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Highlights

- Semi-Empirical Model
- Annular Porous Medium
- 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

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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 interms of average Nusselt number ($\overline{Nu}$), 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

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

Dr. D. Prabhakar[α] & Dr. G. Prabhakararao[σ]

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 interms of average Nusselt number ($\bar{N}u$), 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.

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 etal [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 interms of average Nusselt number ($\bar{N}u$), 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 ri and outer radius r_0 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_∞. 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:

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

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

Velocity in horizontal direction

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

velocity in vertical direction

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

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

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

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

$$\rho = \rho_\infty [\, 1 - \beta_T (T - T_\infty) \qquad (1.2.5)$$

Momentum Equation:

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

Energy equation:

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

The continuity equation (1.2.1) can be satisfied by introducing the stream function ψ as

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

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

The corresponding dimensional boundary conditions are

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

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

(except at z = 0)

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

Non-dimensional Radius

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

Non-dimensional Height

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

Non-dimensional stream function

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

Non-dimensional Temperature

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

Rayleigh number

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

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

Momentum equation:

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

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Energy equation:

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

The corresponding non-dimensional boundary conditions are

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

at $\bar{r} = \bar{r}_0$, $\bar{T}=0$, $\bar{\psi}=0$ (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 :

- 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).

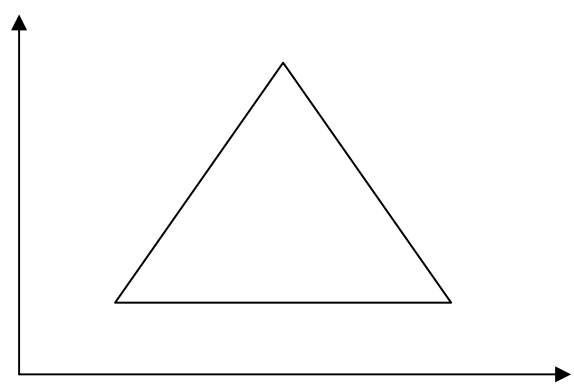

Figure 1 : Typical triangular element

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 co-ordinates 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:

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

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

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

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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

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

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

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

The constants can be expressed in terms of coordinates as

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

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

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

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

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

The differentiation of following term results into

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

Thus

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

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

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

Substitution of (1.2.21) into (1.2.27) gives

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

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

Similarly

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

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The third term of equation (1.2.24) is

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

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).

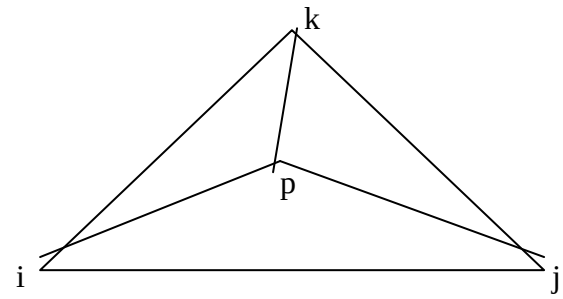

Figure 2 : Showing the sub triangular areas

Defining the new area ratios as

$$M_k = \frac{area\ \ pij}{area\ \ ijk} \qquad M_i = \frac{area\ \ pjk}{area\ \ ijk} \qquad M_j = \frac{area\ \ pki}{area\ \ ijk}$$

It can be shown Elshyab and Beng (33) that

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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

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

Considering the terms individually of the above equation

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

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

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

Following the same above steps

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

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

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

$$\int_A N^T \frac{1}{\overline{r}} \frac{\partial}{\partial \overline{r}} \left(\overline{r} \frac{\partial \overline{T}}{\partial \overline{r}} \right) 2\Pi \overline{r} dA = -\frac{2\Pi \overline{R}}{4A} \begin{bmatrix} b_1^2 & b_1 b_2 & b_1 b_3 \\ b_1 b_2 & b_2^2 & b_2 b_3 \\ b_1 b_3 & b_2 b_3 & b_3^3 \end{bmatrix} \begin{bmatrix} \overline{T}_1 \\ \overline{T}_2 \\ \overline{T}_3 \end{bmatrix}$$

