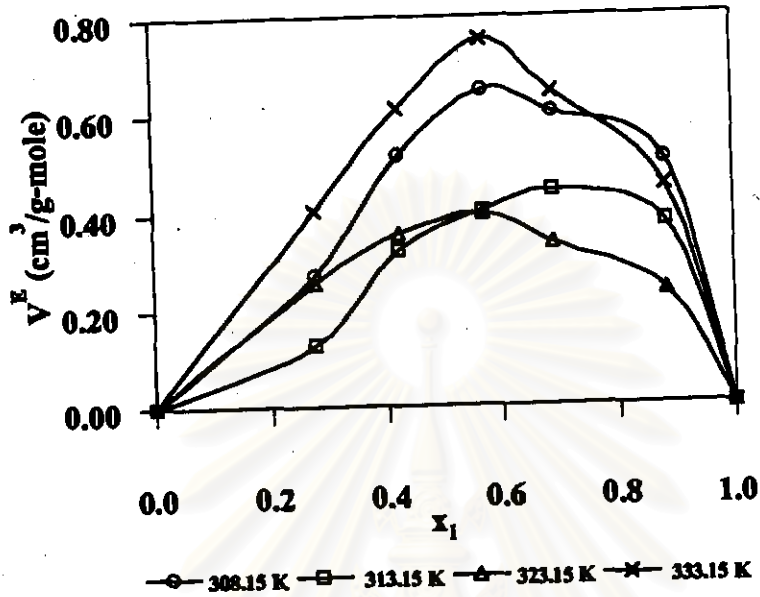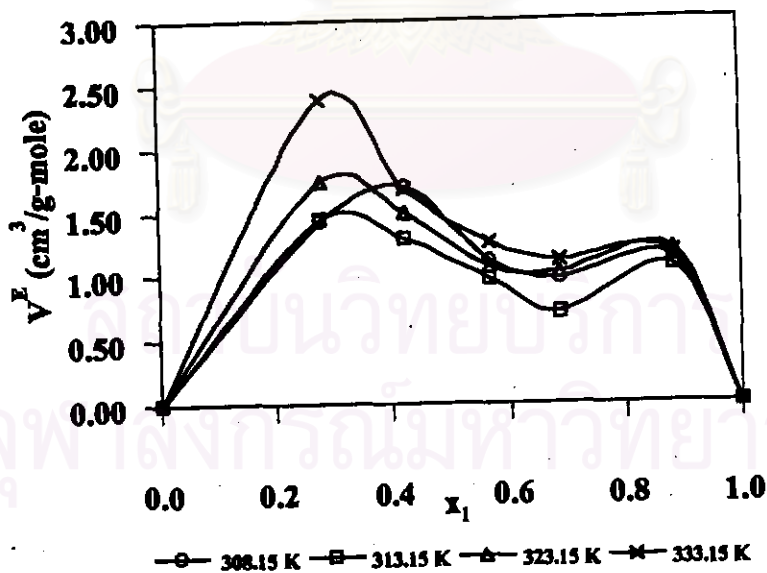Figure 6.27 Excess molar volumes of benzene (1) and n-heptane (2) system at 5 bar.
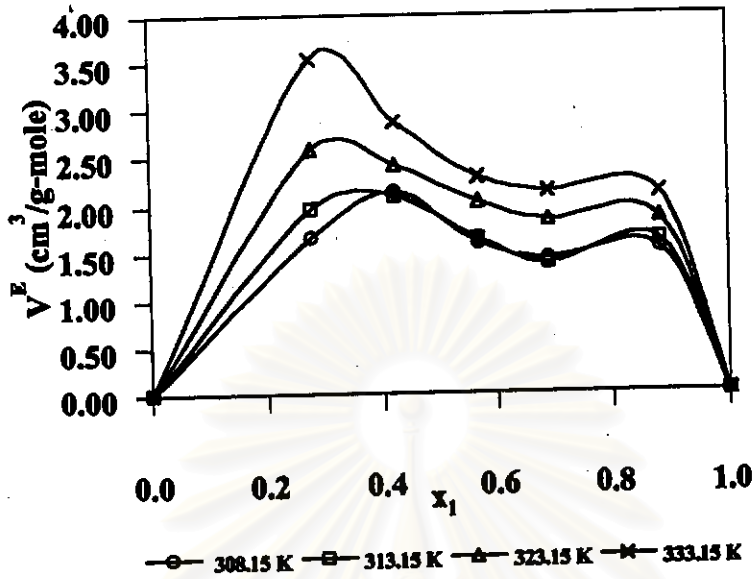
Figure 6.28 Excess molar volumes of benzene (1) and n-heptane (2) system at 10 bar.
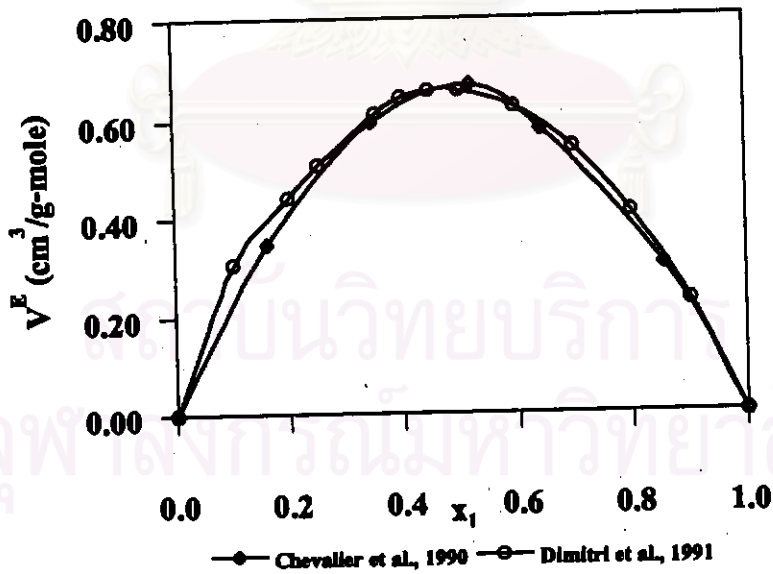
Figure 6.29 Excess molar volumes of benzene (1) and cyclohexane (2) at 298.15 K

and 1.01325 bar, (Dimitri et al., 1991 and Chevalier et al., 1990).
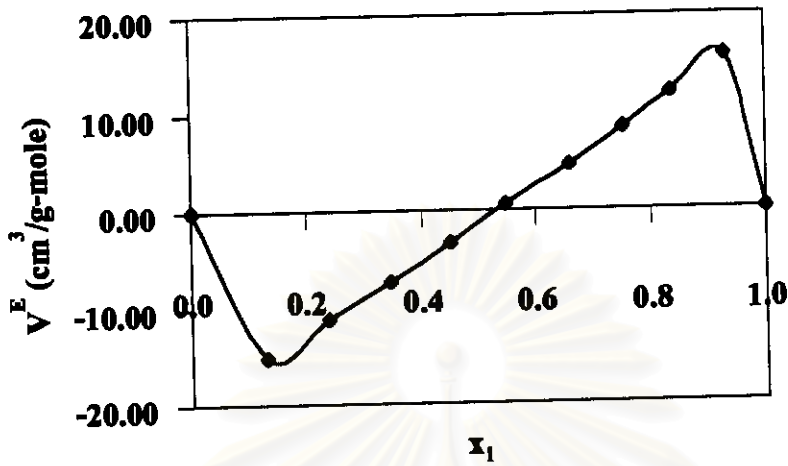
Figure 6.30 Excess molar volumes of benzene (1) and cyclohexane (2) at 293.15 K
and 1.01325 bar, (Anwel et al., 1992).
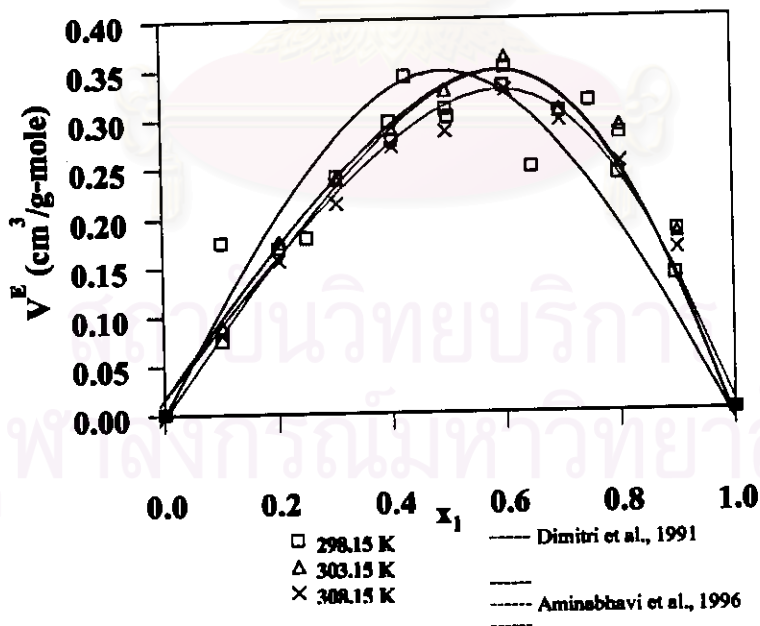
Figure 6.31 Excess molar volumes of cyclohexane (1) and n-heptane (2) at 1.01325
bar, (Dimitri et al., 1991 and Aminabhavi et al., 1996).
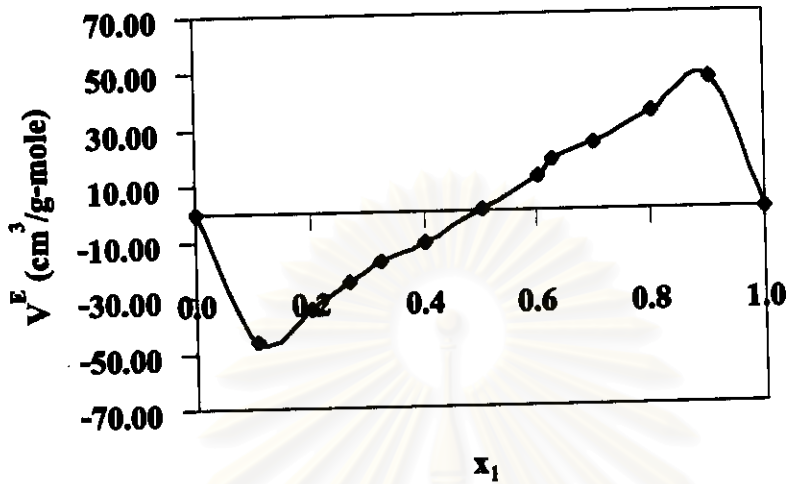
Figure 6.32 Excess molar volumes of benzene (1) and n-heptane (2) system at 298.15 K and 1.01325 bar, (Stefanos et al., 1989).

---- □ Anwel et al., 1992 at 293.15 K
---- X Thomas et al., (1989) at 297.85 K
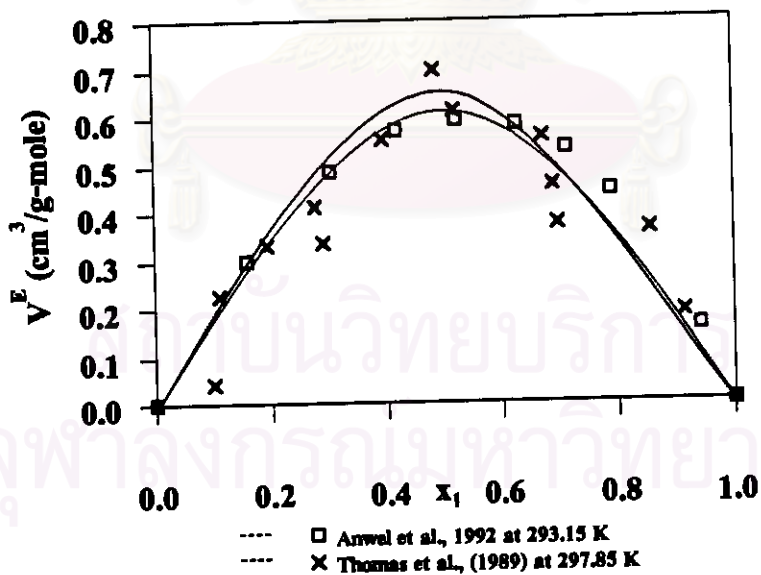
Figure 6.33 Excess molar volumes of benzene (1) and n-heptane (2) system at 1.01325 bar, (Anwel et al., 1992 and Thomas et al., 1989).
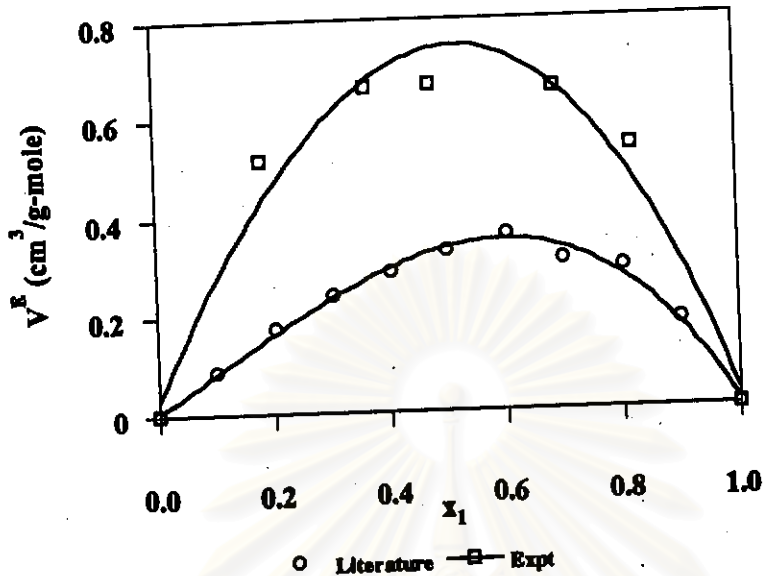
Figure 6.34 Comparison between experimental and literature (Aminabhavi et al., 1996) excess molar volume values of the cyclohexane and n-heptane system at 308.15 K and 1.01325 bar.

For ternary system, excess molar volumes were calculated by using the following equation.

$$V^E = V_{mix} - (x_1 V_1 - x_2 V_2 - x_3 V_3) \qquad (6.3)$$

where V_{mix} is the molar volume of mixture and V_1, V_2 and V_3 are the molar volume of benzene, cyclohexane and n-heptane respectively. Isothermal excess molar volumes of the ternary system as determined via equation 6.3 are shown in Table 6.4. Excess molar volumes are positive over the entire range of composition. The results indicated that the ternary system exhibited nonideal solution because ideal solution must presented molar volume of mixture equal sum of molar volume of pure components ($V^E = 0$) as shown in equation 6.3.

Table 6.4 Excess molar volumes of benzene (1), cyclohexane (2) and n-heptane (3) system.

x_1	x_2	$V^E(cm^3/g\text{-mole})$			
		1.01325 bar	2 bar	5 bar	10 bar
T = 308.15 K					
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2368	0.1774	0.9175	0.7952	0.7986	1.2903
0.2073	0.3413	0.9292	0.8635	0.8364	1.3171
0.2024	0.5063	0.9689	0.9059	0.8718	1.3480
0.1979	0.6526	0.9464	0.9095	0.8388	1.2868
0.3786	0.1792	1.1302	1.0589	1.0041	1.5489
0.3654	0.3361	0.9641	0.9328	0.9456	1.4070
0.3823	0.4742	1.1352	1.0941	1.1312	1.5477
0.5363	0.1391	1.2002	1.0732	1.0445	1.5076
0.5613	0.2956	1.1895	1.1710	1.1545	1.5823
0.6458	0.1980	1.0652	0.9728	0.9864	1.4481
T = 313.15 K					
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2368	0.1774	0.5302	0.5303	0.5768	1.3593
0.2073	0.3413	0.5995	0.5878	0.5738	1.2871
0.2024	0.5063	0.6965	0.6876	0.6019	1.3268
0.1979	0.6526	0.7814	0.7289	0.7452	1.3751
0.3786	0.1792	0.9057	0.8047	0.8581	1.5650
0.3654	0.3361	0.5140	0.7912	0.8093	1.5213
0.3823	0.4742	1.1796	1.0037	1.0030	1.6239
0.5363	0.1391	0.9253	0.9194	0.9720	1.5653
0.5613	0.2956	1.0119	1.0233	1.0573	1.6611
0.6458	0.1980	0.8767	0.8894	0.9638	1.5768

Table 6.7 Excess molar volumes of benzene (1), cyclohexane (2) and n-heptane (3) system (continued).

x_1	x_2	V^E (cm^3/g-mole)			
		1.01325 bar	2 bar	5 bar	10 bar
T = 323.15 K					
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2368	0.1774	0.6973	0.6269	0.6522	1.6008
0.2073	0.3413	0.6332	0.6283	0.6291	1.5833
0.2024	0.5063	0.7174	0.7453	0.6865	1.5285
0.1979	0.6526	0.8158	0.7971	0.7350	1.5639
0.3786	0.1792	0.9884	0.9624	0.9943	1.8032
0.3654	0.3361	0.8978	0.8982	0.8886	1.7140
0.3823	0.4742	1.0514	1.0448	1.0628	1.8505
0.5363	0.1391	1.1011	1.0684	1.0846	1.9277
0.5613	0.2956	1.0622	1.0766	1.0774	1.9083
0.6458	0.1980	1.0757	1.0193	1.0161	1.7935
T = 333.15 K					
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2368	0.1774	0.8823	0.9199	0.8819	2.1025
0.2073	0.3413	0.8751	0.9079	0.8303	2.0534
0.2024	0.5063	0.8879	0.8687	0.8678	1.9935
0.1979	0.6526	0.9376	0.8899	0.8603	1.8564
0.3786	0.1792	1.1456	1.1511	1.0898	2.2075
0.3654	0.3361	1.1393	1.0830	0.9262	2.0936
0.3823	0.4742	1.2214	1.1762	1.1933	2.2136
0.5363	0.1391	1.4778	1.3444	1.2384	2.2792
0.5613	0.2956	1.4670	1.2935	1.2568	2.2580
0.6458	0.1980	1.1823	1.0848	1.0710	2.0760

6.3 Density of Benzene, Cyclohexane and n-Heptane System by Equation of State.

This section consists of two parts. First, prediction of binary systems and second, prediction of ternary systems.

