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Effective characterization of specific hydrocarbon and their mixtures using LIR

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Linear Isotherm Regularity (LIR) is a statistical based valid method for a wide range of applications. This method depends much on the *p-v-T* experimental data. The determined data for certain hydrocarbons and their mixtures studied in this paper are scares. Hence we try to use LIR method for the prediction of the packing fraction $\eta = \dfrac{\pi}{6}\rho\sigma^3$ and structure factor *S(Q)*, of specific pure hydrocarbon compounds and their mixtures. The temperature dependency of the hard-core diameter of the pure hydrocarbon compounds and their mixtures has been determined by the calculated packing fraction values. Even, the temperature dependence of the nano hardcore diameter is taken care by this method. The structure factors, of these compounds have been determined using the calculated packing fraction. The encouraging results, backs the application of LIR.

Key words: LIR, nanoscales, structure factor, packing fraction, hydrocarbons.

INTRODUCTION

The packing factor η is of much importance because of its direct connection with all the important equation of states. Therefore, the dependence of η on pressure, volume and temperature is also evident. Numerous studies are available to handle the variation of η with temperature and volume. The hard sphere model is one of the simplest representations of the condensed matter systems. Such systems are very well described by the estimation of packing fraction of hard spheres which includes colloids, amorphous metals and simple liquids. In most real systems, the hard core diameter of the components is the temperature dependent that must be determined.

There are other quantities in statistical mechanics which are related to the packing fraction. The structure factor, *S(Q)*, is one such important properties (Singh and Holz, 1983 ; Khanna and McLaughlin, 1989 ; Hayter et al. 1983; Nigam and Khanna, 1991), which is a measure of interparticle correlation in reciprocal space. Adopting the hard-sphere model, however, the structure factor has been theoretically derived, dependent on the packing fraction, η, (Wertheim, 1963; Thiele, 1963). So far, the structure factor has been obtained by adjusting the hard core diameter to fit-in the experimentally observed structure factor. A novel and simple method of determining the packing fraction from easily measurable ultrasonic velocity in any liquid or liquid mixture at any given temperature has been established by Ravi et al. (2001). They used the obtained packing fraction in the structure factor expression, assuming the hard sphere model, since the behavior of simple liquids is the same as the hard-sphere fluids in the high density and *S(Q)* is insensitive to details of potential. The method proposed by Ravi et al. has three restrictions, which states that the measurable ultrasonic velocity values and the heat capacity ratio, $\gamma = C_p/C_V$, must be existed in the same temperature, while they are not usually available, and also the experimental ultrasonic velocity values are scares for liquids at high density and high temperature.

In the present paper, an attempt has been made to

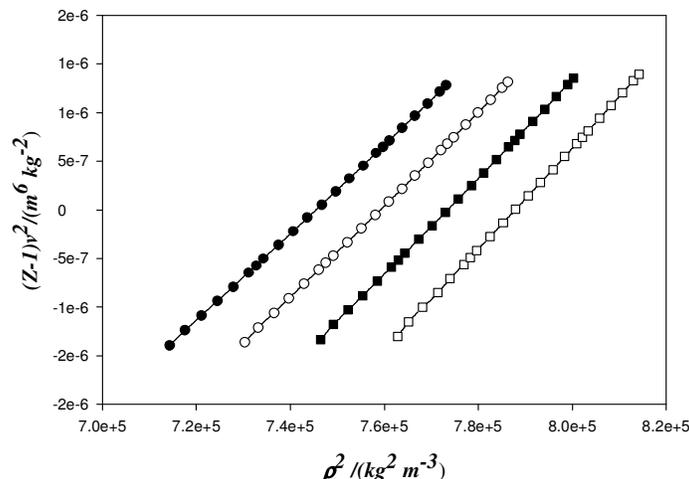*Corresponding author. E-mail: suga_ravi@yahoo.co.in.

Figure 1. The isotherms of $(Z-1)v^2$ vs ρ^2 for chlorohexane at $\bullet$) 328.15K, $\circ$) 318.15K, $\blacksquare$) 308.15K and $\square$) 298.15K.

predict the packing fraction of simple liquids using Linear Isotherm Regularity (LIR). The proposed method is applicable for all fluids that obey the LIR. The parameters existing in LIR are composition and temperature dependent and are also related to the repulsion and the attraction of the intermolecular potential in the dense fluids. The structure factor, $S(Q)$, and the temperature dependency of the hard core diameter of simple hydrocarbons and their mixtures have been predicted using their calculated packing fraction. It is worth noting that the packing fraction of numerous number of dense fluids can be predicted using this method because of the validity of the LIR for the wide range of dense fluids. The paper is organized as follow. The preparation of the LIR for the hydrocarbon compounds and their mixtures are shown in "LIR for simple hydrocarbon compounds and their mixtures". Our method for the estimation of the packing fraction is presented and applied for some of the hydrocarbon compounds in "Determination of the packing fraction using the LIR". We obtain that the hard core diameter of a mixture obeys a mixing rule and can be predicted by our method. In "Prediction of the structure factor of pure and mixture hydrocarbon compounds using the LIR", the structure factor of some of the hydrocarbon compounds is evaluated using the calculated packing fractions.

LIR FOR SIMPLE HYDROCARBON COMPOUNDS AND THEIR MIXTURES

The particles distribution in dense system is not random, like as gases, and not regular, like as solids. For this reason, investigation of such systems is difficult from the molecular point of view. However, it has been proved that all of these systems follow certain general unique rules (Huang and O'Connell, 1987; Song and Mason, 1989).