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$$\int_A N^T \frac{\partial^2 \overline{T}}{\partial \overline{z}^2} 2\Pi \overline{r} dA = -\frac{2\Pi \overline{R}}{4A} \begin{bmatrix} c_1^2 & c_1c_2 & c_1c_3 \\ c_1c_2 & c_2^2 & c_2c_3 \\ c_1c_3 & c_2c_3 & c_3^2 \end{bmatrix} \begin{bmatrix} \overline{T}_1 \\ \overline{T}_2 \\ \overline{T}_3 \end{bmatrix}$$

Thus the stiffness matrix of Energy equation is given by

$$\left[\frac{2\Pi}{12A} \begin{Bmatrix} c_1\overline{\psi}_1 + c_2\overline{\psi}_2 + c_3\overline{\psi}_3 \\ c_1\overline{\psi}_1 + c_2\overline{\psi}_2 + c_3\overline{\psi}_3 \\ c_1\overline{\psi}_1 + c_2\overline{\psi}_2 + c_3\overline{\psi}_3 \end{Bmatrix} [b_1, b_2, b_3] - \frac{2\Pi}{12A} \begin{Bmatrix} b_1\overline{\psi}_1 + b_2\overline{\psi}_2 + b_3\overline{\psi}_3 \\ b_1\overline{\psi}_1 + b_2\overline{\psi}_2 + b_3\overline{\psi}_3 \\ b_1\overline{\psi}_1 + b_2\overline{\psi}_2 + b_3\overline{\psi}_3 \end{Bmatrix} [c_1, c_2, c_3] \right] \begin{bmatrix} \overline{T}_1 \\ \overline{T}_2 \\ \overline{T}_3 \end{bmatrix}$$

$$+ \frac{2\Pi \overline{R}}{4A} \left\{ \begin{bmatrix} b_1^2 & b_1b_2 & b_1b_2 \\ b_1b_2 & b_2^2 & b_2b_3 \\ b_1b_3 & b_2b_3 & b_3^3 \end{bmatrix} \begin{bmatrix} \overline{T}_1 \\ \overline{T}_2 \\ \overline{T}_3 \end{bmatrix} + \begin{bmatrix} c_1^2 & c_1c_2 & c_1c_3 \\ c_1c_2 & c_2^2 & c_2c_3 \\ c_1c_3 & c_2c_3 & c_3^2 \end{bmatrix} \begin{bmatrix} \overline{T}_1 \\ \overline{T}_2 \\ \overline{T}_3 \end{bmatrix} \right\} = 0 \qquad (1.2.43)$$

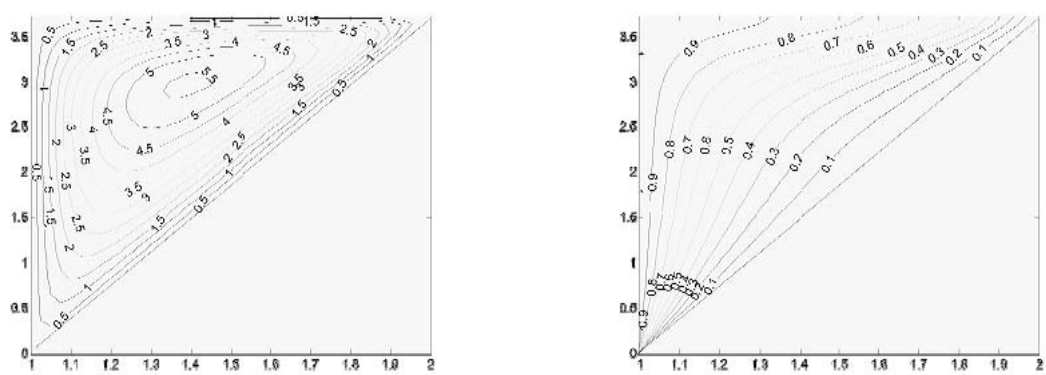
IV. Results and Discussion

Results are obtained in terms of Nusselt number (Nu) at hot wall for various parameters such as Cone angle (C_A), Radius ratio (R_r) and Rayleigh number (Ra), when heat is supplied to vertical conical annular.

