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## Physics and Space Science

Semi-Empirical Model

Annular Porous Medium

Highlights

Gallium-Arsenide Atom

Inverse Dielectric Susceptibility

Discovering Thoughts, Inventing Future

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# Natural Convection of Heat Transfer in a Vertical Conical Annular Porous Medium

By Dr. D. Prabhakar & Dr. G. Prabhakararao

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**Abstract** - In this chapter, we study the natural convection heat transfer in a saturated porous medium confined in a vertical annular porous medium. In this study Finite Element Method (FEM) has been used to solve governing partial differential equations. Results are presented in terms of average Nusselt number ( $\bar{Nu}$ ), streamlines and Isothermal lines for various values of Rayleigh number ( $Ra$ ), Cone angle ( $C_A$ ) and Radius ratio ( $R_r$ ).

**Keywords** : porous medium, pressure, Rayleigh number, boundary-layer, flux.

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# Natural Convection of Heat Transfer in a Vertical Conical Annular Porous Medium

Dr. D. Prabhakar<sup>α</sup> & Dr. G. Prabhakararao<sup>σ</sup>

**Abstract** - In this chapter, we study the natural convection heat transfer in a saturated porous medium confined in a vertical annular porous medium. In this study Finite Element Method (FEM) has been used to solve governing partial differential equations. Results are presented in terms of average Nusselt number ( $\bar{Nu}$ ), streamlines and Isothermal lines for various values of Rayleigh number ( $Ra$ ), Cone angle ( $C_A$ ) and Radius ratio ( $R_r$ ).

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## I. INTRODUCTION

Natural convection heat transfer in a saturated porous medium has a number of important and geophysical applications, such as nuclear reactor cooling system and underground energy transport. The problems of free convection about a vertical impermeable flat plate are studied by Cheng and Minkowycz [1], Cheng [2], Na and Pop [3], Gorla and Zinalabedini [4]. The vertical cylinder cases are investigated by Minkowycz and Cheng [5], Kumari et al [6], Markin [7] and Basson et al [8]. Cheng et al. [9] use the local non-similarity method to analyze the natural convection of Darcial fluid about a cone.

The effect of surface mass flux on a vertical flat plate [10] the similarity solution is possible only when the variations of the wall temperature and the transpiration rate are proportional to power-law of  $x$  measured from the leading edge.

From practical point of view, however, the uniform mass flux may be easily realized. The effect of uniform surface mass flux on a vertical flat plate with uniform wall temperature is investigated by Merkin [11] and Minkowycz and Cheng [12]. Yücel [13], and Hwang and Chen [14] numerically study the vertical cylinder case.

Khan and Zebib [15] studied the double – diffusive instability of the double boundary – layer structure that forms near a vertical wall immersed in temperature and concentration stratified porous medium. Raptis et al. [16] constructed similarity solutions of boundary - layer near a vertical surface wall in porous medium with constant temperature and concentration. Bejan and Khair [17] used Darcy's law to study the vertical natural convective flows driven by

temperature and concentration gradients. Lal and Kulacki [18] studied the natural convection boundary layer flow along a vertical surface with constant heat and mass flux including the effect of wall injection. Nakayama and Hossain [19], and Singh and Queeny [20] applied the integral method to obtain the heat and mass transfer by free convection from a vertical surface with constant wall temperature and concentration. Yih [21] studied the heat and mass transfer characteristics in natural convection flow over a truncated cone subjected to variable wall temperature and concentration or variable heat and mass flux embedded in porous medium.

Comprehensive review on this phenomenon has been recently reported by Trevisan and Bejan [22] for various geometries. Bejan and Khair [23] investigated the vertical natural convection boundary – layer flow in a saturated porous medium due to the combined heat and mass transfer. Jang and Chang [24] studied the buoyancy – induced inclined boundary - layer in porous medium resulting from combined heat and mass buoyancy effects.

Heat and mass transfer about vertical cylinder in saturated porous media is analyzed by Yücel [25] [26]. Nakayama and Hossain [27], and Singh and Queeny [28] used an integral method to solve the problem of Bejan and Khair [23]. Lai et al [29] investigated the coupled heat and mass transfer by natural convection from horizontal line sources in saturated porous media. Nakayama and Ashizawa [32] performed a boundary layer analysis of combined heat and mass transfer by natural convection from a concentrated source in a saturated porous medium.

In this chapter, we study the natural convection heat transfer in a saturated porous medium confined in a vertical annular porous medium. In this study Finite Element Method (FEM) has been used to solve governing partial differential equations. Results are presented in terms of average Nusselt number ( $\bar{Nu}$ ), streamlines and Isothermal lines for various values of Rayleigh number ( $Ra$ ), Cone angle ( $C_A$ ) and Radius ratio ( $R_r$ ).

## II. MATHEMATICAL FORMULATION

A vertical annular cone of inner radius  $r_i$  and outer radius  $r_o$  as depicted by schematic diagram as shown in figure (A) is considered to investigate the heat transfer behavior. The co-ordinate system is chosen

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such that the r-axis points towards the width and z-axis towards the height of the cone respectively. Because of the annular nature, two important parameters emerge which are Cone angle ( $C_A$ ) and Radius ratio ( $R_r$ ) of the annulus. They are defined as

$$C_A = \frac{H_t}{r_0 - r_i}, \quad R_r = \frac{r_0 - r_i}{r_i}$$

where  $H_t$  is the height of the cone.

The inner surface of the cone is maintained at isothermal temperature  $T_h$  and outer surface is at ambient temperature  $T_\infty$ . It may be noted that, due to axisymmetry, only a section on the annulus is sufficient for analysis purpose.

Following assumptions are made:

- The flow inside the porous medium obeys Darcy law and there is no phase change of fluid.
- Porous medium is saturated with fluid.
- The fluid and medium are in local thermal equilibrium in the domain.
- The porous medium is isotropic and homogeneous.
- Fluid properties are constant except the variation of density.

With the above assumptions, the governing equations are given by continuity equation:

$$\frac{\partial(ru)}{\partial r} + \frac{\partial(rw)}{\partial z} = 0 \quad (1.2.1)$$

The velocity in r and z directions can be described by Darcy law as

Velocity in horizontal direction

$$u = -\frac{K}{\mu} \frac{\partial p}{\partial r} \quad (1.2.2)$$

velocity in vertical direction

$$w = -\frac{K}{\mu} \left( \frac{\partial p}{\partial z} + \rho g \right) \quad (1.2.3)$$

the permeability K of porous medium can be expressed as Bejan (33)

$$K = \frac{D_p^2 \phi^3}{180(1-\phi)^2} \quad (1.2.4)$$

The variation of density with respect to temperature can be described by Boussinesq approximation as

$$\rho = \rho_\infty [ 1 - \beta_T (T - T_\infty) ] \quad (1.2.5)$$

Momentum Equation:

$$\frac{\partial w}{\partial r} - \frac{\partial u}{\partial z} = \frac{gK\beta}{\nu} \frac{\partial T}{\partial r} \quad (1.2.6)$$

Energy equation:

$$u \frac{\partial T}{\partial r} + w \frac{\partial T}{\partial z} = \alpha \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right) \quad (1.2.7)$$

The continuity equation (1.2.1) can be satisfied by introducing the stream function  $\psi$  as

$$u = -\frac{1}{r} \frac{\partial \psi}{\partial z} \quad (1.2.8)$$

$$w = \frac{1}{r} \frac{\partial \psi}{\partial r} \quad (1.2.9)$$

The corresponding dimensional boundary conditions are

$$\text{at } r = r_i, \quad T = T_w, \quad \psi = 0 \quad (1.2.10a)$$

$$\text{at } r = r_0, \quad T = T_\infty, \quad \psi = 0 \quad (1.2.10b)$$

(except at  $z = 0$ )

The new parameters arising due to cylindrical co-ordinates system are

Non-dimensional Radius

$$\bar{r} = \frac{r}{L} \quad (1.2.11a)$$

Non-dimensional Height

$$\bar{z} = \frac{z}{L} \quad (1.2.11b)$$

Non-dimensional stream function

$$\bar{\psi} = \frac{\psi}{\alpha L} \quad (1.2.11c)$$

Non-dimensional Temperature

$$\bar{T} = \frac{(T - T_\infty)}{(T_w - T_\infty)} \quad (1.2.11d)$$

Rayleigh number

$$Ra = \frac{g\beta_T \Delta T K L}{\nu \alpha} \quad (1.2.11e)$$

The non-dimensional equations for the heat transfer in vertical cone are

Momentum equation:

$$\frac{\partial^2 \bar{\psi}}{\partial \bar{z}^2} + \bar{r} \left( \frac{1}{\bar{r}} \frac{\partial \bar{\psi}}{\partial \bar{r}} \right) = \bar{r} Ra \frac{\partial \bar{T}}{\partial \bar{r}}$$



Energy equation:

$$\frac{1}{r} \left[ \frac{\partial \bar{\psi}}{\partial r} \frac{\partial \bar{T}}{\partial z} - \frac{\partial \bar{\psi}}{\partial z} \frac{\partial \bar{T}}{\partial r} \right] = \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \bar{T}}{\partial r} \right) + \frac{\partial^2 \bar{T}}{\partial z^2} \right) \quad (1.2.13)$$

The corresponding non-dimensional boundary conditions are

$$\text{at } \bar{r} = \bar{r}_i, \quad \bar{T}=1, \quad \bar{\psi} = 0 \quad (1.2.14)$$

$$\text{at } \bar{r} = \bar{r}_0, \quad \bar{T}=0, \quad \bar{\psi} = 0 \quad (1.2.15)$$

### III. SOLUTION OF GOVERNING EQUATIONS

The partial differential equations, which describe the heat and fluid flow behavior in the vicinity of porous medium are given earlier. There are various numerical methods available to achieve the solution of these equations, but the most popular numerical methods are Finite difference method, Finite volume method and the Finite element method. The selection of these numerical methods is an important decision, which is influenced by variety of factors amongst which the geometry of domain plays a vital role. Other factors include the ease with which these partial differential equations can be transformed into simple forms, the computational time required and the flexibility in development of computer code to solve these equations.

In the present study, we have used Finite Element Method (FEM). The following sections briefly described the Finite Element Method and present its application to solve the above mentioned equations.

The Finite Element Method is a popular method amongst scientific community. This method was originally developed to study the mechanical stresses in a complex air frame structure Clough (36) and popularized by Zienkiewicz and Cheung (37) by applying it to continuum mechanics. Since then the application of finite element method has been exploited to solve the numerous problems in various engineering disciplines.

The great thing about finite element method is its ease with which it can be generalized to engineering problems comprised of different materials. Another admirable feature of the Finite Element Method (FEM) is that it can be applied to wide range of geometries having irregular boundaries, which is highly difficult to achieve with other contemporary methods. FEM can be said to have comprised of roughly 5 steps to solve any particular problem. The steps can be summarized as :

$$\alpha_i = \frac{1}{2A} [(r_j z_k - r_k z_j) T_i + (r_k z_i - r_i z_k) T_j + (r_i z_j - r_j z_i) T_k] \quad (1.2.16)$$

$$\alpha_2 = \frac{1}{2A} [(z_j - z_k) T_i + (z_k - z_i) T_j + (z_i - z_j) T_k] \quad (1.2.17)$$

$$\alpha_3 = \frac{1}{2A} [(r_k - r_j) T_i + (r_i - r_k) T_j + (r_j - r_i) T_k] \quad (1.2.18)$$

- ☞ Descritizing the domain: This step involves the division of whole physical domain into smaller segments known as elements, and then identifying the nodes, coordinates of each node and ensuring proper connectivity between the nodes.
- ☞ Obtaining the characteristics of the element which is written in terms of nodal values
- ☞ Development of Global matrix: The equations are arranged in a global matrix which takes into account the whole domain
- ☞ Solution: The equations are solved to get the desired variable at each node in the domain
- ☞ Evaluate the quantities of interest: After solving the equations a set of values are obtained for each node, which can be further processed to get the quantities of interest.

There are varieties of elements available in FEM, which are distinguished by the presence of number of nodes. The present study is carried out by using a simple 3- noded triangular element as shown in figure (1).

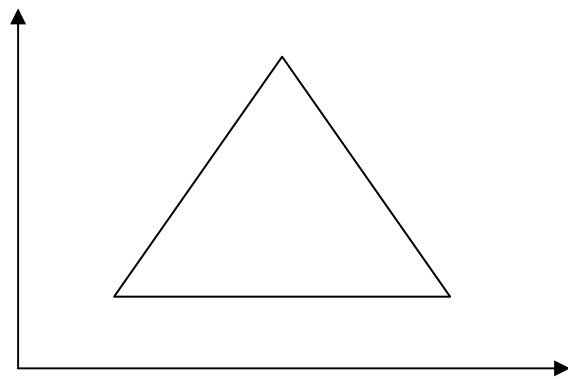


Figure 1 : Typical triangular element

Let us consider that the variable to be determined in the triangular area as "T". The polynomial function for "T" can be expressed as:

$$T = \alpha_1 + \alpha_2 r + \alpha_3 z \quad (1.2.15)$$

The variable T has the value  $T_i, T_j$  &  $T_k$  at the nodal position i, j & k of the element. The r and z coordinates at these points are  $r_i, r_j, r_k$  and  $z_i, z_j, z_k$  respectively. Substitution of these nodal values in the equation (1.2.15) helps in determining the constants  $a_1, a_2, a_3$  which are:

where A is area of the triangle given as

$$2A = \det \begin{vmatrix} 1 & r_i & z_i \\ 1 & r_j & z_j \\ 1 & r_k & z_k \end{vmatrix} \quad (1.2.19)$$

Substitution of  $a_1, a_2, a_3$  in the equation (1.2.15) and mathematical arrangement of the terms results into

The constants can be expressed in terms of coordinates as

$$\left. \begin{aligned} a_i &= r_j z_k - r_k z_j & b_i &= z_j - z_k & c_i &= r_k - r_j \\ a_j &= r_k z_i - r_i z_k & b_j &= z_k - z_i & c_j &= r_i - r_k \\ a_k &= r_i z_j - r_j z_i & b_k &= z_i - z_j & c_k &= r_j - r_i \end{aligned} \right\} \quad (1.2.22)$$

Good insight into the FEM is given in Segerland (35); Elshayed and Beng (33) Lewis et al. (34). Galerkin method is employed to convert the partial differential equations into matrix form of equation for an element. The steps involved are as given below.

Please note that the nodal terms  $i, j$  &  $k$  are replaced by 1,2 & 3 respectively in subsequent discussions for simplicity.

Applying of Galerkin method to momentum equation (1.2.12) yields

$$\{R^e\} = - \int_A N^T \left( \frac{\partial^2 \bar{\psi}}{\partial z^2} + r \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial \bar{\psi}}{\partial r} \right) + rRa \frac{\partial \bar{T}}{\partial r} \right) dV \quad (1.2.23)$$

Thus

$$\int_A N^T \frac{\partial^2 \bar{\psi}}{\partial r^2} dA = \int_A \frac{\partial}{\partial r} \left( [N^T] \frac{\partial^2 \bar{\psi}}{\partial r^2} \right) 2\Pi r dA - \int_A \frac{\partial [N^T]}{\partial r} \frac{\partial \bar{\psi}}{\partial r} \quad (1.2.26)$$

The first term on right hand side of equation (1.2.26) can be transformed into surface integral by the application of Greens theorem and leads to inter-element requirement at boundaries of an element. The boundary conditions are incorporated in the force vector.

Making use of (1.2.20) produces

$$\int_A N^T \frac{\partial^2 \bar{T}}{\partial r^2} 2\Pi r dA = - \int_A \frac{\partial N^T}{\partial r} \frac{\partial N}{\partial r} \begin{Bmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \end{Bmatrix} dA \quad (1.2.27)$$

Similarly

$$\int_A N^T \frac{\partial^2 \bar{\psi}}{\partial z^2} 2\Pi r dA = - \frac{2\Pi R}{4A} \begin{bmatrix} c_1^2 & c_1 c_2 & c_1 c_3 \\ c_1 c_2 & c_2^2 & c_2 c_3 \\ c_1 c_2 & c_2 c_3 & c_3^2 \end{bmatrix} \begin{Bmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \end{Bmatrix} \quad (1.2.29)$$

$$T = N_i T_i + N_j T_j + N_k T_k \quad (1.2.20)$$

In equation (1.2.20)  $N_i, N_j, N_k$  are the shape functions given by

$$N_m = \frac{a_m + b_m r + c_m z}{2A}, m = i, j \text{ \& \ } k \quad (1.2.21)$$

$$\{R^e\} = - \int_A N^T \left( \frac{\partial^2 \bar{\psi}}{\partial z^2} + r \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial \bar{\psi}}{\partial r} \right) + rRa \frac{\partial \bar{T}}{\partial r} \right) 2\Pi r dA \quad (1.2.24)$$

where  $R^e$  is the residue. Considering individual terms of equation (1.2.24)

The differentiation of following term results into

$$\frac{\partial}{\partial r} \left( [N^T] \frac{\partial \bar{\psi}}{\partial r} \right) = [N^T] \frac{\partial^2 \bar{\psi}}{\partial r^2} + \frac{\partial [N^T]}{\partial r} \frac{\partial \bar{\psi}}{\partial r} \quad (1.2.25)$$

Substitution of (1.2.21) into (1.2.27) gives

$$\begin{aligned} &= - \frac{1}{(2A)^2} \int_A \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} [b_1 b_2 b_3] \begin{Bmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \end{Bmatrix} 2\Pi r dA \\ &= - \frac{2\Pi R}{4A} \begin{bmatrix} b_1^2 & b_1 b_2 & b_1 b_3 \\ b_1 b_2 & b_2^2 & b_2 b_3 \\ b_1 b_3 & b_2 b_3 & b_3^2 \end{bmatrix} \begin{Bmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \end{Bmatrix} \quad (1.2.28) \end{aligned}$$



The third term of equation (1.2.24) is

$$\int_A N^T \bar{r} Ra \frac{\partial \bar{T}}{\partial r} \Pi \bar{r} dA = Ra \int_A N^T \bar{r} \frac{\partial \bar{T}}{\partial r} 2\Pi \bar{r} dA \tag{1.2.30}$$

In order to get the matrix equation of (1.2.30), the following method can be applied. The triangular element can be subdivided into three triangles with a point in the center of original triangle as shown in figure (2).

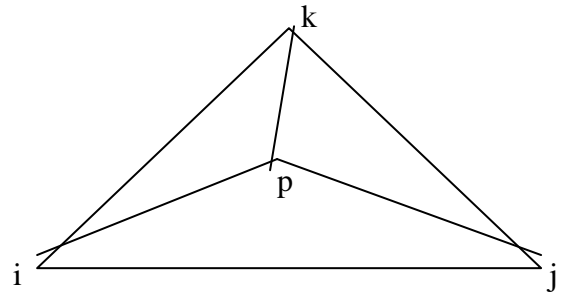


Figure 2 : Showing the sub triangular areas

Defining the new area ratios as

$$M_k = \frac{\text{area } pij}{\text{area } ijk} \quad M_i = \frac{\text{area } pj k}{\text{area } ijk} \quad M_j = \frac{\text{area } pki}{\text{area } ijk}$$

It can be shown Elshyab and Beng (33) that

$$M_i = N_1 \quad M_j = N_2 \quad M_k = N_3 \tag{1.2.31}$$

Replacing shape functions in equation (1.2.30) by (1.1.31) yields

$$\int_A N^T \bar{r} Ra \frac{\partial \bar{T}}{\partial r} 2\Pi \bar{r} dA = \bar{r} Ra \int_A \begin{bmatrix} M_1 \\ M_2 \\ M_3 \end{bmatrix} \frac{\partial(N)}{\partial r} \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} 2\Pi \bar{r} dA \tag{1.2.32}$$

The area integration can be evaluated by a simple relation Segerland (35).

$$\int_A M_1^d M_2^e M_3^f = \frac{d!e!f!}{(d+e+f+2)!} 2A \tag{1.2.33}$$

$$= \frac{2\Pi \bar{R}^2 Ra}{6} \begin{Bmatrix} b_1 \bar{T}_1 + b_2 \bar{T}_2 + b_3 \bar{T}_3 \\ b_1 \bar{T}_1 + b_2 \bar{T}_2 + b_3 \bar{T}_3 \\ b_1 \bar{T}_1 + b_2 \bar{T}_2 + b_3 \bar{T}_3 \end{Bmatrix} \tag{1.2.35}$$

Application of equation (1.2.33) into (1.2.32) gives rise to:

$$= Ra \frac{A}{3} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \frac{2\Pi \bar{R}^2}{2A} [b_1 + b_2 + b_3] \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} \tag{1.2.34}$$

Now the momentum equation (1.2.12) can be written in the matrix form as

$$\frac{2\Pi \bar{R}}{4A} \left\{ \begin{bmatrix} b^2 & b_1 b_2 & b_1 b_3 \\ b_1 b_2 & b_2^2 & b_2 b_3 \\ b_1 b_3 & b_2 b_3 & b_3^2 \end{bmatrix} + \begin{bmatrix} c_1^2 & c_1 c_2 & c_1 c_3 \\ c_1 c_2 & c_2^2 & c_2 c_3 \\ c_1 c_3 & c_2 c_3 & c_3^2 \end{bmatrix} \right\} \begin{Bmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \end{Bmatrix} + \frac{2\Pi \bar{R}^2 Ra}{6} \begin{Bmatrix} b_1 \bar{T}_1 + b_2 \bar{T}_2 + b_3 \bar{T}_3 \\ b_1 \bar{T}_1 + b_2 \bar{T}_2 + b_3 \bar{T}_3 \\ b_1 \bar{T}_1 + b_2 \bar{T}_2 + b_3 \bar{T}_3 \end{Bmatrix} = 0 \tag{1.2.36}$$

In simple form the above equation can be represented as:

$$[K_s] \{ \bar{\psi} \} = \{ f \} \tag{1.2.37}$$

where  $K_s$  is stiffness matrix and  $f$  is the force vector. For equation (1.2.12) they are:

$$[K_s] = \frac{2\Pi \bar{R}}{4A} \left\{ \begin{bmatrix} b_1^2 & b_1 b_2 & b_1 b_3 \\ b_1 b_2 & b_2^2 & b_2 b_3 \\ b_1 b_3 & b_2 b_3 & b_3^2 \end{bmatrix} + \begin{bmatrix} c_1^2 & c_1 c_2 & c_1 c_3 \\ c_1 c_2 & c_2^2 & c_2 c_3 \\ c_1 c_3 & c_2 c_3 & c_3^2 \end{bmatrix} \right\} \tag{1.2.38a}$$

$$\{\bar{\psi}\} = \begin{Bmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \end{Bmatrix} \tag{1.2.38b}$$

$$\{f\} = \frac{2\Pi\bar{R}^2 Ra}{6} \begin{Bmatrix} b_1\bar{T}_1 + b_2\bar{T}_2 + b_3\bar{T}_3 \\ b_1\bar{T}_1 + b_2\bar{T}_2 + b_3\bar{T}_3 \\ b_1\bar{T}_1 + b_2\bar{T}_2 + b_3\bar{T}_3 \end{Bmatrix} \tag{1.2.38c}$$

The radial distance  $\bar{R}$  to the centroid of an element is given by relation

$$\bar{R} = \frac{\bar{r}_1 + \bar{r}_2 + \bar{r}_3}{3}$$

6 Similarly application of Galerkin method to Energy equation (1.2.13) gives

$$\{R^e\} = -\int_A [N]^T \left[ \frac{1}{r} \left( \frac{\partial \bar{\psi}}{\partial r} \frac{\partial \bar{T}}{\partial z} - \frac{\partial \bar{\psi}}{\partial z} \frac{\partial \bar{T}}{\partial r} \right) - \left( \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \frac{\partial \bar{T}}{\partial r} \right\} + \frac{\partial^2 \bar{T}}{\partial z^2} \right) \right] 2\Pi\bar{r}dA \tag{1.2.39}$$

