

Theory for transport properties of molecular fluids of non-spherical molecules

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Abstract : The effective diameter hard sphere theory is employed to estimate the transport properties of molecular fluids of non-spherical molecules interacting *via* the hard Gaussian overlap and Gaussian overlap with constant energy (GOCE) potentials. The transport properties (TP's) of the molecular fluids are expressed in terms of a hard sphere (HS) fluid of properly chosen effective hard sphere diameter. The explicit expressions for the shear viscosity and thermal conductivity for the HS fluid are given. The theory is applied to estimate the TP's of fluids of the hard ellipsoid of revolution, N₂ and C₆H₆. The agreement is found to be fairly good.

Keywords : Molecular fluid, transport properties, non-spherical molecules

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1. Introduction

In recent years, the transport properties (TP's) of molecular fluids composed of non-spherical molecules have been the subject of considerable interest [1,2]. Several potential models have been proposed for molecular fluids of non-spherical molecules [3]. The Gaussian overlap (GO) model of Berne and Pechukas [4] is of special interest because it provides analytically tractable expressions for studying non-spherical molecules. The GO model considers an interaction between molecules whose repulsive parts are basically ellipsoids of revolutions. The hard Gaussian overlap (HGO) model has a considerable similarity with the hard ellipsoids of revolution (HER). Thus, the HER fluid forms an important class of convex bodies and is a useful reference system for molecular fluids of non-spherical molecules.

The effective diameter hard sphere theory (EDHST) [5] is an important method for studying the TP's of dense real fluids in terms of the hard sphere fluid with state-dependent effective hard sphere diameter. Castillo and Orozco [1] and Sinha [2] have employed the EDHST for estimating the TP's of molecular fluids.

These two methods differ in determining the effective hard sphere diameter. Sinha [2] has used the method of Singh *et al* [6] to obtain the effective diameter for non-spherical molecules. This is different from that used by Castillo and Orozco [1].

In the present paper, we employ Sinha's [2] approach along with the use of effective diameter obtained by Singh *et al* [6] to estimate the TP's of some molecular fluids of non-spherical molecules.

The paper is organised as follows. In Section 2, we describe the basic theory for transport properties (TP's) of dense molecular fluids. Section 3 is devoted to estimate the TP's of the HGO fluid model. Section 4 is concerned with the TP's of the GO fluid. The concluding remarks are given in Section 5.

2. Basic theory for transport properties of dense molecular fluids

The basic idea of our approach is that the structure of a dense molecular fluid is very similar to that of a hard convex body (HCB) fluid and attractive forces play a minor role in the

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dense fluid behaviour. The HCB fluid can be expressed in terms of a hard sphere (HS) fluid of properly chosen effective hard sphere diameter de . The HS fluid can be handled with the revised Enskog theory (RET) of van Beijeren and Ernst [7] to predict the TP's such as the shear viscosity μ and thermal conductivity λ . They are expressed as

$$\mu = [g_{HS}(de)]^{-1} \left[1 + (4/5)(4\eta g_{HS}(de)) + 0.7615(4\eta g_{HS}(de))^2 \right] \mu_0, \quad (1)$$

$$\lambda = [g_{HS}(de)]^{-1} \left[1 + (6/5)(4\eta g_{HS}(de)) + 0.7575(4\eta g_{HS}(de))^2 \right] \lambda_0, \quad (2)$$

$$\text{where } \mu_0 = (5/16 \pi de^2)(\pi mkT)^{1/2}, \quad (3)$$

$$\lambda_0 = (75k/64 \pi de^2)(\pi kT/m)^{1/2}. \quad (4)$$

$\eta = (\pi \rho de^3/6)$ is the packing fraction and $g_{HS}(de)$ is the equilibrium radial distribution function (RDF) of HS fluid at the contact. Here ρ is the number density, m is the mass of a particle, T the absolute temperature and k the Boltzmann constant.

The effective hard sphere diameter de depends on the nature of the fluid models.