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

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

a)



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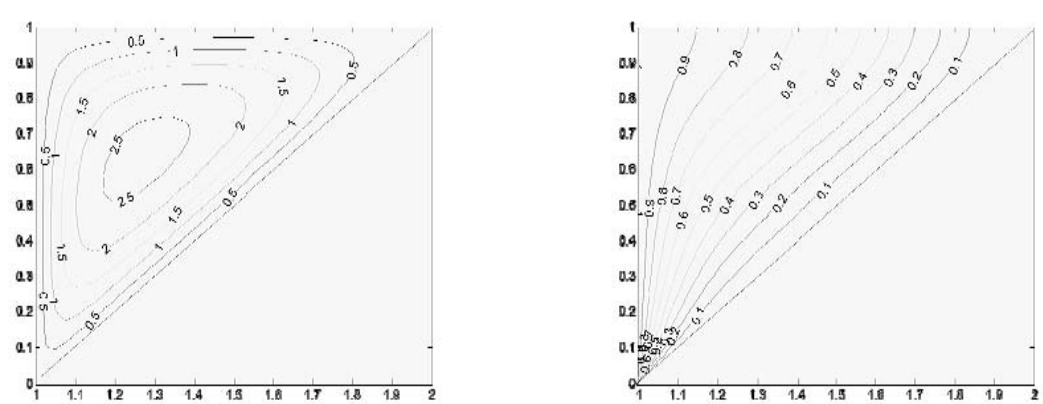

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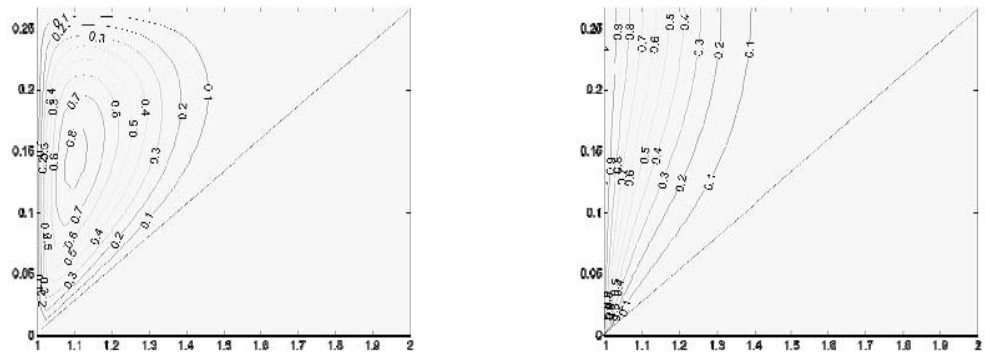

Figure 1.4.1 : Streamlines(left) and Isotherms(Right) for Ra=50, R_r=1
a) C_A =15 b) C_A =45 c) C_A =75

Figure (1.4.1) shows the evaluation of streamlines and isothermal lines inside the porous medium for various values of Cone angle (C_A) at Ra = 50, R_r = 1. The magnitude of the streamlines decreases with the increase in Cone angles (C_A). The thermal bounded layer thickness decreases with the increase of Cone angles (C_A). 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 (C_A). The circulation of the fluid covers almost whole domain at both lower and higher values of Cone angles (C_A) at 15°. Where the relation inversely proportion exists between streamlines and Cone angles (C_A). This trend is also observed with isothermal lines.

