

# Canonical average effective potential for viscosity of Non-polar (SO<sub>2</sub>), Polar (NH<sub>3</sub>) and Complex polar water (H<sub>2</sub>O)

Jeet Singh<sup>1</sup>, Pankaj Pathak<sup>2</sup>, S. P. Singh<sup>3</sup>

Physics Department, L.S.S.S.S.Government Degree College Mant, Mathura, Uttar Pradesh, India<sup>1</sup>

Physics Department, S.S.V.P.G.College, Hapur, Uttar Pradesh, India<sup>2</sup>

Physics Department, Dr.B.R.Ambedkar Government Degree College, Mainpuri, Uttar Pradesh, India<sup>3</sup>

## ABSTRACT

The canonical average effective potential is very useful to computed the viscosity for non polar sulphur dioxide (SO<sub>2</sub>), polar ammonia (NH<sub>3</sub>) and complex polar fluids water (H<sub>2</sub>O). .The agreement between theoretical and experimental results conform the validity of the canonical average effective potential for the viscosity of non polar sulphur dioxide (SO<sub>2</sub>), polar ammonia (NH<sub>3</sub>) and complex polar fluids water(H<sub>2</sub>O).The collision integral  $\Omega^{(2,2)*}$  [1]for the viscosity ( $\eta$ ) of a single dilute polar gas has been obtained for a central pair potential which is an average of the Stockmayer potential [2] over all orientation of the dipoles. The collision integrals show better agreement with the canonical average effective potential as well as experimental value.

**Keywords :** L-J Potential, Canonical Average Potential, Viscosity, Collision integral.

## I. INTRODUCTION

The study of liquid state is done through Statistical mechanics in terms of equilibrium and non-equilibrium phenomena .In equilibrium a given physical property is used to be uniformly distributed throughout the whole system and it does not change with time except for small fluctuations. In case the fluid is not in equilibrium, its properties change with time. Transport properties are Non-equilibrium properties of the system. A transport process in a medium occurs when something is transferred from one part of the medium to another .The most familiar transport processes are Viscosity, Diffusion and Thermal conductivity. In this paper we discuss only viscosity of fluids for Non polar, Polar and complex polar. The success of the Canonical average effective potential has been attained in calculating the transport properties of many dilute gases. Whose molecular interactions may be described by spherically symmetric potential function. Similar calculations for systems which require angular dependent potential have been more limited, probably because of the

difficulty in evaluating the necessary collision integrals  $\Omega^{(L,S)*}$ . We removed this difficulty by the help of canonical average effective potential which permits use of existing tabulations of the collision integral[1] (Joseph O. Hirschfelder, Charles F. Curtiss and R. Byron Bird in 1964 ) for systems with isotropic potential by eliminating the need for a separate calculation of the contribution from the angular dependent part of the potential.

**Theory:** Bae and Reed [3] used the effective potential as the canonical average, over the angular variables of the anisotropic pair potential. In the present study, we have used the orientation-dependent potential has the dipole-dipole and dipole-quadrupole interaction term in addition.

$$\Omega(r, \omega) = \Phi_{L-J}(r) - \frac{\mu^2}{r^3} g_{11}(\omega) + \frac{3\mu Q}{4r^4} g_{12}(\omega) \quad \text{--- (1)}$$

Where  $\Phi_{L-J}(r)$  is the well-known Lennard-Jones potential [4], and

$$g_{11}(\omega) = 2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos \phi \quad \text{----- (2)}$$

$$g_{12}(\omega) = \cos \theta_1 (3 \cos^2 \theta_2 - 1) - 2 \sin \theta_1 \sin \theta_2 \cos \theta_2 \cos \phi \quad \text{----- (3)}$$

Further,  $\mu$  and  $Q$  are the electric dipole and quadrupole moment of the molecules.  $\theta_1$  and  $\theta_2$  are the angle between the axis of the molecular dipoles and the line joining the molecular centres of the two molecules respectively,  $\phi$  is the azimuthal angle in the plane perpendicular to this line, and  $\omega$  is the function of the angular coordinates.

d Joshi (1980) and Pathak et. al (1981) [5] have been used the effective potential as the free-energy average, over the angular variables, of the anisotropic pair potential. But in this paper, we have been taken the canonical average over the angular variables of an isotropic pair potential  $\phi(r, \omega)$  and represented in following manner

$$\langle \phi(r, T) \rangle = \phi_{L-J} - \frac{2\mu^4}{3KT r^6} - \frac{\mu^2 Q^2}{4KT r^8} + \frac{14\mu^8}{225K^3 T^3 r^{12}} \quad \text{----- (4)}$$

Where  $T$  is the temperature and  $k$  is the Boltzmann constant. This hypothesis obviates the consideration at a given temperature, the function  $\langle \phi(r, T) \rangle$  change in the Lennard-Jones potential with temperature dependent parameters.