6.3.1 Prediction of Binary Systems

The main program involves determination of interaction parameters of benzene and cyclohexane, cyclohexane and n-heptane, and benzene and n-heptane systems. Experimental density data were used in form of molar volumes (cm^3/g-mole) for program computer which was described in chapter 5. All optimum interaction parameters can be determined by golden section search method which minimizes the objective function as follows:

$$OBF = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{V_{cal}[i] - V_{expt}[i]}{V_{expt}[i]}\right| \qquad (6.3)$$

A range of these parameters of -0.1-0.6 was chosen in searching procedure. The determinated interaction parameters of three binary systems are present in Table 6.5.

Table 6.5 Interaction parameters.

Systems	T (K)	Equations of state			
		PR	PRSV	PRSV2	MRK
Benzene-cyclohexane	308.15	0.3401	0.3529	0.3520	0.2563
	313.15	0.3298	0.3415	0.3403	0.2483
	323.15	0.3222	0.3320	0.3306	0.2427
	333.15	0.3079	0.3157	0.3143	0.2236
Cyclohexane-n-heptane	308.15	0.0722	0.0825	0.0803	-0.0277
	313.15	0.0676	0.0771	0.0748	-0.0332
	323.15	0.0686	0.0761	0.0740	-0.0367
	333.15	0.0703	0.0761	0.0741	-0.0391
Benzene-n-heptane	308.15	0.0421	0.0532	0.0507	-0.0617
	313.15	0.0396	0.0499	0.0475	-0.0682
	323.15	0.0527	0.0610	0.0587	-0.0635
	333.15	0.0515	0.0587	0.05545	-0.0576

The parameters were found to be dependent on system temperature. The equations studied are Modified Redlich-Kwong (MRK), Peng-Robinson (PR), Peng-Robinson-Stryjek-Vera (PRSV) and Peng-Robinson-Stryjek-Vera2 (PRSV2).

According to studying of interaction parameters, it was found that they depended on temperature. For benzene and cyclohexane system, Figure 6.35 shows that as temperature increase, the parameters decrease. The positive parameters of the system exhibit strong forces which appear between unlike molecules. Value of the parameter of each equation is different from one another, because it depends on characteristic of the equation.

Figure 6.35 Interaction parameters of benzene and cyclohexane system.

For cyclohexane and n-heptane system, interaction parameters slightly varied with temperature like benzene and cyclohexane system of all equations of state as shown in Figure 6.36. The parameters presented interaction of molecule between cyclohexane and n-heptane. Moreover, value of the parameter of each equation is different from one another, because it depends on characteristic of the equation.

Figure 6.36 Interaction parameters of cyclohexane and n-heptane system in this work

and a previous literature of Aminabhavi et al., 1996.

However, it was found that interaction parameters of cyclohexane and n-heptane system for a previous literature (Aminabhavi et al., 1996) are different from the results of this work as presented in Figure 6.36. The parameters of the literature slightly increase with temperature at 1.01325 bar. It may be that the literature determined only three points, insufficient for conclusive results.

But in benzene and n-heptane system, interaction parameters by MRK, PR, PRSV and PRSV2 equations of state tend to increase with temperature increases as presented in Figure 6.37. The cause of these results due to different molecule size and shape of n-heptane (chain molecule) which might have effect on interaction with benzene molecule. The PR, PRSV and PRSV2 equations of state obtained positive parameter; but for the MRK equation of state obtained the negative parameters. Value of the parameter of each equation is different from one another, because it depends on characteristic of the equation.

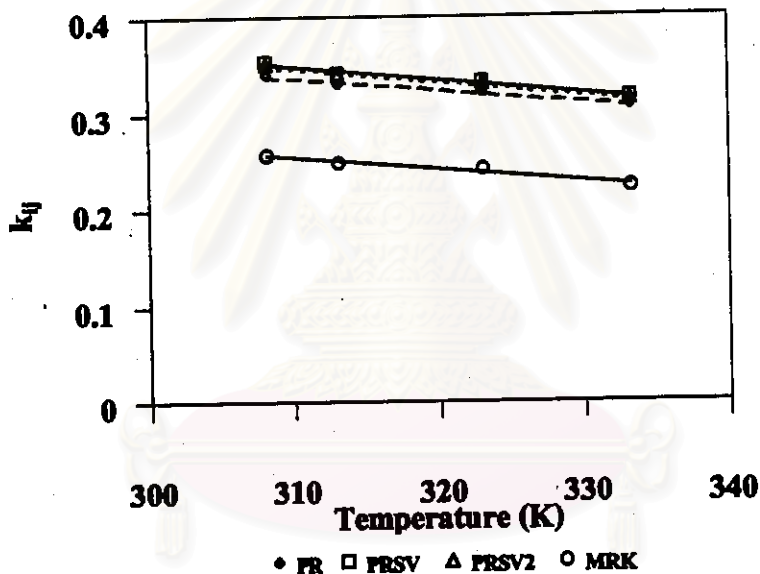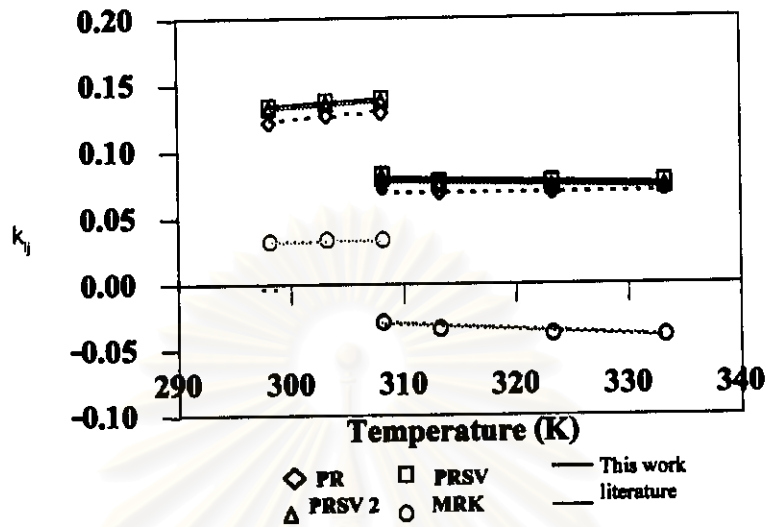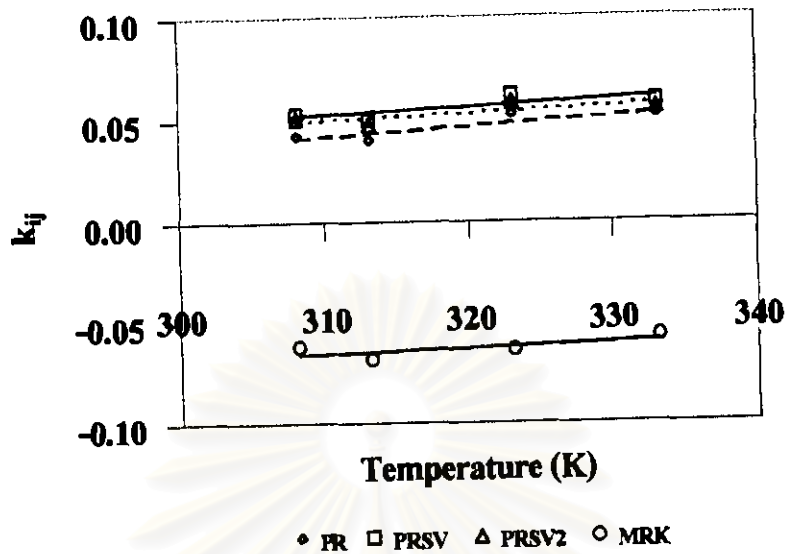Figure 6.37 Interaction parameters of benzene and n-heptane system.

In addition, the binary parameters of the benzene and cyclohexane system are higher than the system of cyclohexane and n-heptane and of benzene and n-heptane respectively for all equations of state. The results indicated that the system of benzene and cyclohexane exhibit strong interaction between unlike molecules more than the system of cyclohexane and n-heptane and of benzene and n-heptane respectively.

Furthermore, this work also determined interaction parameters base on data in literature as shown in Table 6.6. The results of the three binary systems agreed with the results of this work that each the binary system obtained only one interaction parameter by each equation of state and the system of benzene and cyclohexane exhibit strong interaction between unlike molecules more than the system of cyclohexane and n-heptane and of benzene and n-heptane respectively.

Table 6.6 Interaction parameters of benzene, cyclohexane and n-heptane systems in literatures.

Systems	T (K)	PR EOS	PRSV EOS	PRSV2 EOS	MRK EOS	References
Benzene-cyclohexane	293.15	0.3688	0.3889	0.3890	0.2612	Anwel et al. (1992)
	298.15	0.3601	0.3745	0.3741	0.2717	Dimitri et al. (1991)
	298.15	0.3288	0.3439	0.3436	0.2444	Chevalier et al. (1990)
Cyclohexane-n-heptane	298.15	0.1674	0.1796	0.1783	0.0783	Dimitri et al. (1991)
	298.15	0.1218	0.1337	0.1320	0.0323	Aminabhavi et al. (1996)
	303.15	0.1272	0.1380	0.1363	0.0346	Aminabhavi et al. (1996)
	308.15	0.1290	0.1389	0.1369	0.0336	Aminabhavi et al. (1996)
Benzene-n-heptane	293.15	0.0245	0.0385	0.0372	-0.0605	Anwel et al. (1992)
	297.85	0.0437	0.0567	0.0549	-0.0454	Thomas et al (1989)
	298.15	0.0044	0.0183	0.0169	-0.0856	Stefanos et al. (1989)

When interaction parameter of each binary systems was determinated, it can be used to predict molar volumes of each system by equations of state. In Tables 6.7-6.9, results of percentage average absolute deviation (% AAD) of the binary systems are given. The % AAD is used in evaluating models of equation of state; the smaller the deviation, the better the equation of state. The % AAD equation is defined as

$$\% \, AAD = \frac{100}{N} \sum_{i=1}^{N} \left| \frac{V_{cal} - V_{expt}}{V_{expt}} \right| \tag{6.4}$$

For benzene and cyclohexane system, comparing between the calculated molar-volumes by cubic equations of state and experimental molar volumes for the system as shown in Figure 6.38-6.41. It can be seen that the obtained results were closed with experimental results. However, the results that predicted with MRK are better than PR, PRSV2 and PRSV equations of state at all states.

Table 6.7 Percentage average absolute deviations (% AAD) in molar volume of benzene-cyclohexane system calculated with equations of state.

T (K)	P (bar)	% AAD			
		PR	PRSV	PRSV2	MRK
308.15	1.01325	1.3355	1.3862	1.3819	0.9329
	2	1.1376	1.1879	1.1841	0.8070
	5	1.1105	1.1606	1.1569	0.7824
	10	0.9935	1.0434	1.0397	0.6683
313.15	1.01325	1.3206	1.3689	1.3642	0.8749
	2	1.1615	1.2091	1.2042	0.8170
	5	1.1483	1.1957	1.1907	0.8067
	10	1.0327	1.0800	1.0750	0.6942
323.15	1.01325	1.4570	1.4996	1.4931	0.9358
	2	1.2377	1.2804	1.2739	0.8563
	5	1.2267	1.2692	1.2627	0.8484
	10	1.1108	1.1531	1.1467	0.7360
333.15	1.01325	1.4724	1.5095	1.5024	0.9151
	2	1.2714	1.3084	1.3010	0.8431
	5	1.2038	1.2407	1.2333	0.7787
	10	1.1942	1.2310	1.2236	0.7180

Table 6.8 Percentage average absolute deviations (% AAD) in molar volume of cyclohexane-n-heptane system calculated with equations of state.

T (K)	P (bar)	% AAD			
		PR	PRSV	PRSV2	MRK
308.15	1.01325	1.1120	1.1205	1.1266	1.1487
	2	1.0691	1.0774	1.0835	1.1061
	5	1.1291	1.1373	1.1432	1.1528
	10	1.3603	1.3685	1.3744	1.3798
313.15	1.01325	1.1199	1.1276	1.1336	1.1542
	2	1.0593	1.0672	1.0731	1.0940
	5	1.0870	1.0952	1.1008	1.1188
	10	1.3381	1.3463	1.3519	1.3656
323.15	1.01325	1.1600	1.1678	1.1730	1.2006
	2	1.0764	1.0843	1.0894	1.1173
	5	1.0625	1.0699	1.0750	1.1037
	10	1.3369	1.3356	1.3400	1.4055
333.15	1.01325	1.1407	1.1481	1.1527	1.1896
	2	1.0967	1.1040	1.1086	1.1459
	5	1.0647	1.0716	1.0762	1.1143
	10	1.4612	1.4601	1.4636	1.5418

Table 6.9 Percentage average absolute deviations (% AAD) in molar volume of benzene-n-heptane system calculated with equations of state.

T (K)	P (bar)	% AAD			
		PR	PRSV	PRSV2	MRK
308.15	1.01325	0.7348	0.7534	0.7569	0.7081
	2	0.5567	0.5752	0.5788	0.5316
	5	0.6527	0.6703	0.6724	0.5873
	10	1.0187	1.0284	1.0282	0.9343
313.15	1.01325	0.6856	0.7098	0.7063	0.6161
	2	0.5098	0.5271	0.5299	0.4846
	5	0.5715	0.5888	0.5910	0.5012
	10	0.8985	0.9085	0.9098	0.8059
323.15	1.01325	0.8288	0.8506	0.8457	0.7215
	2	0.5772	0.5935	0.5953	0.5570
	5	0.6253	0.6414	0.6429	0.5380
	10	0.8290	0.8384	0.8396	0.7038
333.15	1.01325	0.8642	0.8777	0.8851	0.5948
	2	0.5960	0.6151	0.6115	0.4906
	5	0.5629	0.5792	0.5760	0.5039
	10	0.7725	0.7852	0.7763	0.7326

For cyclohexane and n-heptane system, the calculated molar volumes with PR are better than PRSV, PRSV2 and MRK equations of state at most of states except at 10 bar of temperature of 323.15 and 333.15 K that the calculated molar volume with PRSV are better than PR, PRSV2 and MRK equations of state. The calculated molar volumes by cubic equations of state compared with experimental molar volumes of the system as shown in Figure 6.42-6.45.

For benzene and n-heptane system, Figure 6.46-6.49 shown the calculated molar volumes by cubic equations of state compared with experimental molar volumes of the system. The results with MRK are better than PR, PRSV and PRSV2 equations of state at most of states except at 10 bar, temperature of 308.15 K, 1.01325 bar, temperature of 313.15 and 323.15 K, and 2, 5 and 10 bar, temperature of 333.15 K that the results with MRK are better than PR, PRSV2 and PRSV equations of state.