Considering the terms individually of the above equation

$$\int_A [N]^T \frac{\partial \bar{\psi}}{\partial z} \frac{\partial \bar{T}}{\partial r} 2\Pi dA = \int_A \begin{bmatrix} M_1 \\ M_2 \\ M_3 \end{bmatrix} \frac{\partial [N]}{\partial z} \{\bar{\psi}\} \frac{\partial [N]}{\partial r} \{\bar{T}\} 2\Pi\bar{r}dA \tag{1.2.40}$$

$$= \frac{2\Pi A}{3} \times \frac{1}{4A^2} [c_1\bar{\psi}_1 + c_2\bar{\psi}_2 + c_3\bar{\psi}_3] [b_1, b_2, b_3] \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} \tag{1.2.41}$$

$$= \frac{2\Pi}{12A} \begin{Bmatrix} c_1\bar{\psi}_1 + c_2\bar{\psi}_2 + c_3\bar{\psi}_3 \\ c_1\bar{\psi}_1 + c_2\bar{\psi}_2 + c_3\bar{\psi}_3 \\ c_1\bar{\psi}_1 + c_2\bar{\psi}_2 + c_3\bar{\psi}_3 \end{Bmatrix} [b_1, b_2, b_3] \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} \tag{1.2.42}$$

Following the same above steps

$$\int_A [N]^T \frac{\partial \bar{\psi}}{\partial r} \frac{\partial \bar{T}}{\partial z} 2\Pi dA = \int_A \begin{bmatrix} M_1 \\ M_2 \\ M_3 \end{bmatrix} \frac{\partial [N]}{\partial r} \{\bar{\psi}\} \frac{\partial [N]}{\partial z} \{\bar{T}\} 2\Pi dA$$

$$\int_A N^T \frac{\partial \bar{\psi}}{\partial r} \frac{\partial \bar{T}}{\partial z} 2\Pi dA = \frac{2\Pi}{12A} \begin{Bmatrix} b_1\bar{\psi}_1 + b_2\bar{\psi}_2 + b_3\bar{\psi}_3 \\ b_1\bar{\psi}_1 + b_2\bar{\psi}_2 + b_3\bar{\psi}_3 \\ b_1\bar{\psi}_1 + b_2\bar{\psi}_2 + b_3\bar{\psi}_3 \end{Bmatrix} [c_1, c_2, c_3] \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix}$$

The remaining two terms of Energy equation can be evaluated in similar fashion of equation (1.2.24)

$$\int_A N^T \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \bar{T}}{\partial r} \right) 2\Pi\bar{r}dA = -\frac{2\Pi\bar{R}}{4A} \begin{bmatrix} b_1^2 & b_1b_2 & b_1b_3 \\ b_1b_2 & b_2^2 & b_2b_3 \\ b_1b_3 & b_2b_3 & b_3^2 \end{bmatrix} \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix}$$

$$\int_A N^T \frac{\partial^2 \bar{T}}{\partial z^2} 2\Pi r dA = -\frac{2\Pi R}{4A} \begin{bmatrix} c_1^2 & c_1 c_2 & c_1 c_3 \\ c_1 c_2 & c_2^2 & c_2 c_3 \\ c_1 c_3 & c_2 c_3 & c_3^2 \end{bmatrix} \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix}$$

Thus the stiffness matrix of Energy equation is given by

$$\begin{bmatrix} \frac{2\Pi}{12A} \begin{Bmatrix} c_1 \bar{\psi}_1 + c_2 \bar{\psi}_2 + c_3 \bar{\psi}_3 \\ c_1 \bar{\psi}_1 + c_2 \bar{\psi}_2 + c_3 \bar{\psi}_3 \\ c_1 \bar{\psi}_1 + c_2 \bar{\psi}_2 + c_3 \bar{\psi}_3 \end{Bmatrix} [b_1, b_2, b_3] - \frac{2\Pi}{12A} \begin{Bmatrix} b_1 \bar{\psi}_1 + b_2 \bar{\psi}_2 + b_3 \bar{\psi}_3 \\ b_1 \bar{\psi}_1 + b_2 \bar{\psi}_2 + b_3 \bar{\psi}_3 \\ b_1 \bar{\psi}_1 + b_2 \bar{\psi}_2 + b_3 \bar{\psi}_3 \end{Bmatrix} [c_1, c_2, c_3] \end{bmatrix} \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} + \frac{2\Pi R}{4A} \begin{bmatrix} b_1^2 & b_1 b_2 & b_1 b_2 \\ b_1 b_2 & b_2^2 & b_2 b_3 \\ b_1 b_3 & b_2 b_3 & b_3^2 \end{bmatrix} \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} + \begin{bmatrix} c_1^2 & c_1 c_2 & c_1 c_3 \\ c_1 c_2 & c_2^2 & c_2 c_3 \\ c_1 c_3 & c_2 c_3 & c_3^2 \end{bmatrix} \begin{bmatrix} \bar{T}_1 \\ \bar{T}_2 \\ \bar{T}_3 \end{bmatrix} = 0 \tag{1.2.43}$$

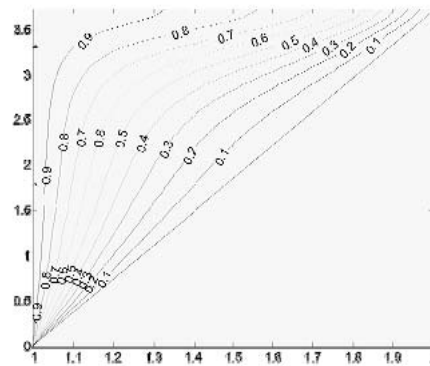
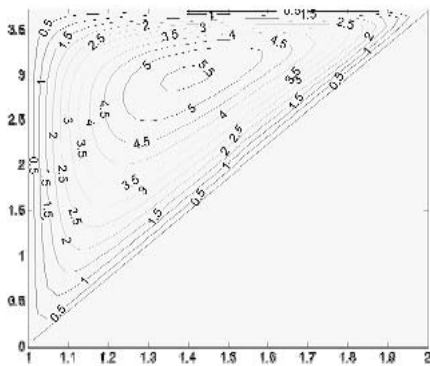
#### IV. RESULTS AND DISCUSSION

Results are obtained in terms of Nusselt number (Nu) at hot wall for various parameters such as Cone angle (C<sub>A</sub>), Radius ratio (R<sub>r</sub>) and Rayleigh number (Ra), when heat is supplied to vertical conical annular.

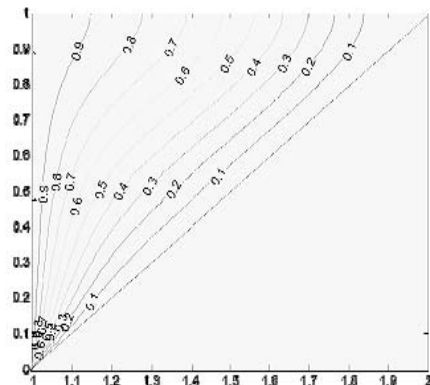
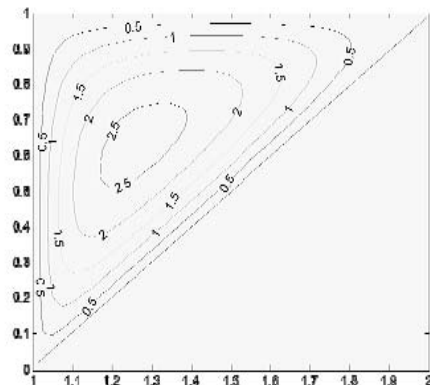
The average Nusselt number ( $\bar{Nu}$ ) is given by

$$\bar{Nu} = \int_0^1 \left( \frac{\partial \bar{T}}{\partial r} \right)$$

a)



b)



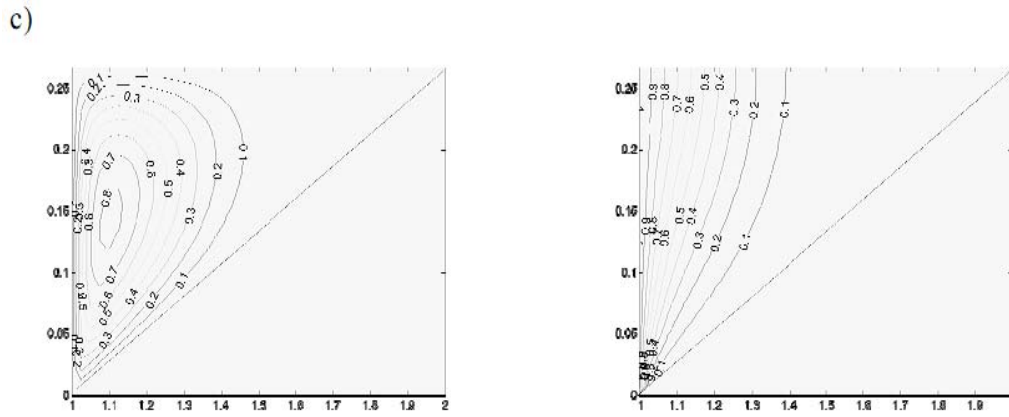


Figure 1.4.1 : Streamlines(left) and Isotherms(Right) for Ra=50, Ri=1  
 a) CA = 15 b) CA = 45 c) CA = 75

Figure (1.4.1) shows the evaluation of streamlines and isothermal lines inside the porous medium for various values of Cone angle (CA) at Ra = 50, Ri = 1. The magnitude of the streamlines decreases with the increase in Cone angles (CA). The thermal bounded layer thickness decreases with the increase of Cone angles (CA). It can be seen from streamlines and isothermal lines that the fluid movements shifts from

lower portion of the hot wall to upper portion of the cold wall of the vertical annual cone with the increase of Cone angles (CA). The circulation of the fluid covers almost whole domain at both lower and higher values of Cone angles (CA) at 15°. Where the relation inversely proportion exists between streamlines and Cone angles (CA). This trend is also observed with isothermal lines.

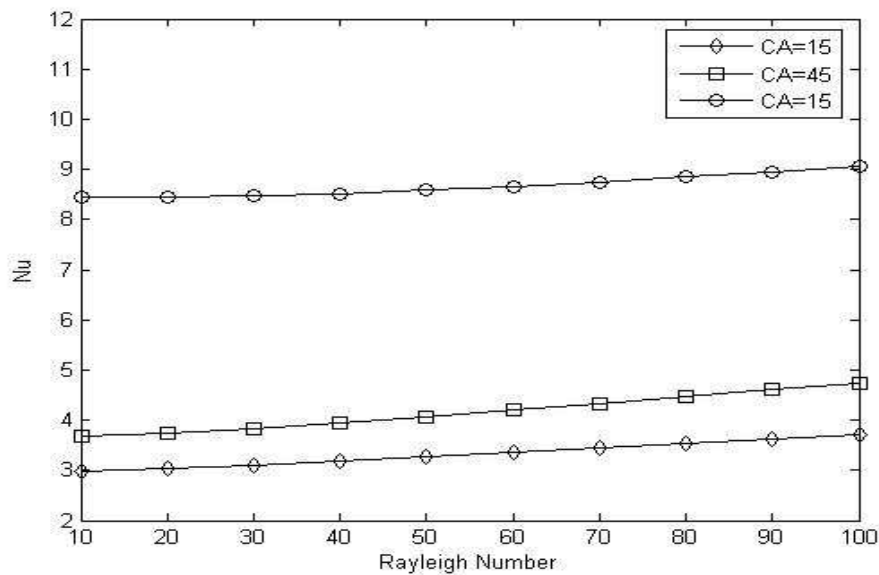
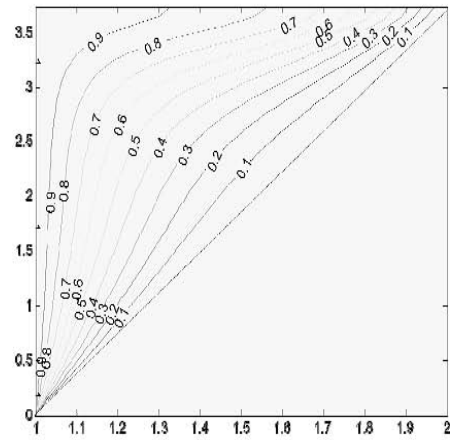
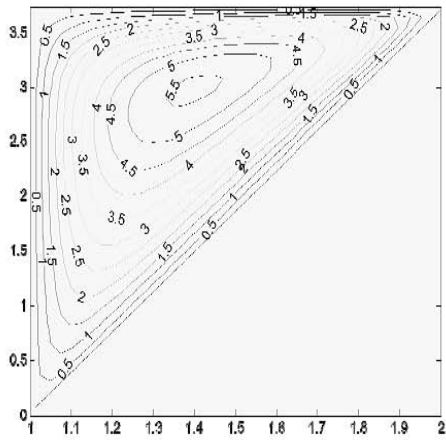


Figure 1.4.2 :  $\bar{Nu}$  variation with Ra at hot surface for different values of CA at Ri=1

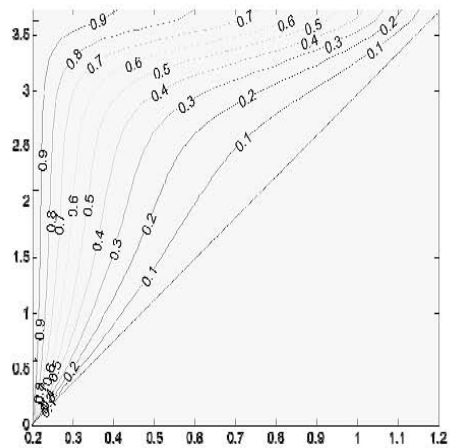
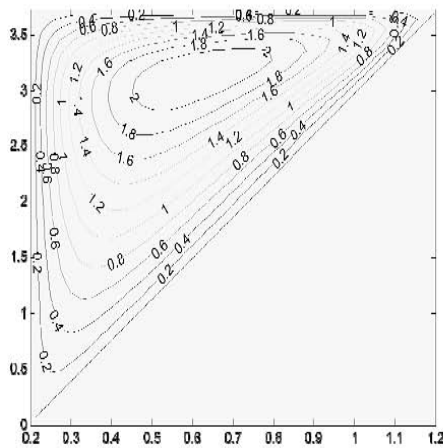
Figure (1.4.2) illustrates the effect of Rayleigh number (Ra) on the average Nusselt number ( $\bar{Nu}$ ). This Figure is obtained for value of Ri = 1. When cone angle is increased from 15 to 75, at the hot wall of the vertical annular cone, it is found that the average Nusselt number ( $\bar{Nu}$ ) at Ra = 10 is increased by 23.3%. The corresponding increase in average Nusselt number ( $\bar{Nu}$ ) at Ra = 100 is found to be 26.3%. The difference

between the average Nusselt number ( $\bar{Nu}$ ) at two different values of Cone angle (CA) increases with increase in Cone angle (CA). This is due to the reason that high cone angle produces high buoyancy force, which leads to increased fluid movements and thus increased the average Nusselt number ( $\bar{Nu}$ ) with Rayleigh number (Ra) as expected. This increase is almost linear for Cone angles (CA) 15 & 45 degrees.

a)



b)



c)

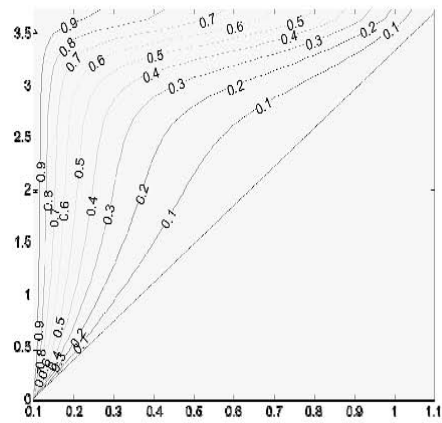
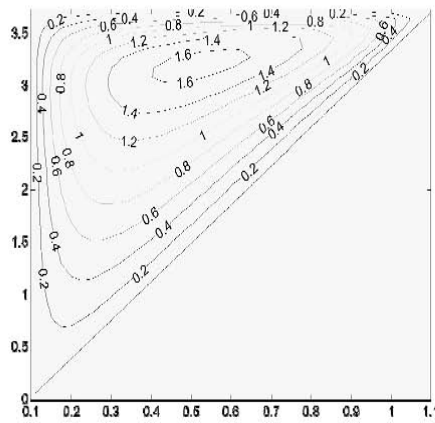


Figure 1.4.3 : Streamlines(left) and Isotherms(: Right) for Ra=50,  $C_A = 15$

a)  $R_r=1$  b)  $R_r=5$  c)  $R_r=10$

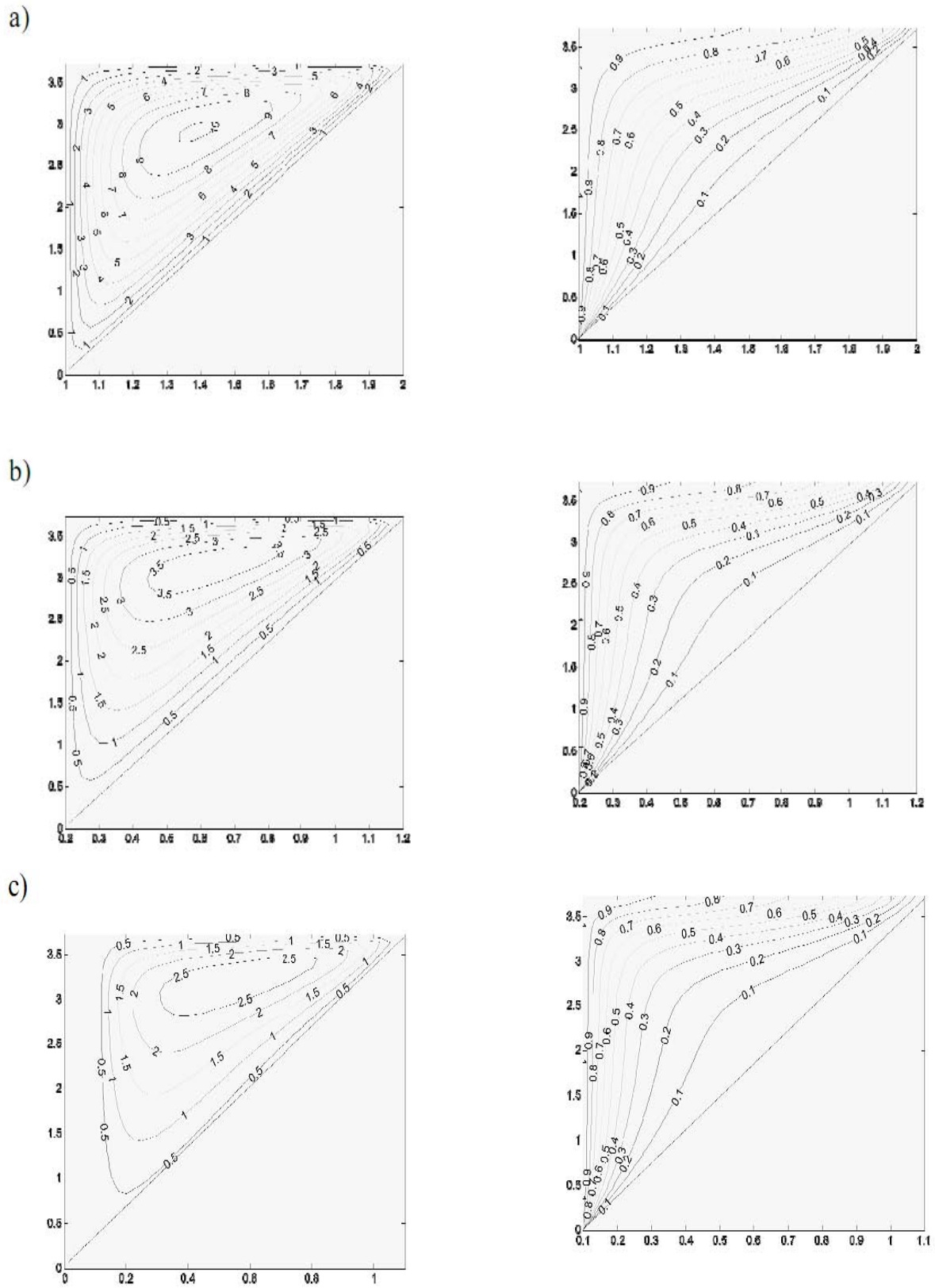


Figure 1.4.4 : Streamlines(left) and Isotherms(: Right) for Ra=100,  $C_A = 15$

a)  $R_r=1$  b)  $R_r=5$  c)  $R_r=10$



Figure (1.4.4) shows the streamlines and isothermal lines inside the porous medium for various values of Radius ratio ( $R_r$ ) at  $Ra = 50$  and  $C_A = 15$ . It can be observed that the horizontal scale changes for various values of Radius Ratio ( $R_r$ ). The magnitude of the streamlines decrease with the increase in Radius ratio ( $R_r$ ). The thermal boundary layer thickness

decreases with the increase in Radius ratio ( $R_r$ ). It can be seen from the streamlines and isothermal lines that the fluid movement shifts from lower portion of the hot wall to the upper portion of the cold of the vertical annular cone with the increase in Radius ratio ( $R_r$ ). The circulation of fluid covers almost whole domain at both lower and higher values of Radius ratio ( $R_r$ ).

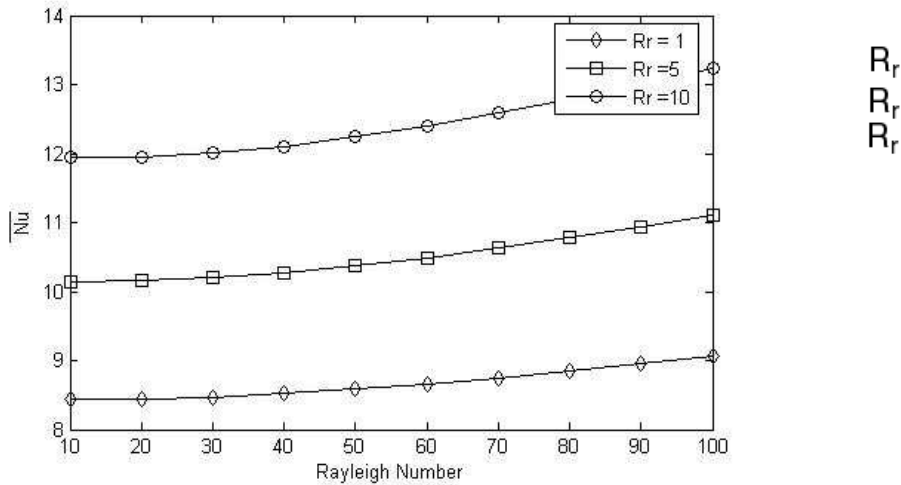


Figure 1.4.5:  $\bar{Nu}$  variation with  $Ra$  at hot surface for different values of  $R_r$  at  $C_A = 75$

Figure (1.4.5) shows the variation of average Nusselt number ( $\bar{Nu}$ ) at hot wall with respect to Rayleigh number ( $Ra$ ). This Figure is obtained for the value of  $C_A = 75$ . When Radius ratio ( $R_r$ ) is increased from 1 to 10 at the hot wall of the vertical annular cone, it is found that the average Nusselt number ( $\bar{Nu}$ ) at  $Ra = 10$  is increased by 20%. The corresponding increases in average Nusselt number ( $\bar{Nu}$ ) at  $Ra = 100$  is found to be 21%. The difference between the average Nusselt number ( $\bar{Nu}$ ) at two different values of Radius ratio ( $R_r$ ) increases with increase in Radius ratio ( $R_r$ ). High Radius

ratio ( $R_r$ ) produces high buoyancy force, which leads to faster fluid movements and thus increased the average Nusselt number ( $\bar{Nu}$ ). i.e., for a given Rayleigh number ( $Ra$ ) Nusselt number ( $\bar{Nu}$ ) increases with Radius ratio ( $R_r$ ).

Figure (1.4.5) shows the streamlines and isothermal lines inside the porous medium for various values of Radius ratio ( $R_r$ ) at  $Ra = 100$  and  $C_A = 75$ . Though the value of Rayleigh number increases ( $Ra = 100$ ), the streamlines and isothermal lines appear almost same as in Figure (1.4.7).