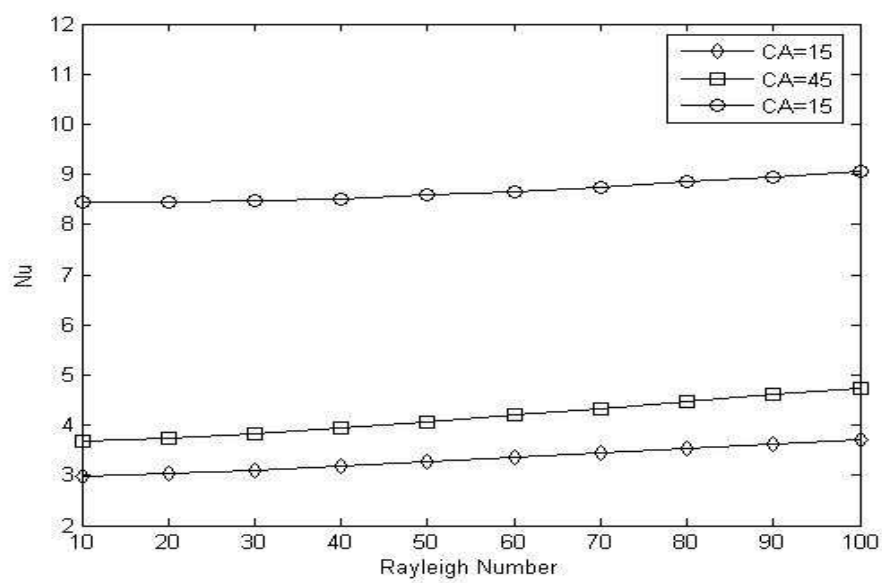

Figure 1.4.2 : $\bar{Nu}$ variation with Ra at hot surface for different values of C_A at R_r=1

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 R_r = 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 (C_A) increases with increase in Cone angle (C_A). 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 (C_A) 15 & 45 degrees.

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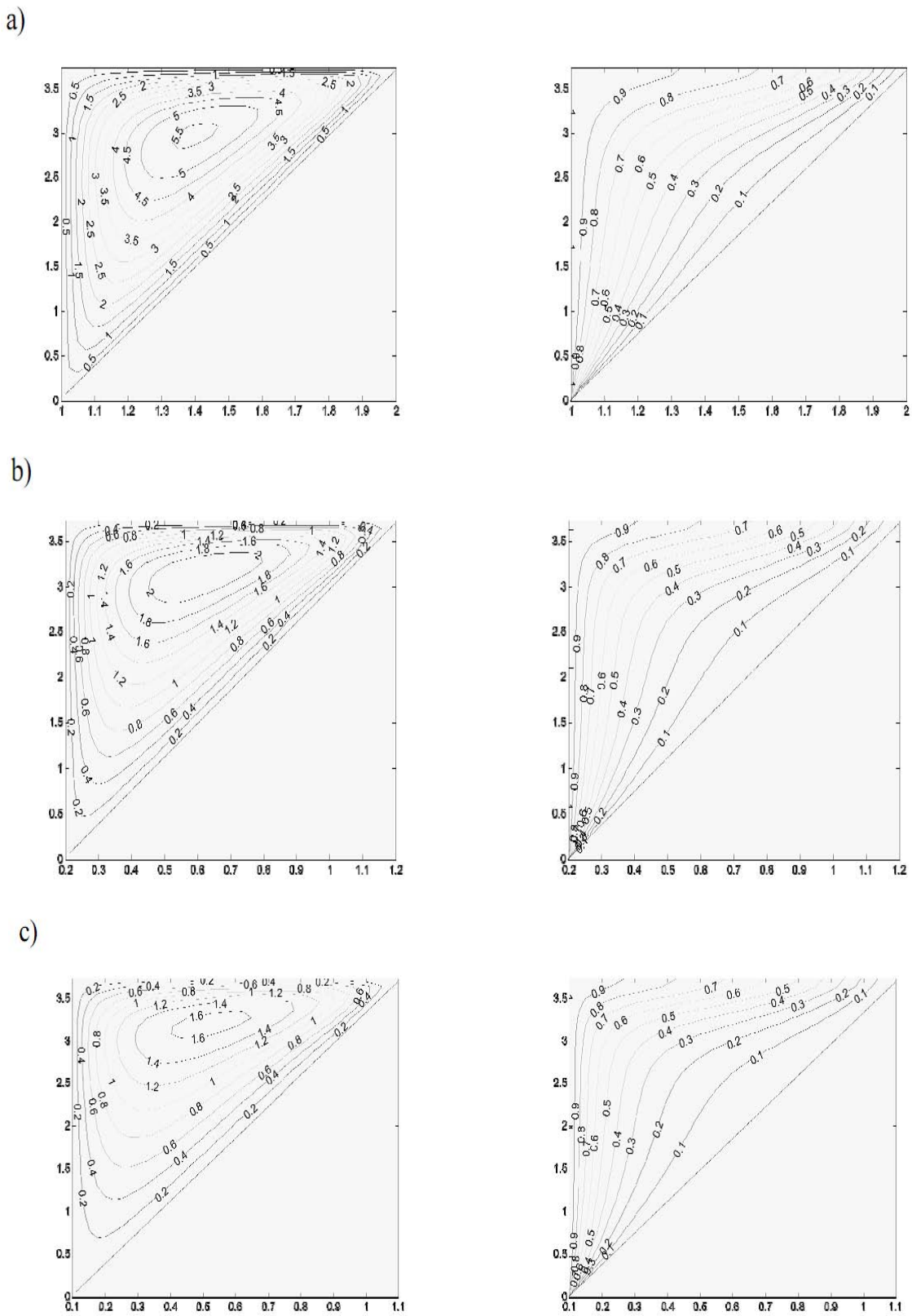