In addition, it appears that the calculated molar volumes of three binary systems are sensitive to the type of cubic equations of state used, when the equations of state were coupled with the conventional one binary interaction parameter rule. However, determination of interaction parameters has to the highest correct provided that the prediction of molar volume by using the equations of state also is high accuracy. Figure 6.50-6.52 shown the molar volumes of previous literatures.

Figure 6.38 Calculated molar volumes of benzene (1) and cyclohexane (2) system at 308.15 K by using equations of state.

Figure 6.39 Calculated molar volumes of benzene (1) and cyclohexane (2) system at 313.15 K by using equations of state.
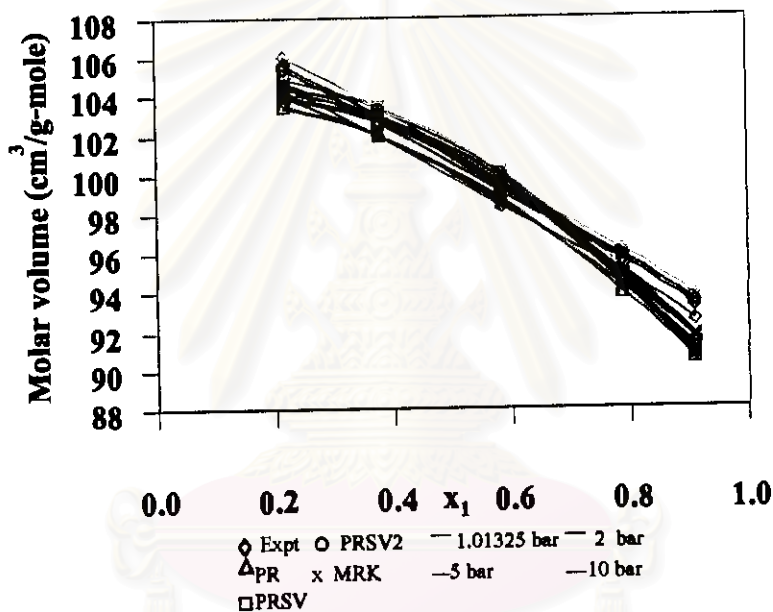

Figure 6.40 Calculated molar volumes of benzene (1) and cyclohexane (2) system at 323.15 K by using equations of state.

Figure 6.41 Calculated molar volumes of benzene (1) and cyclohexane (2) system at 333.15 K by using equations of state.

Figure 6.42 Calculated molar volumes of cyclohexane (1) and n-heptane (2) system at 308.15 K by using equations of state.
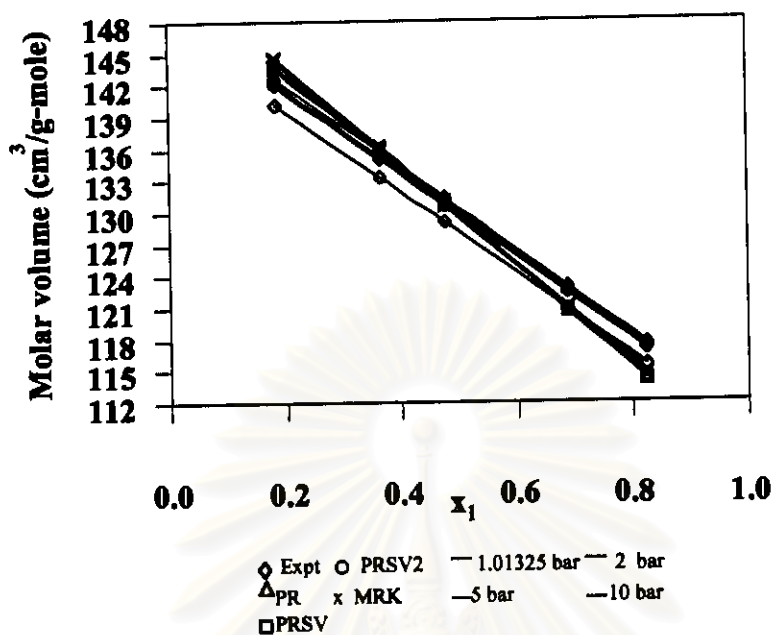
Figure 6.43 Calculated molar volumes of cyclohexane (1) and n-heptane (2) system

at 313.15 K by using equations of state.
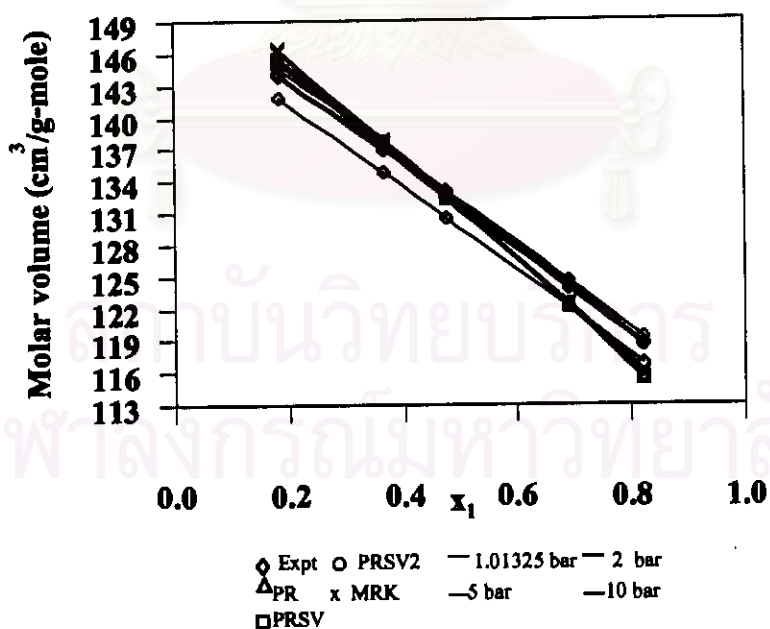
Figure 6.44 Calculated molar volumes of cyclohexane (1) and n-heptane (2) system

at 323.15 K by using equations of state.
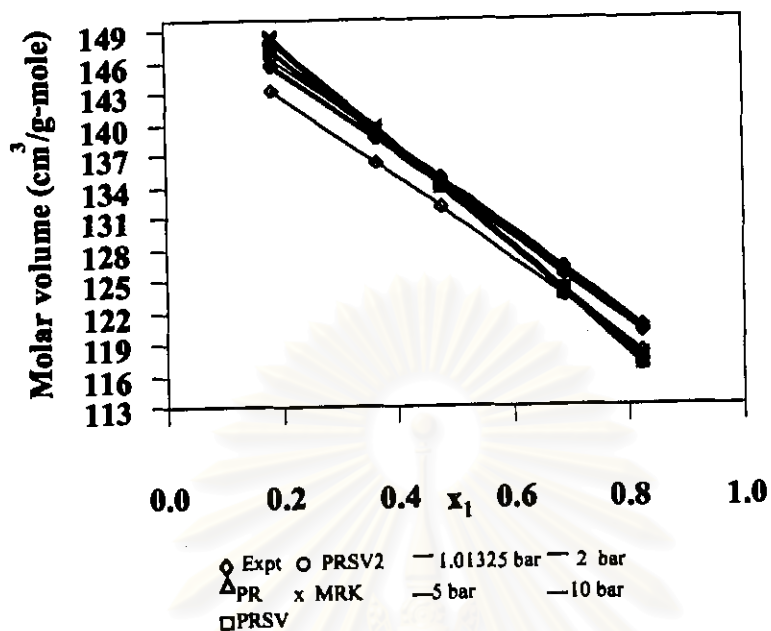
Figure 6.45 Calculated molar volumes of cyclohexane (1) and n-heptane (2) system

at 333.15 K by using equations of state.
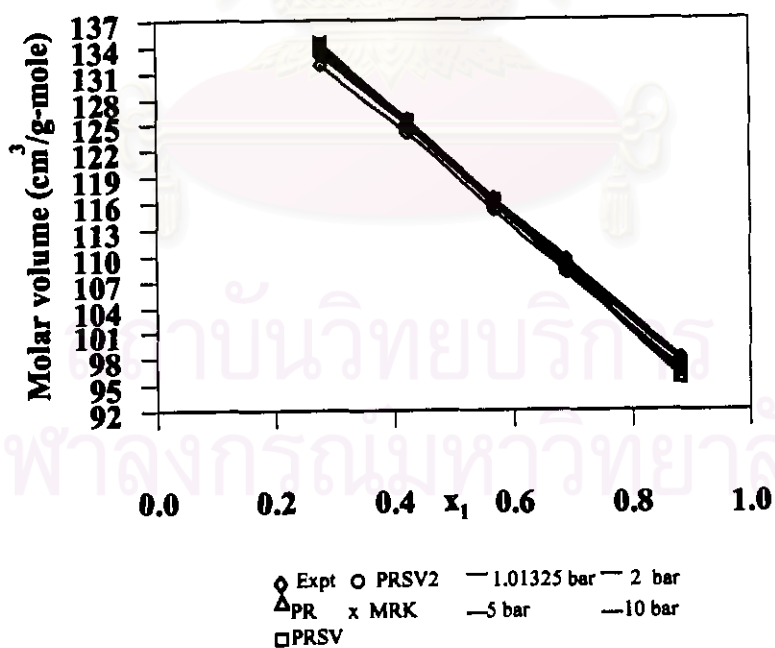
Figure 6.46 Calculated molar volumes of benzene (1) and n-heptane (2) system
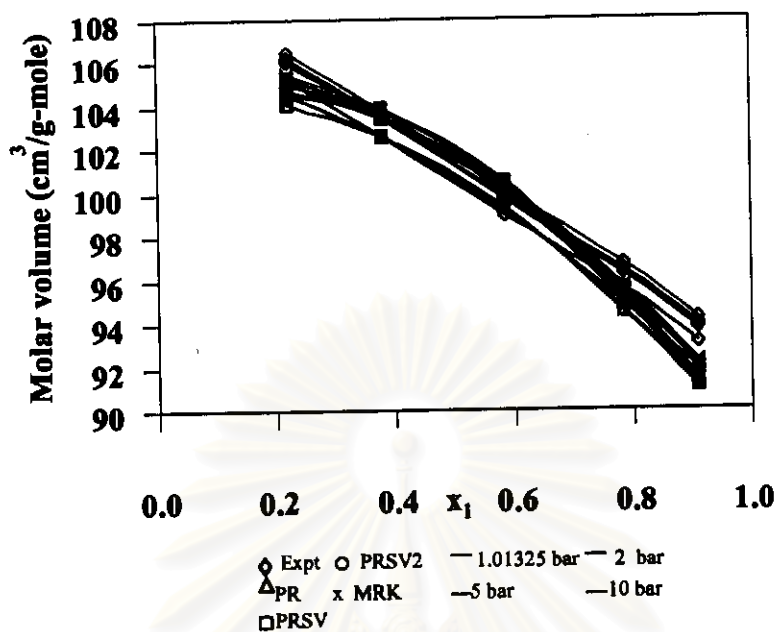
at 308.15 K by using equations of state.
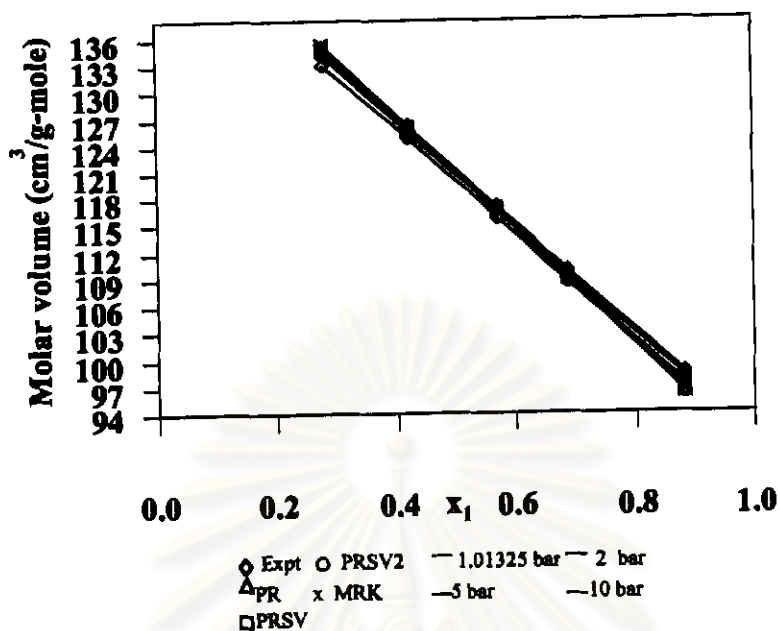
Figure 6.47 Calculated molar volumes of benzene (1) and n-heptane (2) system
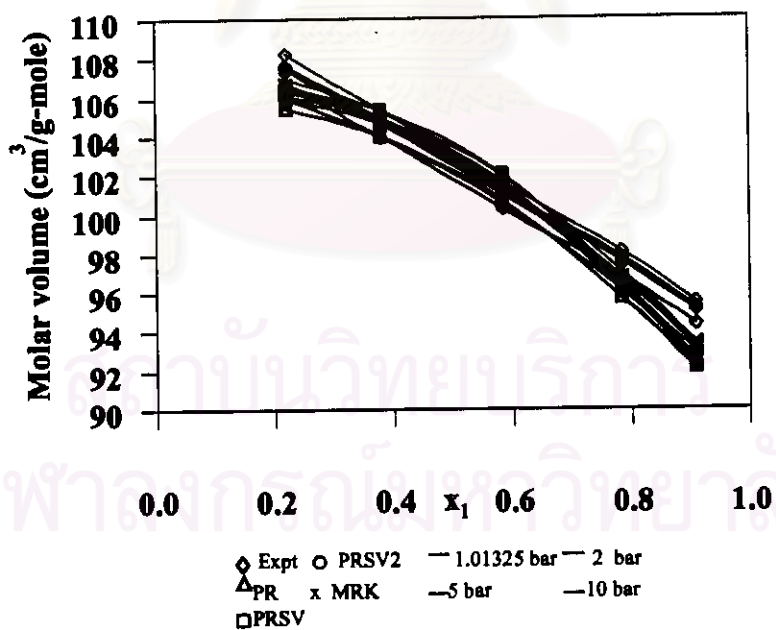
at 313.15 K by using equations of state.
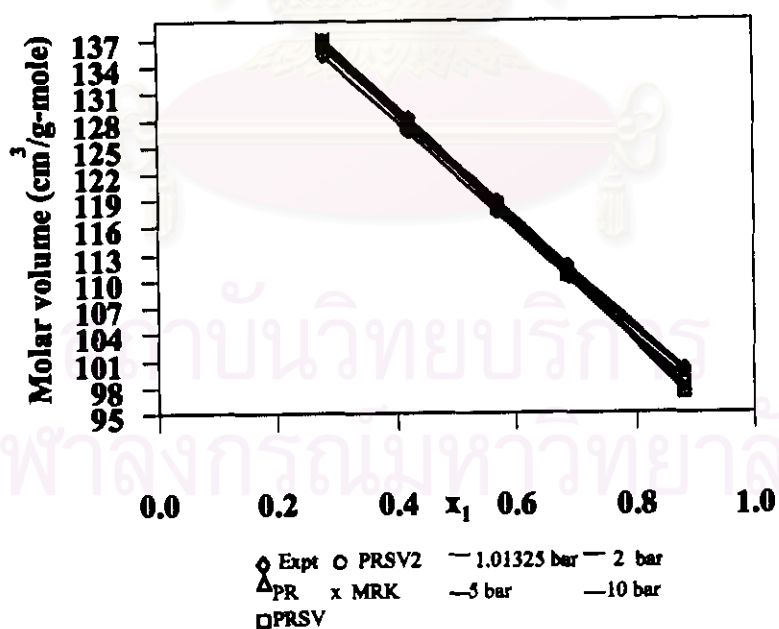
Figure 6.48 Calculated molar volumes of benzene (1) and n-heptane (2 sytem

at 323.15 K by using equations of state.