3. Transport properties of hard Gaussian overlap fluid

We employ this theory to estimate the TP's of a fluid of molecules interacting via the hard Gaussian overlap (HGO) potential defined as

$$U_{HGO}(r\omega_1\omega_2) = \infty, \quad r < d(\omega_1\omega_2), \\ = 0, \quad r > d(\omega_1\omega_2), \quad (5)$$

where $d(\omega_1\omega_2)$ is the distance of closest approach between two hard-core molecules, $r = |\mathbf{r}_1 - \mathbf{r}_2|$ is the centre-to-centre distance and ω_i represents the orientation of molecule i . We may take the expression of $d(\omega_1\omega_2)$ given by Berne and Pechukas [4] in terms of the Euler angles

$$d(\omega_1\omega_2) = d_0 \left[1 - \chi(\cos^2 \theta_1 + \cos^2 \theta_2 - 2\chi \cos \theta_1 \cos \theta_2 \cos \theta_{12}) \times (1 - \chi^2 \cos^2 \theta_{12})^{-1} \right]^{-1/2}, \quad (6)$$

$$\text{where } \chi = (K^2 - 1)/(K^2 + 1) \quad (7)$$

is an anisotropy parameter, K being the length-to-width ratio of a molecule i.e. $K = 2a/2b$. Here, $d_0 = 2b$ is the width of the molecule. This model is valid for oblate ($K < 1$) as well as prolate ($K > 1$) shape of arbitrary symmetry. For $K = 1$, eq. (5) simply reduces to the hard sphere potential for spherical molecules. Due to similarity, the HGO model represents the hard ellipsoid of revolution (HER) fluid.

In this case, the effective hard sphere diameter de is expressed as $de = K^{1/3}d_0$ and the RDF $g_{HS}(de)$ of the HS fluid is given by [8]

$$g_{HS}(de) = (1 - \eta/2)(1 - \eta)^{-3}, \quad (\text{method 1}) \quad (8)$$

$$\text{where } \eta = \rho v_m = (\pi/6)\rho K d_0^3 \quad (9)$$

is the packing fraction of the HGO molecule of volume v_m and density ρ .

The compressibility factor for the HGO fluid is expressed as [9]

$$Z_{HGO} = [1 + (3\alpha - 2)\eta + (3\alpha^2 - 3\alpha + 2)\eta^2 - \alpha^2\eta^2] \times (1 - \eta)^{-3}, \quad (10)$$

where α is the shape factor defined by

$$\alpha = Rs/3v_m. \quad (11)$$

Here, R is the $(1/4\pi)$ multipole of the mean curvature integral, s the surface integral and v_m is the volume of the HGO (or HER). They are given [10] for prolate HER ($K > 1$)

$$R = (1/4) \left[K + (\ln[K + (K^2 - 1)^{1/2}]) \times (K^2 - 1)^{-1/2} \right] d_0, \quad (12a)$$

$$s = (1/2) \left[1 + (K^2 \arccos K^{-1})(K^2 - 1)^{-1/2} \right] \pi d_0^2, \quad (12b)$$

$$v_m = \pi K d_0^3/6, \quad (12c)$$

and for oblate HER ($K < 1$)

$$R = (1/4) \left[K + (\arccos K)(1 - K^2)^{-1/2} \right] d_0, \quad (13a)$$

$$s = (1/4) \left[1 + (K^2(1 - K^2)^{-1/2}) \times (\ln[1 + (1 - K^2)^{-1/2}/K]) \right] \pi d_0^2, \quad (13b)$$

$$v_m = \pi K d_0^3/6. \quad (13c)$$

The compressibility factor of the HGO fluid can also be written in the form [10]

$$Z_{HGO} = 1 + 4\eta\alpha g_{HS}(de) \quad (14)$$

$$\text{or } g_{HS}(de) = (Z_{HGO} - 1)/4\eta\alpha, \quad (\text{method 2}) \quad (15)$$

where Z_{HGO} is given by eq. (10).

The value of α for different values of K are reported in Table 1. For $K \geq 1.0$, α increases with the increase of K . The table shows that α for K is identical to that for $1/K$. For example $\alpha = 1.48458$ for both $K = 3$ and $K = 1/3$.

Table 1. Values of α for different K .