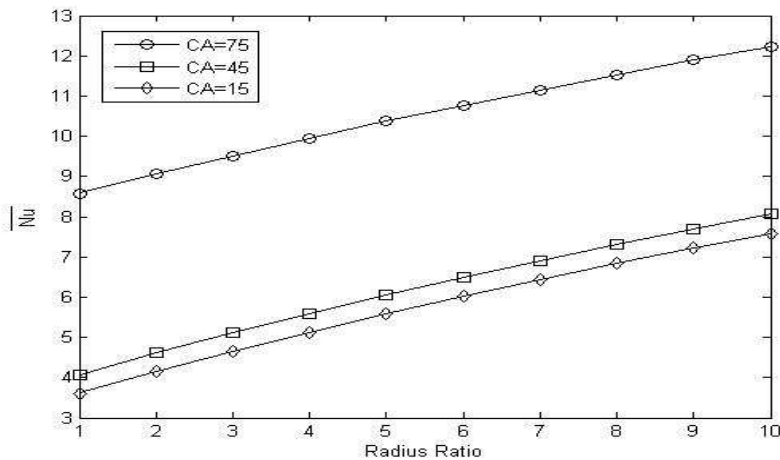


Figure 1.4.6:  $\bar{Nu}$  variation with  $R_r$  at hot surface for different values of  $C_A$  at  $Ra = 50$

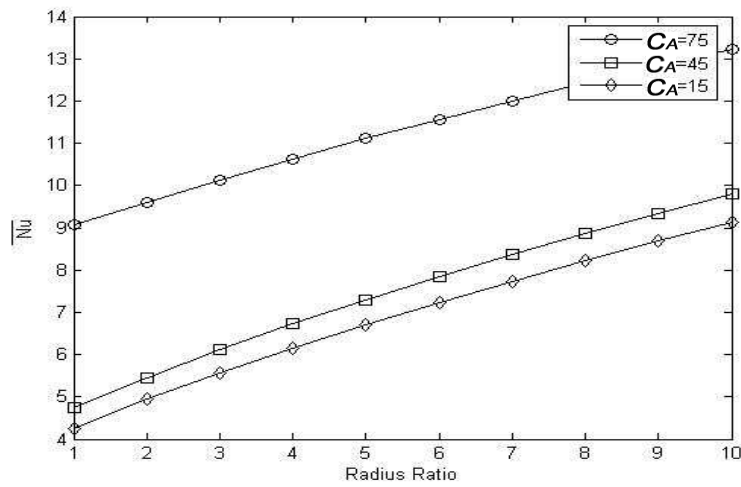
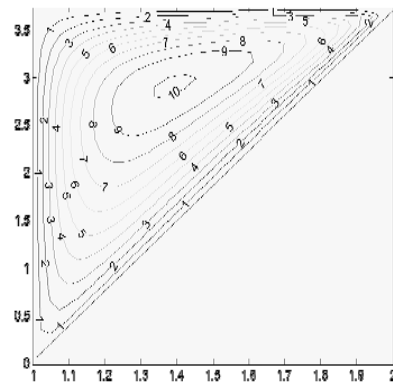
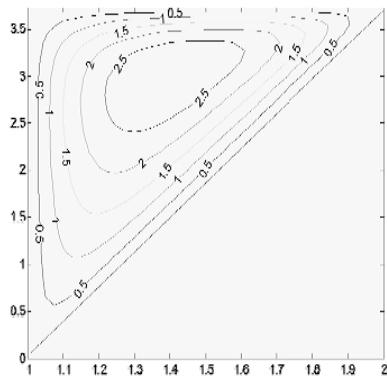


Figure 1.4.7:  $\bar{Nu}$  variation with  $R_r$  at hot surface for different values of  $C_A$  at  $Ra = 100$

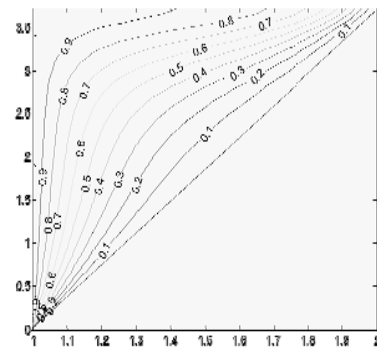
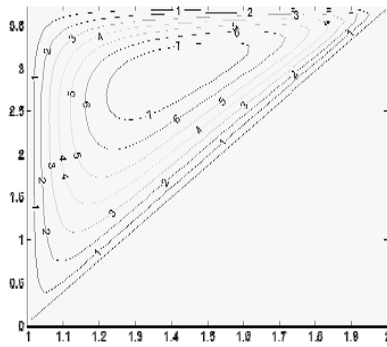
Figure (1.4.7) illustrates the effect of Radius ratio ( $R_r$ ) on average Nusselt number ( $\bar{Nu}$ ). This Figure corresponds to the value  $Ra = 50$ . It is seen that the average Nusselt number ( $\bar{Nu}$ ) at hot wall of the vertical annular cone increases with increase in Radius ratio ( $R_r$ ). It is found that the average Nusselt number ( $\bar{Nu}$ ) at  $R_r = 1$  increases by 9% when Cone angle ( $C_A$ ) increased from 15 to 45. the corresponding increase in average Nusselt number ( $\bar{Nu}$ ) at  $R_r = 10$  is found to be 9.4%. This difference becomes more prominent with the increase in Radius ratio ( $R_r$ ) for higher values of cone angle. For a given Radius ratio ( $R_r$ ) as the Cone angle ( $C_A$ ) increases, the average Nusselt number ( $\bar{Nu}$ ) increases. The increase is marginal when the Cone angle ( $C_A$ ) is increased from  $15^\circ$  to  $45^\circ$  when as we increases is substantial when we Cone angle ( $C_A$ ) increases from  $45^\circ$  to  $75^\circ$ .

Figure (1.4.10) illustrates the effect of Radius ratio ( $R_r$ ) on the average Nusselt number ( $\bar{Nu}$ ). This Figure corresponds to the value  $Ra = 100$ . It is seen that the average Nusselt number ( $\bar{Nu}$ ) at hot wall of the vertical annular cone increases with increase in Radius ratio ( $R_r$ ). It is found that the average Nusselt number ( $\bar{Nu}$ ) at  $R_r = 1$  increased by 9.2% when Cone angle ( $C_A$ ) increased from 15 to 45. The corresponding increase in average Nusselt number ( $\bar{Nu}$ ) at  $R_r = 10$  is found to be 9.8%. This difference between the average Nusselt number ( $\bar{Nu}$ ) at two different value of Cone angle ( $C_A$ ) increases with increase Cone angle ( $C_A$ ). This difference becomes more prominent with the increase in Radius ratio ( $R_r$ ) for higher values of Cone angle ( $C_A$ ).

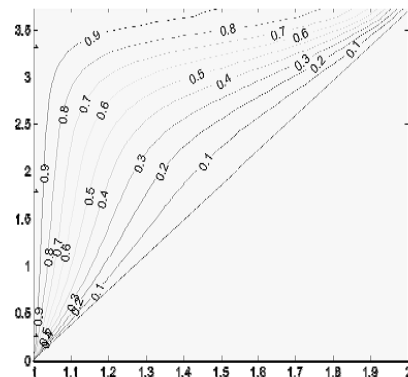
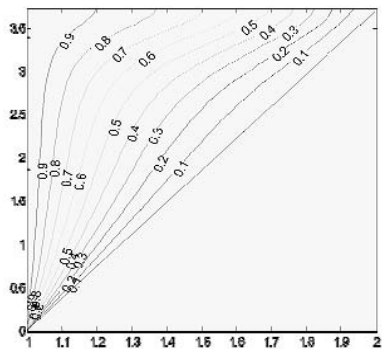
a)



b)



c)



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# Determination and Optimization of Bulk Total Energy for Gallium-Arsenide (GaAs) Atom using FHI98MD Input Variables

By J. A. Owolabi, M. Y. Onimisi & S. G. Abdu

*Kaduna State University, Nigeria*

**Abstract** - The Optimization of bulk total energy Calculations have been performed using the Local Density approximation for the exchange-correlation functional of Perdew Wang, within density-functional theory (DFT) for Gallium-arsenide (GaAs) atom. The optimized values obtained were used to calculate the bulk total energy of Gallium-arsenide. These calculations were performed using the Density Functional Theory method which represents the most popular technique for examining a wide range of structural and electronic properties of semiconductors and its alloys. The DFT code FHI98MD was employed for this computation which contains seventy six input parameters/variables. Some of these variables were determined and calculated while seven parameters that determine electronic convergence were successfully optimized for Local Density Approximation (LDA).

Result shows that the bulk total energies of - 8.6610957 were obtained for GaAs (LDA). This result of GaAs agrees well with the value -8.0691176 Rydberg/atom obtained 1999 by Stadelde et al and -8.364 Rydberg/atom obtained 2003 by Franziska Gizegoizewski.

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**GJSFR-A Classification** : FOR Code: 091305



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## 1. INTRODUCTION

This paper presents the results of first principles calculations of electronic structure by optimization of Bulk total energy for Gallium arsenide (GaAs). This is a compound of the elements gallium and arsenic. It is a III/V semiconductor, and is used in the manufacture of devices such as microwave frequency integrated circuits, monolithic microwave integrated circuits, infrared light-emitting diodes, laser diodes, solar cells and optical windows. (Moss and Ledwith 1987).

The intensive aspect of Hartree-Fock (HF) was circumvented when performing the first principle calculations considering the large system of atoms involved. Over the years, the use of density functional theory (DFT) as a solution towards solving these problems has been highly successful. In this method the electron density is treated as the fundamental variable (Hohenberg and Kohn, 1964; Kohn and Sham 1965) instead of the one-electron wavefunctions as in HF. Here the forces on the ions were calculated and the ion

positions with respect to the total energy were optimised. Fundamentally, we wish to solve the many-body Schrodinger equation for this specific set of atoms in a specific configuration, i.e.

$$H\Psi_i = E_i\Psi_i \quad (1)$$

where H is the many-body Hamiltonian, and  $\Psi$  is the many-body wave-function corresponding to the  $i^{th}$  state which has energy  $E_i$ . The term  $\Psi$  is a function of the electron spin and co-ordinates as well as the nuclear positions. The minimum value of  $E$  therefore represents the ground state of the system.

### a) Theoretical Background

The approach used in this paper for the theory of electronic structure is that of DFT. In this approach, the electron density distribution  $n(\mathbf{r})$  rather than the many electron wave-function plays a central role between the fully interacting many electron system (described by the schrodinger equation) and a fictitious system of non-interacting fermions. The fundamental proof of DFT is of the existence of a local, effective mean field potential,  $V_{eff}$ , which depends only on the electron density and for which, if one solves a set of single particle Schrodinger- like equations,

$$\left(-\frac{1}{2}\nabla^2 + V_{eff}\right)\psi_i = \epsilon_i\psi_i \quad (2)$$

the density of the non-interacting system

$$n(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2 \quad (3)$$

will reproduce the exact density of the fully interacting system. Moreover the energy of the non-interacting system reproduces the exact ground state energy of the interacting system. The existence of such a potential is fascinating but the utility of DFT is dependent on one finding a decent approximation for  $V_{eff}$  that can be used in practical simulations (Parr and Yang, 1989). Typically,  $V_{eff}$  is separated into an electron-nuclear ( $V_{en}$ ), classical (Hartee) electron-electron interaction

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$(V_H)$  and the remaining exchange-correlation potential  $(V_{xc})$ ;

$$V_{eff} = V_{en} + V_H + V_{xc} \quad (4)$$

Where

$$V_H(r) = \int \frac{n(r')}{|r - r'|} dr' \quad (5)$$

a great variety of different approximations to  $V_{xc}$  have been developed.

For many years the local density approximation (LDA) has been used. In the LDA the exchange correlation energy density at a point in space is taken to be that of the homogeneous electron gas with the local electron density,  $\epsilon_{xc}(n)$ . Thus the total exchange correlation energy functional is approximated as

$$E_{xc}^{LDA} = \int n(r)\epsilon_{xc}(n(r))dr \quad (6)$$

from which the potential is obtained as,

$$V_{xc} = \frac{\delta E_{xc}}{\delta n} \quad (7)$$

The LDA has proven to be a remarkably fruitful approximation. However in computing energy differences between different structures, the LDA can have significant errors. For instance, the binding energy of many- systems is overestimated and energy barriers in diffusion or chemical reactions may be too small or absent. Currently, effective potentials that depend on local density approximation are widely used.

## II. METHODOLOGY

In this work the DFT programmed used is fhi98md. It has start utility fhi98start, the input files constraints.ini, inp.mod, start. inp, fort.11 and fort.12 are all placed in a common folder. All 76 parameters / variables in the files inp.mod and start.inp are determined and calculated for this system of interest. The start utility is then run which produces three additional files: inp.ini, balsac and balsacclu.

The fhi98md program is then run which produces seventeen output files. These include the general output file fort.6; the file energy; restart files fort.71, fort.72, fort.73, fort.74, fort.80; control files stopfile, stopprogram and a host of other data files.

To optimize a given parameter, the program is run repeatedly changing the value of the parameter in each run. The total energy, Harris energy, internal energy at zero temperature (zero energy) and the number of iterations are recorded for each run. The values obtained are then used for:

- Convergence test by plotting parameter versus total energy;
- Accuracy test by plotting parameter versus absolute difference between total energy and Harris energy
- Speed test by plotting parameter versus number of iterations.

The optimal value of the parameter is then determined from the three plotted graphs.

For parameters that are logical in nature, the program is run with the parameter set to .true. and then re-run with the parameter set to .false.

We then used all optimal values obtained to calculate total energies for bulk Gallium-arsenide.

The optimal parameters used are as follows

Delt: step length of the electronic iterations

Gamma: damping parameter for the second order electronic minimization scheme

Ecut: plane wave energy cutoff (in Rydberg)

Ecuti: plane wave energy cutoff of the initial wave function

Ekt: temperature of the artificial Fermi smearing of the electrons

idyn: scheme for solving the equation of motion of the nuclei.

i\_edyn: scheme to iterate the wave functions

tmetal: occupy electronic state

force\_eps: convergence criteria for local and total forces

ion\_damp: damping parameter

ion\_fac: mass parameter/ mass of the nuclei

## III. RESULTS AND DISCUSSIONS

The seven parameters that determine electronic convergence were optimized and several data were generated. The software "origin 5.0" was used to plot the graphs. These optimal values were then used to calculate the bulk total energy of Gallium-arsenide for Local Density Approximation.

### a) Tables of Data

Table 1 : Delt Optimization for Gallium-arsenide LDA

Delt	Number of iterations	Total energy ( $E_T$ )	Harris energy ( $E_H$ )	ABS( $E_T - E_H$ )
10	27	-8.6076685	-8.6076687	0.0000002
20	16	-8.6076686	-8.6076688	0.0000002
30	15	-8.6076685	-8.6076686	0.0000001
40	18	-8.6076684	-8.6076686	0.0000002

50	25	-8.6076685	-8.6076686	0.0000001
60	52	-8.6076685	-8.6076687	0.0000002
70	99	-8.6076685	-8.6076687	0.0000002
80	99	-7.7738509	-7.7618081	0.0120428
90	99	-7.5559049	-7.6780074	0.1221025
100	99	-7.5032794	-7.625224	0.1219446

Table 2 : Gamma Optimization for Gallium-arsenide LDA

Gamma	Number of iterations	Total energy ( $E_T$ )	Harris energy ( $E_H$ )	ABS( $E_T-E_H$ )
0.1	99	-7.5657386	-7.5719817	0.0062431
0.2	15	-8.6076685	-8.6076686	0.0000001
0.3	17	-8.6076685	-8.6076687	0.0000002
0.4	23	-8.6076685	-8.6076687	0.0000002
0.5	27	-8.6076686	-8.6076688	0.0000002
0.6	29	-8.6076685	-8.6076688	0.0000003
0.7	31	-8.6076685	-8.6076687	0.0000002
0.8	33	-8.6076685	-8.6076687	0.0000002
0.9	34	-8.6076686	-8.6076687	0.0000001
1	35	-8.6076686	-8.6076687	0.0000001

Table 3 : Ecut Optimization for Gallium-arsenide LDA

Ecuti	Number of iterations	Total energy ( $E_T$ )	Harris energy ( $E_H$ )	ABS( $E_T-E_H$ )
1	20	-8.68585	-8.685852	0.0000003
2	17	-8.68585	-8.685852	0.0000001
3	14	-8.68585	-8.685852	0.0000002
4	13	-8.68585	-8.685852	0.0000000
5	13	-8.68585	-8.685852	0.0000000
6	13	-8.68585	-8.685852	0.0000000
7	13	-8.68585	-8.685852	0.0000000
8	13	-8.68585	-8.685852	0.0000000
9	13	-8.68585	-8.685852	0.0000000
10	13	-8.68585	-8.685852	0.0000000
11	13	-8.68585	-8.685852	0.0000000
12	13	-8.68585	-8.685852	-0.0000001
13	13	-8.68585	-8.685852	-0.0000001
14	13	-8.68585	-8.685852	0.0000000
15	13	-8.68585	-8.685852	-0.0000001
16	13	-8.68585	-8.685852	0.0000001

Table 4 : Ecuti Optimization for Gallium-arsenide LDA

Ecuti	Number of iterations	Total energy ( $E_T$ )	Harris energy ( $E_H$ )	ABS( $E_T-E_H$ )
1	20	-8.68585	-8.685852	0.0000003
2	17	-8.68585	-8.685852	0.0000001
3	14	-8.68585	-8.685852	0.0000002
4	13	-8.68585	-8.685852	0.0000000
5	13	-8.68585	-8.685852	0.0000000
6	13	-8.68585	-8.685852	0.0000000
7	13	-8.68585	-8.685852	0.0000000
8	13	-8.68585	-8.685852	0.0000000
9	13	-8.68585	-8.685852	0.0000000
10	13	-8.68585	-8.685852	0.0000000
11	13	-8.68585	-8.685852	0.0000000

Table 5 : EKT Optimization for Gallium-arsenide LDA

EKT	Number of iterations	Total energy ( $E_T$ )	Harris energy ( $E_H$ )	ABS( $E_T-E_H$ )
0.01	13	-8.6858517	-8.6858517	0.0000000
0.02	13	-8.6858517	-8.6858517	0.0000000
0.03	13	-8.6858516	-8.6858517	0.0000001

0.04	13	-8.6858517	-8.6858517	0.0000000
0.05	13	-8.6858517	-8.6858517	0.0000000
0.06	13	-8.6858516	-8.6858516	0.0000000
0.07	13	-8.6858513	-8.6858514	0.0000001
0.08	13	-8.6858505	-8.6858504	0.0000001
0.09	13	-8.6858485	-8.6858484	0.0000001
0.1	13	-8.6858446	-8.6858446	0.0000000

Table 6 : Summary of Optimal Values

Parameters	Gallium-arsenide
Delt	30
Gamma	0.2
Ecut	17
Ecuti	14
EKT	0.05
ldyn	2
i_dyn	2
t-metal	True
force eps	0.0001
ion_damp	tfor- false tsdp- false
ion_fac	No effect

b) Total energy calculations for GaAs using optimized parameters

Table 7 : Total energy calculation for bulk GaAs LDA

Number of iterations	Total Energy ( $E_T$ )
1	-8.6594317
2	-8.6608468
3	-8.6610073
4	-8.6610704
5	-8.6610831
6	-8.6610916
7	-8.6610937
8	-8.6610951
9	-8.6610935
10	-8.6610938
11	-8.6610948
12	-8.6610955
13	-8.6610957
14	-8.6610958