Linear Isotherm Regularity (LIR) which has a statistical mechanical base is applicable for dense fluids. LIR was derived using the Lennard-Jones potential and a simple lattice model (Parsafar and Mason, 1993). According to this regularity, the isotherms of a dense fluid follow the relation as:

$$(Z-1)v^2 = A(T) + B(T)\rho^2 \qquad (1)$$

where Z is the compressibility factor, $\rho = 1/v$ is the molar density and A and B are the temperature dependent parameters of the LIR which are related to the attraction and the repulsion contributions of the potential, respectively. The temperature dependency of A and B is given as:

$$A = A'' + \frac{A'}{RT} \qquad B = B'' + \frac{B'}{RT} \qquad (2)$$

The constants A' and B' are also related to the intermolecular attraction and repulsion, respectively, and the constants A'' and B'' are related to the non-ideal contribution of the thermal pressure.

LIR is valid for a wide range of compounds like as non-polar, polar, dense, hydrogen-bonded and quantum fluids, as well as fluid mixtures. Parameters A and B are the composition dependent for mixtures of dense fluids as follow (Parsafar and Mason, 1994):

$$B = x_1^2 B_{11} + 2x_1 x_2 B_{12} + x_2^2 B_{22} \qquad (3)$$

$$A/B = x_1^2 \left(A/B\right)_{11} + 2x_1 x_2 \left(A/B\right)_{12} + x_2^2 \left(A/B\right)_{22} \qquad (4)$$

where the index 12 shows a hypothetical pure fluid having 1 to 2 interactions.

Table 1. Temperature dependent parameters of the LIR, *A* and *B*, for pure compounds. R^2 is the coefficient of determination.

Compound	*T* (K)	$A \times 10^5$ (m^6 kg^{-2})	$B \times 10^{11}$ (m^{12} kg^{-4})	R^2
Decane	303	-7.40	1.38	
	323	-6.80	1.32	0.99
	353	-6.04	1.27	
Nonane	298	-6.90	1.31	
	308	-6.46	1.25	0.99
	318	-6.06	1.20	
	328	-5.60	1.13	
Octane	298	-5.59	11.03	
	308	-5.22	10.51	
	318	-4.87	9.99	0.99
	328	-4.57	9.55	
Heptane	298	-2.77	3.40	
	308	-2.59	3.25	
	318	-2.43	3.12	0.99
	328	-2.27	2.97	
Hexane	298	-5.40	1.19	
	323	-4.80	1.11	0.97
	348	-4.10	1.02	
Chlorohexane	298	-2.93	3.68	
	308	-2.75	3.51	
	318	-2.60	3.37	0.99
	328	-2.44	3.22	
Hexadecane	323	-1.17	2.02	
	348	-1.08	1.94	0.98
	373	-1.007	1.87	
Propane	380	-1.35	6.02	
	400	-1.20	5.76	
	420	-1.17	5.53	0.97
	440	-1.12	5.27	
Isobutane	280	-2.94	8.06	
	300	-2.50	7.22	
	320	-2.13	6.52	0.99
	340	-1.84	5.98	
Cyclohexane	288	-3.20	2.96	
	298	-3.32	2.76	0.98
	313	-3.44	2.56	
Benzene	293	-2.83	3.50	
	303	-2.64	3.33	0.99
	313	-2.48	3.19	
Nitrobenzene	293	-3.11	2.10	
	303	-2.93	2.01	0.99
	313	-2.80	1.98	

Application of the LIR for pure hydrocarbon compounds is investigated by plotting the isotherms of $(Z-1)v^2$ versus ρ^2. As an example, Figure 1 shows such plots for chlorohexane in the different temperatures using the *p-v-T* experimental data. The Linear regression of the experimental $(Z-1)v^2$ versus ρ^2 gives the values of *A* and *B*. The resulted data for *A* and *B* are listed in Table 1 for some pure hydrocarbon compounds (Abdulagatov and Azizov, 2006; Glos et al., 2004; Mutalik et al., 2006; Claus et al., 2003). The coefficients of determination of the linear regressions are reported in the last column of Table 1. The temperature dependency of the LIR parameters can be obtained from the plot of *A* and *B* versus $1/T$. Figure 2 represents such plots for chlorohexane and, the values of *A'*, *A''*, *B'* and *B''* in Equation (2) are consequently obtained from the slope and the intercept of these plots. The results are summarized in Table 2 for some hydrocarbon compounds. The coefficient of determination of each plot is also shown in the last column of Table 2.

The investigation is extended for mixtures. The results of such investigations have been listed in Table 3 for heptane-octane, propane-isobutane, octane-chlorohexane, nonane-cyclohexane, benzene-nitrobenzene and octane-benzene mixtures which their *p-v-T* experimental data are available.(Morávková et al., 2006; Miyamoto et al., 2007; Miyamoto and Uematsu, 2007; Naziev et al., 2005; Morávková et al., 2008).

DETERMINATION OF THE PACKING FRACTION USING THE LIR

In the previous part, we have shown that the LIR is applicable for the hydrocarbon compounds which are used in this work as well as the liquids that are previously reported in densities greater than the Boyle density (Farzi and Safari, 2005). It has already been proved that the LIR can predict the thermodynamic properties of the dense fluids in good accordance with the experiment (Parsafar and Kermanpour, 1992). For instance, the isothermal compressibility, $\kappa_T = \frac{1}{\rho}(\frac{\partial \rho}{\partial P})_T$, can be derived from the LIR as:

$$\kappa_T = \frac{1}{k_B T(3A\rho^3 + 5B\rho^5 + \rho)} \tag{5}$$

where k_B is Boltzmann constant.