K	α	K	α
1/2	1.179496	1.1	1.003233
1/3	1.484583	1.3	1.024651
2/3	1.059463	1.5	1.059463
		2.0	1.179496
		3.0	1.484583
		4.0	1.825966
		5.0	2.184001

The RDF $g_{HS}(de)$ can be calculated using either eq. (8) (method 1) or eq. (15) (method 2). When expressed as a function of density $\rho^+ = \rho d_0^3$, the values of the RDF $g_{HS}(de)$ obtained by these two methods depend on K . However, when $g_{HS}(de)$ is calculated as a function of η , the values of $g_{HS}(de)$ obtained by method 1 does not depend on K as K is associated in the expression of η , whereas the values obtained by method 2 depend on K due to the presence of α in the expression [eq. (15)] of $g_{HS}(de)$. The values of RDF $g_{HS}(de)$, obtained by methods 1 and 2, are shown in Table 2 for different densities $\rho^+ / \sqrt{2}$ and K , where $\rho_{cp} = \sqrt{2}$ is the closed packed density in the reduced unit. They are in good agreement at low density ρ^+ and/or low values of K . The deviation increases with an increase of ρ^+ and/or increase of K .

Table 2. The RDF $g_{HS}(de)$ for the HGO fluid.

	$\rho^+ / \sqrt{2}$	$g_{HS}(de)$ (Method 1)	$g_{HS}(de)$ (Method 2)
1.0	0.3	1.8887	1.8887
	0.6	4.5326	4.5326
1.1	0.3	1.8887	1.8891
	0.6	4.5326	4.5626
1.5	0.6	4.5326	4.6057
2.0	0.3	1.8887	1.8987
	0.5	3.2626	3.3772
	0.6	4.5326	4.7611
	0.7	6.6296	7.0672
3.0	0.8	10.3920	11.2437
	0.1	1.2130	1.1579
	0.3	1.8887	1.9427
	0.4	2.4436	2.6059
	0.5	3.2626	3.6053
5.0	0.6	4.5326	5.1873
	0.2	1.4976	1.5408
	0.3	1.8887	2.1026
	0.4	2.4436	2.9310
1/3	0.4	2.4436	2.5812
	0.5	3.2626	3.5574
	0.6	4.5326	5.0996
2/3	0.6	4.5326	4.6057

The RDF $g_{HS}(de)$, obtained by using eqs. (8) and (15) (*i.e.* by methods 1 and 2), can be used to estimate the shear viscosity μ and thermal conductivity λ of the HER fluid. In the present study, we take $m = 1$, $kT = 1$ and unit of length l , where $l^3 = K d_0^3$ in eqs. (1) and (2). We employ the RET [7] with expressions of $g_{HS}(de)$ to estimate μ and λ for the HER fluids.

μ_1 and μ_2 are the shear viscosity obtained from eq. (1) using the RDF $g_{HS}(de)$ by methods 1 and 2. They are compared with the molecular dynamic (MD) [11] and Enskog-Song-Mason (ESM) results [11] in Table 3. The ESM is the prediction of Enskog theory with the Song-Mason expression for g_{HS} [11] which is different from the RET of Beijeren and Ernst [7]. From the table, we find that $\mu_1 < \mu_2$ throughout the density range for different values of K . For low values of K (*i.e.* $K \leq 1.1$), μ_1 and μ_2 are in close agreement, but inferior to the ESM values. Further, μ_1 (or μ_2) is better than μ_{ESM} for large values of K (*i.e.* $K \geq 2$) in general, except at low density when compared with the MD values. The deviation from the MD values increases with the increase of $\rho^+ / \sqrt{2}$ and/or K (or K^{-1}).

Table 3. Shear viscosity μ for HER fluid

	$\rho^+ / \sqrt{2}$	μ_1	μ_2	μ_{ESM}	μ_{MD}
1.0	0.3	0.419	0.419	0.422	0.42
	0.6	2.212	2.212	2.280	2.76
1.1	0.3	0.419	0.419	0.419	0.42
	0.6	2.212	2.224	2.271	2.85
1.5	0.6	2.212	2.242	2.217	1.69
2.0	0.3	0.419	0.419	0.392	0.36
	0.5	1.224	1.256	1.290	1.01
	0.6	2.212	2.307	2.400	2.26
	0.7	4.145	4.396	4.580	2.40
3.0	0.8	8.185	8.826	9.100	4.40
	0.1	0.201	0.208	0.155	0.136
	0.3	0.419	0.422	0.483	0.37
	0.4	0.700	0.726	0.949	0.46
	0.5	1.224	1.319	1.820	0.67
5.0	0.6	2.212	2.484	3.470	1.18
	0.2	0.272	0.271	0.385	0.182
	0.3	0.419	0.432	0.943	0.300
1/3	0.4	0.700	0.780	2.053	0.460
	0.4	0.700	0.722	0.80	0.43
	0.5	1.224	1.306	1.52	0.70
2/3	0.6	2.212	2.448	2.85	1.20
	0.6	2.212	2.242	2.19	2.44