Figure 1.4.3 : Streamlines(left) and Isotherms(: Right) for Ra=50, C_A =15

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

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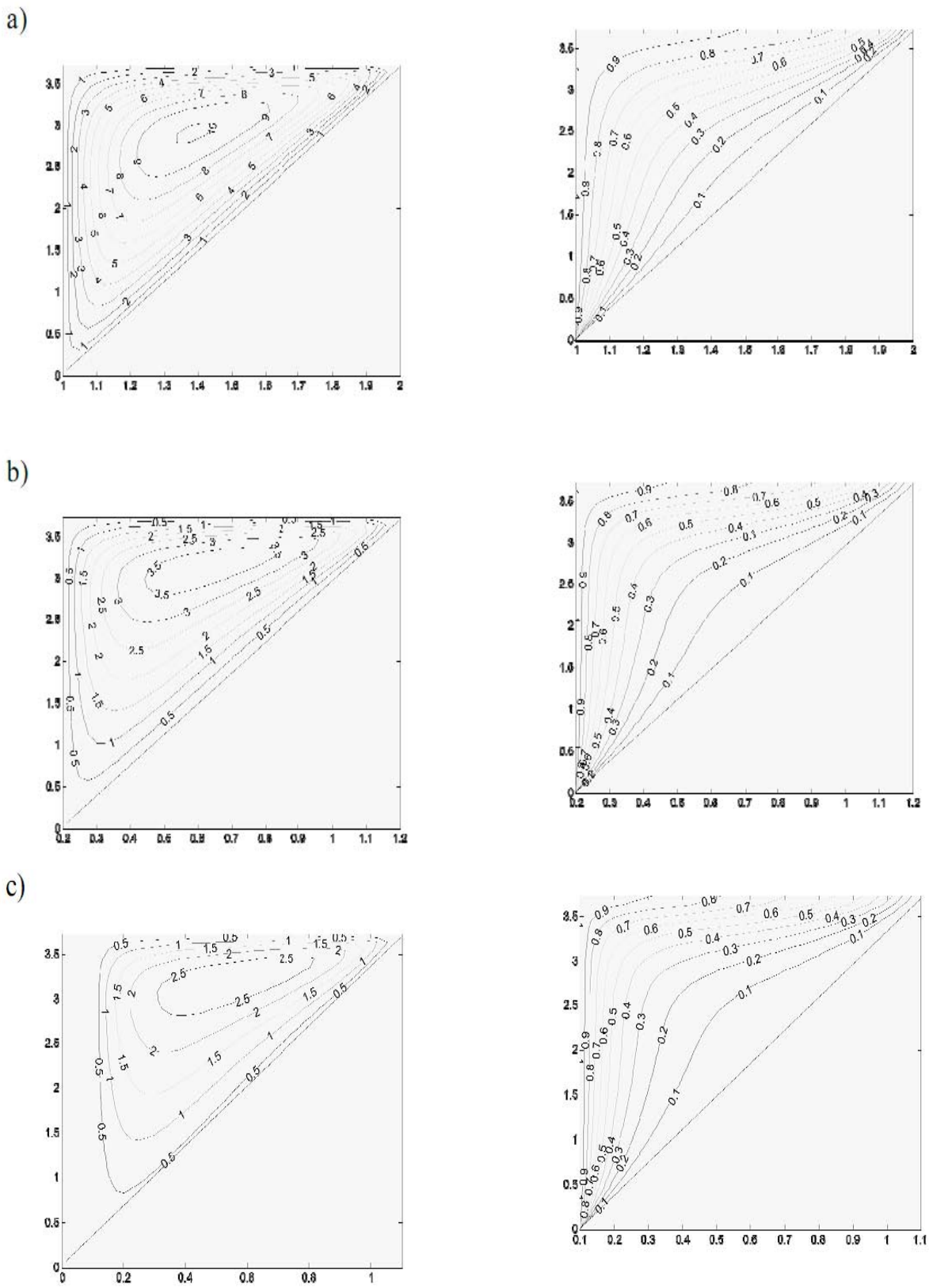