If a reduced dipole moment ( $\delta_{\max}$ ), reduced temperature ( $T_0^*$ ) and reduced dipole quadrupole moment ( $\alpha_{\max}$ ) can be expressed as

$$\delta_{\max} = \frac{\mu^2}{2\epsilon_0 \sigma_0^3} \quad \text{----- (5)}$$

$$T_0^* = \frac{KT}{\epsilon_0} \quad \text{----- (6)}$$

$$\alpha_{\max} = \frac{\mu Q}{2\epsilon_0 \sigma_0^4} \quad \text{----- (7)}$$

The canonical average potential can be written in the form of L-J potential [4] using equation (4), we have

$$\langle \phi(r, T) \rangle = 4\epsilon_0 \left[ \left( \frac{\sigma_0}{r} \right)^{12} \left( 1 + \frac{56\delta_{\max}^4}{225T_0^{*3}} \right) - \left( \frac{\sigma_0}{r} \right)^6 \left\{ 1 + \frac{2\delta_{\max}^2}{3T_0^*} + \left( \frac{\sigma_0}{r} \right)^2 \frac{\alpha_{\max}^2}{4T_0^{*2}} \right\} \right] \quad \text{----- (8)}$$

This equation (8) can be express as a temperature-dependent canonical average potential in the L-J potential format

$$\phi_{\text{eff}}(r, T) = 4\epsilon_T \left[ \left( \frac{\sigma_T}{r} \right)^{12} - \left( \frac{\sigma_T}{r} \right)^6 \right] \quad \text{----- (9)}$$

Where  $\epsilon_T$  and  $\sigma_T$  are new temperature-dependent parameter to be related to  $\epsilon_0$  and  $\sigma_0$ .

By equating the coefficient of  $r^{-12}$  and  $r^{-6}$  in equation L-J potential.

We have obtained the following relation between the two sets of parameters

$$\sigma_T = \sigma_0 \left( \frac{\epsilon_0}{\epsilon_T} \right)^{1/12} \left( \frac{56\delta_{\max}^4}{225T_0^{*3}} \right)^{1/12} \quad \text{----- (10)}$$

$$\epsilon_T = \epsilon_0 \left( 1 + \frac{56\delta_{\max}^4}{225T_0^{*3}} \right)^{-1} \left[ 1 + \frac{2\delta_{\max}^2}{3T_0^*} + \frac{\alpha_{\max}^2}{5T_0^{*2}} \right] \quad \text{----- (11)}$$

Such a formal introduction of temperature in this potential is quite logical because it involves a regular variation of the characterises parameters of L-J potential.

The numerical values given in table-1 used, to compute the values of  $\epsilon_T$  and  $\sigma_T$ .

**Table-1:**

Fluids	$\sigma_0$ (A <sup>0</sup> )	$\epsilon_0/K$ (°K)	$\mu^*10^{18}$ (esu)	$Q^*10^{-26}$ (esu)	M (gm)
NH <sub>3</sub>	3.13	340	1.47	-2.32	17.032
H <sub>2</sub> O	2.725	356	1.85	0.45	18.02
SO <sub>2</sub>	4.026	363	1.70	-4.24	64

## Determination of Viscosity:

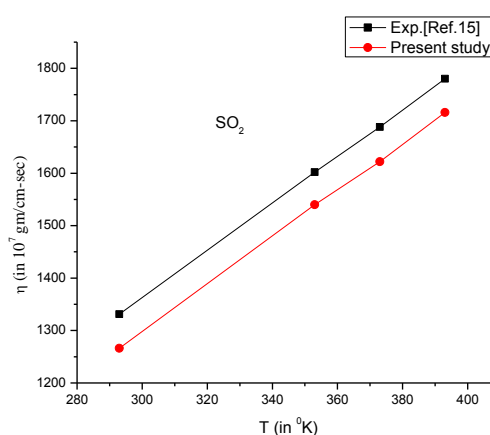
The main purpose of the investigation is to compare collision integral for viscosity obtained from canonical average potential with the average collision integral based on the fixed –orientation. It is interesting to note that, the calculated the numerical values of the parameters of the canonical average potential from experimental viscosity of non-polar, polar and complex polar fluids. The procedure is essentially given by Hirshfelder, Curtiss, and Bird and also used by others. The Chapman and Enskog[12]show that mass transfer results not only from a concentration gradient, but also from a temperature gradient, similarly .The energy transfer results not only from a temperature gradient ,but also from a concentration gradient .These and other second order effects ,which cannot be described in terms of simple kinetic theory ,energy quite naturally from the rigorous approach .The Chapman and Enskog show that solution of the Boltzmann equation provides one with a complete solution of the problem of describing the transport properties of dilute gases. In particular, one obtains expressions which relate the transport coefficients appearing in the experimental phenomenological flow equations to the intermolecular potential. The expression for the viscosity in g/cm/sec for Non-polar, Polar and Complex polar [16] fluids according to Chapman-Enskog (1952), is given by