The thermal conductivity λ_1 and λ_2 obtained from eq. (2) with eqs. (8) and (15) are compared with the MD [11] and ESM [11] values in Table 4. In this case also $\lambda_1 < \lambda_2$ throughout the density range for different values of K except for $K = 1.0$ (hard spheres) where $\lambda_1 = \lambda_2$. λ_1 (or λ_2) is smaller than λ_{ESM} except for $K = 1.1$ and 1.5 (or 2/3), where $\lambda_1 > \lambda_{ESM}$. For $K = 2.0$, λ_1 is better than λ_2 as well as λ_{ESM} , when compared with the MD values. However, for $K > 2.0$, the situation is just reversed *i.e.* λ_2 is better particularly at high

density. The deviation from the MD values increases with the increase of $\rho^*/\sqrt{2}$ and/or K (or K^{-1}).

Table 4. Thermal conductivity λ for HER fluid

K	$\rho^*/\sqrt{2}$	λ_1	λ_2	λ_{LSM}	λ_{MD}
1.0	0.3	1.802	1.802	1.814	1.81
	0.6	8.725	8.725	8.984	9.048
1.1	0.3	1.802	1.802	1.748	1.90
	0.6	8.725	8.772	7.796	8.5
1.5	0.6	8.725	8.939	8.53	7.20
2.0	0.3	1.802	1.804	1.89	1.93
	0.5	4.961	5.080	5.85	4.7
	0.6	8.725	9.080	10.65	7.90
	0.7	16.018	16.954	19.96	14.0
3.0	0.8	31.166	33.556	39.13	28.0
	0.1	0.833	0.857	0.710	0.66
	0.3	1.802	1.814	2.49	2.24
	0.4	2.928	3.026	4.78	3.24
5.0	0.5	4.961	5.319	9.01	6.00
	0.6	8.725	9.743	16.78	10.8
	0.2	1.175	1.176	1.91	1.16
	0.3	1.802	1.851	4.56	2.61
1/3	0.4	2.928	3.228	9.71	5.20
	0.4	2.928	3.011	4.40	3.2
	0.5	4.961	5.268	8.20	5.8
2/3	0.6	8.725	9.606	15.14	10.3
	0.6	8.725	8.839	8.47	7.59

4. Transport properties of Gaussian overlap fluid

In this section, we apply our theory to estimate the TP's of molecular fluid of non-spherical molecules with axial symmetry, such molecules interact *via* the GO potential [4]

$$u_{GO}(r\omega_1\omega_2) = 4 \epsilon(\omega_1\omega_2) \left[(\sigma(\omega_1\omega_2)/2)^{12} - (\sigma(\omega_1\omega_2)/r)^6 \right], \quad (16)$$

$$\text{where } \epsilon(\omega_1\omega_2)/\epsilon_0 = [1 - \chi^2 \cos^2 \theta_{12}]^{-1/2}, \quad (17a)$$

$$\sigma(\omega_1\omega_2)/\sigma_0 = d(\omega_1\omega_2)/d_0. \quad (17b)$$

Here, the constants ϵ_0 and σ_0 have the dimensions of energy and length respectively; the anisotropy parameter χ is defined by eq. (7) and $d(\omega_1\omega_2)/d_0$ is given by eq. (6). Thus, the GO model is a three parameter one $\{\epsilon_0, \sigma_0$ and $\chi\}$, where χ determines the shape. For $K = 1$, eq. (16) simply reduces to the Lennard-Jones (LJ) (12-6) potential for spherical molecules. In the special case of the Gaussian overlap with the constant energy (GOCE) model [12], $\epsilon(\omega_1\omega_2) = \epsilon_0$. It is expected that use of ϵ_0 instead of $\epsilon(\omega_1\omega_2)$ does not change the TP's much like the thermodynamic properties [12]. In the present calculation, we use the GOCE model.