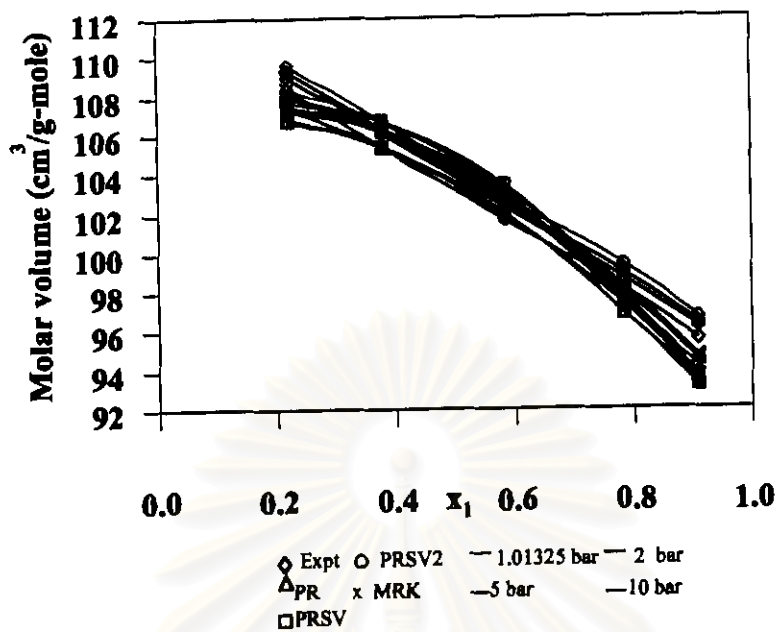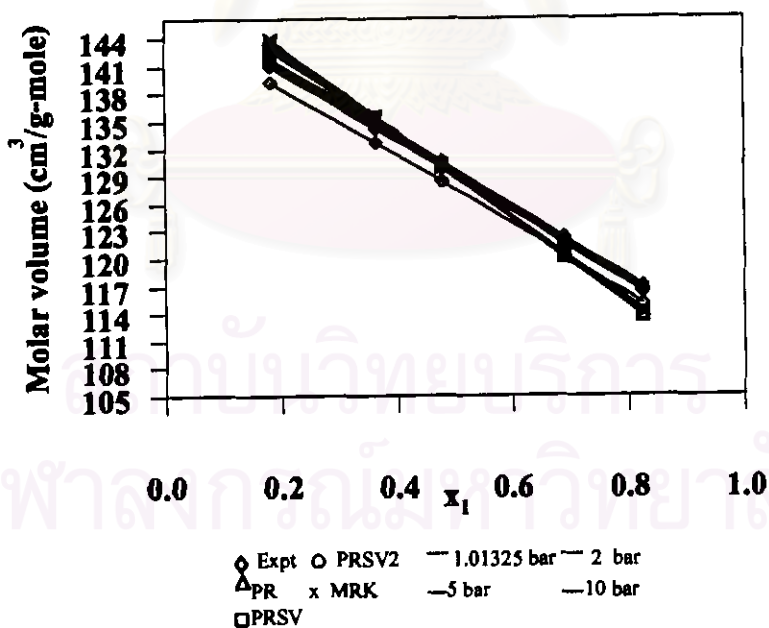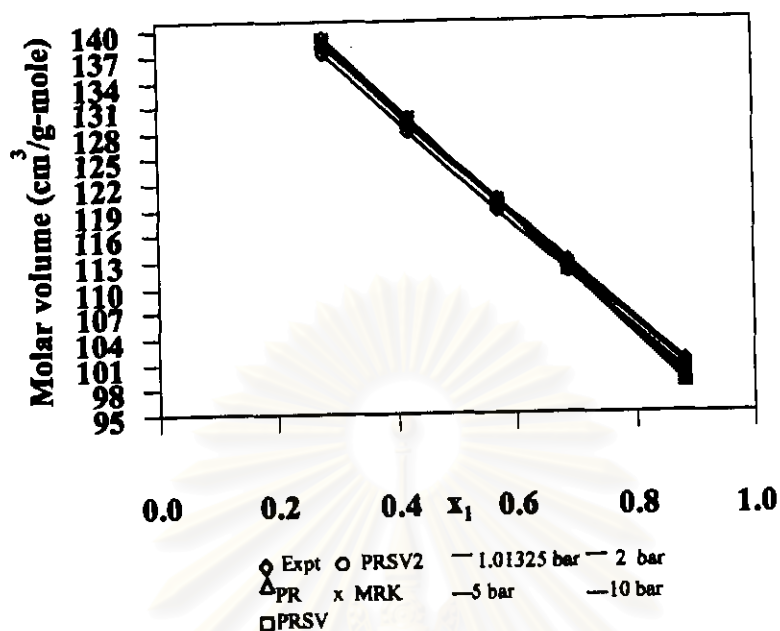Figure 6.49 Calculated molar volumes of benzene (1) and n-heptane (2) system at 333.15 K by using equations of state.
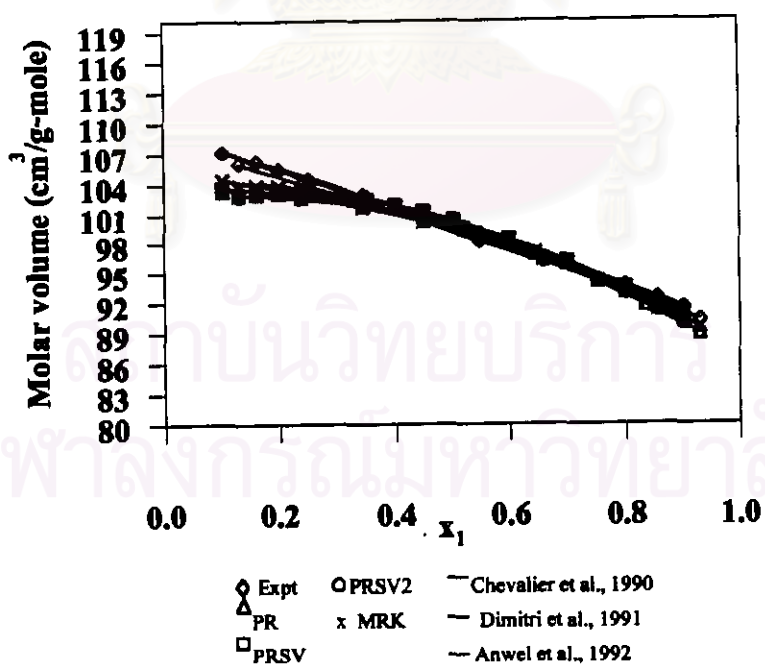
Figure 6.50 Calculated molar volumes of benzene (1) and cyclohexane (2) system, (Chevalier et al., 1990, Dimitri et al., 1991 and Anwel et al., 1992).
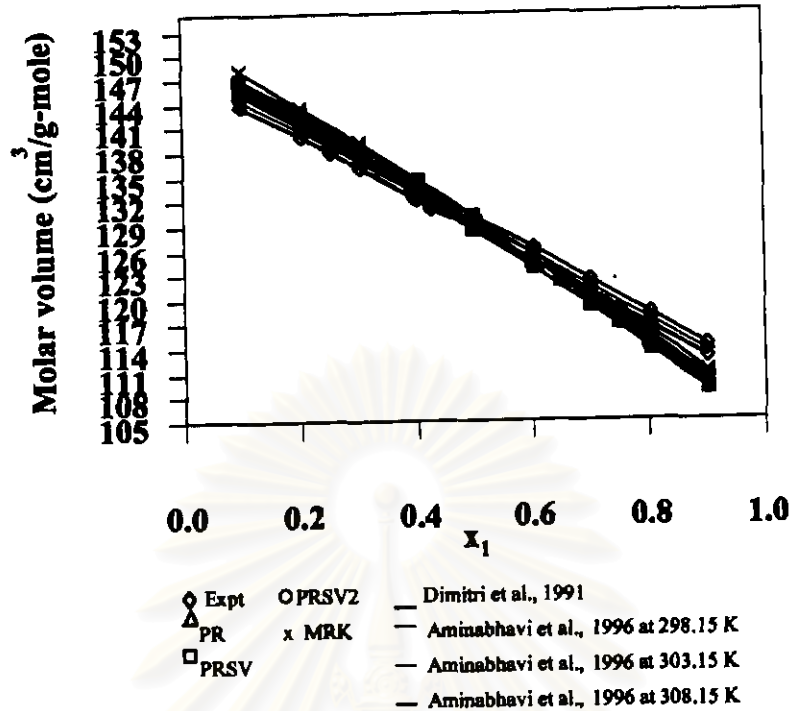
Figure 6.51 Calculated molar volumes of cyclohexane (1) and n-heptane (2) system, (Dimitri et al., 1991 and Aminabhavi et al., 1996).
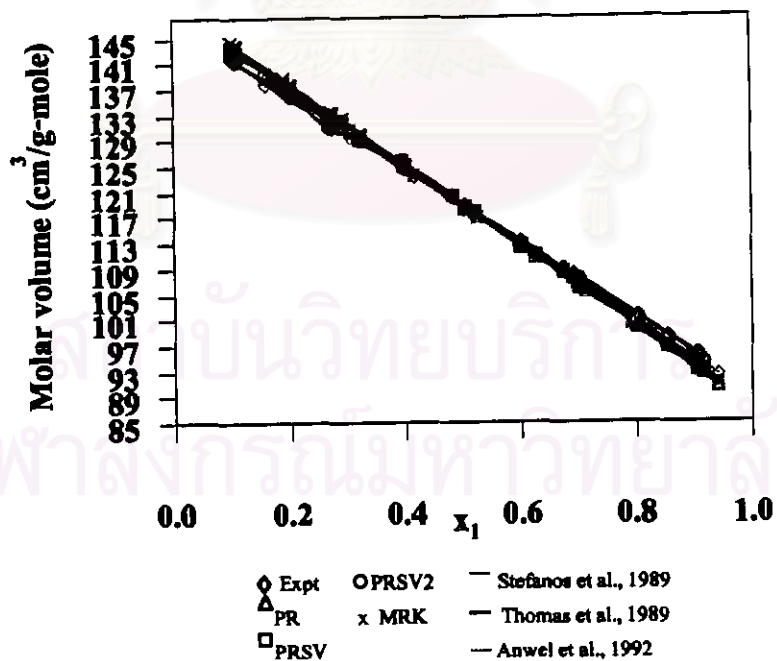
Figure 6.52 Calculated molar volumes of benzene (1) and n-heptane (2) system, (Stefanos et al., 1989, Thomas et al., 1989 and Anwel et al., 1992).

6.3.2 Prediction of Ternary Systems

Binary interaction parameters can be used to predict molar volume of a ternary system. Percentage average absolute deviation in molar volume of the ternary system is shown in Table 6.10. % AAD values are very closed for all equations of state. However, the results indicated that prediction of the ternary system with MRK is better than PR, PRSV2 and PRSV equations of state, respectively at all temperatures and pressures. The calculated molar volumes by cubic equations of state of the ternary system are shown in Table 6.11-6.26.

Table 6.10 Percentage average absolute deviations (% AAD) in molar volume of ternary system calculated with equations of state.

T (K)	P (bar)	% AAD			
		PR	PRSV	PRSV2	MRK
308.15	1.01325	0.3687	0.3928	0.3897	0.3112
	2	0.6225	0.6586	0.6517	0.3721
	5	0.7719	0.8078	0.8009	0.4854
	10	1.3405	1.3777	1.3694	1.0251
313.15	1.01325	0.3816	0.4049	0.4019	0.3240
	2	0.5790	0.6140	0.6073	0.3353
	5	0.6675	0.7022	0.6956	0.3857
	10	1.1686	1.2047	1.1965	0.8647
323.15	1.01325	0.3868	0.4075	0.4044	0.3079
	2	0.6011	0.6316	0.6251	0.3306
	5	0.7089	0.7392	0.7328	0.3970
	10	1.1973	1.2284	1.2207	0.8569
333.15	1.01325	0.3884	0.4045	0.3982	0.3390
	2	0.6450	0.6742	0.6596	0.3646
	5	0.7523	0.7812	0.7667	0.4495
	10	1.2382	1.2681	1.2518	0.9147

Table 6.11 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 308.15 K and 1.01325 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt.	PR	PRSV	PRSV2	MRK
0.2368	0.1774	128.6948	129.5644	129.5925	129.5932	129.4150
0.2073	0.3413	124.0045	124.5089	124.5639	124.5553	124.0953
0.2024	0.5063	117.8619	117.6790	117.7301	117.7174	117.2598
0.1979	0.6526	112.3670	111.3390	111.3477	111.3395	111.2575
0.3786	0.1792	120.5382	121.0676	121.1197	121.1107	120.6584
0.3654	0.3361	115.0072	115.6217	115.6970	115.6824	115.0461
0.3823	0.4742	108.7770	109.0206	109.0820	109.0700	108.6044
0.5363	0.1391	112.9824	113.0012	113.0389	113.0279	112.6365
0.5613	0.2956	105.3760	105.6098	105.6559	105.6455	105.2651
0.6458	0.1980	104.1266	104.0242	104.0410	104.0328	103.8377

Table 6.12 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 308.15 K and 2 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	128.1506	129.5409	129.5689	129.5696	129.3880
0.2073	0.3413	123.5338	124.4854	124.5402	124.5316	124.0691
0.2024	0.5063	117.4149	117.6564	117.7073	117.6947	117.2349
0.1979	0.6526	111.9646	111.3179	111.3265	111.3183	111.2335
0.3786	0.1792	120.0679	121.0457	121.0976	121.0887	120.6340
0.3654	0.3361	114.5954	115.5993	115.6744	115.6598	115.0218
0.3823	0.4742	108.3764	108.9982	109.0595	109.0475	108.5800
0.5363	0.1391	112.4763	112.9818	113.0194	113.0084	112.6149
0.5613	0.2956	105.0030	105.5895	105.6355	105.6252	105.2429
0.6458	0.1980	103.6804	104.0061	104.0228	104.0146	103.8173

Table 6.13 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 308.15 K and 5 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	127.8606	129.4696	129.4974	129.4981	129.3060
0.2073	0.3413	123.2231	124.4141	124.4684	124.4599	123.9899
0.2024	0.5063	117.1088	117.5878	117.6383	117.6257	117.1593
0.1979	0.6526	111.6322	111.2537	111.2622	111.2541	111.1608
0.3786	0.1792	119.7302	120.9793	121.0308	121.0219	120.5602
0.3654	0.3361	114.3356	115.5312	115.6057	115.5912	114.9483
0.3823	0.4742	108.1521	108.9303	108.9911	108.9791	108.5064
0.5363	0.1391	112.1730	112.9229	112.9603	112.9493	112.5494
0.5613	0.2956	104.7250	105.5280	105.5737	105.5634	105.1756
0.6458	0.1980	103.4315	103.9510	103.9677	103.9595	103.7556

Table 6.14 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 308.15 K and 10 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	126.9095	129.3512	129.3786	129.3793	129.1705
0.2073	0.3413	122.3119	124.2957	124.3492	124.3408	123.8588
0.2024	0.5063	116.2603	117.4739	117.5238	117.5113	117.0345
0.1979	0.6526	110.8149	111.1473	111.1556	111.1476	111.0407
0.3786	0.1792	118.9234	120.8691	120.9199	120.9111	120.4381
0.3654	0.3361	113.5037	115.4182	115.4917	115.4774	114.8267
0.3823	0.4742	107.3450	108.8177	108.8776	108.8658	108.3847
0.5363	0.1391	111.3680	112.8252	112.8620	112.8512	112.4411
0.5613	0.2956	103.9673	105.4261	105.4711	105.4609	105.0643
0.6458	0.1980	102.7202	103.8597	103.8761	103.8681	103.6536

Table 6.15 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 313.15 K and 1.01325 bar.

| x_1 | x_2 | Molar volume (cm^3/g-mole) | | | | |
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	129.3162	130.2624	130.2913	130.2929	130.1212
0.2073	0.3413	124.6078	125.1744	125.2290	125.2200	124.7664
0.2024	0.5063	118.4275	118.3067	118.3571	118.3434	117.9018
0.1979	0.6526	112.9558	111.9377	111.9470	111.9379	111.8934
0.3786	0.1792	121.2132	121.7198	121.7711	121.7632	121.3006
0.3654	0.3361	115.3728	116.2416	116.3147	116.2996	115.6655
0.3823	0.4742	109.5417	109.6058	109.6647	109.6511	109.2161
0.5363	0.1391	113.5111	113.6093	113.6464	113.6370	113.2334
0.5613	0.2956	105.8892	106.1767	106.2208	106.2100	105.8516
0.6458	0.1980	104.6229	104.5826	104.5989	104.5915	104.4112

Table 6.16 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 313.15 K and 2 bar.

| x_1 | x_2 | Molar volume (cm^3/g-mole) | | | | |
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	128.9325	130.2376	130.2664	130.2680	130.0928
0.2073	0.3413	124.2283	125.1496	125.2040	125.1950	124.7389
0.2024	0.5063	118.0700	118.2829	118.3332	118.3195	117.8756
0.1979	0.6526	112.5715	111.9154	111.9247	111.9157	111.8682
0.3786	0.1792	120.7460	121.6967	121.7479	121.7400	121.2751
0.3654	0.3361	115.3007	116.2180	116.2909	116.2758	115.6400
0.3823	0.4742	109.0350	109.5823	109.6410	109.6275	109.1906
0.5363	0.1391	113.1531	113.5888	113.6258	113.6164	113.2107
0.5613	0.2956	105.5702	106.1554	106.1994	106.1886	105.8284
0.6458	0.1980	104.3038	104.5636	104.5798	104.5724	104.3898