The standard relation for structure factor in the zero limit of the momentum transfer parameter that is, Q→0 *S(0)* is (Wertheim, 1963; Thiele, 1963);
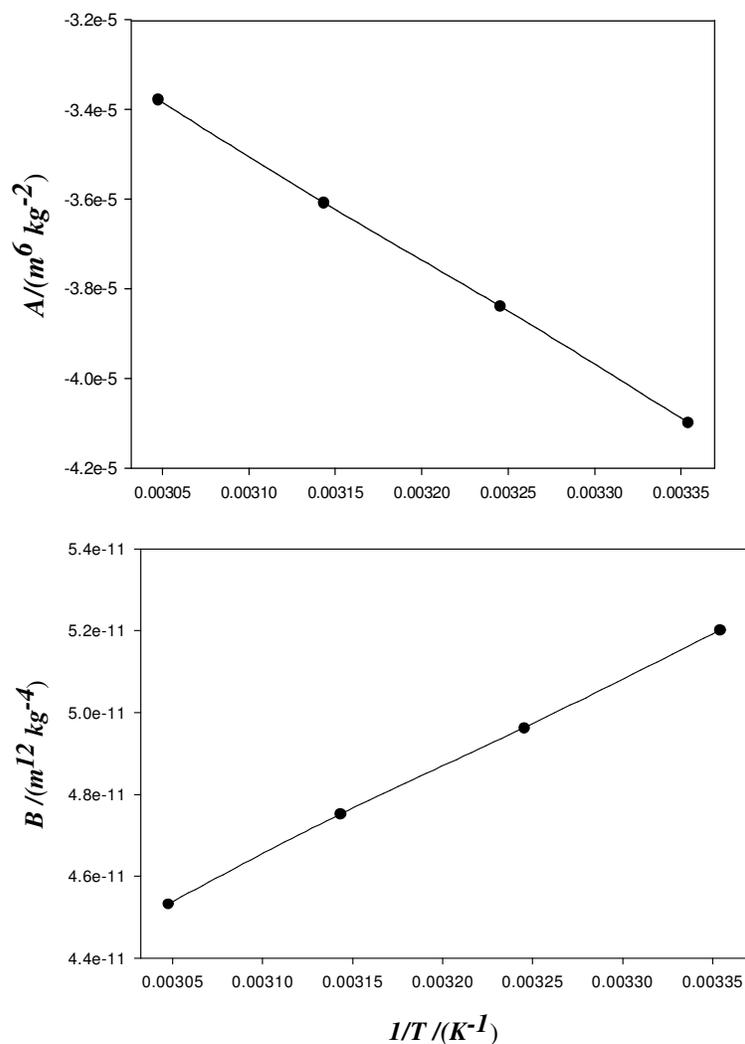
$$S(0) = \rho k_B T \kappa_T \tag{6}$$

Figure 2. Temperature dependency of the LIR parameters *A* and *B*.

Table 2. The constants of equation (2) for pure compounds.

Compound	A"× 10^5 (m^6 kg^{-2})	B"× 10^{11} (m^{12} kg^{-4})	A'/R (m^6 kg^{-2} K)	B'/R × 10^8 (m^1 kg^{-4} K)	R^2
Decane	2.540	-6.00	0.300	-2.33	0.999
Nonane	7.200	-6.87	0.042	-5.98	0.999
Octane	3.240	-1.69	0.019	-1.68	0.998
Heptane	2.670	-1.25	0.016	-3.80	0.999
Hexane	4.096	-1.11	0.028	-3.92	0.999
Chlorohexane	3.740	-2.07	0.023	-2.17	0.998
Hexadecane	5.076	-2.49	0.039	3.52	0.999
Propane	2.037	-2.62	0.012	-3.38	0.999
Isobutane	3.840	-4.34	0.019	-3.48	0.998

Equation (5) into Equation (6) leads to

$$S(0) = \frac{1}{3A\rho^2 + 5B\rho^4 + 1} \tag{7}$$

On the other hand, Carnahan and Starling (1969) derived an expression for *S(0)* of the hard-sphere fluid as:

$$S(0) = \frac{(1-\eta)^4}{(1+2\eta)^2} \tag{8}$$

Table 3. The temperature dependent parameters of the LIR and the constants of equation (2) for some mixtures in the different mole fractions (x).

Compounds	x	T(K)	$A \times 10^5$ (m^6 kg^{-2})	$B \times 10^{11}$ (m^{12} kg^{-4})	$A' \times 10^5$ (m^6 kg^{-2})	$B' \times 10^{11}$ (m^{12} kg^{-4})	A'/R (m^6 kg^{-2} K)	$B'/R \times 10^s$ (m^{12} kg^{-4} K)	R^2
Heptane (x) $_+$ Octane(1-x)	0.28	401	-2.90	7.19	4.26	-5.77	-0.02876	5.22	0.98
		429	-2.38	6.26					
		451	-2.16	5.99					
		475	-1.78	5.22					
	0.54	409	-2.52	6.40	5.87	-1.04	-0.3595	7.34	0.99
		424	-2.55	6.75					
		447	-2.26	6.34					
		466	-1.77	5.14					
Propane(x) + Isobutane (1-x)	0.27	320	-2.54	8.04	2.56	-1.35	-0.01630	3.00	0.98
		360	-1.94	6.94					
		400	-1.50	6.15					
		420	-1.15	5.47					
	0.50	380	-1.50	6.08	6.83	-5.58	-0.01525	1.91	0.96
		400	-1.41	6.12					
		420	-1.29	6.05					
		440	-1.21	6.07					
Octane(x) + Chlorohexane (1-x)	0.39	298	-3.79	5.73	3.49	-2.38	-0.02169	2.42	0.99
		308	-3.55	5.46					
		318	-3.33	5.22					
		328	-3.12	4.98					
	0.59	298	-4.31	7.12	4.07	-3.06	-0.02497	3.04	0.99
		308	-4.03	6.79					
		318	-3.77	6.47					
		328	-3.54	6.19					
	0.79	298	-4.90	8.86	4.80	-4.03	-0.02891	3.84	0.99
		308	-4.58	8.44					
		318	-4.28	8.02					
		328	-4.02	7.69					
Octane(x) + Benzene (1-x)	0.41	298	-3.86	6.19	3.65	-2.54	-0.02237	2.61	0.99
		308	-3.61	5.91					
		318	-3.38	5.63					
		328	-3.17	5.40					

Table 3. Contd.