In order to obtain the TP's of the GOCE fluid, we divide the GOCE potential u_{GOCE} into a reference part u_0 and perturbation part u_p such that [6] :

$$u_{GOCE}(r\omega_1\omega_2) = u_0(r\omega_1\omega_2) + u_p(r\omega_1\omega_2), \quad (18)$$

$$\text{where } u_0(r\omega_1\omega_2) = u_{GOCE}(r\omega_1\omega_2) + \epsilon_0, \quad r < r_{\min}(\omega_1\omega_2), \\ = 0, \quad r > r_{\min}(\omega_1\omega_2) \quad (19a)$$

$$\text{and } u_0(r\omega_1\omega_2) = -\epsilon_0, \quad r < r_{\min}(\omega_1\omega_2), \\ = u_{GOCE}(r\omega_1\omega_2), \quad r > r_{\min}(\omega_1\omega_2) \quad (19b)$$

Here, $r_{\min}(\omega_1\omega_2) = 2^{1/6} \epsilon(\omega_1\omega_2)$. Using this perturbation scheme, the Helmholtz free energy of the GOCE fluid is given by

$$A/NkT = A_0/NkT + (1/2)\beta\rho \int dr \langle g_0(r\omega_1\omega_2)u_p(r\omega_1\omega_2) \rangle_{\omega_1\omega_2}, \quad (20)$$

where A_0 and $g_0(r\omega_1\omega_2)$ are, respectively, the Helmholtz free energy and pair correlation function (PCF) of the reference fluid.

The properties of the reference system can be obtained by a blip function expansion about a suitably chosen HGO system defined by eq. (5), where d_0 is a function of density and temperature.

For the GOCE model, Singh *et al* [6] have given the expression for $d_0^* = d_0/\sigma_0$ as

$$d_0^* = d_B^* [1 - (\sigma_{11}/2\sigma_{00})\delta] \approx d_B^* [1 + (\sigma_{11}/2\sigma_{00})\delta], \quad (21)$$

where

$$d_B^* = \int_0^\infty (1 - \exp[-\beta u_0(r^*)]) dr^*, \quad (22a)$$

$$\delta = \int_0^\infty (r^*/d_B^* - 1)^2 (d/dr^*) (\exp[-\beta u_0(r^*)]) dr^*, \quad (22b)$$

$$\sigma_{00} = (1 - \eta/2)(1 - \eta)^{-3}, \quad (23a)$$

$$\sigma_{11} = [2 - 7.5\eta + 0.5\eta^2 - 5.7865\eta^3 - 1.51\eta^4](1 - \eta)^{-4} \quad (23b)$$

$$\text{with } \eta = \rho v_m = (\pi/6)\rho^* d_0^3 K. \quad (24)$$

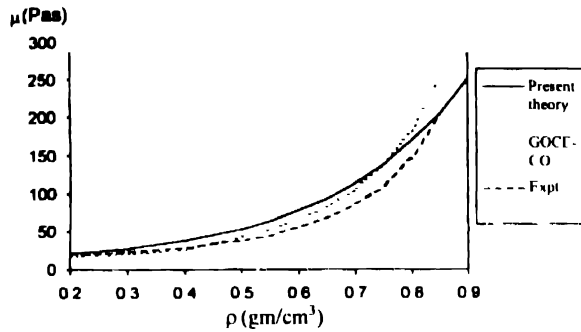
η is the packing fraction of the HGO fluid of the reduced density $\rho^* = \rho\sigma_0^3$. Hence, the effective hard sphere diameter de is given by $de = K^{1/3} d_0$. Thus de , which is a function of η , depends on the shape parameter. In this case, we employ eq. (8) to calculate the RDF $g_{HS}(de)$ of the HS fluid.

We calculate the TP's of molecular fluids of prolate ($K > 1$) and oblate ($K < 1$) shaped molecules. We consider N_2 and C_6H_6 using the GOCE model potentials whose force parameters are available [13,14] and reported in Table 5.