c) Graphs of Optimized Bulk Gallium-Arsenide using Fhi98md Input Variables

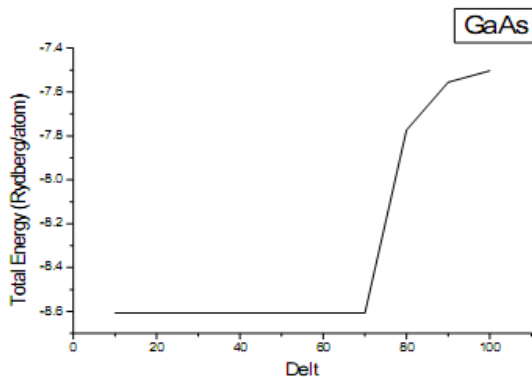


Figure 1 : Delt vs total energy (LDA) for GaAs

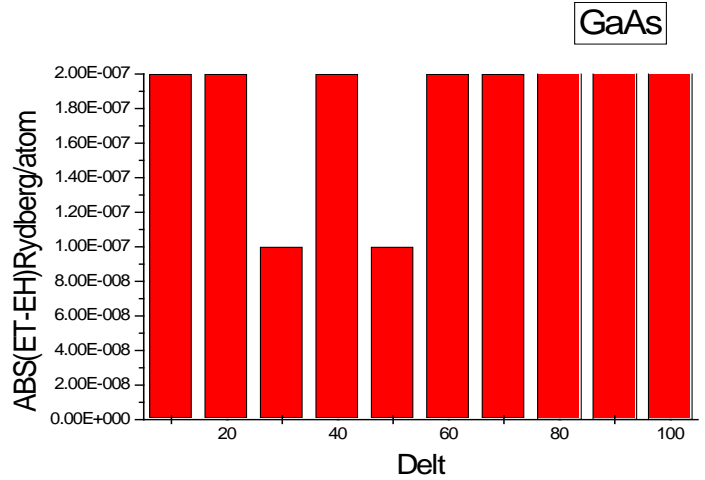


Figure 2 : Delt Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

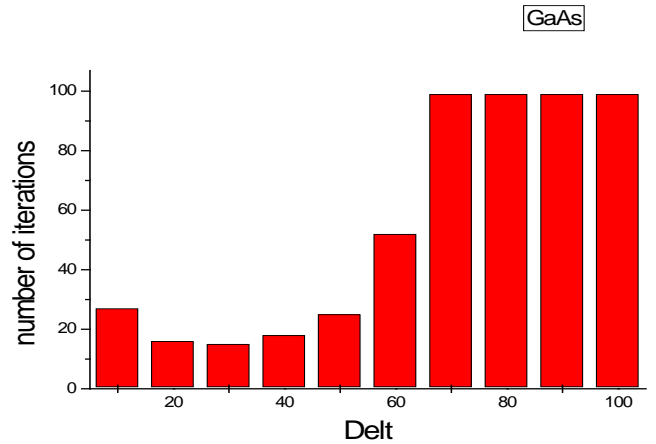


Figure 3 : Delt Vs number of iteration (LDA) for GaAs

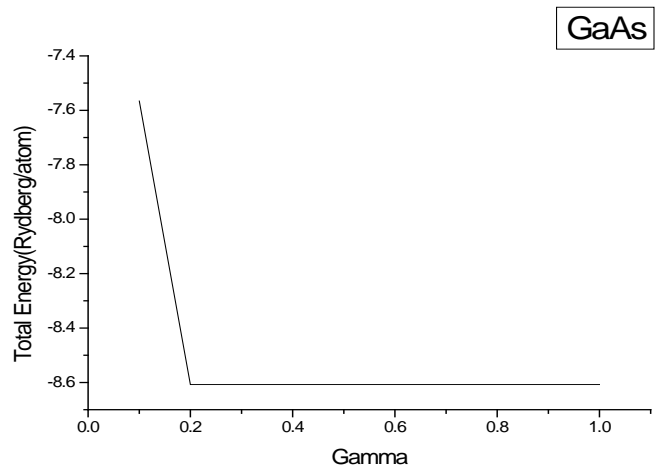


Figure 4 : Gamma vs. total energy (LDA) for GaAs

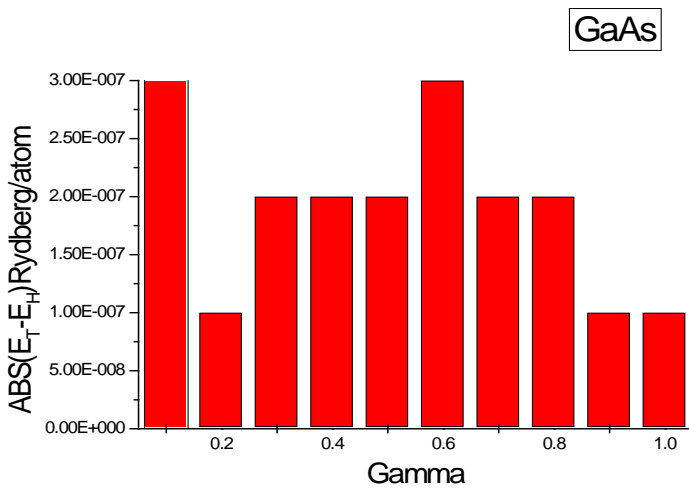


Figure 5 : Gamma Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

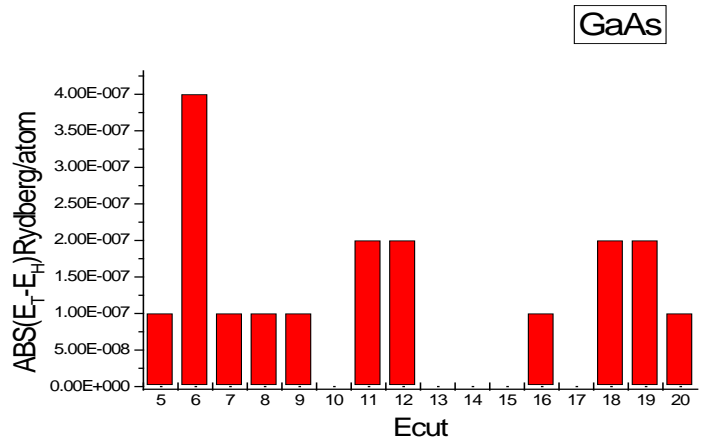


Figure 8 : Ecut Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

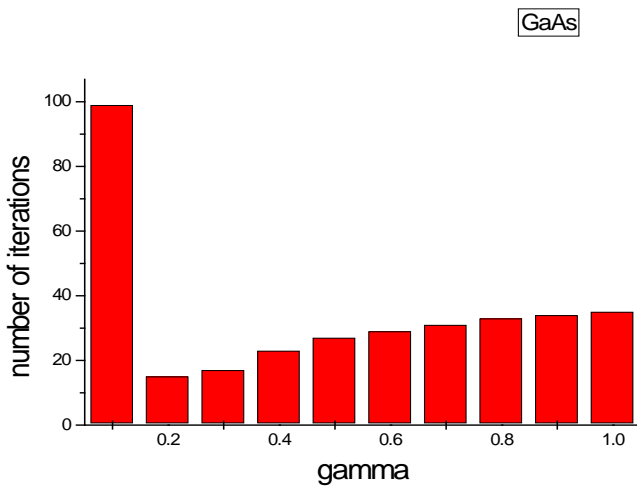


Figure 6 : Gamma Vs number of iterations (LDA) for GaAs

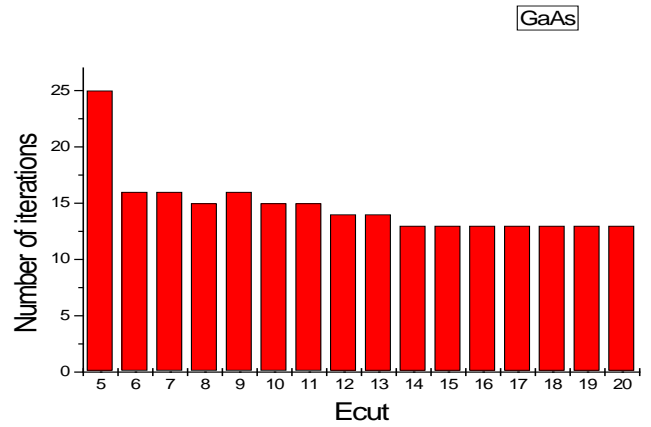


Figure 9 : Ecut Vs number of iterations (LDA) for GaAs

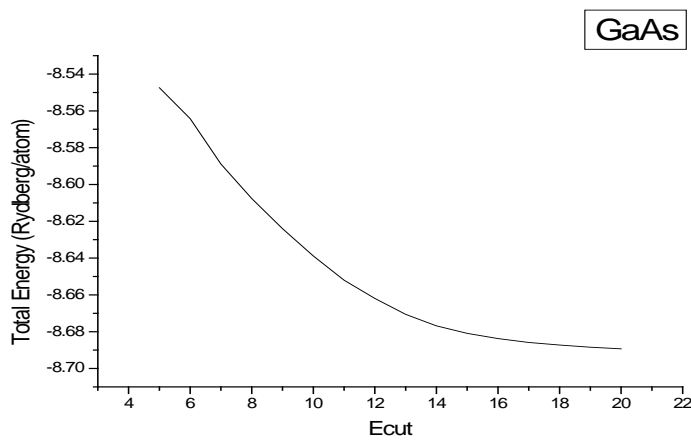


Figure 7 : Ecut Vs total energy (LDA) for GaAs

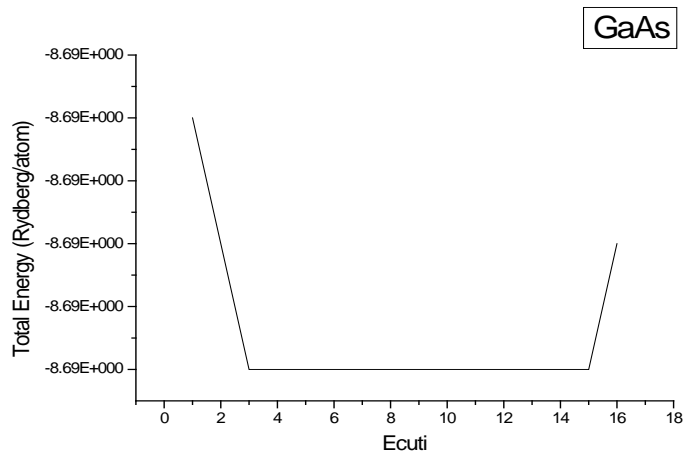


Figure 10 : Ecuti vs Total energy (LDA) for GaAs

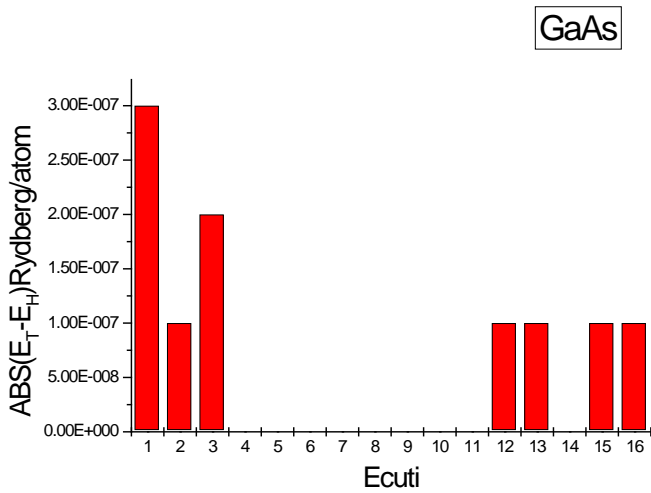


Figure 11 : Ecuti Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

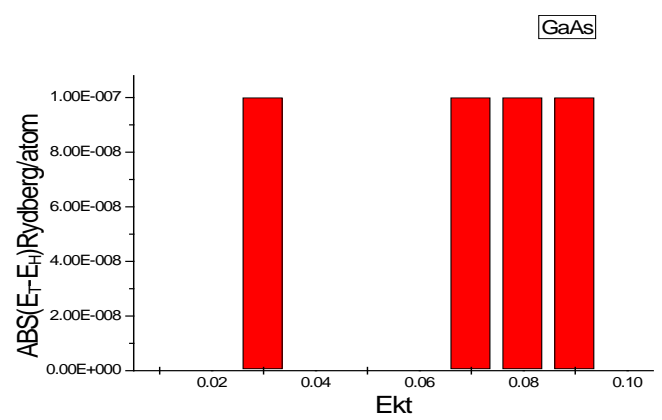


Figure 14 : Ekt Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

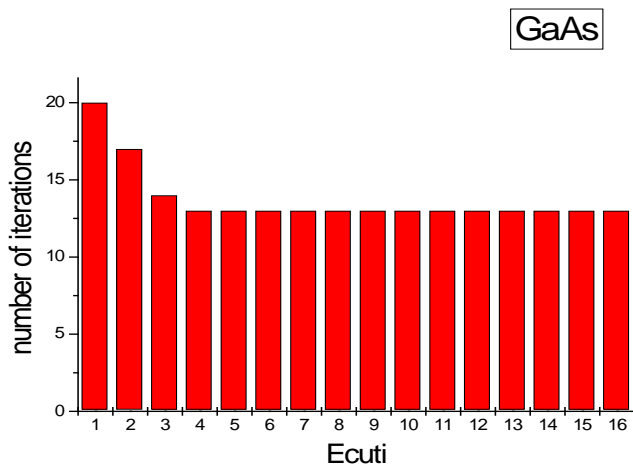


Figure 12 : Ecuti Vs number of iterations (LDA) for GaAs

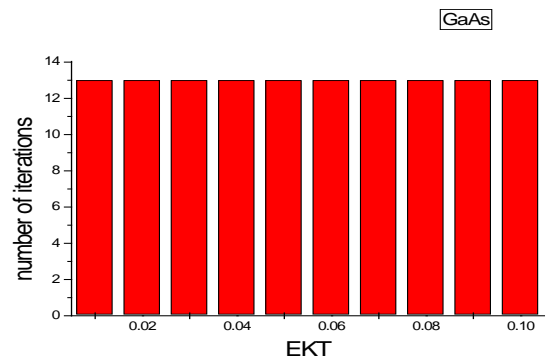


Figure 15 : Ekt Vs number of iterations (LDA) for GaAs

i. Total energy calculations for bulk GaAs

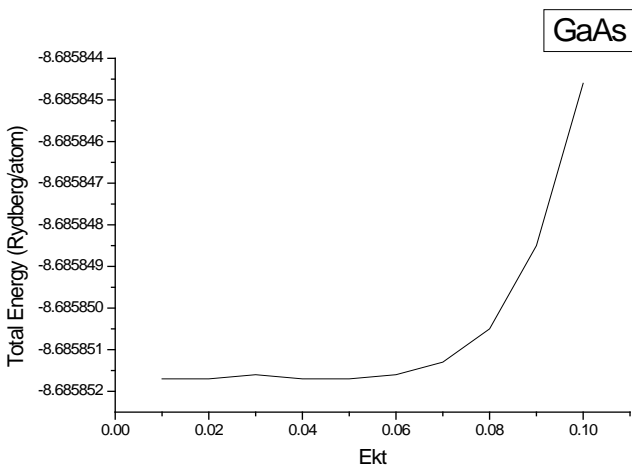


Figure 13 : Ekt vs Total energy (LDA) for GaAs

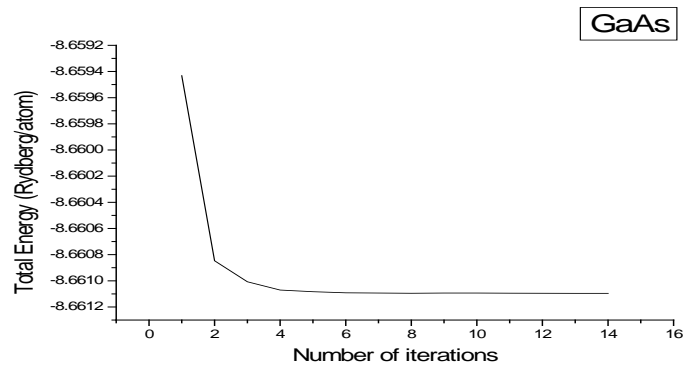


Figure 16 : Bulk Gallium-Arsenide convergence test (LDA)

#### IV. DISCUSSIONS

Fig1. Shows that Delt has a minimum energy between 10 and 70 while in Fig 2, Delt gave a more accurate result at 30 and 50. But from Fig 3 we can see that Delt has the least number of iterations at 30. This implies that 30 is the optimal value for Delt. However, fig 4 gave the minimum energy between 0.2 to 1.0 for Gamma, while fig 6 shows the least number of iterations

at 0.2 indicating that the optimal value for Gamma is 0.2. Fig 7-9 show that 17 is the optimal value for Ecut, while in figs 10-12 we can see that 14 is the optimal value for Ecuti. Fig: 16 show the bulk convergence test for GaAs which shows that the computations converged with total energy of -8.6610957 Rydberg/atom for GaAs.

This optimal values obtained for the parameters were used to calculate the total energy for bulk Gallium-arsenide. The energy -8.6610957 Rydberg/atom obtained for GaAs is in agreement with previously reported local density approximation (LDA) values of -8.0691176 Rydberg/atom (Stadele et al, 1999); and -8.364 Rydberg/atom. (Grzegoizewski, 2003).

## V. CONCLUSION

The seven main parameters that determine electronic as well as structural convergence have been successfully optimized and the optimal values were used to calculate the bulk total energy of Gallium-arsenide: -8.6610757 Rydberg / atom for LDA. This is in agreement with previously reported theoretical values.

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# Temperature Dependence of Inverse Dielectric Susceptibility in KDP-Type Crystals

By V. S. Bist & N. S. Panwar

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**Abstract** - By using four particle cluster model Hamiltonian along with third and fourth order phonon anharmonic interaction terms for KDP-type crystals, expressions for renormalized soft mode frequency, and inverse dielectric susceptibility have been obtained. The method of double time temperature dependent Green's function has been used for calculation. Fitting the values of model parameters, the temperature dependence of soft mode frequency and inverse dielectric susceptibility has been evaluated. The inverse dielectric susceptibility was observed increases linearly with temperature, for KDP crystal, in its paraelectric phase. Theoretical results are compared with experimental results of Kim et al [Physics Review B73, 134114 (2006), and Current Applied Physics 9(2009) 1307]. A good agreement has been found between the reported and present results.

**Keywords** : *soft mode frequency, inverse dielectric susceptibility, anharmonic interaction.*

**GJSFR-A Classification** : *FOR Code: 020199, 020109*



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# Temperature Dependence of Inverse Dielectric Susceptibility in KDP-Type Crystals

V. S. Bist<sup>α</sup> & N. S. Panwar<sup>σ</sup>

**Abstract** - By using four particle cluster model Hamiltonian along with third and fourth order phonon anharmonic interaction terms for KDP-type crystals, expressions for renormalized soft mode frequency, and inverse dielectric susceptibility have been obtained. The method of double time temperature dependent Green's function has been used for calculation. Fitting the values of model parameters, the temperature dependence of soft mode frequency and inverse dielectric susceptibility has been evaluated. The inverse dielectric susceptibility was observed increases linearly with temperature, for KDP crystal, in its paraelectric phase. Theoretical results are compared with experimental results of Kim et al [Physics Review B73, 134114 (2006), and Current Applied Physics 9(2009) 1307]. A good agreement has been found between the reported and present results.

**Keywords** : soft mode frequency, inverse dielectric susceptibility, anharmonic interaction.

## I. INTRODUCTION

Potassium dihydrogen phosphate ( $\text{KH}_2\text{PO}_4$ ), potassium dihydrogen arsenate ( $\text{KH}_2\text{AsO}_4$ ) and their deuterated forms, generally called KDP-type ferroelectrics, have been extensively studied due to their promising applications in optical communication, memory display and electro-optic devices. Much theoretical work has been done on KDP-type ferroelectrics as compared to ADP-type antiferroelectrics. KDP crystal undergoes a first order transition at 123 K, accompanied by tetragonal  $I\bar{4}2d(D_{2d}^{12})$ , at room temperature; and orthorhombic  $Fdd2(CD_{2v}^{19})$ , below transition temperature ( $T_c$ ). The  $(\text{H}_2\text{PO}_4^-)$  network, in which each phosphate group is linked by O-H-O bonds to a tetrahedron arrangement of phosphate group neighbors. All KDP-type ferroelectrics and selenites show a nearly two-fold increase (isotope effect) in transition temperature ( $T_c$ ) on deuteration.

The  $\text{KH}_2\text{PO}_4$  (KDP)-type crystals are interesting hydrogen-bonded materials undergoing structural phase transition accompanied by ferroelectricity or antiferroelectricity. In these crystals, it is known that

proton in the double well potentials on the hydrogen bonds are involved in a phase transition accompanied by displacements in the heavy atom (K, P, O) structure. KDP undergoes the ferroelectric phase transition at 123K<sup>1</sup>. An outstanding peculiarity with KDP is the proton-deuteron "isotope effect", that raises the transition temperature by about 100 K mainly due to the change in the O-O separation rather than to a change in the tunneling frequency by the mass change<sup>2</sup>. The protons are self-trapped in one or the other of its equivalent positions according to recent neutron Compton scattering experiments<sup>3</sup>. While the tunneling model does not consider the hydrogen-bond geometry, the  $\text{PO}_4$  tetrahedral distortion has theoretically been shown to give rise to a change in the ground state energy<sup>4,5</sup>.

Earlier Havlin, Litov, and Uehling<sup>6</sup>, using a mean field approximation, a Curie-type transverse susceptibility was theoretically obtained for  $T > T_c$ , and Semwal and Sharma<sup>7</sup> using Green's function method have studied ferroelectric transition and dielectric properties of KDP-type crystals. Many workers<sup>8-12</sup> have experimentally studied the dielectric properties of these crystals. Expressions for different physical parameters were developed to explain ferroelectric transitions in displacive<sup>13-16</sup> and order-disorder<sup>17-21</sup> type crystals.

In our previous works<sup>20-21</sup> we used the Blinc's Hamiltonian including the lattice anharmonicity upto fourth order, for the stochastic motion of  $\text{H}_2\text{PO}_4^-$  groups. Applying Green's functions techniques and Dyson's equation the higher order correlations were evaluated using the renormalized Hamiltonian. The proton renormalized frequency of the coupled system and collective proton wave half widths have been evaluated. Temperature dependence of relaxation time in KDP-type ferroelectrics, and dielectric properties of order-disorder type crystals, were studied above  $T_c$ . In the present study the same Hamiltonian, same techniques have been used to obtain expressions for renormalized soft mode frequency and inverse dielectric susceptibility. Fitting the values of model parameters in the obtained expressions, the temperature dependence of soft mode frequency and inverse dielectric susceptibility has been evaluated. The inverse dielectric susceptibility increased linearly with temperature for KDP crystal in its paraelectric phase. Theoretical results are compared with experimental result of Kim *et al*<sup>8-9</sup>.

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## II. DIELECTRIC SUSCEPTIBILITY

The response of a dielectric field is conveniently described by the dielectric susceptibility. Following Kubo<sup>22</sup> and Zubarev<sup>23</sup>, the general expression for complex dielectric susceptibility tensor  $\chi_{mn}(\omega)$  can be expressed as

$$\chi_{mn}(\omega) = \lim_{\varepsilon \rightarrow 0} -2\pi G_{mn}(\omega + j\varepsilon). \quad (1)$$

Where  $G_{mn}(\omega)$  is the Fourier transform of the retarded double-time thermal Green's function between the  $m^{\text{th}}$  and  $n^{\text{th}}$  components of the crystal dipole moment operators  $\vec{M}(t)$  in the Heisenberg representation, and is defined as

$$G_{mn}(t-t') = \langle\langle M_m(t); M_n(t') \rangle\rangle = -j\theta(t-t') \langle [M_m(t); M_n(t')] \rangle. \quad (2)$$

Where  $\theta(t-t')$  is the Heaviside step function and the angular brackets  $\langle \dots \rangle$  denote the thermal ensemble average. The crystal dipole moment  $\vec{M}(t)$  depends on the ionic co-ordinates, like potential energy, and can be expanded in a Taylor's series in terms of ionic displacements. Because of the periodic boundary conditions, i.e., symmetry considerations, imposed on the ionic motions, only the low lying relaxational modes have non-zero polarization associated with them. Thus only the expansion coefficients which correspond to lowest frequency mode, i.e.,  $\vec{M}(q, j)$  (where  $q = 0$  for ferroelectrics, and  $j$  relates the modes of spectrum) contribute to the dielectric susceptibility, significantly. Thus we can write the dielectric susceptibility as

$$\chi_{mn}(\omega) = \lim_{\varepsilon \rightarrow 0} -2\pi N\mu^2 G_{mn}(\omega + j\varepsilon), \quad (3)$$

where  $N$  is the number of unit cells in the sample and  $\mu$  is the effective dipole moment per unit cell, and

$$G_{mn}(\omega + j\varepsilon) = \langle\langle A_q(t); A_q(t') \rangle\rangle = G'(\omega) - jG''(\omega). \quad (4)$$

Where  $G'(\omega)$  and  $G''(\omega)$  are real and imaginary parts of the Green's function defined by<sup>20</sup>. The dielectric constant can be evaluated using the relation

$$\varepsilon(\omega) = 1 + 4\pi\chi = \varepsilon'(\omega) - j\varepsilon''(\omega), \quad (5)$$

where  $\varepsilon'(\omega)$  and  $\varepsilon''(\omega)$  are real and imaginary parts of the dielectric constant. The real part of the dielectric constant can be expressed as

$$\varepsilon'(\omega) - 1 = -8\pi N\mu^2 G'(\omega), \quad (6)$$

and the imaginary part

$$\varepsilon''(\omega) = -8\pi N\mu^2 G''(\omega). \quad (7)$$

Using equation (3) and acoustic phonon Green's function by<sup>20</sup>. The dielectric susceptibility for KDP - system can be obtained as

$$\chi(\omega) = \frac{-2N\mu^2 \tilde{\omega}}{[\omega^2 - \tilde{\omega}^2 + 2j\omega \Gamma_P(\omega)]}. \quad (8)$$

Where  $\tilde{\omega}$ ,  $\Gamma_P(\omega)$  are the collective mode frequency, and damping constant, respectively is given by<sup>20</sup>. The range of frequencies used in ultrasound<sup>24</sup>, Brillouin<sup>25</sup> and susceptibility<sup>24</sup> measurement experiments are such that  $\omega \ll \tilde{\omega}$ . Thus equation (8) reduces to

$$\chi(\omega) = \frac{2N\mu^2 \tilde{\omega}}{\tilde{\omega}^2 [1 - j\omega\tau_P]}. \quad (9)$$

Where the polarization relaxation time ( $\tau_P$ ) is given by<sup>26</sup>. This approximation of equation (9) is equivalent to Debye relaxation susceptibility. Furthermore, if  $\omega\tau_P \ll 1$ , which is true for KDP-system<sup>22</sup>, equation (9) can be further reduced to

$$\chi(\omega) = \frac{2N\mu^2 \tilde{\omega}}{\tilde{\omega}^2} (1 + j\omega\tau_P), \quad (10)$$

Using equation (5) in equation (8) expression for dielectric constant, can be obtained as

$$\varepsilon(\omega) - 1 = \frac{-8\pi N\mu^2 \tilde{\omega} \left[ (\omega^2 - \tilde{\omega}^2) - 2j\omega\Gamma_P(\omega) \right]}{\left[ (\omega^2 - \tilde{\omega}^2)^2 + 4\omega^2 \Gamma_P^2(\omega) \right]}. \quad (11)$$

The imaginary part of which can be written as

$$\varepsilon''(\omega) = -\frac{8\pi N\mu^2 \tilde{\omega} 2\omega\Gamma_P(\omega)}{\left( \omega^2 - \tilde{\omega}^2 \right)^2 + 4\omega^2 \Gamma_P^2(\omega)}. \quad (12)$$

and the real part as

$$\varepsilon'(\omega) - 1 = -\frac{8\pi N\mu^2 \tilde{\omega} (\omega^2 - \tilde{\omega}^2)}{\left( \omega^2 - \tilde{\omega}^2 \right)^2 + 4\omega^2 \Gamma_P^2(\omega)}, \quad (13)$$

for the experimental range of frequencies,  $\omega \ll \tilde{\omega}$  and ( $\omega\tau_P \ll 1$  for KDP), equation (13) can be reduced to ( $\varepsilon' \gg 1$ )

$$\varepsilon'(\omega) = \frac{8\pi N\mu^2 \tilde{\omega}}{\tilde{\omega}^2 + \omega^2 \tau_p^2} = \frac{8\pi N\mu^2 \tilde{\omega}}{\tilde{\omega}^2}, \quad (14)$$

where  $\tilde{\omega}_\pm^2$ ,  $\tilde{\omega}_+$ ,  $\tilde{\omega}_-$ , and  $\tilde{\omega}$  are represented by<sup>20-21</sup>. The inverse susceptibilities, obtained from  $\varepsilon(\omega) = 1 + 4\pi\chi$ .

$$\chi_a^{-1}(\omega) = \frac{\tilde{\omega}^2}{2N\mu^2 \tilde{\omega} - \tilde{\omega}^2}. \quad (15)$$

The dielectric loss ( $\tan \delta$ ), for the dissipation of power in the dielectric crystal is defined as the ratio of imaginary and real parts of the dielectric constant, i.e.,

$$\tan \delta = \frac{\varepsilon''(\omega)}{\varepsilon'(\omega)} = \frac{G''(\omega)}{G'(\omega)}. \quad (16)$$

The dielectric loss tangent ( $\tan \delta$ ) in a dielectric sample given by equation (16), can be further written as

$$\tan \delta = \frac{-\omega\Gamma_p}{(\omega^2 - \tilde{\omega}_\pm^2)}. \quad (17)$$

The  $\tilde{\omega}_+$  mode gives the contribution for a weakly temperature dependent transverse relaxation behavior of the observed transverse tangent loss ( $\tan \delta_a$ ), can be written as

$$\tan \delta_a = \frac{-\omega\Gamma_p}{(\omega^2 - \tilde{\omega}_+^2)}, \quad (18)$$

$\tilde{\omega}_-$  mode contributes to the longitudinal relaxational behavior of the longitudinal tangent loss ( $\tan \delta_c$ ), which can be written as

$$\tan \delta_c = \frac{-\omega\Gamma_p}{(\omega^2 - \tilde{\omega}_-^2)}. \quad (19)$$

### III. NUMERICAL CALCULATIONS

By using Blinc-de Gennes model parameters for KDP as given by Ganguli et al<sup>28</sup>. We have calculated width, shift, collective phonon mode frequency, transverse dielectric constant  $\varepsilon_a(0)$ , observed dielectric constant  $\varepsilon_c(0)$ , loss tangent and the inverse susceptibilities are calculated using respective equations are tabulated in table 1.