	0.59	298	-4.37	7.58	4.21	-3.25	-0.02557	3.23	0.99
		308	-4.09	7.24					
		318	-3.82	6.88					
		328	-3.59	6.60					
	0.79	298	-4.95	9.22	4.86	-4.13	-0.02924	3.98	0.99
		308	-4.64	8.81					
		318	-4.33	8.37					
		328	-4.06	8.01					
Nonane(x) + Cyclohexane (1-x)	0.30	298	5.06	9.27	5.07	-4.61	-0.03022	4.14	0.99
		308	4.73	8.83					
		318	4.45	8.46					
		328	4.12	7.98					
	0.59	298	5.41	9.55	5.77	-5.029	-0.03334	4.35	0.97
		308	5.05	9.09					
		318	4.73	8.69					
		328	4.38	8.20					
Benzene(x) + Nitrobenzene (1-x)	0.2	293	2.78	2.93	0.975	-5.79	-0.01101	0.69	0.99
		303	2.66	2.85					
		313	2.54	2.78					
	0.4	293	3.08	2.85	1.30	-1.86	-1.01284	0.78	0.99
		303	2.95	2.76					
		313	2.80	2.68					
	0.6	293	2.60	2.09	1.16	-5.79	-0.01102	0.60	0.99
		303	2.47	2.03					
		313	2.36	1.96					

where η is the packing fraction, $\eta = \frac{\pi}{6}\rho\sigma^3$.

The structure factor $S(Q)$ is insensitive to details of the potential and in the high density the simple liquids behave like as the hard sphere fluids.

Therefore, in this work by adopting the hard sphere model for the structure factor of the hydrocarbon compounds in the high density which the LIR is satisfied, the packing fraction, η, can be obtained by replacing Equation (7) into left side of Equation (8), namely:

$$\frac{1}{3A\rho^2 + 5B\rho^4 + 1} = \frac{(1-\eta)^4}{(1+2\eta)^2} \tag{9}$$

Equation (9) has four important features:

a) Since A and B parameters of the LIR are

temperature and composition dependent, the packing fraction can also be obtained as a function of temperature and composition.

b) *A* and *B* parameters have been resulted from the *p-v-T* experimental data which is available for most compounds. Therefore the packing fraction of these compounds can also be obtained in a wide range of temperature and density.

c) Replacing *A′*, *A″*, *B′* and *B″* in Equation (2), and the results in Equation (1), the density or the pressure and consequently, the packing fraction of each interested compound can be calculated in each temperature which are not reported in literatures.

d) In this method the packing fraction indirectly adjusts itself to produce the experimental values of *S(0)*, thus the calculated packing fraction is not the hard sphere packing fraction, however, it is a special value for each fluid.

e) Since *A* and *B* are related to the attraction and the repulsion parts of the potential, this relation shows the correlation of the packing fraction to such forces.

When the calculated *A* and *B* of some simple hydrocarbons, which are listed in Table 1, are replaced into Equation (9), the packing fraction in each temperature has been obtained. The results of these calculations are summarized in Table 4 for some pure hydrocarbon compounds. The results show that the packing fraction decreases by the temperature.

It is interesting to note that the temperature dependency of the hard core diameter can also be determined using the calculated packing fraction value for each temperature. Such calculations are extended for the mixtures of hydrocarbon compounds. The structure factor of the mixtures, *S(0)$_{mix}$* can be obtained using Carnahan and Starling (1969) relation as:

$$S_{mix}(0) = \zeta_0 \left[\frac{\zeta_0}{(1-\zeta_3)^2} + \frac{6\zeta_1\zeta_2}{(1-\zeta_3)^3} + \frac{\zeta_2^3(9-4\zeta_3\zeta_3^2)}{(1-\zeta_3)^4} \right]^{-1} \quad (10)$$

where

$$\zeta_m = \frac{\pi}{6} \sum_{i=1}^{2} x_i \sigma_i^m \quad (11)$$

where *m*=0, 1, 2, 3 and *x$_i$* is the mole fraction of each components (*i*) of the mixture. Also Equation (8) can safely be used for mixtures as factors in the zero limit of momentum transfer which is calculated by the experimental data, our assumption and Carnahan and Starling expression, respectively.

$$S_{mix}(0) = \frac{(1-\eta_{mix})^4}{(1+2\eta_{mix})^2} \quad (12)$$

In most cases, this assumption gives the better results for

Table 4. The calculated packing fractions and the hard core diameters of some pure hydrocarbon compounds.

Compound	*T*(K)	*P* (kg m^{-3})	η	σ (A^o)
Heptane	401.4	882.6	0.4500	5.44
	429.3	871.8	0.4396	5.42
	451.2	860.9	0.4287	5.40
	475.8	840.6	0.4087	5.36
Decane	303.5	722.5	0.5259	6.84
	323.5	707.4	0.5181	6.87
	353.5	703.0	0.5113	6.86
Propane	320	613.6	0.4149	4.55
	360	604.2	0.4057	4.54
	400	595.6	0.4000	4.54
	420	587.6	0.3892	4.48
Isobutane	380	575.58	0.3495	4.81
	400	551.78	0.3119	4.70
	420	525.78	0.2623	4.49
	440	503.72	0.2352	4.38
Chlorohexane	298.15	873.4	0.4915	5.98
	308.15	864.0	0.4857	5.97
	318.15	856.6	0.4748	5.95
	328.15	845.2	0.4649	5.93
Nonane	298.15	713.6	0.5035	6.61
	308.15	705.8	0.4942	6.59
	318.15	698.2	0.4843	6.64
	328.15	690.5	0.4734	6.66

Table 5 shows such results for octane-chlorohaxane and octane- benzene mixtures in the different mole fractions. In this table *S$_{mix}$(0)$_1$*, *S$_{mix}$(0)$_2$* and *S$_{mix}$(0)$_3$* are the structure in the zero limit of momentum transfer which is calculated by the experimental data, our assumption and Carnahan and Starling expression, respectively.