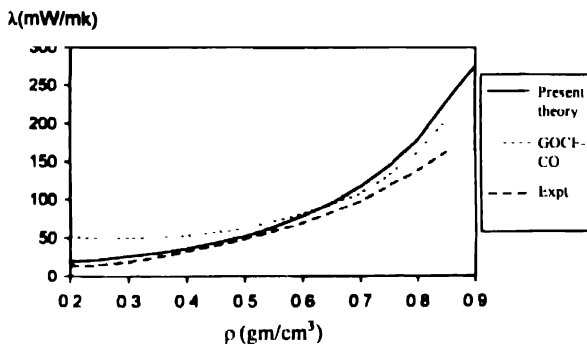
Table 5. Force parameters of the GOCE model

System	$\sigma_0(A)$	$\epsilon_0/k(K)$	
N ₂	3.37	94	1.3
C ₆ H ₆	6.30	300	0.5

We calculate the TP's such as μ and λ of fluid N₂ using the GOCE parameters used by Castillo and Orozco [1]. These results were obtained previously [2] but have been found to contain numerical errors. We have repeated the calculations here. We compare the shear viscosity μ of fluid N₂ at $T = 250$ K with the experimental data [13] and the results of Castillo and Orozco [1] with the GOCE model (GOCE-CO) in Figure 1. Our theory overestimates while the GOCE-CO underestimates μ at low density. At high densities, our theory predicts better.

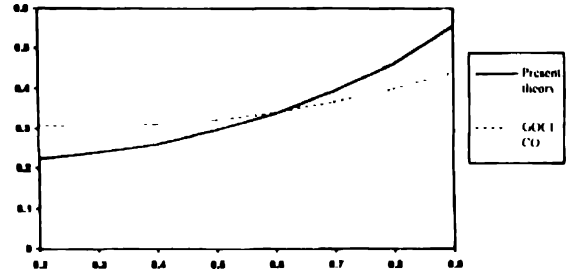
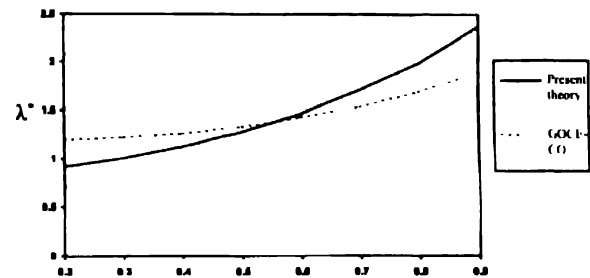

Figure 1. Shear viscosity μ (Pas) for N₂ (with $K = 1.3$) as a function of ρ (gm/cm³) at $T = 250$ K using GOCE model

The values of thermal conductivity λ of fluid N₂ are demonstrated in Figure 2 at $T = 130$ K along with the experimental [13] as well as the GOCE-CO data [1]. The agreement is good except at high density.


Figure 2. Thermal conductivity λ (mW/mK) for N₂ (with $K = 1.3$) as a function of ρ (gm/cm³) at $T = 130$ K using GOCE model

Next, we calculate the shear viscosity μ and thermal conductivity λ for benzene (C₆H₆) using the GOCE model with $K = 0.5$. The values of $\mu^* = \mu\sigma_0^2/(m\epsilon_0)^{1/2}$ and $\lambda^* = \lambda\sigma_0^2/k(m/\epsilon_0)^{1/2}$ for C₆H₆ at $T^* = 1.4$ are compared

with the results obtained by Castillo and Orozco [1] in Figures 3 and 4, respectively. They are in good agreement in the intermediate range of density ρ^* . Our values are lower


Figure 3. Values of $\mu^* = \mu\sigma_0^2/(m\epsilon_0)^{1/2}$ for C₆H₆ with $K = 0.5$ as a function of ρ^* at $T^* = 1.4$ using GOCE model

Figure 4. Values of $\lambda^* = \lambda\sigma_0^2/k(m/\epsilon_0)^{1/2}$ for C₆H₆ with $K = 0.5$ as a function of ρ^* at $T^* = 1.4$ using GOCE model

than those of Castilla and Orozco [1] at low densities and greater at high density. The deviation increases with the decrease as well as increase of density. Since the simulation results are not available, no definite conclusion can be drawn. However, it is expected to provide good results at low values of ρ^* .

5. Concluding remarks

We have employed the EDHST to calculate the TP's of molecular fluids made-up of non-spherical molecules interacting *via* GOCE potential model. This model has certain deficiencies [15]. Even then, it is sufficiently realistic [16] and may be employed to fluids of non-spherical molecules [17]. For the GOCE model, we have used the simpler approach of Singh *et al* [6] to calculate the effective hard sphere diameter.

From the study, it is clear that our approach provides in general, fairly good estimates of the shear viscosity and thermal conductivity of non-spherical molecule fluids.

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