Table 1: Calculated values for KDP crystal in PE phase

Temperature (K)	125	130	135	140	145	150	Reference
$\Gamma_p(\omega) \times 10^{-4}$ ( $\text{cm}^{-1}$ )	2.87	2.31	1.76	1.88	1.90	1.92	20
$\tilde{\omega}$ ( $\text{cm}^{-1}$ )	45.65	57.04	58.69	63.04	64.91	65.85	20
$\varepsilon_a(0)$	63	62	61	60	59	58	21
$\varepsilon_c(0)$	35714	6144	2286	874	486	359	21
$\tan \delta_a$	0.004	0.00398	0.00397	0.00396	0.00395	0.00394	21
$\tan \delta_c$	0.067	0.035	0.0261	0.0255	0.0250	0.02	21
$\tilde{\omega} \times 10^3$ (MHz)	1.3685	1.7104	1.7594	1.8898	1.9459	1.9476	<i>Present study</i>
$\chi_a^{-1} \times 10^{-3}$	202.68	206	209.4	212.9	216.6	220.04	<i>Present study</i>
$\chi_c^{-1} \times 10^{-4}$	3.518	20.45	54.99	143.78	259.13	408.49	<i>Present study</i>

### IV. TEMPERATURE DEPENDENCE OF INVERSE DIELECTRIC SUSCEPTIBILITY

The inverse dielectric susceptibility has been calculated in the paraelectric phase at 10 GHz for KDP crystal obtained from  $\varepsilon(\omega) = 1 + 4\pi\chi$ . The temperature variations of inverse dielectric susceptibility have also

shown in figures 1 and 2. The theoretical results are in fair agreement with experimental result of Kim et al<sup>8</sup>. The solid lines are linear fits above  $T_c$ .

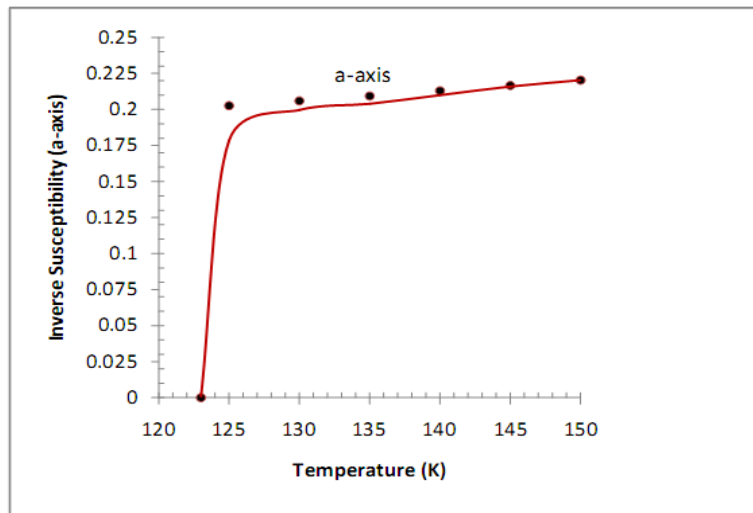


Figure 1 : Temperature dependence of inverse susceptibility in KDP crystal (a-axis)

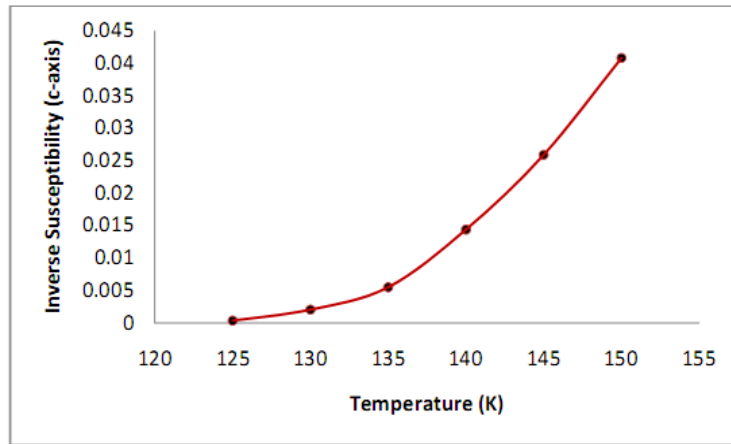


Figure 2 : Temperature dependence of inverse susceptibility in KDP crystal (c-axis)

### V. FREQUENCY DEPENDENCE OF DIELECTRIC LOSS

Putting calculated value of  $\Gamma_p(\omega)$ ,  $\tilde{\omega}$ , in the temperatures region  $T > T_c$ , into equations (18) and

(19), dielectric loss is obtained for KDP crystals at 9.2 GHz at 123K. The variations are shown in figure 3. The increase in loss is followed by an increase in frequency in KDP crystal. The dielectric loss versus  $(T-T_c)^{-1}$  for KDP crystal is shown in figure 4.

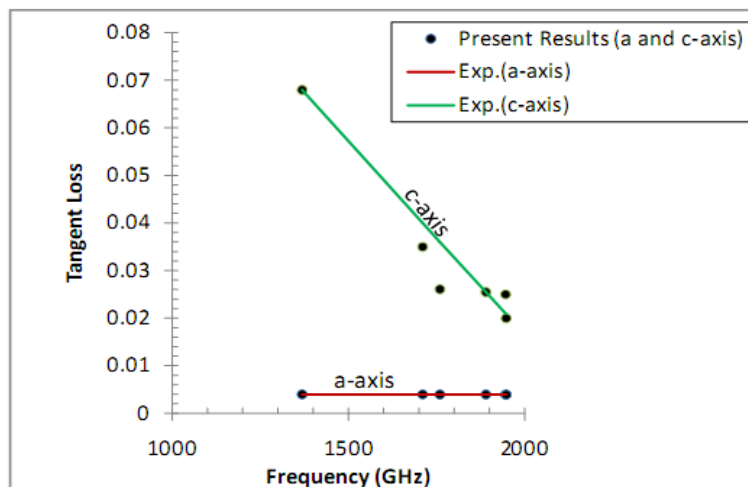


Figure 3 : Frequency dependence of dielectric loss in KDP crystal



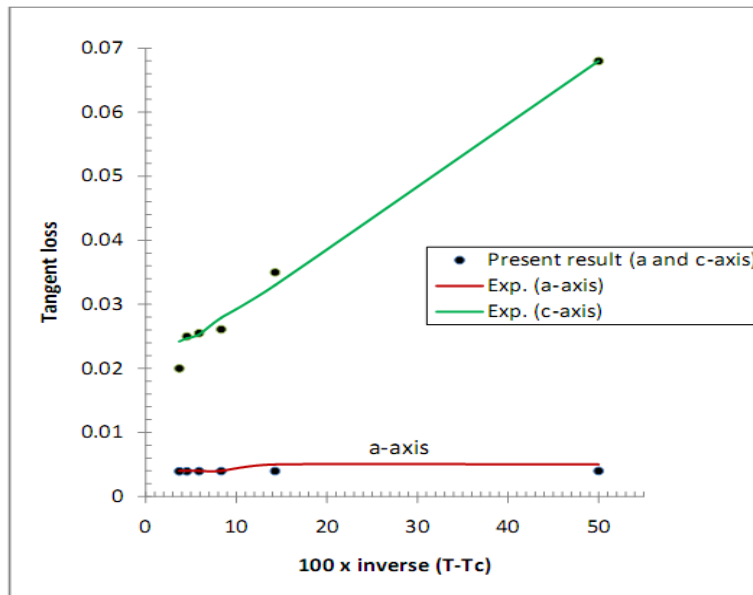


Figure 4 : Temperature dependence of dielectric loss in KDP crystal

## VI. RESULT AND DISCUSSION

In this paper, the four-particle cluster model Hamiltonian for KDP-type ferroelectric crystals has been modified by adding the third and fourth order phonon anharmonic interaction terms. Expressions for the inverse susceptibility and tangent loss are evaluated theoretically. Using model value as given by Ganguli<sup>28</sup>, temperature variations of these quantities for KDP crystal were calculated. Present work differs with the earlier works in the sense of that phonon anharmonic terms are not considered in that work. Ganguli et al<sup>28</sup> have considered the higher order anharmonic phonon-interaction terms and find the exact isotope dependence of Curie-Weiss constant, specific heat and electrical susceptibility, but they could not explain the behavior of loss parameter, width and shift in pseudospin-lattice coupled mode (PLCM) frequency due to early decoupling of correlation functions.

Ramakrishnan and Tanaka<sup>29</sup>, using the fermions Green's function, showed that with Tyablikov-type decoupling<sup>30</sup> the transverse susceptibility of KDP reproduces, the result of Havlin, Litov and Uehling<sup>6</sup>. They concluded that the use of Green's function offers a systematic approach to the study of both static and dynamical aspects of ferroelectric phase transition in KDP and showed the superiority of Green's-function method over the usual mean-field and linearized Bloch equation of motion method.

Due to anharmonic phonon interactions, decay processes takes place. For example, third order interaction leads to the decay of a virtual phonon into two real phonons or the virtual phonon may be destroyed by scattering a thermally excited phonon. Similar processes occur for fourth-and higher order interactions.

In figure 4, the loss shows Curie-Weiss behavior, i.e., losses are proportional to  $(T-T_c)^{-1}$  in the vicinity of  $T_c$  which is in agreement with earlier experiments<sup>32</sup>. The phonon anharmonic interactions significantly contribute to temperature dependence of soft mode, dielectric constant and loss, at and above  $T_c$ .

## VII. CONCLUSIONS

Present study shows that soft mode theory successfully explains the dynamics of ferroelectric transition in KDP in a quite similar way as the antiferroelectric transition in ADP, which shows the possibility of a unified theory of ferroelectric and antiferroelectric transitions. It reveals that four particle cluster mode Hamiltonian, alongwith third and fourth order anharmonic interactions, explains phase transition and the dielectric properties of KDP-type ferroelectric crystals. The result of present calculation can also be extended to explain phase transition and the dielectric properties of other ferroelectric crystals such as Cs H<sub>2</sub>PO<sub>4</sub>, RbH<sub>2</sub>PO<sub>4</sub>, PbH<sub>2</sub>PO<sub>4</sub>, TiH<sub>2</sub>PO<sub>4</sub><sup>8-11</sup>.

The observed dielectric susceptibility may be expressed as a linear combination of the susceptibility originating due to the two relaxation times ( $\tau_1$ , and  $\tau_2$ ):  $\tau_1$  corresponding to  $\tilde{\omega}_-$ , tends to infinity as  $T \rightarrow T_c$  and the other  $\tau_2$ , corresponding to a  $\tilde{\omega}_+$ , is weakly temperature dependent.

$$\chi = \frac{\chi_1}{1 + j\omega\tau_1} + \frac{\chi_2}{1 + j\omega\tau_2}$$

$\chi_1$  and  $\chi_2$  represent the contribution of the static susceptibility ( $\chi_0$ ) from the two relaxation

modes. From these results we conclude the following properties of the susceptibility  $\chi(\omega)$  in the present approximation: (i) the static susceptibility is mainly contributed from  $\chi_1$ . (ii) in the dynamic susceptibility  $\chi(\omega)$ , the first part contributes significantly, i.e., contribution from the first mode which vanishes at  $T = T_c$ , just as in Mason theory<sup>27</sup>, because of the fact that  $\chi_1 \rightarrow \infty$ , as  $\tau_1 \rightarrow \infty$  at  $T \rightarrow T_c$ . (iii) The contribution to  $\text{Re } \chi(\omega)$  from the second mode remains finite at  $T_c$ , although its magnitude is of negligible order.

The inverse dielectric susceptibility increases linearly with temperature for KDP crystal in its paraelectric phase.

## VIII. ACKNOWLEDGEMENT

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## Some Observable Effects of Heat Flow in Response to Thermal Potentials at the Boundary

By C.I. Okoro

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**Abstract** - When heat flow is subject to temperature dependent thermal potential at the boundary, the associated local temperature field responds significantly, while the neighboring field is marginally influenced. This response results into effects quite intriguing. This paper examines these effects over a pure metallic plate. By considering both linear and non-linear thermal potentials induced at the edge of the plate as test cases, governed by Poisson Equation in 2-dimensions, finite element algorithm is employed to compute the temperature profiles. A control model is set-up, which admits Laplace Equation in 2-dimensions, and the outputs from the test models and the control model are examined and compared. The MATLAB results show notable effects. These results are discussed which are invaluable design factors for optimum efficiency of thermally driven systems such as in nuclear power plants, thermo-chemical plants, thermo-mechanical industries, lasers, solid state plasma, e.t.c. This paper, when incorporated with our previous work [9], serves as good theoretical grounds for believing the notable physical anomalies in heat transfer processes, such as the paradox of moving medium detected in the non-Fourier DPL heat conduction model [10].

*GJSFR-A Classification : FOR Code: 091505*



SOME OBSERVABLE EFFECTS OF HEAT FLOW IN RESPONSE TO THERMAL POTENTIALS AT THE BOUNDARY

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# Some Observable Effects of Heat Flow in Response to Thermal Potentials at the Boundary

C.I. Okoro

**Abstract** - When heat flow is subject to temperature dependent thermal potential at the boundary, the associated local temperature field responds significantly, while the neighboring field is marginally influenced. This response results into effects quite intriguing. This paper examines these effects over a pure metallic plate. By considering both linear and non-linear thermal potentials induced at the edge of the plate as test cases, governed by Poisson Equation in 2-dimensions, finite element algorithm is employed to compute the temperature profiles. A control model is set-up, which admits Laplace Equation in 2-dimensions, and the outputs from the test models and the control model are examined and compared. The MATLAB results show notable effects. These results are discussed which are invaluable design factors for optimum efficiency of thermally driven systems such as in nuclear power plants, thermo-chemical plants, thermo-mechanical industries, lasers, solid state plasma, e.t.c. This paper, when incorporated with our previous work [9], serves as good theoretical grounds for believing the notable physical anomalies in heat transfer processes, such as the paradox of moving medium detected in the non-Fourier DPL heat conduction model [10].

## I. INTRODUCTION

The response of heat flow to any external thermal field is best understood at the molecular level. The original heat flow profile is significantly influenced by the particular form of induced potential at the boundary. Ideally these external thermal fields must cause significant changes to the system under study. Such changes yield certain effects which require qualitative treatments and analytic studies, either by laboratory experiments or by computer simulations.

Analysis of heat flow problems in the presence of external thermal fields finds applications in numerous systems. Thermal effects on Magnetohydrodynamics Rayleigh flow were studied [1] by varying the radiation-conduction parameter which significantly alters the heat flux and temperature. Heat reservoir for real transformer was shown to provide guidance for optimum design of absorption heat transformer [2] in which the resultant heat sink was found to decrease cost and noise and increasing reliability. The ground, as a source of heat pump systems and as a loop heat exchanger has been demonstrated to be efficient [3] that allows connection to both heating and chilled water plant loops. Induced Gaussian bump was shown to have yielded the shifting

surface kinks [4] that yield discontinuous changes in the interface orientation. Thermal resonances were observed in signal transmission [5], in neutron capture [6] and in energy propagation in oscillators [7]. Non-linear temperature dependent magnetization is used [8] in the study of Biomagnetic fluid flow. Thermal stability in response to non-linear potential was recently studied [9] in which the simulations pose strong stability due to the insufficiency of the applied potentials to permanently distort the saddle point. It is worth pointing out that all these researches conducted were centered on thermal radiation.

The primary goal of this paper is to complement our previous work [9] so as pave way for understanding some noticeable physical anomalies of heat flow. Closely similar to the earlier literatures, this paper includes both linear and logarithmic potentials, in addition to the radiation potential studied in our previous work, aimed at exploring more potential effects of heat flow in response to boundary formulations. The main appealing feature of this study is its mathematical simplicity and elegance, in that similar effects observed in the literatures have been achieved without necessarily employing any mathematical rigor. Based on previous experience, we have adopted similar computational data and numerical results obtained [9]. The remanding part of this paper is structured as follows: In section 2, the mathematical problem is formulated. The finite element theory is discussed and the basic mathematical equations employed are transformed into finite element numerical scheme, in section 3. In sections 4, the simulation test is discussed and the results presented in graphic form. The effects observed are also discussed explicitly.

## II. THE MATHEMATICAL PROBLEM

Consider a solid plate bounded by a surface S as shown in fig 1 below. At any point in the plate the rate of heat flow per unit area in any given direction is proportional to the temperature gradient in that direction. The 2-dimensional steady state heat diffusion in the presence of heat sources is known to follow the familiar Poisson's equation in two dimensions given as;

$$\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} = \rho(r), \quad (1a)$$

In the absence of heat source term,  $\rho(r)$ , the equation reduces into Laplace's equation

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$$\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} = 0 \quad (1b)$$

The boundary fixed temperatures are as follows;

$$\begin{aligned} \theta(1,1) = 750K, \theta(1,6) = 700K, \theta(1,12) = 700K, \theta(1,19) = 700K, \\ \theta(2,6) = 700K, \theta(1,11) = 700K, \theta(2,1) = 800K, \theta(3,1) = 800K, \\ \theta(4,1) = 800K, \theta(5,1) = 800K, \theta(2,33) = 500K, \theta(3,34) = 500K, \\ \theta(4,35) = 500K, \theta(5,36) = 500, \theta(11,37) = 600K \end{aligned} \quad (2a)$$

The imposed linear, radiation and logarithmic differential boundary conditions are as follows:

$$\frac{\partial \theta}{\partial n} = \begin{cases} \frac{-M\theta + S}{\kappa}, \\ 4E\sigma\theta_r^3(\theta - \theta_r), \\ \frac{-h\theta}{b} \ln\left(1 + \frac{bg}{K_o\theta_o}\right) \end{cases} \quad (2b)$$

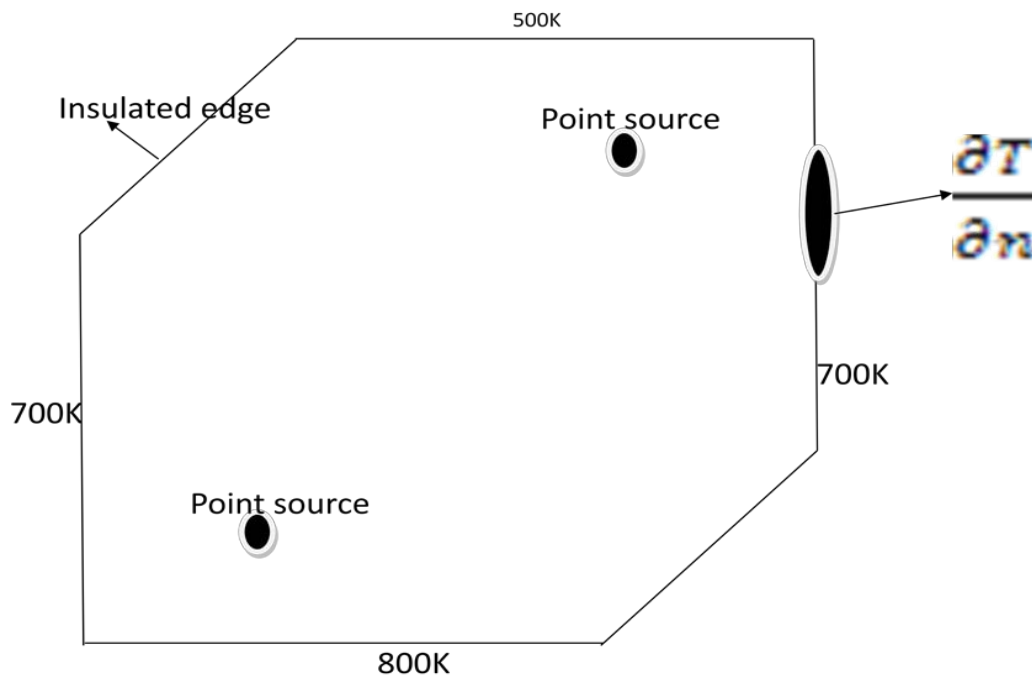


Figure 1 : The physical hexagonal pure metal for the simulation of heat flow

From equation (2a) above we have as follows:  
 $E$  is surface emissivity,  $h$  is thermal conductivity,  $\sigma$  is Stefan-Boltzmann constant,  $\theta_r$  is the temperature of external radiation source,  $\theta_o$  assumed lower limit temperature and  $M, S, b, g, K_o$  are constants.

### III. FINITE ELEMENT FORMULATION

A class of physical problems arising in realistic systems can be expressed in terms of quantity minimization. These variational problems must be

stationary and must be of second order in their differential forms. Such a variational problem can be expressed as the functional

$$I(\Theta) = \int_a^b f(r, \Theta, \Theta') dr, \tag{3}$$

where  $\Theta$  is the temperature field,  $\Theta'$  is the temperature derivative,  $I$  is the integrable functional,  $f$  is a continuous function of temperature and position which minimizes the integral,  $a$  and  $b$  are extremities of the element.

The crux is to determine the solution of equation (3) in some closed bounded region. To achieve this, the finite element method is a very convenient tool. The use of finite element methods to simulate heat flow has gained attention over its finite difference counterpart. The popularity in the finite element methods comes from the fact that it is suitable in solving problems of higher dimensions with complex boundaries and little symmetry, contrary to the finite difference methods. In the Finite Element (FE) theory, it is usual to set-up the interpolation scheme and to choose the appropriate shape function,  $N$ , for the domain problem [11]. Also suitable element is used to span the entire domain.

To obtain the corresponding 2-D finite element scheme for the heat flow problem defined in Equations (1) and (2) we have as follows. As a strategy, we have simulated the finite element domain using triangular elements spanning the plate shown in Figure (1) thereby looping over the elements in a counterclockwise sense. From equation (3) we have the action,

$$dI = \int_a^b \left( \frac{\partial G}{\partial \Theta} d\Theta + \frac{\partial G}{\partial \Theta'} d\Theta' \right) dS = 0, a < S < b. \tag{4}$$

$$\begin{aligned} & \left[ h \iint \begin{pmatrix} \frac{\partial h_1}{\partial x} & 0 & \frac{\partial h_2}{\partial x} & 0 \\ 0 & \frac{\partial h_1}{\partial y} & 0 & \frac{\partial h_2}{\partial y} \\ \frac{\partial h_1}{\partial y} & \frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial y} & \frac{\partial h_2}{\partial x} \end{pmatrix}^T \begin{pmatrix} \kappa & 0 & 0 \\ 0 & \kappa & 0 \\ 0 & 0 & \kappa \end{pmatrix} \begin{pmatrix} \frac{\partial h_1}{\partial x} & 0 & \frac{\partial h_2}{\partial x} & 0 \\ 0 & \frac{\partial h_1}{\partial y} & 0 & \frac{\partial h_2}{\partial y} \\ \frac{\partial h_1}{\partial y} & \frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial y} & \frac{\partial h_2}{\partial x} \end{pmatrix} \begin{vmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} dxdy \right] \begin{pmatrix} \Theta_i \\ \Theta_j \\ \Theta_k \end{pmatrix} = \\ & h \iint \begin{pmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{pmatrix}^T Q \begin{vmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} dxdy + \\ & \int_S \begin{pmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{pmatrix}^T \frac{\partial \Theta}{\partial n} \begin{vmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} ds + \\ & \sum_i \begin{pmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{pmatrix}^T Q_p \frac{\Theta_p}{k}. \tag{7} \end{aligned}$$

The above equilibrium equation can be written in compact form as

$$[h \iint B^{(e)T} C B^e |J^e| dA] \Theta = h \iint H^{(e)T} Q |J^e| dA + \int_S H^{(e)T} \frac{\partial \Theta}{\partial n} |J^e| ds + \sum_i H^{(e)T} Q_p \frac{\Theta_p}{k}. \tag{8}$$

To preserve the boundary conditions we have  $\Delta\Theta(a) = \Delta\Theta(b) = 0$ .