The percent deviations of *S$_{mix}$(0)$_2$* and *S$_{mix}$(0)$_3$* from the experimental values show that our assumption gives the better results with respect to Carnahan and Starling expression. Therefore, the packing fraction and the hard core diameter of some mixtures have been calculated using this assumption. The results are given in Table 6.

Similarly the mixing rule can be applied to the hard core diameter as:

$$\sigma_{mix} = \sum_i \sum_j \sigma_{ij} x_i x_j = \sigma_{11} x_1^2 + 2\sigma_{12} x_1 x_2 + \sigma_{22} x_2^2 \quad (13)$$

where *x$_1$*, *x$_2$* are the mole fractions of components 1 and 2, respectively, and *σ$_{mix}$* is the hard core diameter of

Table 5. Comparison of the experimental structure factor with the calculated structure factors by our procedure (equation (12)) and Carnahan Starling expression (equation (10)) for mixtures.

Mixture	x	$S_{mix}(0)_1$	$S_{mix}(0)_2$	$S_{mix}(0)_3$	|deviation| (%) of $S_{mix}(0)_2$	|deviation| (%) of $S_{mix}(0)_3$
	0.39	0.022994	0.022641	0.023278	1.321	1.456
Octane(x) + Chlorohexane(1-x)	0.59	0.022263	0.021728	0.022442	3.986	0.831
	0.79	0.021367	0.020751	0.022048	2.883	3.187
	0.41	0.025004	0.023860	0.031039	4.575	24.14
Octane(x)+Benzene(1-x)	0.59	0.024011	0.022641	0.027999	5.706	16.61
	0.79	0.022834	0.021256	0.024800	6.911	8.61

their mixture. The hard core diameters of the pure components 1 and 2 are σ_{11} and σ_{22}, respectively, and σ_{12} can be calculated from the combining rule, $\frac{\sigma_{11}+\sigma_{22}}{2}$.

In order to test the validity of Equation (13) for our results in each mole fraction, σ_{mix} is calculated by σ_{11} and σ_{22} which are given in the last column of Table 4. The comparison of σ_{mix} which is obtained by our procedure (last column, Table 6) with those are calculated by Equation (13) is given in Table 7 for benzene-nitrobenzene, octane-chlorohexane and octane-benzene mixtures in the different mole fractions. The percent deviation of Equation (13) from the listed values in Table 4 is reported in the last column of Table 7. It must be noticed that these deviations are very small and they confirm the good precision of our procedure in the calculation of the packing fraction.

PREDICTION OF THE STRUCTURE FACTOR OF PURE AND MIXTURE HYDROCARBON COMPOUNDS USING THE LIR

In this part, the structure factor of the pure and the mixture hydrocarbon compounds has been calculated using the values of η which are obtained in the previous part. Ashcroft and Lekner (1966) have established an expression for direct correlation function $C(Q)$ of the hard sphere fluid as:

$$C_{PY}(Q)=\frac{-4\eta}{Q(1-\eta)^4}\int_0^\sigma r\sin Qr\left[\alpha+\beta\left(\frac{r}{\sigma}\right)+\gamma\left(\frac{r}{\sigma}\right)^3\right]dr \quad (14)$$

where

$$\alpha=(1+2\eta)^2, \quad \beta=-6\eta(1+\eta/2)^2, \quad \gamma=(\eta/2)(1+2\eta)^2 \quad (15)$$

The result of integration in Equation (14) was given as (Block et al., 1976)

$$C_{PY}(Q)=\frac{-24\eta}{x^6\rho}\left\{\begin{array}{l}\alpha x^3(\sin x-x\cos x)+\beta x^2[2x\sin x-(x^2-2)\cos x-2]\\+\gamma(4x^3-24x)\sin x-(x^4-12x^2+24)\cos x-24]\end{array}\right\} \quad (16)$$

where $x=Q\sigma$ and Q is the momentum transfer parameter.

The static structure factor $S(Q)$ is related to $C(Q)$ as:

$$S(Q)=[1-\rho C(Q)]^{-1} \quad (17)$$

When the calculated values of the packing fraction of the pure hydrocarbon compounds and their mixtures which is given in Tables 4 and 6 are fitted Equation (15) and the result in Equation (17), their structure factor can be obtained as a function of Q. Figure 3 represents the calculated structure factors for the pure compounds such as decane, nonane, octane,…..The position of the principal maximum, Q_{max}, for the pure compounds are given in Table 8 along with their packing fractions. From Figure 3 and Table 8, it is found that $S(Q)_{max}$ gradually shifts as the chain length of the hydrocarbons and the packing fraction increased. The variation of $S(Q)_{max}$ with Q_{max} is plotted in Figure 4. The nearest neighbor particle distance, d_c, is related to the main peak position of $S(Q)$ by Bragg's relation as:

$$d_c=(3/2)^{0.5}\frac{2\pi}{Q_{max}} \quad (18)$$

It is expected that the nearest neighbor particle distance, d_c, decreases when the packing fraction or increases. The calculated values of d_c using Bragg's relation are given in the last column of Table 8. It is observable that

Table 6. The calculated packing fraction and the hard core diameter of some mixtures in the different mole fractions and the different temperatures.