Table 6.17 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 313.15 K and 5 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	128.7577	130.1622	130.1907	130.1923	130.0066
0.2073	0.3413	124.0028	125.0744	125.1283	125.1194	124.6557
0.2024	0.5063	117.7827	118.2107	118.2606	118.2470	117.7964
0.1979	0.6526	112.3951	111.8480	111.8572	111.8482	111.7919
0.3786	0.1792	120.5790	121.6266	121.6774	121.6696	121.1976
0.3654	0.3361	115.1079	116.1464	116.2187	116.2037	115.5630
0.3823	0.4742	108.8319	109.5110	109.5693	109.5558	109.1135
0.5363	0.1391	112.9839	113.5267	113.5634	113.5541	113.1420
0.5613	0.2956	105.3920	106.0909	106.1345	106.1238	105.7579
0.6458	0.1980	104.1606	104.5057	104.5218	104.5145	104.3252

Table 6.18 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 313.15 K and 10 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	127.8677	130.0371	130.0652	130.0668	129.8642
0.2073	0.3413	123.1204	124.9496	125.0028	124.9940	124.5182
0.2024	0.5063	117.0103	118.0909	118.1401	118.1267	117.6656
0.1979	0.6526	111.6147	111.7361	111.7451	111.7362	111.6658
0.3786	0.1792	119.7350	121.5104	121.5605	121.5527	121.0696
0.3654	0.3361	114.3552	116.0276	116.0989	116.0842	115.4357
0.3823	0.4742	108.0882	109.3929	109.4503	109.4371	108.9861
0.5363	0.1391	112.1351	113.4236	113.4598	113.4507	113.0285
0.5613	0.2956	104.6722	105.9839	106.0269	106.0163	105.6414
0.6458	0.1980	103.4613	104.4097	104.4255	104.4183	104.2182

Table 6.19 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 323.15 K and 1.01325 bar.

x_1	x_2	Molar volume (cm³/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	131.1909	132.0022	132.0278	132.0296	131.8238
0.2073	0.3413	126.3332	126.8689	126.9163	126.9076	126.3954
0.2024	0.5063	120.1030	119.9144	119.9575	119.9444	119.4580
0.1979	0.6526	114.6119	113.4314	113.4380	113.4302	113.4020
0.3786	0.1792	122.8827	123.4181	123.4641	123.4561	122.9106
0.3654	0.3361	117.3156	117.8909	117.9557	117.9403	117.2256
0.3823	0.4742	110.9236	111.1579	111.2099	111.1964	110.7390
0.5363	0.1391	115.1502	115.2069	115.2399	115.2309	114.7468
0.5613	0.2956	107.3425	107.6806	107.7194	107.7092	107.3235
0.6458	0.1980	106.1775	106.0323	106.0458	106.0397	105.8370

Table 6.20 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 323.15 K and 2 bar.

x_1	x_2	Molar volume (cm³/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	130.6643	131.9736	131.9991	132.0009	131.7917
0.2073	0.3413	125.8815	126.8405	126.8878	126.8790	126.3645
0.2024	0.5063	119.6993	119.8872	119.9302	119.9171	119.4286
0.1979	0.6526	114.1750	113.4061	113.4127	113.4049	113.3737
0.3786	0.1792	122.4328	123.3914	123.4374	123.4293	122.8817
0.3654	0.3361	116.9045	117.8637	117.9284	117.9131	117.1969
0.3823	0.4742	110.5229	111.1311	111.1829	111.1695	110.7104
0.5363	0.1391	114.7253	115.1832	115.2162	115.2072	114.7212
0.5613	0.2956	106.9858	107.6563	107.6950	107.6848	107.2973
0.6458	0.1980	105.7595	106.0104	106.0240	106.0179	105.8129

Table 6.21 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 323.15 K and 5 bar.

x_1	x_2	Molar volume (cm³/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	130.4036	131.8870	131.9123	131.9141	131.6944
0.2073	0.3413	125.6149	126.7543	126.8012	126.7925	126.2708
0.2024	0.5063	119.3959	119.8048	119.8474	119.8344	119.3396
0.1979	0.6526	113.8887	113.3295	113.3360	113.3283	113.2880
0.3786	0.1792	122.2024	123.3107	123.3562	123.3482	122.7943
0.3654	0.3361	116.6529	117.7816	117.8456	117.8304	117.1102
0.3823	0.4742	110.3215	111.0499	111.1012	111.0879	110.6236
0.5363	0.1391	114.4995	115.1117	115.1443	115.1354	114.6437
0.5613	0.2956	106.7712	107.5826	107.6209	107.6108	107.2180
0.6458	0.1980	105.5410	105.9443	105.9577	105.9516	105.7401

Table 6.22 Calculated molar volumes of benzene (1), cyclohexane (2) and n-heptane (3) system at 323.15 K and 10 bar.

x_1	x_2	Molar volume (cm³/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	129.5017	131.7435	131.7683	131.7701	131.5337
0.2073	0.3413	124.7924	126.6115	126.6576	126.6490	126.1162
0.2024	0.5063	118.5557	119.6683	119.7102	119.6974	119.1926
0.1979	0.6526	113.1189	113.2025	113.2089	113.2013	113.1465
0.3786	0.1792	121.2777	123.1768	123.2217	123.2138	122.6498
0.3654	0.3361	115.8273	117.6454	117.7085	117.6935	116.9669
0.3823	0.4742	109.5545	110.9153	110.9659	110.9528	110.4803
0.5363	0.1391	113.7134	114.9929	115.0252	115.0163	114.5155
0.5613	0.2956	106.0866	107.4604	107.4982	107.4882	107.0869
0.6458	0.1980	104.8137	105.8345	105.8477	105.8417	105.6196

Table 6.23 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 333.15 K and 1.01325 bar.

x_1	x_2	Molar volume (cm³/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	132.7295	133.7282	133.7561	133.7448	133.6323
0.2073	0.3413	127.8997	128.5713	128.6162	128.5973	128.0975
0.2024	0.5063	121.5612	121.5356	121.5752	121.5550	121.0457
0.1979	0.6526	115.9886	114.9399	114.9467	114.9354	114.8998
0.3786	0.1792	124.3480	125.0459	125.0926	125.0684	124.5992
0.3654	0.3361	118.8328	119.4817	119.5425	119.5149	118.8018
0.3823	0.4742	112.3317	112.6550	112.7024	112.6816	112.1938
0.5363	0.1391	116.7946	116.7086	116.7437	116.7186	116.3236
0.5613	0.2956	108.9705	109.1055	109.1422	109.1227	108.7448
0.6458	0.1980	107.5031	107.4076	107.4227	107.4068	107.2545

Table 6.24 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 333.15 K and 2 bar.

x_1	x_2	Molar volume (cm³/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	132.3007	133.6957	133.7236	133.7122	133.5960
0.2073	0.3413	127.4855	128.5390	128.5838	128.5649	128.0627
0.2024	0.5063	121.1209	121.5048	121.5442	121.5242	121.0128
0.1979	0.6526	115.5428	114.9114	114.9182	114.9069	114.8683
0.3786	0.1792	123.9236	125.0157	125.0622	125.0381	124.5666
0.3654	0.3361	118.3690	119.4511	119.5117	119.4841	118.7697
0.3823	0.4742	111.9060	112.6248	112.6721	112.6514	112.1620
0.5363	0.1391	116.2648	116.6819	116.7169	116.6918	116.2947
0.5613	0.2956	108.4327	109.0782	109.1147	109.0953	108.7156
0.6458	0.1980	107.0469	107.3830	107.3981	107.3822	107.2276

Table 6.25 Calculated molar volumes of benzene(1), cyclohexane(2) and n-heptane (3) system at 333.15 K and 5 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	132.0560	133.5974	133.6249	133.6137	133.4861
0.2073	0.3413	127.2013	128.4411	128.4855	128.4668	127.9575
0.2024	0.5063	120.9152	121.4114	121.4505	121.4306	120.9133
0.1979	0.6526	115.3102	114.8250	114.8317	114.8205	114.7729
0.3786	0.1792	123.6669	124.9242	124.9703	124.9463	124.4680
0.3654	0.3361	118.0179	119.3581	119.4182	119.3908	118.6726
0.3823	0.4742	111.7321	112.5335	112.5804	112.5598	112.0657
0.5363	0.1391	115.9751	116.6010	116.6356	116.6108	116.2073
0.5613	0.2956	108.2166	108.9954	109.0316	109.0123	108.6274
0.6458	0.1980	106.8589	107.3086	107.3235	107.3078	107.1462

Table 6.26 Calculated molar volume of benzene(1), cyclohexane(2) and n-heptane (3) system at 333.15 K and 10 bar.

x_1	x_2	Molar volume (cm^3/g-mole)				
		Expt	PR	PRSV	PRSV2	MRK
0.2368	0.1774	131.1704	133.4345	133.4615	133.4504	133.3047
0.2073	0.3413	126.3828	128.2790	128.3226	128.3042	127.7838
0.2024	0.5063	120.0865	121.2568	121.2952	121.2756	120.7491
0.1979	0.6526	114.4291	114.6819	114.6884	114.6774	114.6153
0.3786	0.1792	122.8064	124.7726	124.8179	124.7943	124.3052
0.3654	0.3361	117.2823	119.2042	119.2633	119.2364	118.5123
0.3823	0.4742	110.9411	112.3824	112.4285	112.4082	111.9068
0.5363	0.1391	115.1563	116.4668	116.5010	116.4765	116.0630
0.5613	0.2956	107.4675	108.8582	108.8939	108.8749	108.4816
0.6458	0.1980	106.1352	107.1853	107.1999	107.1844	107.0117

6.4 Partial Molar Volumes of Benzene, Cyclohexane and n-Heptane.

In this work, partial molar volumes were determined by using Peng-Robinson equation of state based on molar volume data. The equation of state is widely used to predict thermodynamic properties of mixtures. Correlations of both binary and ternary system were presented in Appendix D. Partial molar volumes of binary systems are shown in Figure 6.53-6.76 and of ternary system are shown in Table 6.27-6.30. For all mixtures, at a given pressure, partial molar volume increases with increasing temperature, while an increase of pressure results in a decrease of partial molar volume. However, temperature effected the partial molar volumes more pronounced than at low pressure. When the molecules in mixtures were slightly pressured with low pressure, interaction of intermolecular rarely could change.

Furthermore, when the results of this work were compared with the results of literatures, it appears that the results of Chevalier et al., 1990; Dimitri et al., 1991; Anwel et al., 1992 for system of benzene and cyclohexane, of Dimitri et al., 1990; Aminabhavi et al., 1996 for system of cyclohexane and n-heptane, and of Stefanos et al., 1989; Anwel et al., 1992; Thomas et al., 1989 for system of benzene and n-heptane agree well with the results of all the binary systems for this work as illustrated in Figure 6.77-6.79. Considering effect of temperature on partial molar volumes of Aminabhavi et al., 1996, it indicated that the partial molar volumes related to temperature like the results of this work as shown in Figure 6.78.
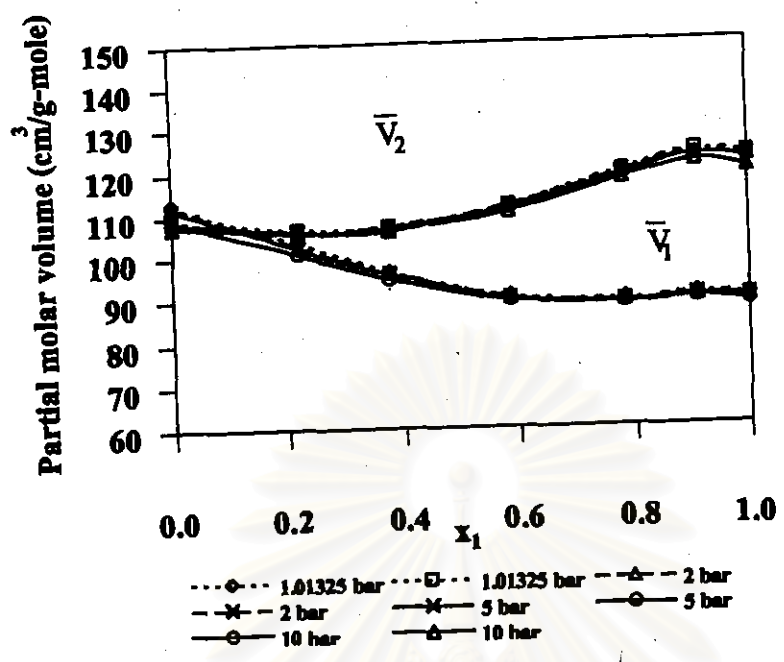
Figure 6.53 Partial molar volumes of benzene(1) and cyclohexane(2) system at 308.15 K.
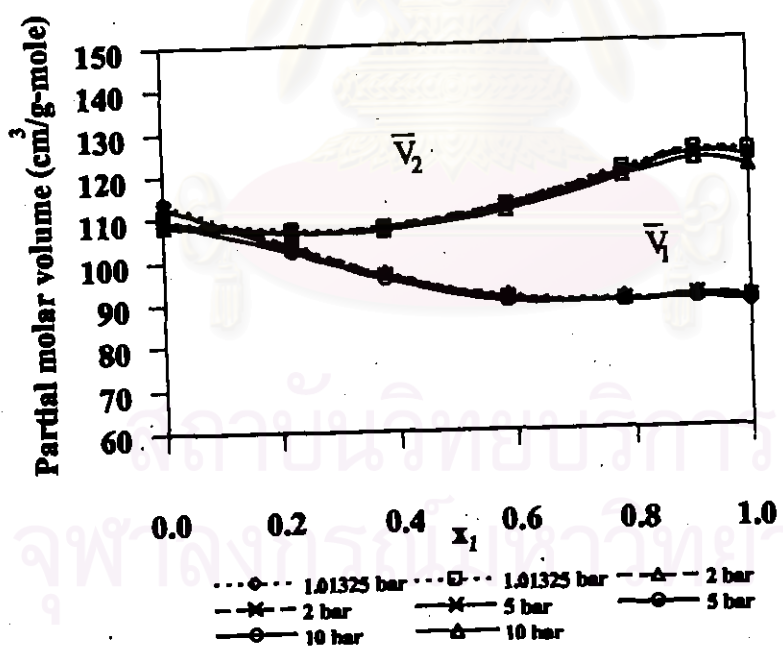
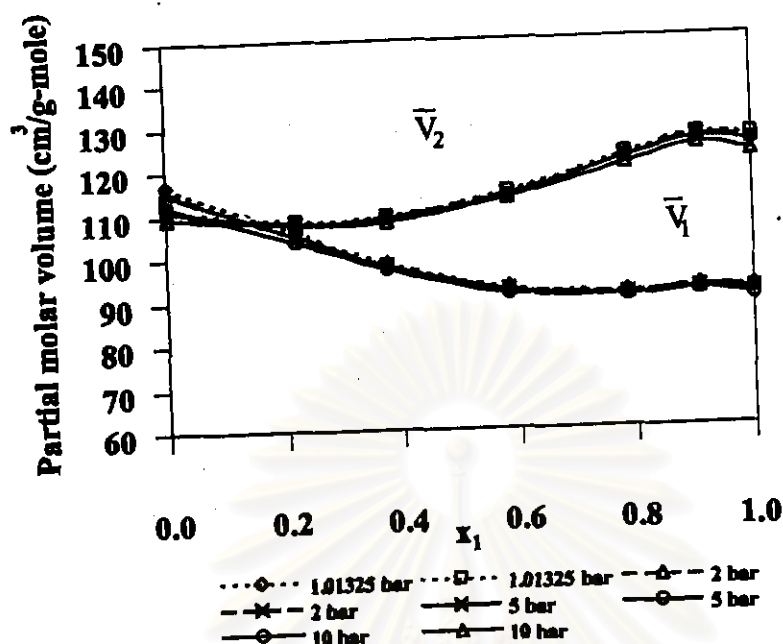Figure 6.54 Partial molar volumes of benzene(1) and cyclohexane(2) system at 313.15 K.