The coefficient of viscosity of a pure gas

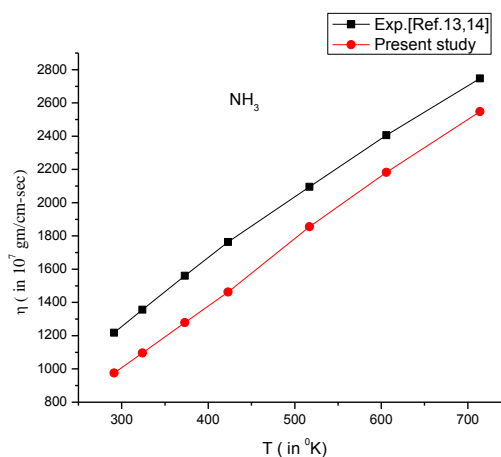
$$(\eta) \times 10^7 = 266.3 \left( \frac{\sqrt{MT}}{\sigma_T \Omega^{(2,2)*} (T_d^*)} \right) \text{ ---- (12)}$$

Where M is the molecular weight in atomic mass unit and T is the absolute temperature in °K.  $\sigma_T$  is the collision diameter of a molecules of the gas. The temperature dependent parameter of the canonical average effective potential is given by (7). The  $\Omega^{(2,2)*}$  is the appropriate collision integral which is a function of reduced temperature  $T_d^*$  which is defined

as  $T_d^* = KT / \epsilon_T$  .The temperature-dependent parameters, We calculated from equation(8) and (9) have been used to calculate the viscosity of Non polar ,polar and complex polar. We calculated the values of viscosity by canonical average effective Potential temperature dependent parameter with experimental value of viscosity for Non-polar ,polar and complex polar .We draw a graph between experimental value of viscosity with Cannonical average effective potential present work temperature dependent have good agreement as shown in graph (1) for non polar SO<sub>2</sub>.

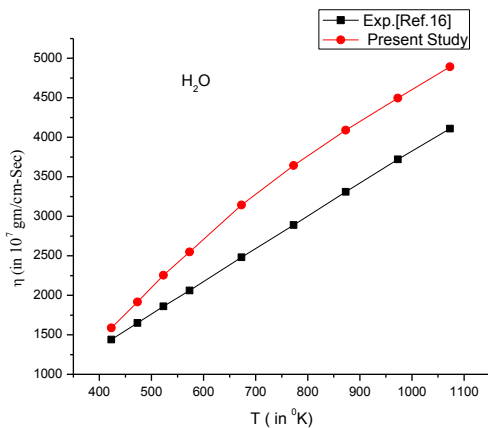


**Figure 1:** Graph showing coefficient of viscosity  $\eta$  ( in 10<sup>7</sup> gm/cm-sec) with Temperature T (in °K) for pure SO<sub>2</sub> vapour.



**Figure 2:** Graph showing coefficient of viscosity  $\eta$  ( in 10<sup>7</sup> gm/cm-sec) with Temperature T (in °K) for Polar gas NH<sub>3</sub>.

**Figure 3:** Graph showing coefficient of viscosity  $\eta$  ( in  $10^7$  gm/cm-sec) with Temperature T (in  $^{\circ}$ K) for Water H<sub>2</sub>O.



## II. Conclusion

It is important to realise that agreement between calculated and experimental values of a single property, such as viscosity, does not of itself indicate that either the form of the potential or its parameters are realistic. This is a good agreement with experimental result obtained by using canonical average potential result. The effective canonical average potential obtained by taking the canonical average of the Rowlinson potential is correlating with the viscosity of non-polar, polar and complex polar fluids using temperature-dependent parameters are shown in the tables of reduced collision integrals for the 12-6 Lennard-Jones potential.

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