Compound	x	T(K)	P (Kgm^{-3})	η	σ (A°)
Heptane(x) + Octane(1-x)	0.28	401.4	585.6	0.3268	5.80
		429.3	565.6	0.3029	5.72
		451.2	539.5	0.2577	5.50
		475.8	515.8	0.2127	5.24
	0.54	409.5	598.0	0.3400	5.76
		424.4	588.7	0.3411	5.79
		447.3	566.0	0.3124	5.70
		466.7	538.3	0.2514	5.39
Propane(x) + Isobutane(1-x)	0.27	320	673.0	0.4727	4.93
		360	654.6	0.4508	4.90
		400	636.1	0.4312	4.87
		420	620.8	0.4139	4.85
	0.50	380	636.2	0.4292	4.74
		400	627.0	0.4262	4.76
		420	619.2	0.4226	4.77
		440	611.3	0.4197	4.78
Octane(x) + Chlorohexane(1-x)	0.39	298.15	796.69	0.4876	6.11
		308.15	787.75	0.4773	6.09
		318.15	778.92	0.4675	6.07
		328.15	770.08	0.4572	6.05
	0.59	298.15	762.0	0.4857	6.16
		308.15	753.3	0.4754	6.15
		318.15	744.8	0.4785	6.14
Benzene(x) + Nitrobenzene(1-x)	0.2	293.15	954.6	0.4676	5.64
		303.15	954.8	0.4607	5.63
		313.15	935.4	0.4534	5.62
	0.4	293.15	1024.2	0.4949	5.44
		303.15	1013.9	0.4826	5.41
		313.15	1004.4	0.4771	5.40
	0.6	293.15	1096.5	0.4905	5.14
		303.15	1085.7	0.4838	5.13
		313.15	1076.7	0.4760	5.12

the greater d_c is related to the smaller Q_{max} which is related to the greater packing fraction, as we expected. Then, our procedure can at least predict the packing fraction qualitatively.

The structure factors of ethanol-methylcyclohexan and hexane-hexadecane,… are calculated as a function of x (or Q) through this procedure. For example, $S(Q)_{max}$ versus Q_{max} and mole fraction (x) are plotted forethanol-methylcyclohexane mixture in different temperatures and mole fractions in Figures 5 and 6,

respectively. It is observable that the $S(Q)$ increases when Q_{max} and the mole fraction increase.

EXTENSION TO NANOSCALES

As indicated in the equation for the packing fraction $\eta = \dfrac{\pi}{6} \rho \sigma^3$, the value of hardcore diameter σ swings

Table 7. The calculated σ_{mix} (1) by our procedure and those are calculated by equation (13), σ_{mix} (2). The absolute percent deviation is given in the last column.

Mixture	x	T(K)	σ_{mix} (1), A	σ_{mix} (2), A	|deviation| (%)
Benzene (x) + Nitrobenzene (1-x)	0.2	293.15	5.647	5.450	3.49
		303.15	5.636	5.439	3.50
		313.15	5.627	5.774	2.62
	0.4	293.15	5.441	5.344	1.79
		303.15	5.413	5.330	1.53
		313.15	5.410	5.286	2.29
	0.6	293.15	5.146	5.235	1.73
		303.15	5.140	5.222	1.60
		313.15	5.127	5.152	0.49
Octane (x) + Chlorohexane (1-x)	0.39	298.15	5.530	5.532	0.03
		308.15	5.509	5.512	0.05
		318.15	5.489	5.491	0.03
		328.15	5.465	5.468	0.06
	0.59	298.15	5.710	5.713	0.04
		308.15	5.690	5.692	0.08
		318.15	5.667	5.670	0.06
		328.15	5.645	5.648	0.05
	0.79	298.15	5.893	5.894	0.01
		308.15	6.819	5.874	0.03
		318.15	5.849	5.851	0.04
		328.15	5.827	5.829	0.03
Octane (x)+Benzene (1-x)	0.41	298.15	5.690	5.642	0.84
		308.15	5.478	5.436	0.77
		318.15	5.455	5.452	0.06
		328.15	5.432	5.392	0.74
	0.59	298.15	5.891	5.857	0.57
		308.15	5.670	5.629	0.72
		318.15	5.645	5.661	0.28
		328.15	5.623	5.585	0.68
	0.79	298.15	6.081	6.070	0.18
		308.15	5.871	5.846	0.42
		318.15	5.847	5.700	0.86
		328.15	5.824	5.801	0.38

around the value of the density ρ and η. The direct estimation of the η through LIR is more reliable and it helps us to handle σ with relative ease. Hence this leads to the idea that, by adjusting the density of study we can synthesis systems with a require diameters. Also LIR study needs only the P-V-T data of the specific system of study. There are numerous studies to establish that

hydrocarbons play an important role in the synthesis of gels, materials in the nano range.

CONCLUSION

Because of the theoretical and experimental importance

Table 8. S (Q_{max}), Q_{max} and the nearest neighbor particle distance, d_c, for some hydrocarbon compounds.