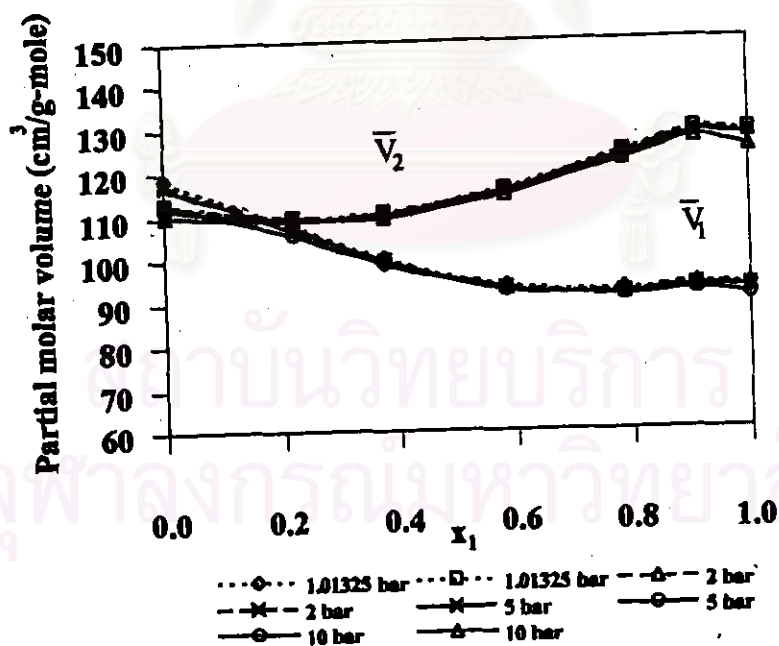Figure 6.55 Partial molar volumes of benzene(1) and cyclohexane(2) system at 323.15 K.

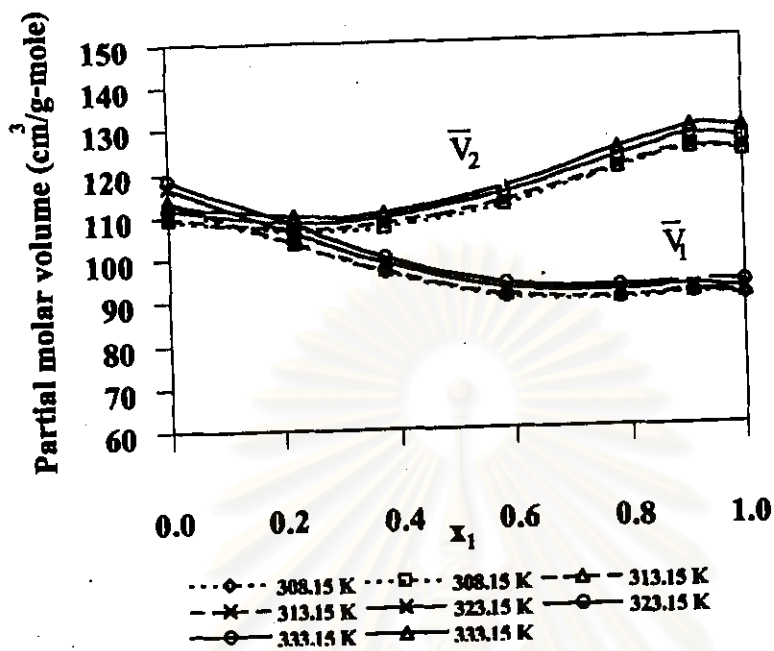Figure 6.56 Partial molar volumes of benzene(1) and cyclohexane(2) system at 333.15.

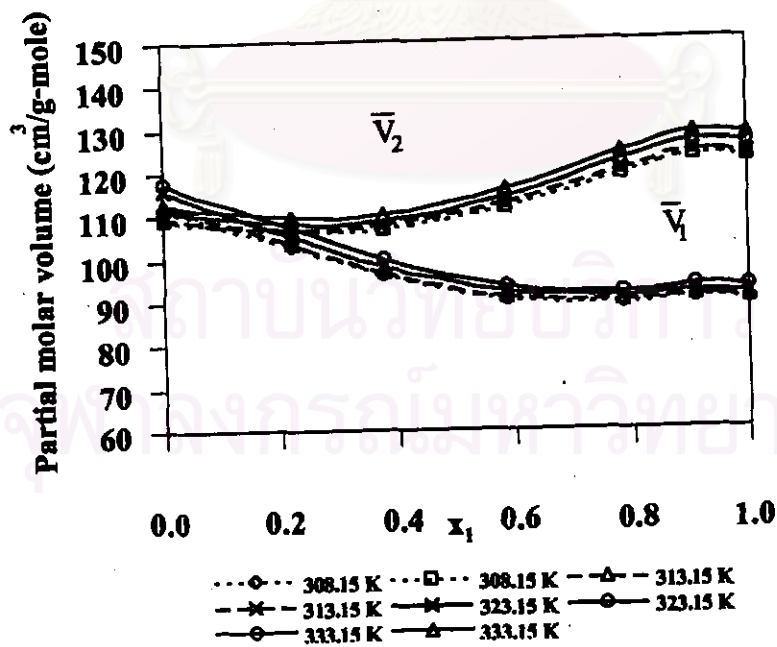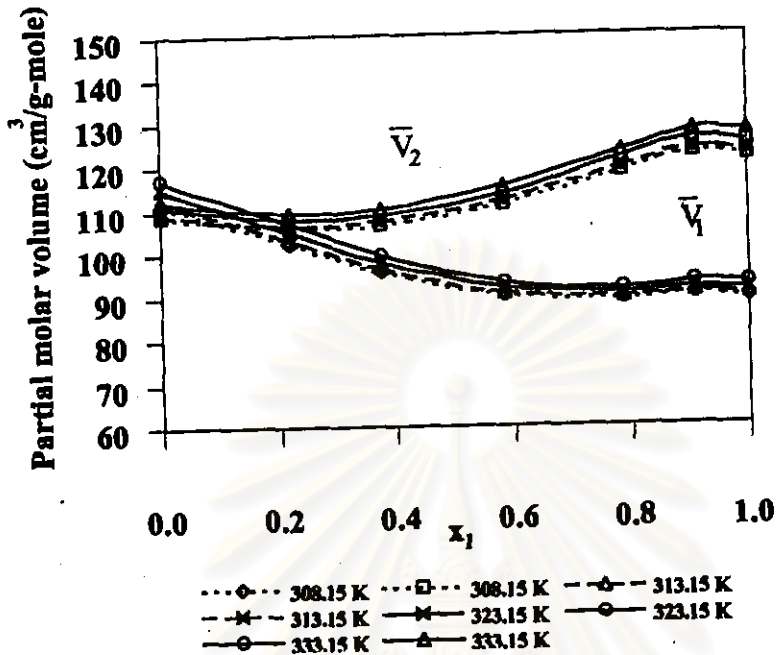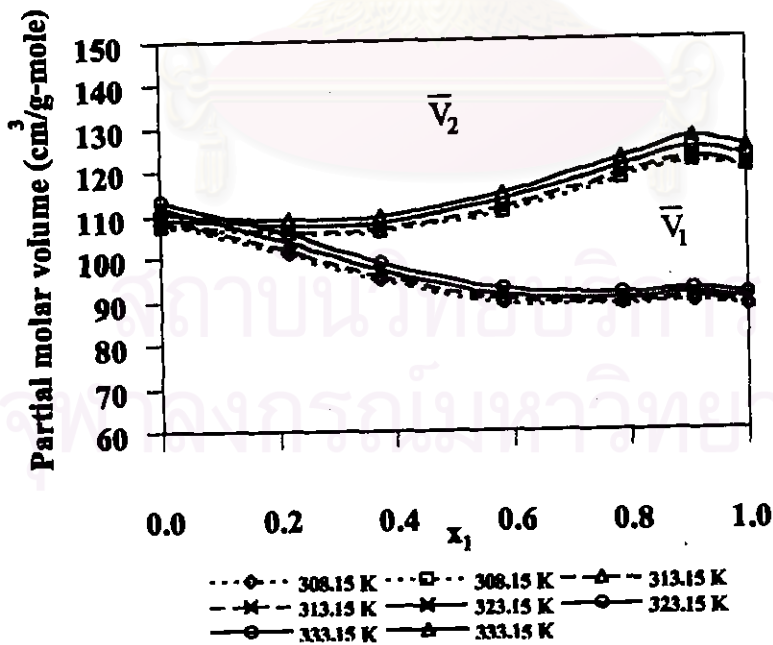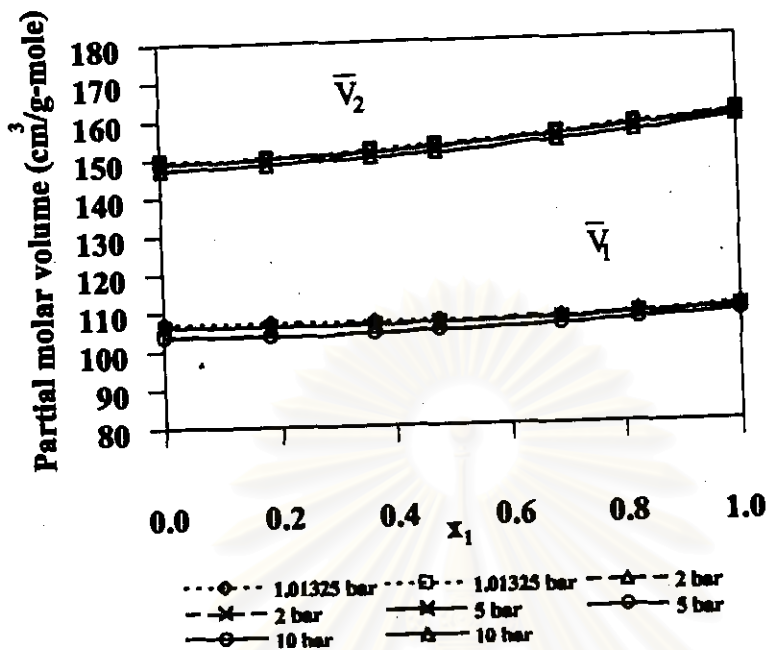Figure 6.57 Partial molar volumes of benzene (1) and cyclohexane (2) system at 1.01325 bar.

Figure 6.58 Partial molar volumes of benzene (1) and cyclohexane (2) system at 2 bar.

Figure 6.59 Partial molar volumes of benzene (1) and cyclohexane (2) system at 5 bar.

Figure 6.60 Partial molar volumes of benzene (1) and cyclohexane (2) system at 10 bar.

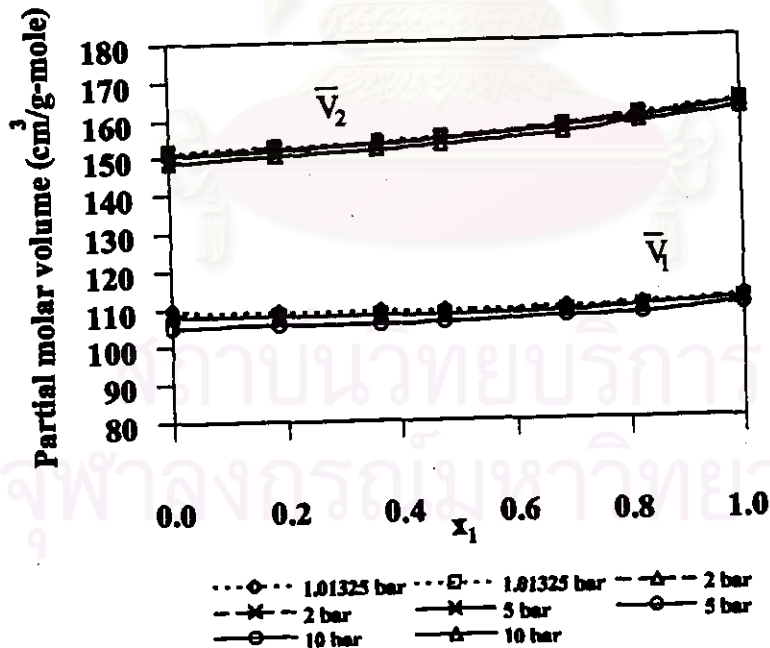Figure 6.61 Partial molar volume of cyclohexane (1) and n-heptane (2) system at 308.15 K.

Figure 6.62 Partial molar volumes of cyclohexane (1) and n-heptane (2) system at 313.15 K.
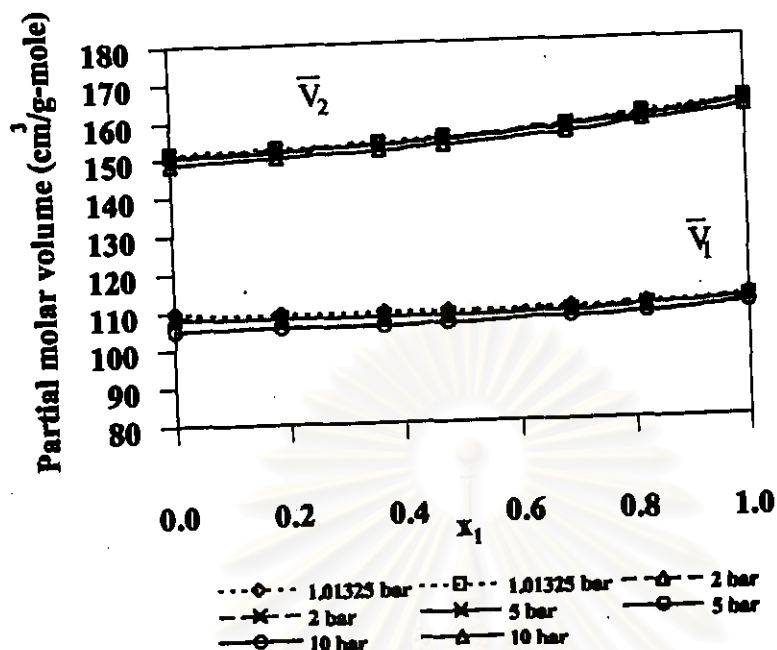
Figure 6.63 Partial molar volumes of cyclohexane (1) and n-heptane(2) system at 323.15 K
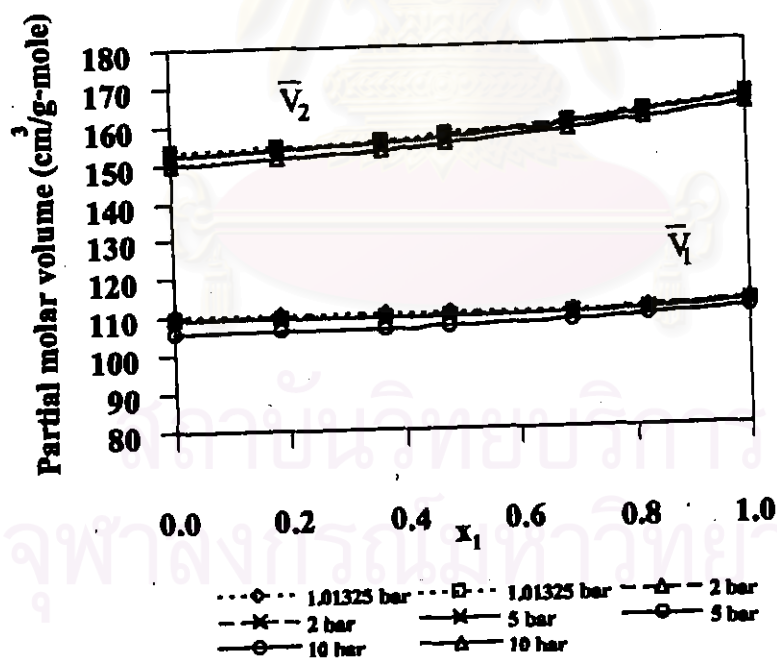

Figure 6.64 Partial molar volumes of cyclohexane (1) and n-heptane (2) system
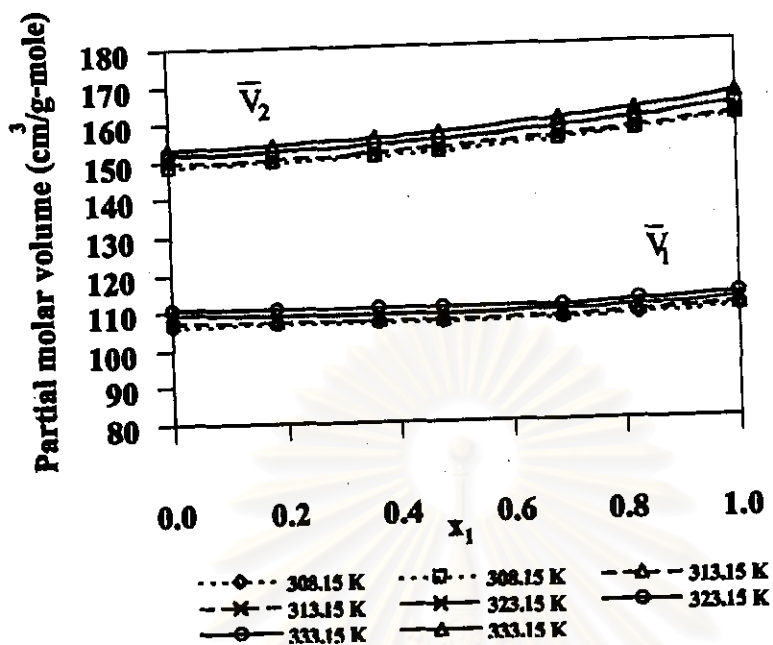
at 333.15 K.