We employ the general functional for heat flow given [12] as;

$$G(x, y, \Theta, \Theta') = \frac{1}{2} \gamma \left[ \left( \frac{d\Theta}{dy} \right)^2 \right] - \frac{1}{2} H\Theta^2 + \frac{1}{k} Q\Theta. \tag{5}$$

Putting Equation (5) into (3) and carrying out the integration gives,

$$I = \iint_A \frac{1}{2} \gamma \nabla^2 \Theta dA + \int_S \frac{1}{2} H\Theta^2 dS - \iint_A \frac{1}{k} Q\Theta dA, \tag{6}$$

for some edge  $S$  over which the plate losses heat to the surrounding,  $A$  is the plate area,  $\gamma$  is some constant coefficient,  $\nabla^2$  is Laplacian operator,  $k$  is thermal diffusivity.

The following relations follow:  $x = \sum_{i=1}^3 N_i x_i, y = \sum_{i=1}^3 N_i y_i$  and in the natural coordinate we have  $x = \sum_{i=1}^3 h_i x_i, y = \sum_{i=1}^3 h_i y_i, h_1 = 1 - r - s, h_2 = r, h_3 = s$ , provide  $\sum_{i=1}^3 h_i = 1$  holds.

Several algorithms have been discussed to assemble the resultant equations [12-17]. In the present work, it is convenient and consistent to strictly adhere to the principle of virtual temperature, discussed in the standard text book [18], and obtain the following equilibrium equation.



The term enclosed in the left hand side constitute the stiffness matrix. The terms in the right hand side are the contributions from the extended heat source, the applied thermal potential and the point sources, respectively. The matrices embedded in these terms are computed and defined [18] as follows:  $B^e$  is the temperature gradient interpolation matrix,  $C$  is the material property matrix,  $J^e$  is the Jacobian and  $H$  is the generalized element temperature matrix. The other

matrices are:  $Q$  the extended heat source,  $Q_p$  the point source, and  $\frac{\partial \theta}{\partial n}$  the applied potential (defined in equation 2),  $H^T$  is the transpose of  $H$ .

Contrary to the test models, we ignore the applied external thermal potentials and the heat sources for the control mode, thus resulting into Laplace's equation as

$$h \iint \begin{pmatrix} \frac{\partial h_1}{\partial x} & 0 & \frac{\partial h_2}{\partial x} & 0 \\ 0 & \frac{\partial h_1}{\partial y} & 0 & \frac{\partial h_2}{\partial y} \\ \frac{\partial h_1}{\partial y} & \frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial y} & \frac{\partial h_2}{\partial x} \end{pmatrix}^T \begin{pmatrix} \kappa & 0 & 0 \\ 0 & \kappa & 0 \\ 0 & 0 & \kappa \end{pmatrix} \begin{pmatrix} \frac{\partial h_1}{\partial x} & 0 & \frac{\partial h_2}{\partial x} & 0 \\ 0 & \frac{\partial h_1}{\partial y} & 0 & \frac{\partial h_2}{\partial y} \\ \frac{\partial h_1}{\partial y} & \frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial y} & \frac{\partial h_2}{\partial x} \end{pmatrix} \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} dx dy \begin{pmatrix} \Theta_i \\ \Theta_j \\ \Theta_k \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (9)$$

Equations (7) and (9) give the contributions for the individual element. To obtain the resultant system of linear equations, we carry out the iterations for the entire elements, and thereafter assemble the equations. In practice, the finite element scheme results into large system of equations. Within this general arrangement, some additional steps must be taken to reduce the computational load. In particular, by judicious selection of the node numbers the stiffness matrix can be arranged into a symmetric band of finite width about the diagonal with zeros elsewhere. This can be used to reduce both the required memory and the computational load needed to solve the simultaneous equations. To solve the resultant set of linear equations, we have employed the well known Gauss-Jordan algorithm. However computer programs have been designed to ease the difficulty in handling finite element problems for large domain. Sample of these programs can be found in reference [19].

#### IV. SIMULATION RESULTS AND DISCUSSION

We employed the simulation data used in our earlier work following our previous experience. The radiation potential is approximated using Newton's law of cooling similar to that used in [16] and suggested in [19], rather than the traditional 4<sup>th</sup> power law, so as the preserve the linearity of the resultant system of equations. However, this approximation is precise only for specific range of temperature difference between the interacting thermal fields. In the standard text [19], it is specified that this temperature difference be at most 10%. To permit this approximation we have arbitrarily taken the value of the external radiation temperature to be 820K.

The results for the simulation are firstly obtained numerically and then we used Matrix Laboratory to obtain the graphs (Figure 3). While solving the resultant system of equations, we have simplified redundancies by eliminating any equation that resurfaced. For details

of the computational data and the numerical results see [9].

The finite element methods have been shown to give efficient, reliable, stable and converging solutions. The temperature profiles for the test cases have been computed and presented in tabular form shown in reference [9]. These results yield significant variations when compared with that of the control model as shown in the graphs (fig.3 data 4). The resultant variations are thus examined as effects manifesting due to the induction of the potential at the boundary. These effects are explicitly pointed out and discussed as follows.

Inducing the linear thermal potential at the boundary on the hexagonal plate has yielded results quite interesting. The temperature limits for the control model (Fig.3, data 4) have been significantly deviated as exhibited by the test models (Fig.3, data 1, 2 and 3). The linear potential (data 1) induces an 'artificial sink' at node 28 where the temperature drops to 483.45K. In principle since heat flow in the direction of lower temperature limit, this drop in the lower temperature limit for the control model could induce thermal cold reservoir. In the realm of Statistical Mechanics, the associated local fields are considered as system while the other particles and their degrees of freedom are considered as heat reservoirs, thus resulting into heat sinks.

Contrary to the graph (data 4) for the control model, the graphs for the test cases (data 1, 2 and 3) show deviations in the upper limit temperature at nodes 7, 8, 13, 14 and 19 due to the induced potentials. Ideally the deviations could have been expected at only the nodes where the potential is concentrated. However the deviations posed by the internal nodes, as well, confirms that the induced external thermal field also influences the neighborhood particles. These results are in agreement with the theoretical treatments discussed in the text book [20]. Depending on physical properties of the material solid (such as thermal resistivity, elongation temperature and melting point), these

deviations can pose overheating of the material surface which in turn pose the tendency of formation of surface bumps or deformation on cooling. Cadwell and Kwan [21] predicted that such cooling or solidification primarily results to boundary perturbation.

Heat in certain continuous processes is studied [22] and it was noted that the difficulty is due to interaction of fluid flow and heat conduction. The non-linear potentials exhibit strong non-linearity. These are simply likened to the oscillatory behavior in thermally interacting packets in the direction of the heat flux, influenced by the induced potentials which results into locally flute-clarinet-like nascent marginally unstable heat flux (figure 3 data 2 and 3). Our results are strongly in confirmation of earlier results obtained [22-24].

More interestingly is the double peaks exhibited by the induction of the non-linear potentials. In particular the logarithmic potential exhibits the peaks at nodes 22 and 28, where the upper temperature limits are largely deviated giving the magnitudes of 1035.88 K and 1150K, respectively. The peaks result due to high pulse heating thermal resonances, a notable effect very useful in lacers and thin films, in which the thermal waves travel with finite speed and extreme temperature gradient at the lowest possible spatial mode. Obviously every oscillating system is capable of exhibiting resonance. The resonance occurs in the event that thermal energy

of the applied potential equals the spontaneous internal energy of the system, thereby temporarily eliminating nascent flute-clarinet like modes manifesting due to marginally unstable vibration at the nodal points closer to the boundary.

## V. CONCLUSION

The finite element method is employed to compute the temperature profiles. We have assessed the response of heat flow profiles to boundary formulations. By comparing the results from the test cases and a control model, significant effects are observed. The associated local fields have been significantly influenced while the neighboring fields are marginally influenced. It could be deduced that the influenced packet is excited thereby interacting with other neighboring packets. We propose the results of this study as invaluable design consideration for optimum efficiency of thermally driven systems such as in nuclear power plants, thermo-chemical plants, thermo-mechanical industries, lasers, plasma e.t.c. This paper, when incorporated with our previous work [9], serves as good theoretical grounds for believing the notable physical anomalies in heat transfer processes, such as the paradox of moving medium detected in the non-Fourier DPL heat conduction model [10].

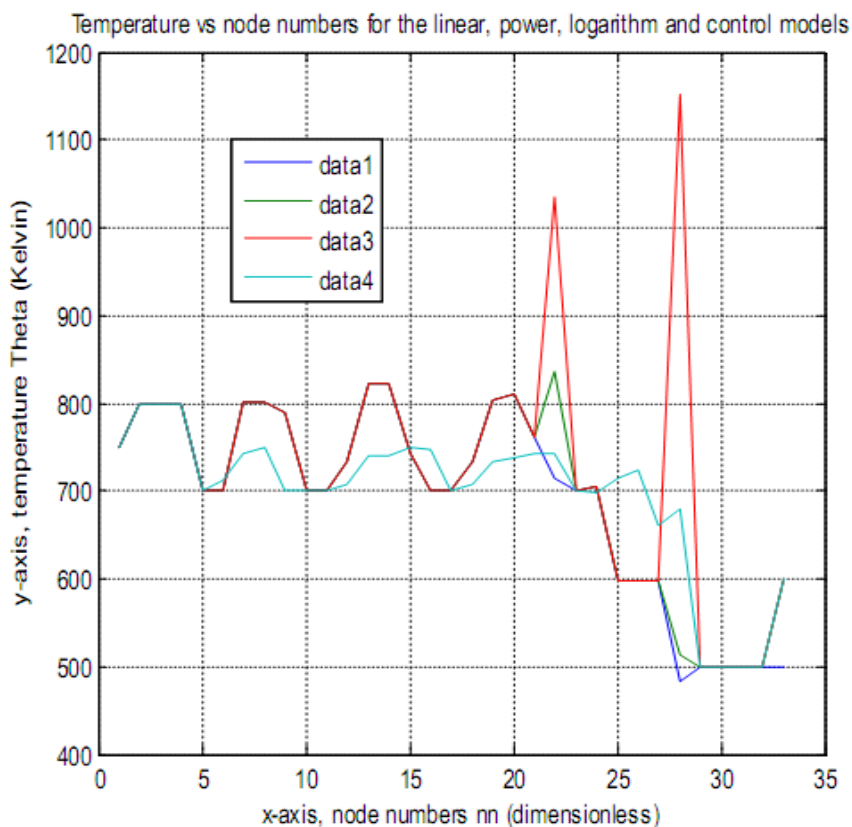


Figure 3 : MATLAB simulation results of the temperature Vs node numbers. Data 1 is the graph for the linear potential; Data 2 is the graph for the radiation potential; Data 3 is the graph for the logarithmic potential; Data 4 is the graph for the control model

## VI. ACKNOWLEDGEMENT

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## Rotating Light House Effect

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**Abstract** - We clarify as to how a precession period appears in the analysis of periodic phenomenon in Astrophysics. The observed redshift that is related to this phenomenon is shown to be  $2a/V = 2/T$ , where 'a' is the relative acceleration between the emitter and receiver and 'V' the relative transverse velocity.

We find that the Hubble relation can equally well be a consequence of galaxies rotating differentially around a common center of mass. It is shown that New-tonian mechanics can account for all major anomalies quoted against it when space-time relationship involving acceleration is properly taken into account.

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# Rotating Light House Effect

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**Abstract** - We clarify as to how a precession period appears in the analysis of periodic phenomenon in Astrophysics. The observed redshift that is related to this phenomenon is shown to be  $2a/V = 2 / T$ , where 'a' is the relative acceleration between the emitter and receiver and 'V' the relative transverse velocity.

We find that the Hubble relation can equally well be a consequence of galaxies rotating differentially around a common center of mass. It is shown that Newtonian mechanics can account for all major anomalies quoted against it when space-time relationship involving acceleration is properly taken into account.

## I. INTRODUCTION

In continuation of our earlier papers (Rajamohan and Satya Narayanan [1], [2]) and references therein, we derive in section 4, a direct solution for the rate of change of redshift for an accelerating observer. This effect is also shown to account for the observed redshift from the center of the Sun's disk.

## II. RELATION BETWEEN PERIODS

In this section we introduce the simple concept of a rotating light source. Let us assume that the period of a rotating light source be  $P_e$  (need not be unity). Also the distance between two consecutive pulses is  $CP_e$ , where  $C$  is the velocity of light. The distance  $D_0$  travelled by the  $N^{\text{th}}$  pulse to meet the receiver will be  $NCP_e$ .

$$D_0 = NCP_e = Ct_0 \quad (1)$$

Here  $t_0$  is the time. The period  $P_e$  is related to the distance travelled and the number of pulses by the relation

$$P_e = \frac{d_0}{NC} = \frac{t_0}{N} \quad (2)$$

For an observer in relative motion, the period is given by

$$P = \frac{P_e}{(1 - \bar{V}/C)} \quad (3)$$

Here  $\bar{V}$  is the average velocity. It is easy to see that

$$NP = NP_e + \frac{\bar{V}}{C} \frac{P_e}{(1 - \bar{V}/C)} N \quad (4)$$

$$= NP_e + \frac{\bar{V}P_e}{C - \bar{V}} N \quad (5)$$

Thus for uniform motion

$$P = P_e + \frac{P_e}{N} \quad (6)$$

Also

$$P_{\text{Observed}} = P_e + \Delta P_e = P_e + \frac{P_e}{N} \quad (7)$$

For an accelerating observer, we can write

$$P = P_e + \frac{1}{2} \frac{2P_e}{N} \quad (8)$$

Here we wish to make an important statement about the periods and period derivatives. For a moving observer with uniform velocity  $V$ , the difference in the periods at different time intervals will remain the same. This would imply that the variation in the periods, or the period derivatives would simply be identically zero. However, for an accelerating observer, the difference in the periods at different time intervals would be different. Such a difference would produce period derivatives. It is important to realize that a pulse which has met an accelerating observer who has moved  $CP_e$  kms, an additional time interval of  $P_e$  seconds has to be accounted for. This additional time interval  $P_e$  will contribute significantly to period derivatives.

The first term in the above equation is the contribution due to uniform motion, while the second term contributes to the change in the period due to acceleration of the moving observer, as  $P_e$  seconds has to be accounted for every  $CP_e$  km due to acceleration. As mentioned above the contribution to the period derivative would come from the second term. For an accelerating observer,  $\bar{V}$  is the average velocity so that the contribution due to acceleration would be of the order of  $2\bar{V}$ . A simple calculation would yield the following relation for the variation in the period.

$$\dot{P} = \frac{2P_e}{N} \quad (9)$$

$$= \frac{2P_e^2}{t_0} = \frac{2CP_e^2}{D_0} \quad (10)$$

Thus

$$\frac{\dot{P}}{P_e} = \frac{2}{t_0} \quad (11)$$

In terms of time, we can write as follows: The total time interval  $T$ ,

$$T = \frac{d_0}{\bar{V}} + \left[ \frac{d_0 + (d - d_0)}{C} \right] \quad (12)$$

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$d/C$  contains  $N$  - intervals of  $\bar{P}$  so that

$$\left[\frac{T}{N}\right]N = \left[\frac{T_0}{N}\right]N + \left[\frac{\bar{P}}{N}\right]N^2 \quad (13)$$

Therefore the period derivative is

$$\dot{P} = \frac{P_e}{T_0(1 - V/C)} \quad (14)$$

As  $V \rightarrow 0$

$$\dot{P} = \frac{P_e}{T_0} \quad (15)$$

It is important to realise that when we calculate the variation in the periods, we have to divide the period with time intervals  $(t - t_e)$  and then subsequently take the limit of  $t_e \rightarrow 0$ . Whenever we say that we are measuring time, one must remember that we actually measure time intervals. A more detailed derivation of the relation between the period and period derivatives is provided in section 4. The simple relation between the periods and period derivative have interesting applications in astrophysics as discussed in the following sections. We first clarify in section 3, as to how a precession period appears in the observed periodic phenomenon in Astrophysics. As the two phenomena are related, it is shown that the observed result can be accounted for by differential rotation of objects around a common center of mass.

### III. PRECESSION

Let two objects A (e.g. Earth) and B (e.g. Mercury) revolve around a common center of Mass (e.g. Sun) with periods  $P_A$  and  $P_B$ , respectively. Let at time  $t = 0$ , A, B and C be aligned and let this line point to a distant object (quasar). The difference in angular motion will again lead to a similar alignment given by the well known Synodic period  $P_S$ . However, this alignment will be pointing towards a different distant object. Let us ask the question when will a given alignment with respect to the same distant object repeat itself. The question is, considered as two clocks with two different periods, were to start in phase at  $t = 0$ , what would be the time interval taken for them to come in phase again.

Let  $P_L$  be this time interval.  $P_L$  is obviously related to the relative acceleration in the angles involved for which a simple solution can be found. In the synodic period  $P_S$  given by

$$2\pi/P_S = 2\pi/P_B - 2\pi/P_A \quad (16)$$

Object A moves through an angle  $\Delta\theta$  given by

$$\Delta\theta = \frac{V_A}{R_A} \cdot P_S \quad (17)$$

In the same time interval, object B moves through an angle

$$2\pi + \Delta\theta = \frac{V_B}{R_B} \cdot P_S \quad (18)$$

Thus

$$2\pi = (\dot{\theta}_B - \dot{\theta}_A)P_S = \dot{\theta}_{rel} \cdot P_S \quad (19)$$

Squaring the above equation, we get

$$2\pi = \frac{(\dot{\theta}_B - \dot{\theta}_A)^2}{2\pi} \cdot P_S^2 = \frac{\dot{\theta}_{rel}^2}{2\pi} \cdot P_S^2 \quad (20)$$

Hence two hypothetical objects moving along the same circle with  $\dot{\theta}$  and  $\dot{\theta}^2/2\pi$  will be aligned in phase again and again at intervals of  $P_S^2$  seconds. Hence this precession period will be reflected in the data as

$$\frac{2\pi}{P_S^2} / \text{ per second} \quad (21)$$

$$= \frac{2\pi}{10^{14}} \times 3.1 \times 10^9 \times 2.063 \times 10^5 \text{ arcsec/century} \quad (22)$$

$$\approx 41 \text{ arcsec/century} \quad (23)$$

This is in good agreement with the observed value of 43 arcsec/century. Orbital inclinations and eccentricity will lead to higher order terms.

A similar situation occurs in the case of binary pulsars. In the determination of orbital parameters of a binary system for example, the position angle of the semimajor axis and the time of periastron passage assumes that the observer is stationary. The relative motion of the Sun is not taken into account. This effect of rotation of the axis leads to a precession of the orbit (spurious) when not taken into account. The signal emitted [(e.g) from velocity maximum] towards the Sun cannot repeat after one orbital period unless the ratio P-orbital to P-emission is an integer. The time required for such a repetition can be calculated as follows.

The height through which the pulsar drops in its orbit is  $(1/2)V^2P_e^2/D$  in  $P_e$  seconds, where 'V' is the orbital velocity and 'D' is the radius of the orbit. For a circular orbit, the number of divisions of  $(1/2)V^2P_e^2/D$  in '4D' is

$$\frac{8D^2}{V^2P_e^2} \quad (24)$$

This would be the time interval needed for repetition of the same phenomenon in phase; for the signal to originate from the same position in its orbit. The observed precession per pulse would then be

$$\frac{2\pi V^2 P_e^2}{8D^2} = \frac{\pi V^2 P_e^2}{4D^2} = \frac{\pi^3 V^2 P_e^2}{4\pi^2 D^2} = \frac{\pi^3 P_e^2}{P_{orb}^2} \quad (25)$$

This result is in good agreement with the observed value of precession of binary pulsars. We can obtain the same result by introducing  $\pi/2$  as a scale factor. As acceleration is  $V^2P_e^2/D^2$ , the precession observed per pulse would be



$$\frac{1}{2} \cdot \frac{\pi}{2} \cdot \frac{V^2 P_e^2}{D^2} \tag{26}$$

#### IV. REDSHIFTS

##### a) Redshift for unit light travel time

Transverse motion involves acceleration given by  $(V^2/d)$  where 'V' is the relative transverse velocity, 'd' is the distance that separates the emitter and the receiver at time  $t = 0$ .

Let an accelerating observer starting from  $x = 0$  be at station A at time  $t_A$  and station B ahead at time  $t_B$ . Let  $X_B - X_A = CP_e$  kms. Let one of the signals emitted at intervals of ' $P_e$ ' seconds by a relatively stationary emitter meet the observer at station B at time  $t_1$ . The next signal will be ' $CP_e$ ' kms behind at station  $X_A$  as  $X_B - X_A = CP_e$  where 'C' is the signal speed.

Let this second signal meet the moving observer at  $X_2$  at time  $t_2$ . Then the observed period is  $(t_2 - t_1)$ . The time ' $t_2$ ' must satisfy the following two relations.

$$t_2 = t_a + \frac{X_2 - X_a}{(1/2)a(t_2 + t_A)} \tag{27}$$

as

$$X_2 - X_a = (1/2)a(t_2^2 - t_A^2) = (1/2)a(t_2 + t_A)(t_2 - t_A)$$

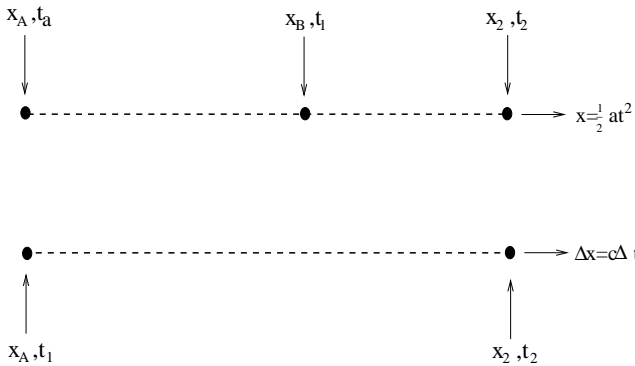


Figure 1 : The relative positions of the two signals

$$t_2 = t_1 + \frac{X_2 - X_a}{C} \tag{28}$$

as

$$C(t_2 - t_1) = X_2 - X_a$$

Subtracting equation (23) from equation (24) we get

$$(t_1 - t_a) - \frac{X_2 - X_a}{(1/2)a(t_2 + t_A)} \left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right) = 0$$

$$(t_1 - t_a) = (t_2 - t_A) \left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)$$

as

$$\frac{X_2 - X_a}{(1/2)a(t_2 + t_A)} = (t_2 - t_A)$$

Therefore

$$(t_2 - t_A) = \frac{(t_1 - t_A)}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)} \tag{29}$$

$$(t_2 - t_1) = \frac{(1/2)a(t_2 + t_A)}{C} \cdot \frac{(t_1 - t_A)}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)} \tag{30}$$

It is important to note that the time interval  $(t_2 - t_1)$  must satisfy the condition

$$(t_2 - t_1) = \frac{V}{C}(t_2 - t_A)$$

where  $\bar{V}$  is the average velocity in the time interval  $(t_2 - t_A)$ .