Compound	S(Q_{max})	Q_{max}	η	d_c
Hexane	2.52	6.7	0.4699	1.1486
Heptane	2.84	6.8	0.4500	1.1317
Octane	3.68	6.9	0.5125	1.1153
Nonane	4.53	7.0	0.5035	1.0993
Decane	6.21	7.1	0.5259	1.0830
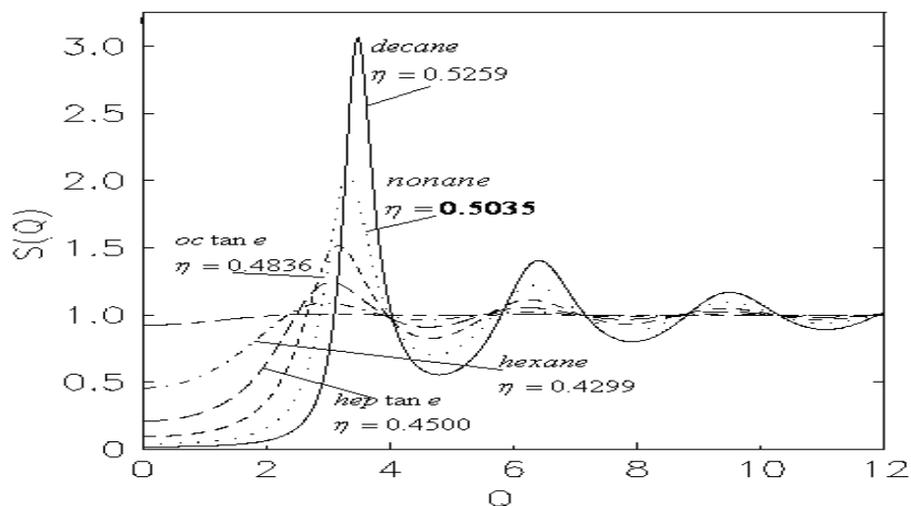
Figure 3. $S(Q)$ vs Q for decane (η = 0.5259), nonane ($\eta = 0.5035$), octane ($\eta = 0.4836$), heptane ($\eta = 0.45$) and hexane ($\eta = 0.4299$).
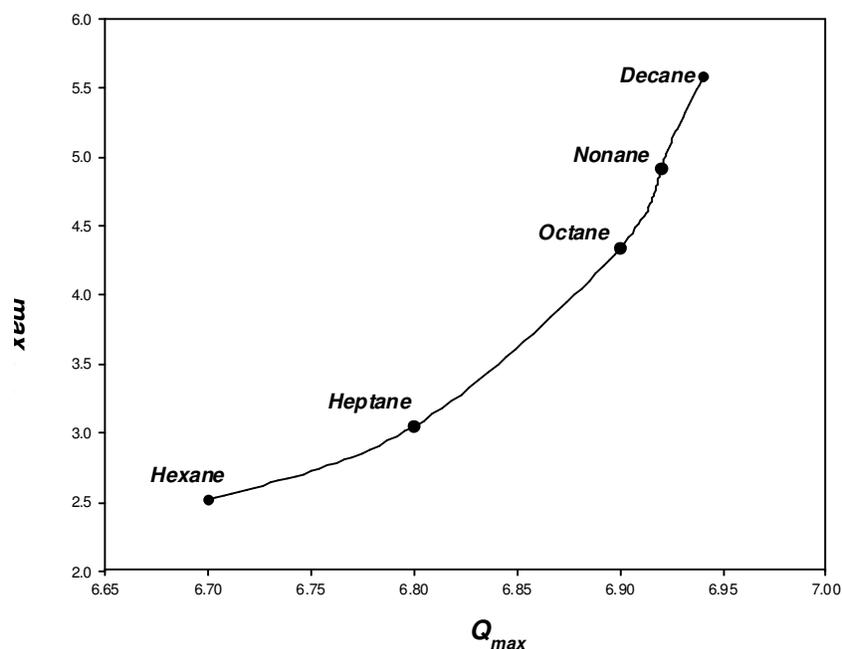
Figure 4. S(Q)$_{max}$ of some pure compounds vs. Q_{max} at T= 298.15K.
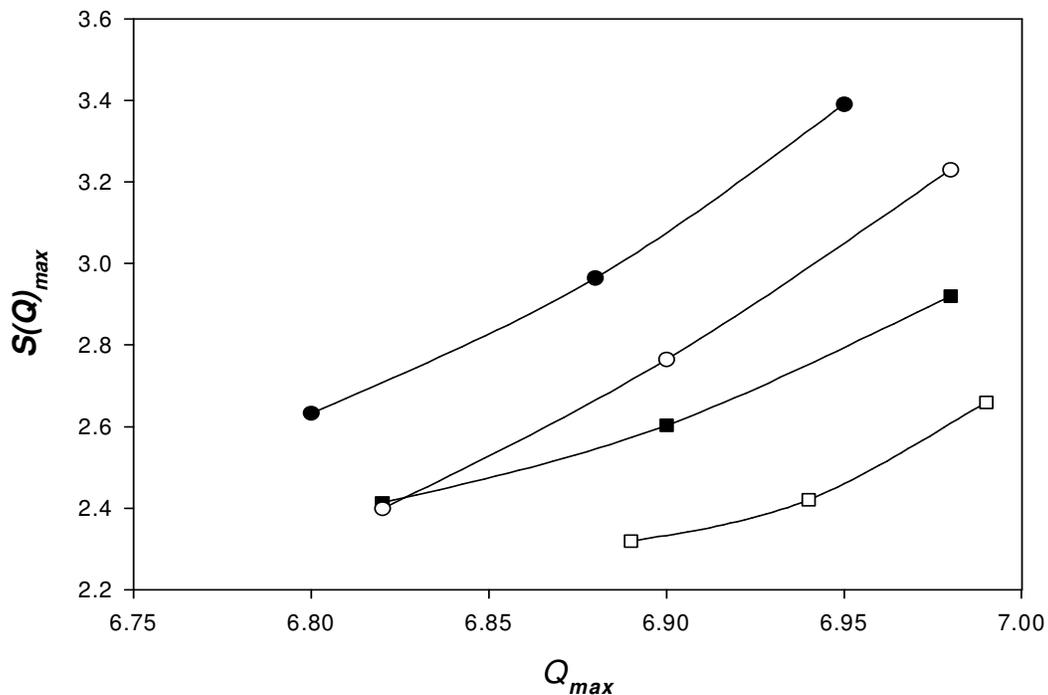
Figure 5. The plot of $S(Q)_{max}$ vs Q_{max} for ethanol (x) - methylcyclohexane(1-x) mixture in the different mole fraction and in □) 283.15K, ■) 298.15K, ○) 303.15K and ●) 313.15K.