Figure 6.65 Partial molar volume of cyclohexane (1) and n-heptane (2) system
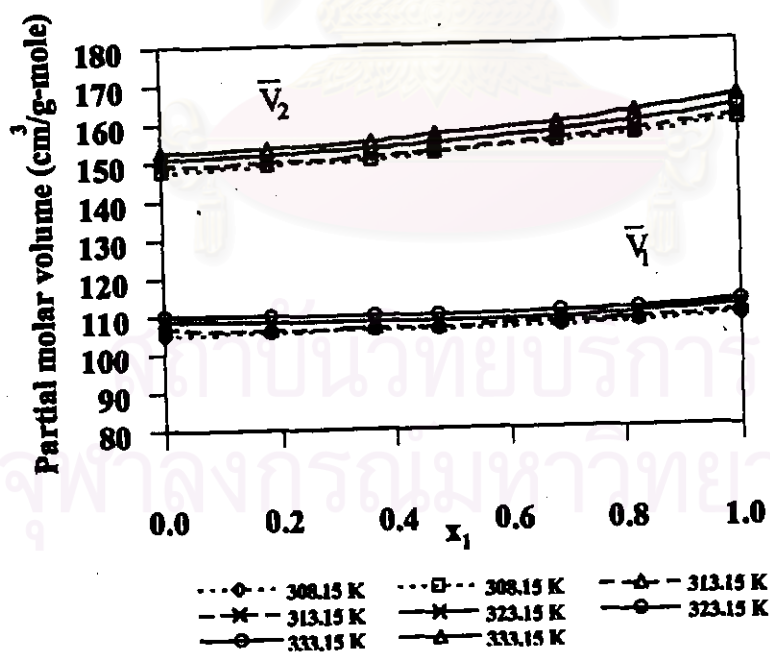
at 1.01325 bar.

Figure 6.66 Partial molar volumes of cyclohexane (1) and n-heptane (2) system at 2 bar.
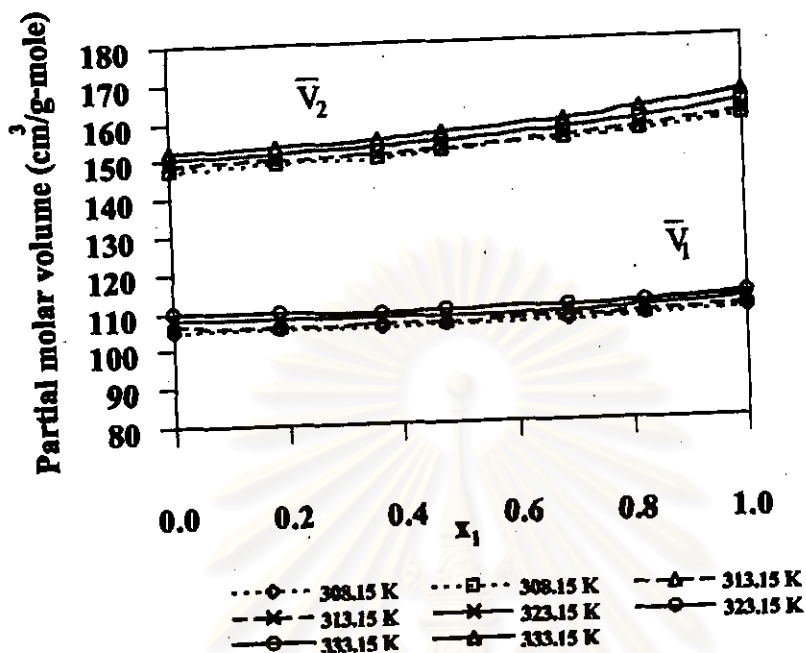
Figure 6.67 Partial molar volumes of cyclohexane (1) and n-heptane (2) system at 5 bar.
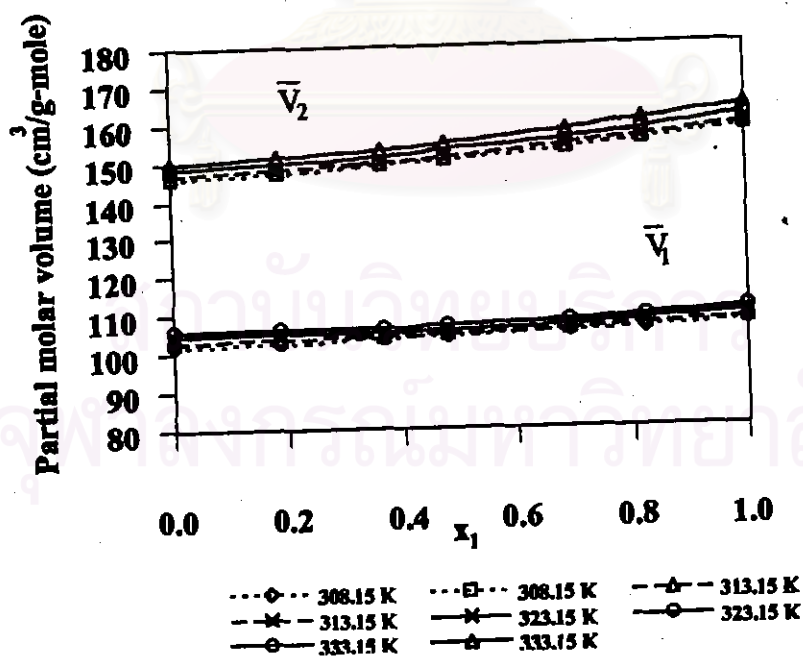

Figure 6.68 Partial molar volumes of cyclohexane (1) and n-heptane (2) system at 10 bar.

Figure 6.69 Partial molar volumes of benzene (1) and n-heptane (2) system at 308.15 K.

Figure 6.70 Partial molar volumes of benzene (1) and n-heptane (2) system at 313.15 K.
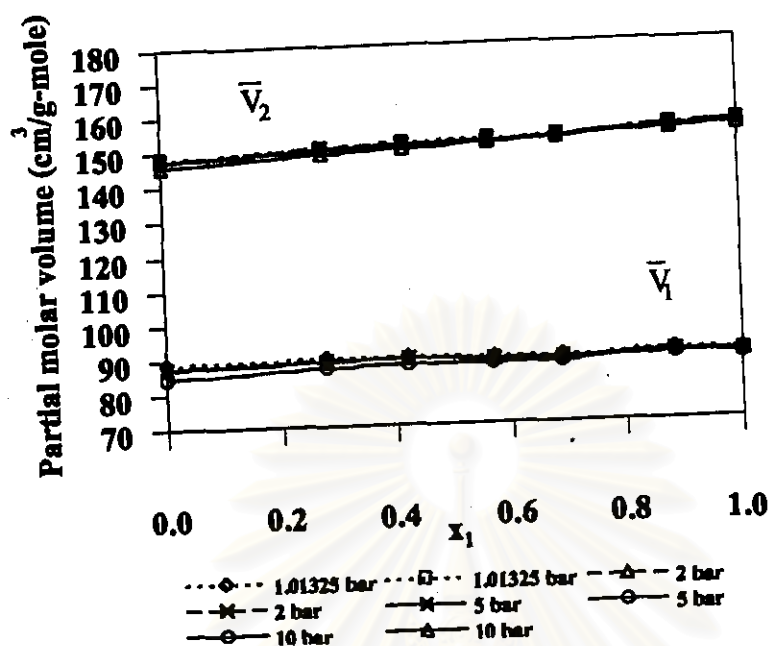
Figure 6.71 Partial molar volumes of benzene (1) and n-heptane (2) system at 323.15 K.

Figure 6.72 Partial molar volumes of benzene (1) and n-heptane (2) system at 333.15 K.

Figure 6.73 Partial molar volumes of benzene (1) and n-heptane (2) system at 1.01325 bar.

Figure 6.74 Partial molar volumes of benzene (1) and n-heptane (2) system at 2 bar.
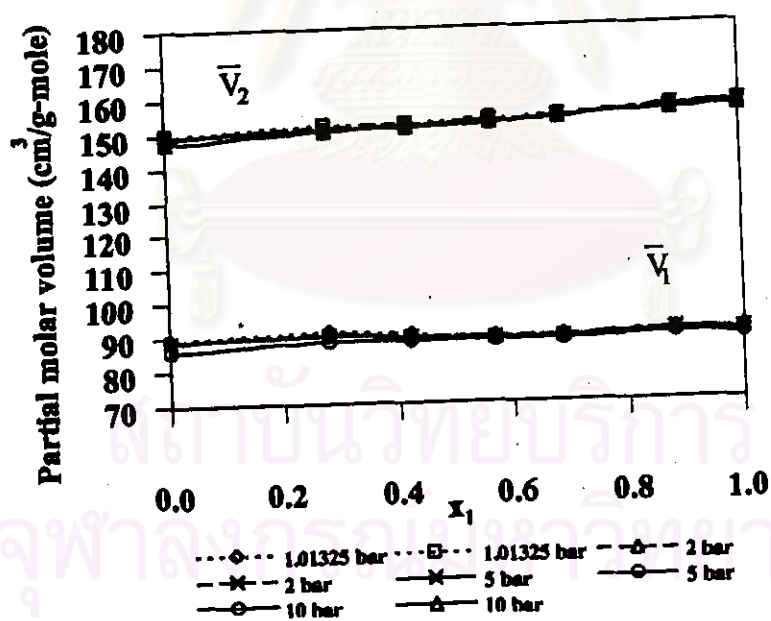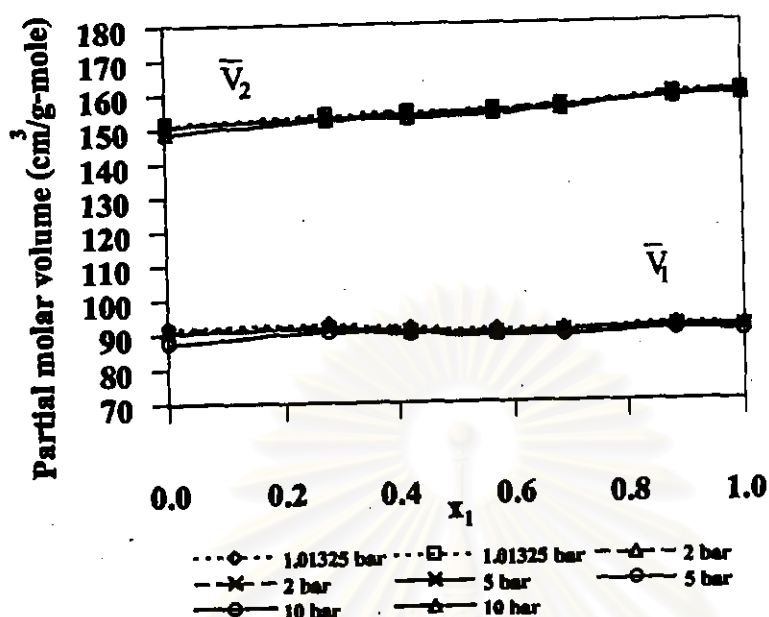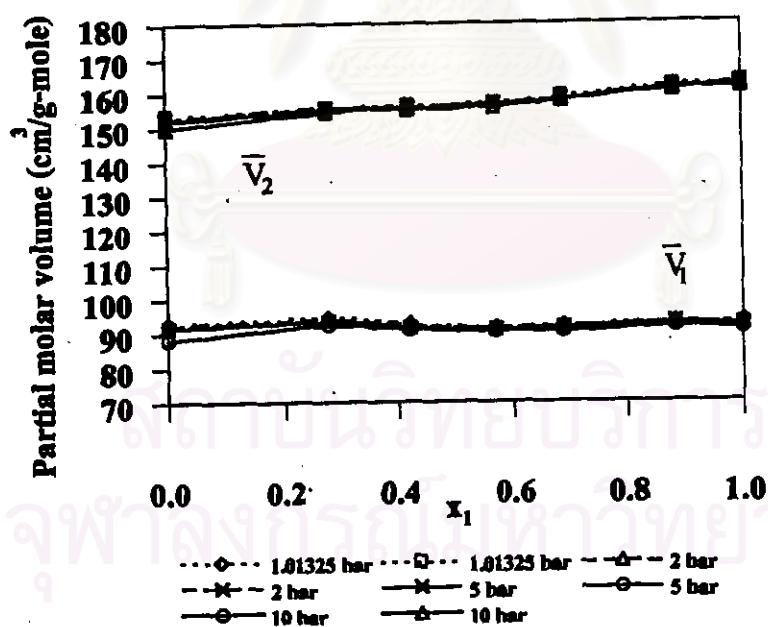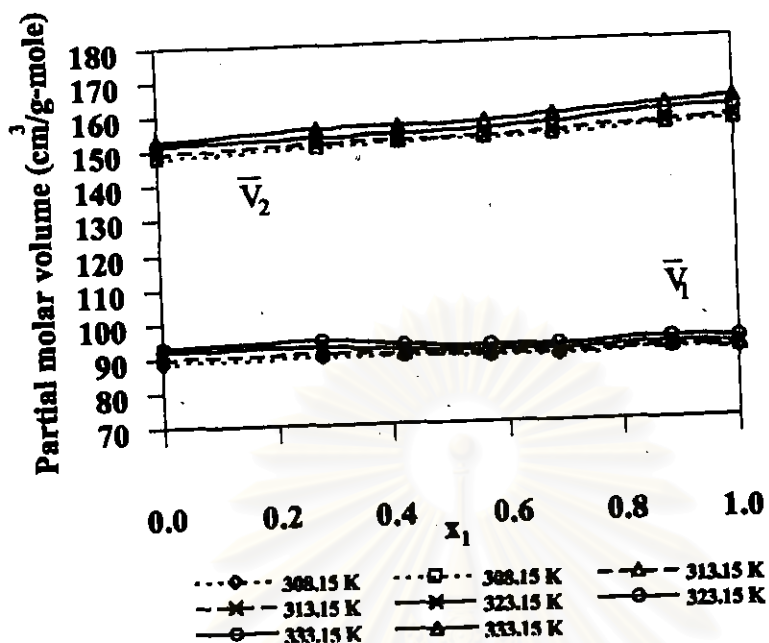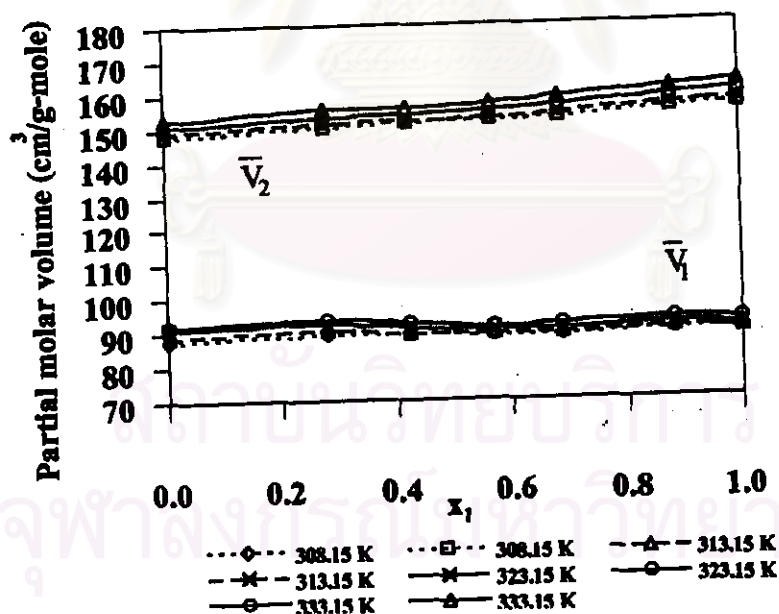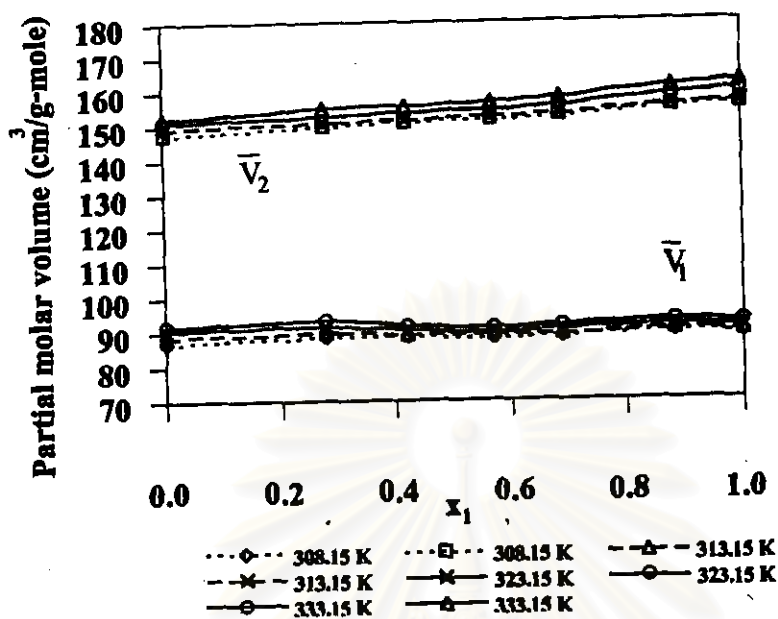
Figure 6.75 Partial molar volumes of benzene (1) and n-heptane (2) system at 5 bar.
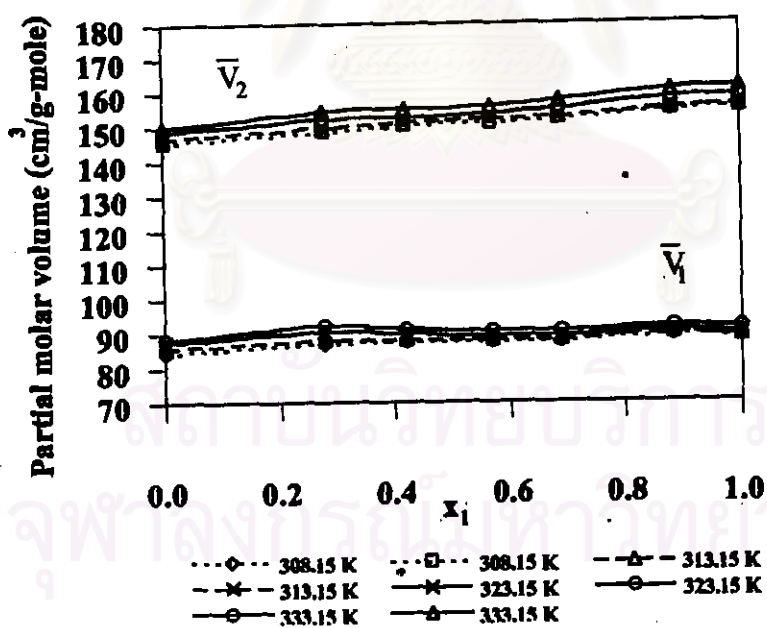