For uniform motion

$$(t_2 - t_1) = \frac{V}{C} \cdot \frac{CP_e}{V(1 - V/C)}$$

or

$$(t_2 - t_1) = \frac{V}{C} \cdot \frac{(t_1 - t_A)}{(1 - V/C)}$$

and

$$X_2 - X_A = \frac{X_1 - X_a}{(1 - V/C)}$$

When acceleration is involved the same relationship is as that given by equation (30).

$$(t_2 - t_1) = P = \frac{(1/2)a(t_2 + t_A)}{C} \cdot \frac{(t_1 - t_A)}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)}$$

$$P = \frac{(t_2 + t_A)}{(t_1 + t_A)} \cdot \frac{P_e}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)}$$

Setting  $t_A = 0$ , we get

$$P = \frac{t_2}{t_1} \cdot \frac{P_e}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)} \tag{31}$$

$$P = \frac{t_1 + (t_2 - t_1)}{t_1} \cdot \frac{P_e}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)}$$

$$P = \frac{P_e}{\left(1 - \frac{(1/2)a(t_2)}{C}\right)} + \frac{PP_e}{\left(1 - \frac{(1/2)a(t_2 + t_A)}{C}\right)t_1} \tag{32}$$

Hence the rate of change of P is

$$\dot{P} \approx 2P_e/t \tag{33}$$

##### b) The Redshift in General

Let  $d_0$  be the distance between the emitter and the receiver at time  $t = 0$ . If the receiver and emitter are relatively stationary, the observed period  $P_E$  will be the same as the emitter period. If the observer is moving towards or away from the receiver, with uniform velocity, the observed period would be  $P_e/(1 + V/C)$  or

$P_e/(1-V/C)$ , respectively. When acceleration is involved, the common error made is to assume that the rate of change of observed period is  $\dot{P} = \dot{V}P_e/C$ . We will show that this is not true and  $\dot{P}$  is given by  $2\dot{V}P_e/V$ . The simplest way of approach is  $V$  (average)  $\Delta T = CP_e$  where  $V$  is the average velocity in the time interval  $\Delta T$ .

$$\frac{1}{\Delta T} = \frac{V}{CP_e}; -\frac{\Delta \dot{T}}{\Delta T^2} = \frac{\dot{V}}{CP_e} \text{ or } -\frac{\Delta \dot{T}}{\Delta T} = \frac{\dot{V}}{CP_e} \Delta T = \frac{\dot{V}}{V} \quad (34)$$

That is, as the observer accelerates, the time interval in  $CP_e$  kms is smaller and smaller and is a function of time. The similarity with frequency and wavelength of light is to be noted.

$$\lambda \nu = C; \frac{1}{\nu} = \frac{\lambda}{C}; -\frac{\dot{\nu}}{\nu^2} = \frac{\dot{\lambda}}{C}; -\frac{\dot{\nu}}{\nu} = \frac{\dot{\lambda}}{C} \nu = \frac{\dot{\lambda}}{\lambda} \quad (35)$$

Consider an observer moving away from the emitter and is at a distance  $d_0$  at time  $T_0$  from the origin ( $d=0$ ).

$$d_0 = (1/2)aT_0^2 \quad (36)$$

Let one of the signal meet the receiver at  $d_0$  at time  $T_0$  and let the  $n$ th signal be at  $d=0$  at  $T=T_0$ . Let the  $n$ th signal meet the receiver at a distance  $d_1$  at time  $T_1$ .

$$T_1 = T_0 + (T_1 - T_0)$$

and

$$d_1 = d_0 + d_1 - d_0 = (1/2)aT_0^2 + [(1/2)aT_1^2 - (1/2)aT_0^2] \quad (37)$$

$$T_1 = T_0 + d/C = T_0 + \frac{d_0}{C(1-\bar{V}/C)} \quad (38)$$

where  $\bar{V}$  is the average velocity in the time interval 0 to  $T_1$ , and  $C(T_1 - T_0) = d_1$ . Therefore

$$T = \left[ \frac{CP_e}{(1/2)aT_0} + \frac{P_e}{1-\bar{V}/C} \right] \frac{d_0}{CP_e} \quad (39)$$

Since the number of signal  $n$  occupies the same space  $d_0$ , between two signals, the number of seconds on an average is  $CP_e/(1/2)aT_0$ . The relationship is of the kind

$$X = (u + (1/2)at)t$$

where 't' is the time interval corresponding to the space interval X. Equation (17) can be written as

$$T_1 = \frac{CP_e}{(1/2)aT_0} \cdot \frac{d_0}{CP_e} + \frac{CP_e^2}{d_0(1-\frac{(1/2)a(T+T_0)}{C})} \cdot \frac{d_0^2}{C^2P_e^2}$$

Hence the acceleration in arrival times is  $CP_e^2/d_0$  per cycle, per  $CP_e/(1/2)aT_0$  seconds. Thus

$$\dot{P} = \frac{CP_e}{d_0} \cdot \frac{(1/2)aT_0}{C} = \frac{(1/2)aT_0 \cdot P_e}{(1/2)aT_0^2} = \frac{P_e}{T_0}$$

$$\frac{\dot{P}}{P_e} = \frac{1}{T_0}$$

In terms of the light travel times, equation (39) gets modified as

$$T_1 - T_0 \approx P_e \cdot \frac{d_0}{CP_e} + \frac{(1/2)aT_0}{C} \cdot \frac{d_0}{CP_e}$$

$$\dot{P} = \frac{(1/2)aT}{C} \cdot \frac{cP_e}{d_0} = \frac{(1/2)aT_0}{(1/2)aT_0^2} \cdot P_e = \frac{P_e}{T_0}$$

Introducing a factor 2 for acceleration, as  $NP = P_i N + (1/2)\dot{P}P_i N^2$  where N is the number of cycles and is the initial period

$$\frac{\dot{P}}{P_e} = \frac{2}{T_0} \quad (40)$$

Note that the change in the velocity by ' $aP_e$ ' occurs for every ' $VP_e$ ' kms. In the length interval  $CP_e$ , the change in 'V' is therefore

$$\frac{CP_e}{VP_e} \cdot aP_e$$

Hence the rate of change of period per unit light travel time is given by

$$\dot{P} = \frac{aP_e}{V} = \frac{P_e}{T}$$

Introducing 2 as a factor for acceleration

$$\frac{\dot{P}}{P_e} = \frac{2}{T}$$

This result can be directly obtained from equation (38) by replacing  $t_1$  by  $T_0$  which satisfies the relation  $d_0 = (1/2)aT_0^2$ .

### c) Comparison with observations

The relative transverse velocity of two objects A and B moving around a massive common center of mass is given by

$$V_A - V_B = \left(\frac{GM}{R_A}\right)^{1/2} - \left(\frac{GM}{R_B}\right)^{1/2}$$

where  $R_A$  and  $R_B$  are the radius vectors.

$$V_{rel} = (GM)^{1/2} \left\{ \frac{1}{R_A^{1/2}} - \frac{1}{R_B^{1/2}} \right\}$$

Let  $R_B = |R_A - d|$ , where  $d = |R_A - R_B|$ .

$$\begin{aligned}
 V_{rel} &= (GM)^{1/2} \left\{ \frac{1}{R_A^{1/2}} - \frac{1}{(R_A - d)^{1/2}} \right\} \\
 &= (GM)^{1/2} \left\{ \frac{1}{R_A^{1/2}} - \frac{1}{R_A^{1/2} (1 - d/R_A)^{1/2}} \right\} \\
 &= (GM)^{1/2} \left\{ \frac{1}{R_A^{1/2}} - \frac{1}{R_A^{1/2}} \left\{ 1 + \frac{d}{2R_A} + \frac{3d^2}{8R_A^2} \right\} \right\} \\
 &= (GM)^{1/2} \left\{ \frac{1}{R_A^{1/2}} \cdot \frac{d}{R_A} + \frac{1}{R_A^{1/2}} \frac{3d^2}{8R_A^2} \right\}
 \end{aligned}$$

The redshift  $\dot{P}/P_e$  is

$$\begin{aligned}
 \frac{1}{2} \sqrt{2} \frac{V_{rel}}{d} &= \frac{1}{\sqrt{2}} \left[ \left( \frac{GM}{R_A} \right)^{1/2} - \left( \frac{GM}{R_B} \right)^{1/2} \right] / |R_A - R_B| \\
 &\approx \frac{1}{\sqrt{2}} \frac{(GM)^{1/2}}{R_A^{3/2}} + \frac{1}{\sqrt{2}} \cdot \frac{3}{8} \frac{(GM)^{1/2}}{R_A^{3/2}} \cdot \frac{d}{R_A}
 \end{aligned}$$

$\frac{(GM)^{1/2}}{R^{3/2}}$  is proportional to the reciprocal of the orbital period. Identifying  $R_A$  with  $R_{Sun}$ , we expect the observed period derivatives of pulsars to be proportional to the distance of pulsars from Sun. This is well corroborated as shown in Rajamohan and Satya Narayanan [2]. This result is in good agreement with the observed period derivatives of pulsars and its relation to the distance from the Sun.

$$d_0 = (1/2) a T_0^2 \quad (41)$$

Therefore

$$\frac{2}{T_0} = \sqrt{2} \frac{v_\tau}{d_0} \quad (42)$$

$\sqrt{2}$  is an approximation to  $\pi/2$ . The redshift therefore observed from the center of Sun's disk is given by

$$\pi/2 \frac{407}{1.5 \times 10^8} \approx 4.24 \times 10^{-6}$$

which is in close agreement with observed values (Weinberg [3]). We can therefore speculate that the Hubble relation is a consequence of this effect if galaxies were to be differentially rotating about a common center of mass. Then the reciprocal of  $H_0$  is proportional to the rotation period of the Milky Way galaxy around such a center.

## V. CONCLUSION

The relationship between space and time as defined by the law of Gravitation and Galilean transformation can account for major anomalies quoted against the law.

The observed precession is an artifact and can be accounted for by differential rotation effects. The same is true of period derivatives of pulsars since the observed  $P$  is not intrinsic to the pulsar. The period derivatives being proportional to the distance can be again accounted for by differential rotation of objects around a common center of mass (Rajamohan and Satya Narayanan [2]).

As acceleration, and in turn rotation appears to be fundamental in nature (i.e., satellites around planets, planets around Sun, Sun and stars around the Milky Way), we suggest that the Hubble relation is a consequence of differential rotation of galaxies around a common center of mass. Many such local universes might exist in infinite space.

The effect derived in this paper shows that the average observed period of pulsars and their dependence on their distance from the Sun is a kinematic effect caused by differential rotation of the galaxy. It leads to the conclusion that Newton's law of gravitation is true to one part in  $10^{16}$ . It also shows that the velocity of light is constant to the same degree of accuracy. The Hubble relation interpreted as differential rotation of galaxies around a common massive center indicates that the above conclusions are true to one part in  $10^{19}$ .

This effect also mitigates the requirement of a large amount of missing mass in the observable universe that are proposed to account for the observed relation between velocity and distance.

The general design of the Nature appears to repeat the same phenomenon of a massive bulge (core) with differentially revolving smaller objects around it - from satellites of planets around the mother planet, planets around the Sun, Sun and stars around the galactic center, and the galactic center with its entire family of Milky Way members around a distant center. Such a center appears to be in the constellation of Virgo, where a clustering of clusters of galaxies is seen.

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## A Stochastic Semi-Empirical Model for First Order Decay Pharmacokinetics

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**Abstract** - A first order stochastic semi-empirical model for pharmacokinetics is presented and the real response of drug concentration to vital pharmacokinetics parameters studied. By invoking Gaussian kinetics and the residual drug concentration eliminated, the probability densities and the response of concentration profiles are theoretically simulated, using empirical data based on our experience. The drug is administered for 3 days at regular time intervals of 3hr and 6hr, respectively, by refreshing the drug half-life. Results show that the amount of drug residue decreases with increasing dose, but increases with increase in ingestion time interval for corresponding dose. It is also shown that the real drug concentration increases to a threshold and decreases marginally for subsequent dose. However it is difficult to predict the response of drug concentration with changes in ingestion time interval. We recommend that for higher drug concentration the half-life be increased. Our simulation results qualitatively agree with those documented in the literatures.

**Keywords** : *real drug concentration; residue; first order pharmacokinetics; gaussian kinetics; drug half-life; stochastic dynamics.*

**GJSFR-A Classification** : FOR Code: 029999



*Strictly as per the compliance and regulations of :*



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# A Stochastic Semi-Empirical Model for First Order Decay Pharmacokinetics

I.C., Okoro

**Abstract** - A first order stochastic semi-empirical model for pharmacokinetics is presented and the real response of drug concentration to vital pharmacokinetics parameters studied. By invoking Gaussian kinetics and the residual drug concentration eliminated, the probability densities and the response of concentration profiles are theoretically simulated, using empirical data based on our experience. The drug is administered for 3 days at regular time intervals of 3hr and 6hr, respectively, by refreshing the drug half-life. Results show that the amount of drug residue decreases with increasing dose, but increases with increase in ingestion time interval for corresponding dose. It is also shown that the real drug concentration increases to a threshold and decreases marginally for subsequent dose. However it is difficult to predict the response of drug concentration with changes in ingestion time interval. We recommend that for higher drug concentration the half-life be increased. Our simulation results qualitatively agree with those documented in the literatures.

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## I. INTRODUCTION

Pharmacokinetics is a branch of pharmacology dedicated to the study of time course of substances relationship with an organism. In practice it is applied mainly to drug substances. It concerns itself with all manner of compounds residing within the organism or system, such as nutrients, hormones and toxins, while pharmacodynamics explores what the drug does; pharmacokinetics considers what the body does with the drug.

Authorized drugs are those drugs commonly used by people for the treatment to their illnesses. The human body passes through various stages to process and distribute both authorised and prohibited drugs. These stages involve drug absorption into the body, drug distribution to various tissues and then the elimination or excretion (Pratt and Taylor, 1990; Amdur and Klaassen, 1991).

Absorption is the first process when we take in drugs. This is the process in which the drugs pass through the administration into the bloodstream. Blood transmit the drugs to the various parts of the organ of the organ. In this stage all the nutrients are absorbed by the blood and may have good or adverse effects to the body (Ellenhorn and Barceloux, 1998). The next stage is

the distribution of the drugs. The blood is responsible for transporting the drugs to the organs in the body. The heart, the kidneys and the brain are organs in the human system that contains large capacity of blood. Due to this they are that main transporters of drugs in the human system. The last stage is the elimination. Drugs can be eliminated, as residue, through urinating, faeces, liver and even the mother's milk. These channels of drug excretion are essential in the execution of our body system.

Drugs help in repairing the strength of an individual. Unfortunately, those harmful drugs may lead to various illnesses resulting into death. Prohibited drugs affect the brain and the body mechanisms (Pratt and Taylor, 1990). Patients commonly receive two or more drugs concurrently and most individuals who abuse drugs are poly-drug users. Multiple drug use may result in drug interactions. This occurs when the pharmacokinetics or pharmacodynamics of one drug is altered by another. This concept is important to consider because interaction may result in decreased therapeutic efficacy or increased risk of toxicity. The degree of drug interaction depends on the relative concentrations and therefore dose and time (Roland and Tozer, 1989).

Blood plasma is an essential fluid in understanding the transport of drugs in the human body. The packets transported by the human circulatory system are mainly contained in the blood plasma. This yellow liquid component of the blood constitutes about 55% of the total blood capacity. It contains dissolved food substances and also serves as a medium for excretory product transportation. The blood flow is very important or decisive part of the human circulatory activities. Blood is transported to all the body tissues through an intrinsic network of blood vessels (Salloum, et al., 2005). In the body tissue, the blood exiting the arteries and flowing into the capillaries is divided into blood in the core and blood flowing into other peripheral part of the human body such as the skin.

Among the dissolved contents in the blood plasma, distribution of drugs is of utmost importance. The mathematical treatment of drug distribution requires a thorough knowledge of the pharmacokinetics profile (Derendorf and Hochhaus, 1995). Along with the experimental approach, mathematical modelling has become a popular tool for analysis of drugs and cardiovascular systems (Eun et al., 1995). Global Dynamic Model (Gordon, 1959) has been developed for

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cardiovascular system; the Lumped Parameter Model (Hardy et al., 1982; Masunzawa et al., 1992) have been employed for controlling heart mechanisms and vessel hemodynamic; a model-based understanding of the fundamental of blood flow dynamics, or hemodynamic (Eun et al., 2004) is important for the diagnosis and management of diseases of the cardiovascular system, including coronary artery and heart muscle dysfunction, vascular disorders, and pulmonary disease; the One- and Two-Compartments Models, with advances in computer software, have been described (Hagan, 1996); Physiological Models, in contrast to the Compartment Models, have been proposed (Rowland and Tozer, 1989); linear system theory has been employed to model many pharmacokinetics systems (Guyton et al., 1984); the Capillary System Model was used to predict the blood flow in the arteries and veins (Salloum et al., 2005). HPLC and fluorescence detection (Samanidou, et al., 2005) have been employed in the simultaneous determination of quinine and Chloroquine by carrying out statistical evaluation with high accuracy.

The concept of zero or first order kinetics may be utilized to describe any rate process in pharmacokinetics (Pratt and Taylor, 1990). Therefore if we are discussing drug absorption, a drug exhibits zero order kinetics if a constant amount of drug is absorbed regardless of the dose. Conversely a drug exhibits first order absorption kinetics if the amount absorbed depends on the dose. Most drugs exhibit first order elimination kinetics in which a constant fraction of drug is eliminated per unit time.

This paper adopts the features of the one-compartment model (Hagan, 1996) and is somewhat in close comparison with the documented model (SDI Review team, unpublished). Unlike the previous models we explore the dynamic behaviour of the drug concentration equation commonly derived in the literatures. The uniqueness in the present formulation is the elimination of the residue, using mathematical tools. This yields the real concentration of the drug. In the frame of stochastic dynamics, we firstly formulate the probability density for the residue, which facilitates the derivation of the probability density for the real drug concentration as a complementary function. The isolated singularity is explored, which gives the residue, using the well known residue formula adopted from complex variable theory. We invoke Gaussian kinetics, based on the assumption of the Central Limit Theorem (Harry and Steven, 1994). Such an assumption allows the formulation of the first-order stochastic model from which the drug concentration profile evolves. Our model permits theoretical simulation of the real response of drug concentration to vital pharmacokinetics parameters.

The remaining part of this paper is structured as follows: in section 2 the probability densities and the stochastic model are formulated. The simulation results

are discussed in section 3 and conclusion made in section 4.

## II. MODEL FORMULATIONS

### a) *The Physical Model*

Similar to the One-Compartment model (Hagan, 1996) in which the entire human body is considered a single unit, the present model further describes the various stages of the drug dynamics in the body volume as shown in Fig. 1, in comparison with the One-Compartment model (Hagan et al., 1996). We assume that the ingestion and the absorption of drug are contemporaneous and that the ingestion is at regular interval of time  $I$  hours, in doses of quantity  $C_0$ , which is also the initial concentration, for a period of time.

#### i. *The Absorption Stage*

In this stage the initial concentration of the drug sample  $C_0$  is taken to be at time  $t = 0$ . The drug is absorbed at time  $t > 0$ , the drug sample begins to react and its rate of reaction per time is the concentration  $C(t)$ .

#### ii. *The Distribution Stage*

We consider that the drug sample is distributed through the entire body as a single channel. At time  $t > 0$ , the total concentration of the drug obeys the linear super-imposition:

$$C(t) = C_0 + C(nI), \quad (1)$$

where  $n$  denote a particular dose count. After a certain time, the drug begins to decay. Salloum et al. (2005) considered that the drug is distributed at different channels in the system, contrary to the One-Compartment model.

#### iii. *The Elimination Stage*

At this stage, due to certain processes (Derendorf and Hochhaus, 1995), which include elimination, the concentration is the sum of the pure and residual samples. This residue is eliminated from the system. The concentration of the sample to the entire system to carry out certain action is thus a stochastic process. It is thus necessary to determine the probability density for the distribution of the residue. We try, in this paper, to derive the theoretical probability density which facilitates further mathematical derivations. Firstly we impose the mutual exclusiveness axiom:

$$P_r + P_p = 1 \quad (2)$$

Here  $P_r$  and  $P_p$  denote the probabilities of residue and dissolved drug samples respectively. For preference we define the dissolved drug sample as the 'real' drug concentration, in our nomenclature.

### b) *Mathematical Formulations*

#### i. *Analysis of Residue*

Consider a drug sample of known half-life  $T_{1/2}$  given every interval of time  $I$  in doses of quantity  $C_0$ , for

an extended period of time. For an initial dose  $C_0$  the concentration  $C(t)$  of drug at any time  $t > 0$  is known to be described by the popularly known first order ordinary differential equation written as

$$\frac{dC(t)}{dt} = -kC(t), t > 0 \tag{3a}$$

$$C(0) = C_0, \tag{3b}$$

where  $k$  is the elimination time rate or decay rate of drug sample.

The analytic solution of this equation can be straight forwardly be obtained by direct integration. This yields the solution;

$$C(t) = C_0 e^{-kt} \tag{4}$$

At time  $t = I$ , the second dose of  $C_0$  is taken, increasing the concentration to

$$C(I) = C_0(1 + e^{-kt}) \tag{5}$$

The drug level immediately begins to decay. The mathematical expression due to this decay becomes

$$\frac{dC(t)}{dt} = -kC(t), t > 0 \tag{6a}$$

$$C(I) = C_0(1 + e^{-kt}) \tag{6b}$$

Similarly the solution to this initial value problem (IVP) is

$$C(t) = C_0(1 + e^{-kt})e^{-k(t-I)} \tag{7}$$

The next dose is taken at time  $t = 2I$ . This yields the particular solution

$$C(2I) = C_0(1 + e^{-kt})e^{-kI} \tag{8a}$$

The level increases to

$$C(t) = C_0(1 + e^{-kt} + e^{-2kt}) \tag{8b}$$

For successive doses, after  $(N+1)$  ingestion, the drug concentration is

$$C(NI) = C_0(1 + e^{-kt} + e^{-2kt} + \dots + e^{-Nkt}). \tag{9}$$

This is the general solution popularly found in the literatures. Equ.(9) can be written in compact form as

$$C(NI) = \frac{C_0(1 - e^{-(N+1)Ik})}{1 - e^{-Ik}} \tag{10}$$

By partial fraction decomposition, this equation can be expressed as

$$C(NI) = \frac{C_0}{1 - e^{-Ik}} + \frac{C_0 e^{-(N+1)Ik}}{e^{-Ik} - 1} \tag{11}$$

In the  $\lim_{N \rightarrow \infty} C(NI)$  we obtain the saturation concentration of drug given as

$$C_s = \frac{C_0}{1 - e^{-Ik}} \tag{12}$$

It is needful to remark that, albeit this saturation term has been given much attention in the literatures,

the other term has never been explored. Interestingly, the mathematical formula, Equ.(10), permits the synthesis of the residue. Denote this term as  $C_r$ . Thus

$$C_r = \frac{C_0 e^{-(N+1)Ik}}{e^{-Ik} - 1} \tag{13a}$$

For successive dose we can express this term as a series of the first  $n$  terms

$$C_r = \sum_{n=1}^N \frac{C_0}{e^{-nk} (e^{-Ik} - 1)} \tag{13b}$$

For the moment we conjecture that the residue is insitu in Equ. (13) and later justify that this residue is non-negative. It has been predicted (SDI Review team, suggested model) that for increasing time decay rate, larger than the injection time interval, it is possible that the residue of the drug increases. More interesting is that analysis of drug in the human body needs to include the residue. In order to extract this residue, it is naturally assumed that the time course of drug (in the plasma) is linear. We admit this deduction and employ the linear transformation;

$$e^{nx} \cong 1 + nx \tag{14}$$

This transformation reduces Equ.(13) into

$$\dot{C}_r = - \sum_{n=1}^N \frac{C_0}{(1+nkI)(kI)} \tag{15}$$

Here the accented variable  $\dot{C}_r$  denote the linearized form of  $C_r$ .

In the literature (CRC Press, 1998) a plot of  $\ln C(NI)$  against  $t$  gives a linear graph of the form

$$C(t) = \alpha C(nI) + \beta, \tag{16}$$

Where the slope  $\alpha$  coincides with  $\ln C_0$  and  $\beta$  is the intercept.