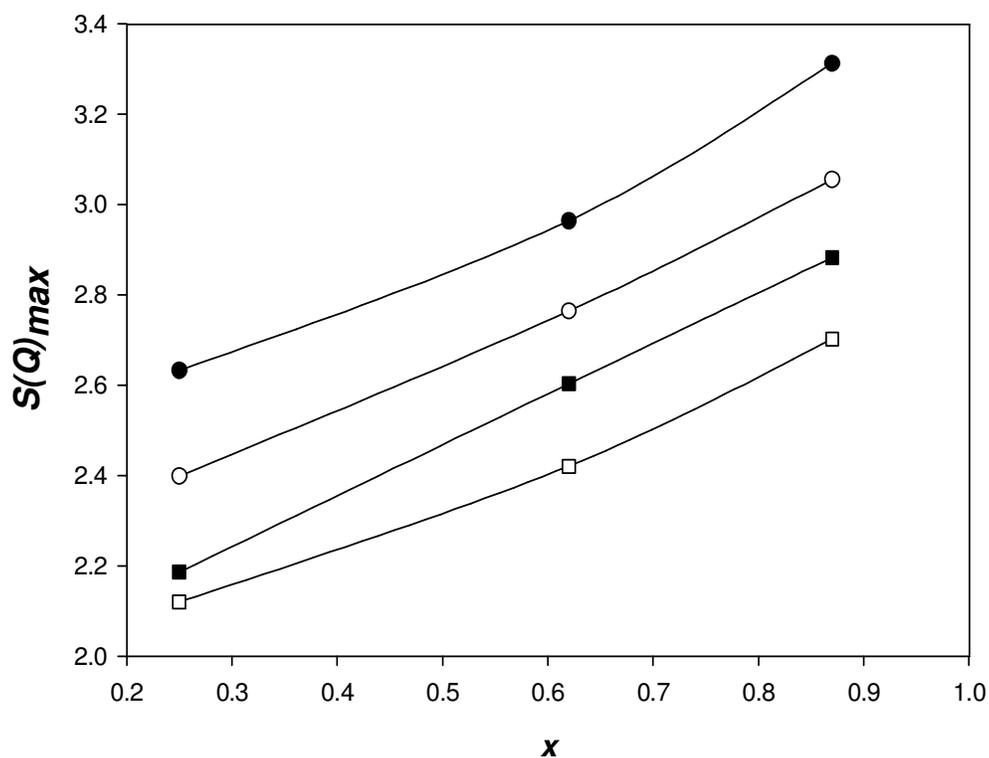**Figure 6.** The plot of $S(Q)_{max}$ vs the mole fraction (x) for ethanol (x)- methylcyclohexane(1-x) mixture in □) 283.15K, ■) 298.15K, ○) 303.15K and ●) 313.15K.

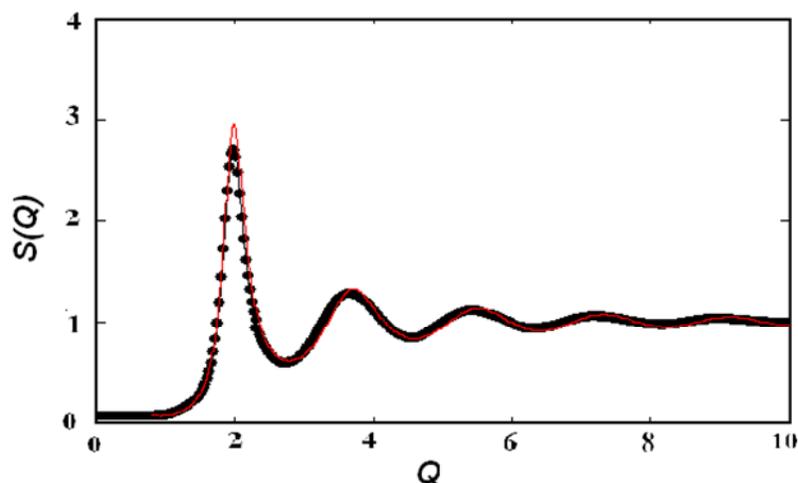**Figure 7.** The plot of calculated (—) and experimental (●) $S(Q)$ vs Q for Argon in T= 85K.

of the packing fraction in the different states, the study on the packing fraction and their dependencies on the temperature and the density through LIR are valuable. In addition, using the LIR, we have obtained the packing fraction in temperatures that the *p-v-T* experimental data are not available. Adopting the hard sphere model for these compounds, we have calculated the value of the structure factor on zero wave vectors ($Q \longrightarrow 0$) using the LIR and then it has been replaced into the same relation for the even non hard sphere model (Equation 6).

The hard core diameter has been determined as a function of temperature, using the value of the packing fraction and the density in each temperature. The hard core diameter of the pure and the mixture hydrocarbon compounds decrease with temperature. This is realizable, since when the temperature is increased, the kinetic energy of the molecules of the fluid increase and can rise to the repulsion branch of the potential curve and consequently, the hard core diameter will educe. Figures 5 to11 explains the variation of maximum value of S(Q) and the maximum Q value. It is evident from the figures that the maximum value is linear with regarding to the increase in number of carbon atoms.

We have shown that the hard core diameters of the mixtures which are determined in this method, obey from a mixing rule which is given in Equation (13). Therefore, the hard core diameter of the mixture can be estimated using the hard core diameters of its pure components which are calculated by our method. To make the method more reliable, the experimental values of S(Q) for Argon (Yarnell et al., 1973) is compared to our theoretical data in Figure 7. A perfect correlation is observed. The structure factor, *S(Q)*, can also be determined using the calculated packing fraction value. Using the calculated packing fraction the *S(Q)* versus *Q* is plotted for the

hydrocarbon compounds, those have been studied in this work. Thus we prefer to conclude that the application of LIR can safely be held good.

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