Figure 6.76 Partial molar volumes of benzene (1) and n-heptane (2) system at 10 bar.

Table 6.27 Partial molar volumes (cm^3/g-mole) of benzene (1), cyclohexane (2) and n-heptane (3) system at 308.15 K.

x_1	x_2	1.01325 bar			2 bar			5 bar			10 bar		
		$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$
0.2368	0.1774	90.5268	108.9809	150.0936	89.7613	108.2181	149.7050	89.4027	107.8304	149.4725	88.1278	106.5240	149.1317
0.2073	0.3413	92.8970	107.9316	150.4428	92.2203	107.3452	150.1541	91.8107	106.9766	149.9326	90.5494	105.8660	149.1495
0.2024	0.5063	96.1548	107.3189	151.2689	95.4879	106.8329	151.0423	95.0524	106.5155	150.8459	93.8175	105.6125	148.6381
0.1979	0.6526	99.9238	106.9580	152.4498	99.2873	106.5753	152.2717	98.7646	106.2695	152.0751	97.4821	105.5041	147.5514
0.3786	0.1792	90.0820	110.9352	150.5055	89.4777	110.2745	150.2273	89.0822	109.8026	149.9933	88.0985	108.6766	149.2064
0.3654	0.3361	91.4714	109.3619	150.1742	90.9480	108.8610	149.9993	90.6498	108.5478	149.8467	89.6315	107.5415	148.0903
0.3823	0.4742	93.5352	108.5569	150.1105	93.0319	108.1455	150.0185	92.7710	107.9148	149.9133	91.7829	107.0859	146.0479
0.5363	0.1391	89.4924	113.9257	151.3881	88.9007	113.1729	151.1290	88.5786	112.7062	150.9271	87.6807	111.4935	149.2684
0.5613	0.2956	89.9454	112.8271	150.5098	89.5530	112.3520	150.4239	89.2845	111.9781	150.3065	88.5162	110.9926	146.7550
0.6458	0.1980	89.2075	115.3473	151.5850	88.7490	114.7015	151.4429	88.5172	114.3103	151.3041	87.8168	113.2454	147.9644

Table 6.28 Partial molar volumes (cm^3/g-mole) of benzene (1), cyclohexane (2) and n-heptane (3) system at 313.15 K.

x_1	x_2	1.01325 bar			2 bar			5 bar			10 bar		
		$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$
0.2368	0.1774	90.9200	109.4424	150.8558	90.3885	108.9100	150.5769	90.2004	108.6880	150.4217	89.0223	107.4766	149.7455
0.2073	0.3413	93.3285	108.4152	151.2156	92.7881	107.9458	150.9780	92.5073	107.6870	150.8029	91.2958	106.6184	150.2125
0.2024	0.5063	96.5933	107.8193	152.0360	96.0639	107.4325	151.8488	95.6599	107.1370	151.6568	94.5464	106.3200	151.1990
0.1979	0.6526	100.4416	107.5275	153.2170	99.8368	107.1616	153.0440	99.5627	107.0066	152.9038	98.3448	106.2766	152.4824
0.3786	0.1792	90.6005	111.5566	151.3364	90.0017	110.9036	151.0570	89.8353	110.6734	150.9152	88.8086	109.5018	150.3604
0.3654	0.3361	91.6417	109.6357	150.8823	91.5620	109.5493	150.8356	91.3539	109.3187	150.7042	90.4436	108.4118	150.3180
0.3823	0.4742	94.2660	109.3312	150.9334	93.6289	108.8110	150.8185	93.3970	108.6020	150.7119	92.4938	107.8382	150.4595
0.5363	0.1391	89.8711	114.4266	152.1763	89.4575	113.8951	151.9848	89.2982	113.6260	151.8420	88.3520	112.3549	151.3349
0.5613	0.2956	90.3692	113.3697	151.3125	90.0354	112.9635	151.2320	89.8765	112.7139	151.1260	89.1512	111.7771	150.8755
0.6458	0.1980	89.6151	115.8883	152.3918	89.2900	115.4248	152.2802	89.1708	115.1824	152.1642	88.4847	114.1369	151.8485

Table 6.29 Partial molar volumes (cm^3/g-mole) of benzene (1), cyclohexane (2) and n-heptane (3) system at 323.15 K.

x_1	x_2	1.01325 bar			2 bar			5 bar			10 bar		
		$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$
0.2368	0.1774	92.7852	111.2468	152.7556	92.0438	110.5177	152.3772	91.7371	110.1805	152.1581	90.5444	108.9653	151.4686
0.2073	0.3413	95.1218	109.9038	153.0887	94.4724	109.3483	152.8065	94.1346	109.0443	152.6008	93.0119	108.0642	152.0353
0.2024	0.5063	98.4992	109.2043	154.0564	97.8975	108.7709	153.8420	97.4695	108.4638	153.6315	96.2519	107.5845	153.1216
0.1979	0.6526	102.5526	108.9108	155.4623	101.8611	108.4977	155.2585	101.4113	108.2409	155.0593	100.2044	107.5300	154.6113
0.3786	0.1792	91.9952	113.2117	153.2470	91.4201	112.5875	152.9749	91.1771	112.2718	152.7897	90.0532	110.9986	152.1769
0.3654	0.3361	93.4926	111.5213	153.0019	92.9723	111.0271	152.8180	92.6933	110.7290	152.6525	91.6960	109.7439	152.2165
0.3823	0.4742	95.5206	110.5752	153.1099	95.0196	110.1669	153.0019	94.7934	109.9618	152.8789	93.8660	109.1806	152.5862
0.5363	0.1391	91.1133	116.3658	154.3427	90.6231	115.7389	154.1122	90.4041	115.3863	153.9297	89.5467	114.2092	153.4288
0.5613	0.2956	91.4626	115.0696	153.6682	91.0912	114.6172	153.5669	90.8992	114.3198	153.4348	90.2236	113.4249	153.1497
0.6458	0.1980	90.7779	117.9833	154.8808	90.3530	117.3802	154.7261	90.1610	117.0267	154.5691	89.4579	115.9364	154.2023

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Table 6.30 Partial molar volumes (cm^3/g-mole) of benzene (1), cyclohexane (2) and n-heptane (3) system at 333.15 K.

x_1	x_2	1.01325 bar			2 bar			5 bar			10 bar		
		$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$	$\overline{V_1}$	$\overline{V_2}$	$\overline{V_3}$
0.2368	0.1774	93.7882	112.7363	154.5256	93.1946	112.1450	154.2125	92.9235	111.8339	153.9986	91.7764	110.6467	153.3100
0.2073	0.3413	96.2543	111.3175	154.9702	95.6664	110.8106	154.7059	95.3137	110.4891	154.4812	94.2176	109.5216	153.9028
0.2024	0.5063	99.6582	110.4561	156.0813	99.0069	109.9846	155.8416	98.7347	109.7887	155.6653	97.5512	108.9295	155.1362
0.1979	0.6526	103.8308	110.1168	157.7144	103.1302	109.6964	157.4946	102.7695	109.4942	157.2992	101.3991	108.6811	156.7688
0.3786	0.1792	92.9558	114.7605	155.1105	92.4196	114.1723	154.8481	92.1525	113.8211	154.6386	91.1328	112.6390	154.0447
0.3654	0.3361	94.6071	113.0412	155.0091	94.0236	112.4846	154.7964	93.6245	112.0681	154.5776	92.7618	111.1945	154.1529
0.3823	0.4742	96.6603	111.9629	155.3008	96.1315	111.5297	155.1744	95.9465	111.3530	155.0399	95.0012	110.5484	154.7044
0.5363	0.1391	92.3699	118.4219	156.4514	91.7590	117.6424	156.1625	91.4723	117.1943	155.9359	90.5908	115.9675	155.3956
0.5613	0.2956	92.7722	117.0143	155.8910	92.2092	116.3378	155.7388	92.0219	116.0350	155.5884	91.2879	115.0567	155.2537
0.6458	0.1980	91.7744	119.7252	157.0393	91.3124	119.0688	156.8614	91.1579	118.7532	156.6967	90.4683	117.6625	156.2973

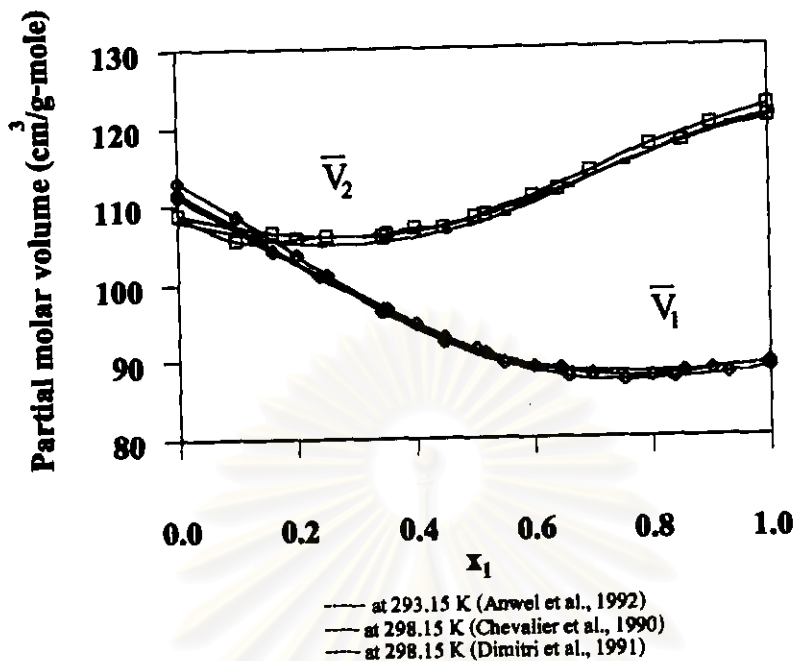สถาบันวิทยบริการ
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Figure 6.77 Partial molar volumes of benzene (1) and cyclohexane (2) system at 1.01325 bar, (Chevalier et al., 1990, Dimitri et al., 1991 and Anwel et al., 1992).
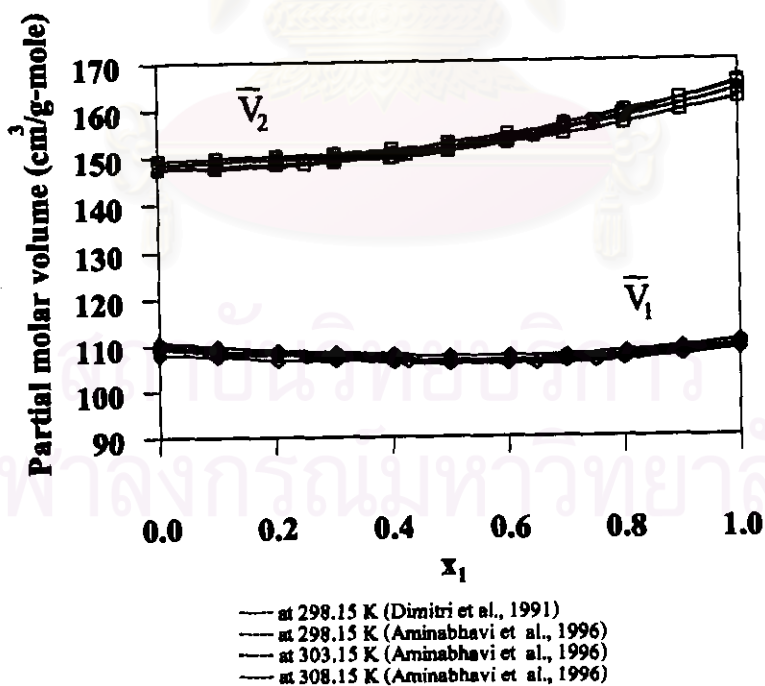

Figure 6.78 Partial molar volumes of cyclohexane (1) and n-heptane (2) system at 1.01325 bar, (Dimitri et al.,1991 and Aminabhavi et al., 1996).
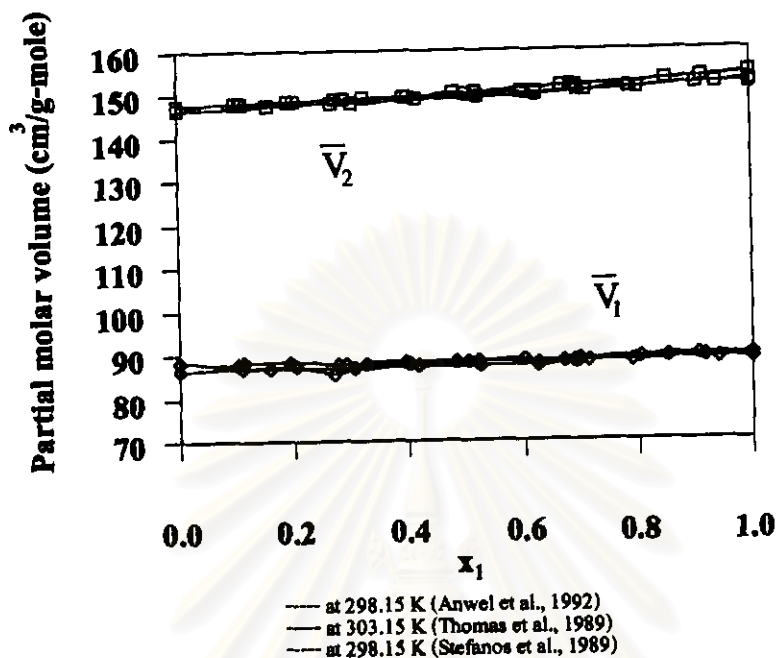
Figure 6.79   Partial molar volumes of benzene (1) and n-heptane (2) system

at 1.01325 bar, (Stefanos et al., 1989, Thomas et al., 1989 and

Anwel et al., 1992).