In the realm of stochastic dynamics we define the moment generating function (MGF),  $\Psi(t)_l$ , in terms of  $\alpha$  and  $\beta$ . Thus;

$$\Psi(t)_l = E(e^{tC}) = e^{\beta l n} \Psi(\alpha l n) \tag{17a}$$

For generality we can define the characteristic function in terms of the set C as

$$\Psi(t)_c = E(e^{\gamma C}), \tag{17b}$$

where  $\gamma$  is a complex number given as;

$$\gamma = inIC(nI) \tag{17c}$$

To preserve the linearity of the model, we freely admit that the characteristic function be defined by;

$$\Psi(t)_c = 1, t \geq 0 \text{ (but zero else where)} \tag{18}$$

This characteristic function is immediately invoked into Equ.(15) as follows:

$$\dot{C}_r = - \sum_{n=1}^N \frac{C_0}{(1+nkI)(kI)} \Psi(t)_c \tag{19}$$

To allow the convergence of Equ.(19), a transformation of the form is necessary, as follows:

$$\dot{C}_r = - \sum_{n=1}^N \frac{C_0}{(lk)^2(n+\frac{1}{lk})} \Psi(nl)_C \quad (20)$$

Here the convergence is achieved such that  $\frac{1}{lk}$  decreases monotonically.

It is compelling to remark that the regularity in the injection time interval is a special case of the model described in the work (SDI Review team, suggested model). In their model, we appreciate that for equal time interval, the Heavy-side function invoked physically describes an integrated sharp impulse of unit magnitude. This is in coincidence with the form of characteristic function invoked in the present work.

As an implication, Equ. (20) shows that  $\dot{C}_r$  has an isolated singularity at  $n = \lfloor \frac{-1}{lk} \rfloor$  with a pole of order 1.

Following the well-known standard complex variable theory, we can calculate the residue, R, by the formula;

$$R = \lim_{n \rightarrow \lfloor \frac{-1}{lk} \rfloor} \left\{ \frac{d^{p-1}}{dn^{p-1}} \left[ n + \frac{1}{lk} \dot{C}_r(nl) \right] \right\}^p, \quad (21)$$

Where p is the order of the pole. Here p=1. We can immediately calculate the concentration of residue from this formula for the nth dose as;

$$C_r(nl) = \frac{C_0}{(lk)^2}; t \geq 0 \quad (22)$$

ii. *The Probability Density Functions*

At any time t the theoretical probability function for the residue can be defined as

$$P_r = \frac{C_0}{C_s(nlk)^2}; t \geq 0 \quad (23)$$

Following the axiom, Equ. (2), the probability function for the real drug concentration can be obtained as;

$$P_p = 1 - \frac{C_0}{C_s(nlk)^2}; t \geq 0 \quad (24)$$

We now invoke Gaussian kinetics thereby permitting the approximation of the probability of real drug concentration to Gaussian distribution, based on the Central Limit Theorem. This approximation is motivated by our conjecture that the eliminated residue is interpreted, in stochastic terms, as decreasing the skewness of the distribution.

Recall that the normalized Gaussian distribution with fluctuation  $\sigma = 1$ , can be written as;

$$f(C(t)) = \int_{entire\ space} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(C(t))^2} = 1 \quad (25)$$

In the realm of our earlier conjecture, the probability function, Equ. (24), can be normalized as;

$$\int_{entire\ space} \left( 1 - \frac{C_0}{C_s(nlk)^2} \right) = 1 \quad (26)$$

iii. *The Stochastic Model*

Equating the last two equations and manipulating the resultant equation yields;

$$C(t) = \ln\left(\frac{1}{\sqrt{2\pi}}\right) - \ln\left(1 - \frac{C_0}{C_s(tk)^2}\right) \quad (27)$$

To formulate the first order stochastic model, Equ. (27) is simply differentiated once with respect to time and setting  $T_{1/2} = \frac{\ln 2}{k}$  (Hagan, 1996) we obtain;

$$\frac{dC(t)}{dt} = \frac{-2\pi l C_0 (T_{1/2})^2}{[(\ln 2t)^2 C_s - C_0 (T_{1/2})^2] t} \quad (28)$$

This equation is the differential equation for the real concentration of drug, indexed in time.

### III. RESULTS AND DISCUSSION

a) *Results*

A numerical algorithm was employed to compute the concentration profiles, formulated in Equ. (28), using the familiar Euler's method. The advantage of this method is due its simplicity in solving first order boundary value problems, in comparison with other existing numerical methods. The formula for the algorithm is given as:

$$C_{t+1} = C_t + \left( \frac{-2\pi l C_0 (T_{1/2})^2}{[(\ln 2t)^2 C_s - C_0 (T_{1/2})^2] t} \right) \quad (29)$$

The probability densities for the residue and the dissolved drug samples, as well as the numerical values of drug concentration profiles are calculated and the obtained results presented graphically (Fig. 1-6). The simulations are carried out theoretically by using the following data, based on our experience:  $C_0 = \frac{190mg}{kg}$ ,

$I = 3hr, 6hr$ . The simulations are refreshed, for each value of I, using the following drug half lives.

$T_{1/2} = 7.5hr, 15hr, 30hr, 60hr$ . All calculations are considered for 3 days of drug administration.

In order to circumvent possible discontinuity in the numerical result at  $t = 0$ , we assumed that  $C_0 = C_1$ . The values of  $C_s$ , shown on table 1, were calculated using Equ.(12). Care must be taken that the saturation concentration does not imply the threshold concentration referred herein. To clarify this, one may consider that while the saturation term refers to the global optimum of the drug concentration the threshold term refers to the local optimum of the drug concentration.

It is worth remarking that the values of the first dose probabilities were taken to be zero, to relegate spuriously values. Albeit, this has no effect on the overall simulation result. The simulations for  $I = 3hr$  are labelled  $A_1 - A_4$  while for  $I = 6hr$  are labelled  $B_1 - B_4$  for clarity (Table 1).



Table 1 : Summary of simulation data

l(hr)	label	$T_{1/2}(hr)$	$C_0(\frac{mg}{kg})$	$C_s(\frac{mg}{kg})$	Duration (days)
3	$A_1$	7.5	190	783.58	3
	$A_2$	15	190	1468.05	3
	$A_3$	30	190	380.06	3
	$A_4$	60	190	5571.05	3
6	$B_1$	7.5	190	446.43	3
	$B_2$	15	190	784.48	3
	$B_3$	30	190	1468.32	3
	$B_4$	60	190	6052.41	3

#### IV. DISCUSSION

The reliability of our model can be seen already in the simulations of the probability densities (Tables 2 and 3) for residues, the probability densities for real drug concentration (Fig. 2 and 3), and more importantly the real drug concentration profiles (Fig. 4 and 5).

Tables 2 and 3 show that the residues decrease with increase in dose, but increases with increase in drug half-life. Comparing the figures, it can be observed that the residue is higher for larger ingestion time interval. This may be likened to susceptibility of drug to other foreign substances due to prolonged decay time. This is in agreement with the influence of active metabolites interacting with the parent drug (CRC Press, 1998; Rowland and Tozer, 1989). It is simply expected that the corresponding probabilities (Fig 2 and 3) for the real drug concentration show complementary features to their respective residues. However one can probably deduce that the amount of residue becomes insignificant for higher dose at regular interval.

The real drug concentration profiles (Fig. 4 and 5) show significant results. The drug concentration shows initial decline after peaking. The threshold time (time-to-peak) can be seen to vary with drug half-life and ingestion time interval. These are in good agreement with earlier findings (e.g., Hagan 1996; Rowland and Tozer 1989). Rowland Tozer (1989) confirmed the decline in drug concentration as drug tolerance which is

influenced by ingestion time. Our simulations also confirm that the degree of tolerance is not consistent with drug half-life. This can be easily observed by the inconsistency shown (Fig. 4 and 5) for  $T_{1/2} = 30 hrs$ . This inconsistency infers that drug concentration is sensitive to the correlation between drug half-life and ingestion time-interval.

Our simulations are not consistent with response real drug concentration to variation in ingestion time interval (Fig. 4 and 5). This can be observed by comparing the numerical values for  $I = 3hr$  and  $I = 6hr$  (Fig 4 and 5) at corresponding ingestion time. Fortunately it has been documented in the literature (CRC Press, 1998) that such difficulty may be likened to factors such as irregular change in blood pressure with time which possibly results in misinterpretation of clinic picture. However it is probable that the difference in drug concentration at different ingestion time is insignificant for very large half-lives.

Our numerical findings are less consistent with models simulating response of drug concentration at unequal ingestion time interval (e.g., SDI Review suggested model). It would be interesting to understand what assumptions of these models differ. Finally our model is amenable to simulate response of free drug concentration of specific drugs with known empirical data.

Table 2 : Probability values for residue sample at 3hr ingestion interval

N	Ingestion time (hr)	Probability values at half life 7.5hr	Probability values at half life 15hr	Probability values at half life 30hr
1	3	0.000	0.000	0.000
2	6	0.789	0.000	0.000
3	9	0.351	0.748	0.000
4	12	0.197	0.421	0.871
5	15	0.126	0.269	0.557
6	18	0.088	0.187	0.387
7	21	0.064	0.137	0.248

8	24	0.049	0.105	0.218
9	27	0.039	0.083	0.172
10	30	0.032	0.067	0.139
11	33	0.026	0.056	0.115
12	36	0.022	0.047	0.097
13	39	0.019	0.040	0.083
14	42	0.016	0.034	0.071
15	45	0.014	0.030	0.062
16	48	0.012	0.026	0.054
17	51	0.011	0.023	0.048
18	54	0.010	0.021	0.043
19	57	0.009	0.019	0.039
20	60	0.008	0.017	0.035
21	63	0.007	0.015	0.032
22	66	0.007	0.014	0.029
23	69	0.006	0.013	0.026
24	72	0.006	0.012	0.024

Table 3 : Probability values for residue sample at 6hr ingestion interval

N	Ingestion time (hr)	Probability values at half life 7.5hr	Probability values at half life 15hr	Probability values at half life 30hr
1	6	0.000	0.000	0.000
2	12	0.346	0.785	0.000
3	18	0.154	0.350	0.749
4	24	0.087	0.197	0.421
5	30	0.055	0.126	0.270
6	36	0.039	0.088	0.187
7	42	0.028	0.064	0.135
8	48	0.022	0.049	0.105
9	54	0.017	0.039	0.083
10	60	0.014	0.032	0.067
11	66	0.011	0.026	0.056
12	72	0.010	0.022	0.047
13	78	0.008	0.019	0.040

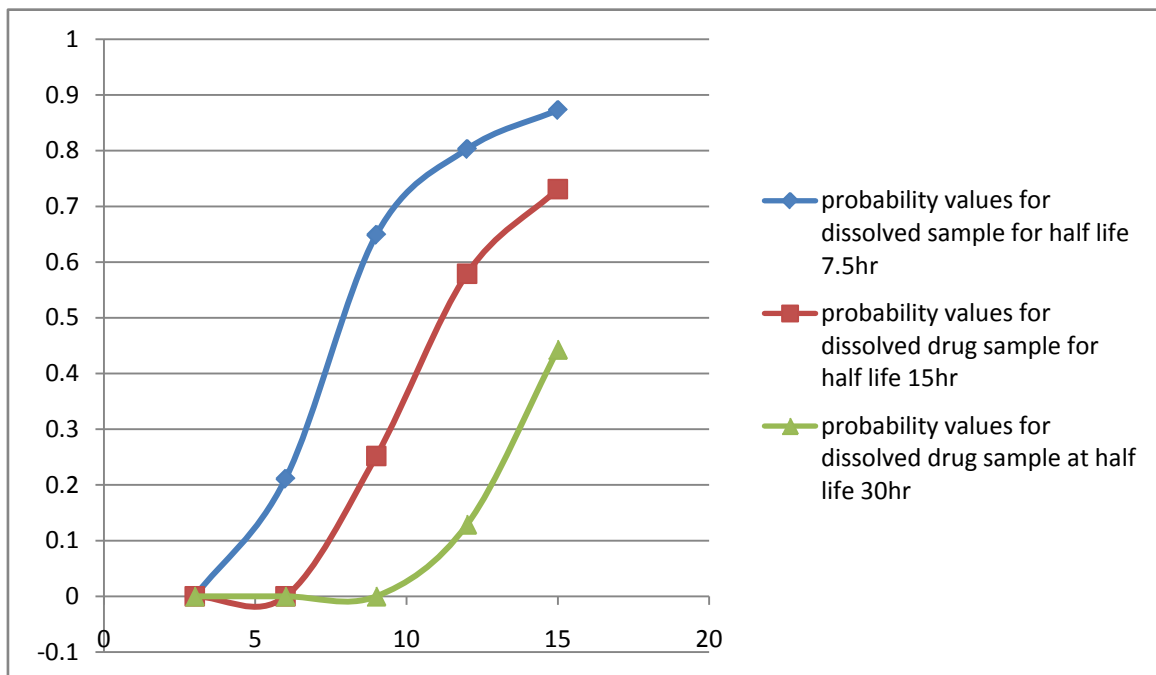


Figure 2 : Probability densities for real drug concentration profiles against time for ingestion time interval of 3hr

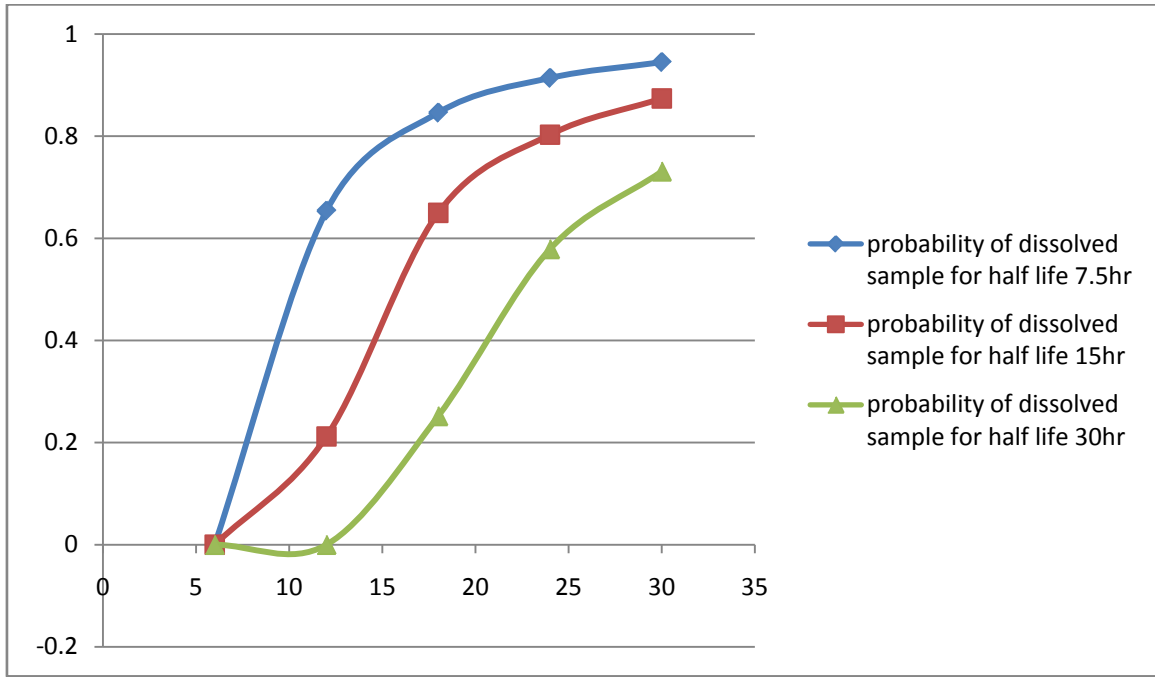


Figure 3 : Probability densities for real drug concentration profiles against time for ingestion time interval of 6hr

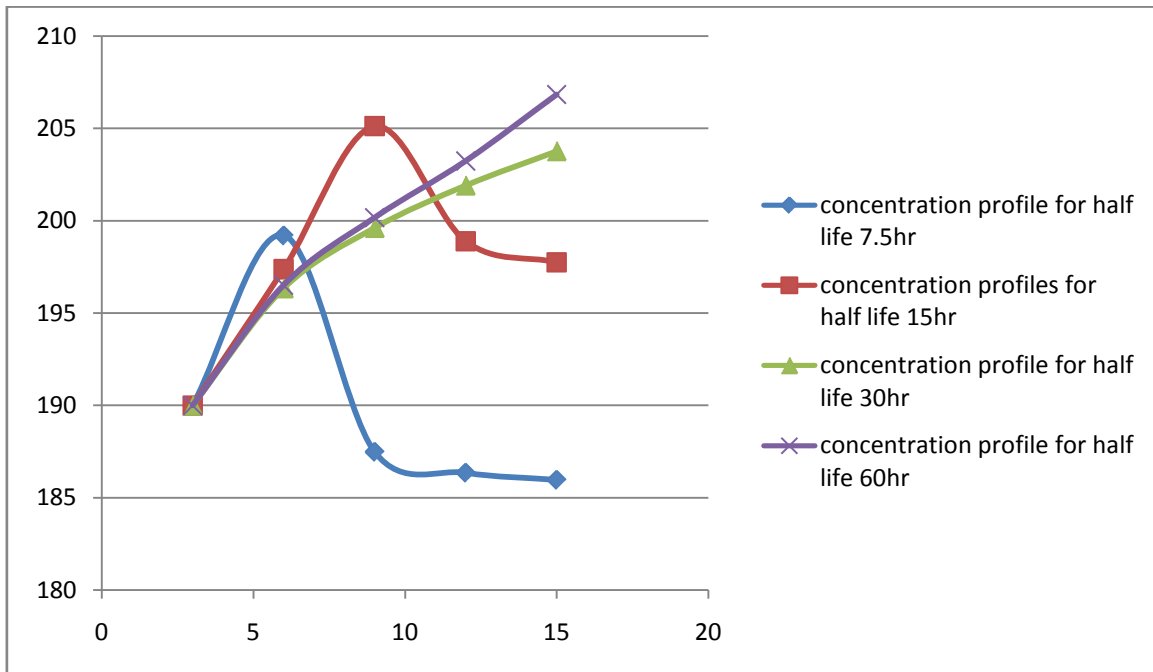


Figure 4 : Real drug concentration (mg/kg) profiles against ingestion time for ingestion time interval of 3hr

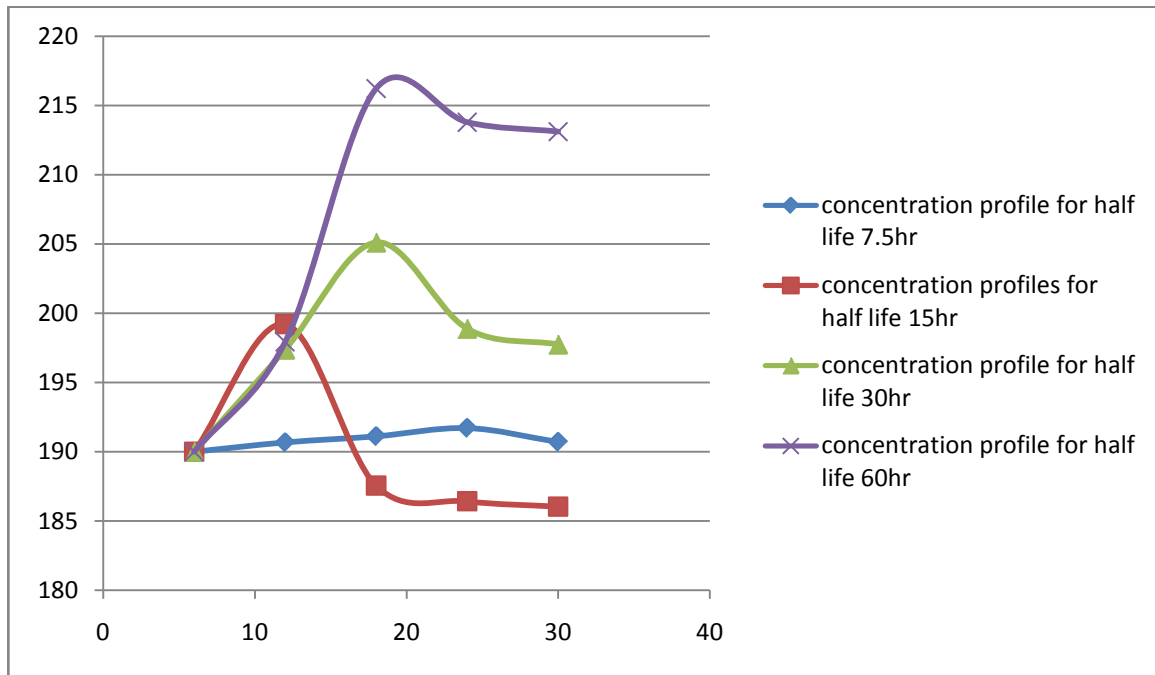


Figure 5 : Real concentration of drug (mg/kg) against ingestion time (hr) for ingestion time interval of 6hr

## V. CONCLUSIONS

Validity of our model for first order decay pharmacokinetics has been shown. The probability densities and the real response of drug concentration to drug half life and ingestion time interval have been theoretically studied. Irrespective of the half life, all simulations have given consistent and reliable results. The eliminated residue has significant influence on the drug concentration profile, but the quantitative difference in the values of the drug concentration is not very important. The major discrepancy lays in the sensitivity of drug concentration profiles to half life. It is thus necessary to analyse the drug residue. This gives quantitative information about the real concentration of the drug in the human body. We admit that the use of such mathematical models should not be treated in absolute terms. They are only attempts to understand the behaviour of the drugs in the human body.

## VI. ACKNOWLEDGEMENT

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The page length of this segment is set by the sum and types of data to be reported. Carry on to be to the point, by means of statistics and tables, if suitable, to present consequences most efficiently. You must obviously differentiate material that would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matter should not be submitted at all except requested by the instructor.



## Content

- Sum up your conclusion in text and demonstrate them, if suitable, with figures and tables.
- In manuscript, explain each of your consequences, point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation an exacting study.
- Explain results of control experiments and comprise remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or in manuscript form.

### What to stay away from

- Do not discuss or infer your outcome, report surroundings information, or try to explain anything.
- Not at all, take in raw data or intermediate calculations in a research manuscript.
- Do not present the similar data more than once.
- Manuscript should complement any figures or tables, not duplicate the identical information.
- Never confuse figures with tables - there is a difference.

### Approach

- As forever, use past tense when you submit to your results, and put the whole thing in a reasonable order.
- Put figures and tables, appropriately numbered, in order at the end of the report
- If you desire, you may place your figures and tables properly within the text of your results part.

### Figures and tables

- If you put figures and tables at the end of the details, make certain that they are visibly distinguished from any attach appendix materials, such as raw facts
- Despite of position, each figure must be numbered one after the other and complete with subtitle
- In spite of position, each table must be titled, numbered one after the other and complete with heading
- All figure and table must be adequately complete that it could situate on its own, divide from text

### Discussion:

The Discussion is expected the trickiest segment to write and describe. A lot of papers submitted for journal are discarded based on problems with the Discussion. There is no head of state for how long a argument should be. Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implication of the study. The purpose here is to offer an understanding of your results and hold up for all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of result should be visibly described. Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved with prospect, and let it drop at that.

- Make a decision if each premise is supported, discarded, or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."
- Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work
- You may propose future guidelines, such as how the experiment might be personalized to accomplish a new idea.
- Give details all of your remarks as much as possible, focus on mechanisms.
- Make a decision if the tentative design sufficiently addressed the theory, and whether or not it was correctly restricted.
- Try to present substitute explanations if sensible alternatives be present.
- One research will not counter an overall question, so maintain the large picture in mind, where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

### Approach:

- When you refer to information, differentiate data generated by your own studies from available information
- Submit to work done by specific persons (including you) in past tense.
- Submit to generally acknowledged facts and main beliefs in present tense.





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<i>References</i>	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring



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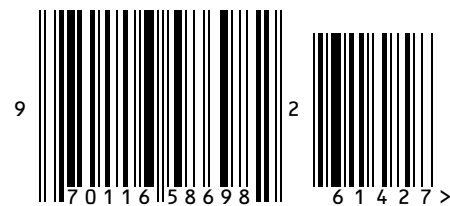


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