Figure 1.4.4 : Streamlines(left) and Isotherms(: Right) for Ra=100, C_A =15

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

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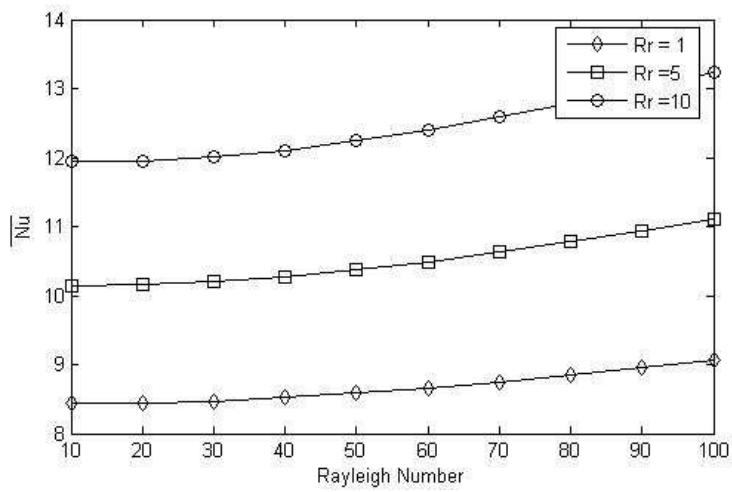
Figure (1.4.4) shows the streamlines and isothermal lines inside the porous medium for various values of Radius ratio (R_r) at Ra = 50 and C_A = 15. It can be observed that be horizontal scale changes for various values of Radius Ratio (R_r). The magnitude of the streamlines decrease with the increase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



R_r
R_r
R_r

Figure 1.4.5 : $\bar{N}u$ 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 ($\bar{N}u$) 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 ($\bar{N}u$) at Ra = 10 is increased by 20%. The corresponding increases in average Nusselt number ($\bar{N}u$) at Ra = 100 is found to be 21%. The difference between the average Nusselt number ($\bar{N}u$) at two difference 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 ($\bar{N}u$). i.e., for a given Rayleigh number (Ra) Nusselt number ($\bar{N}u$) 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 appears almost same as in Figure (1.4.7).

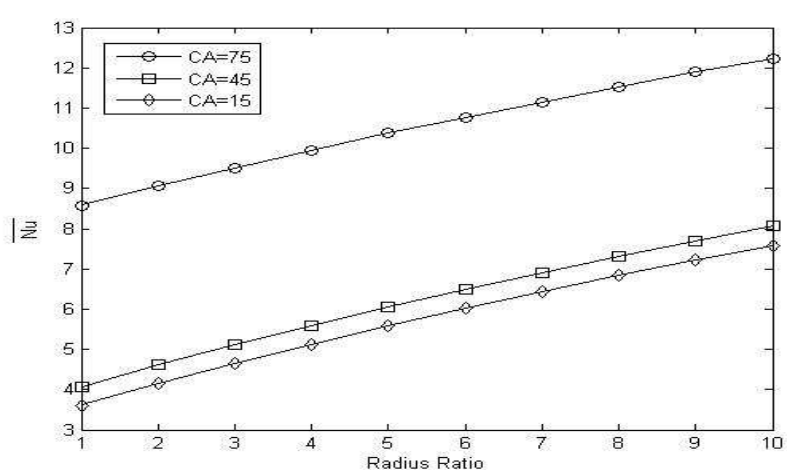


Figure 1.4.6 : $\bar{N}u$ variation with R_r at hot surface for different values of C_A at Ra = 50

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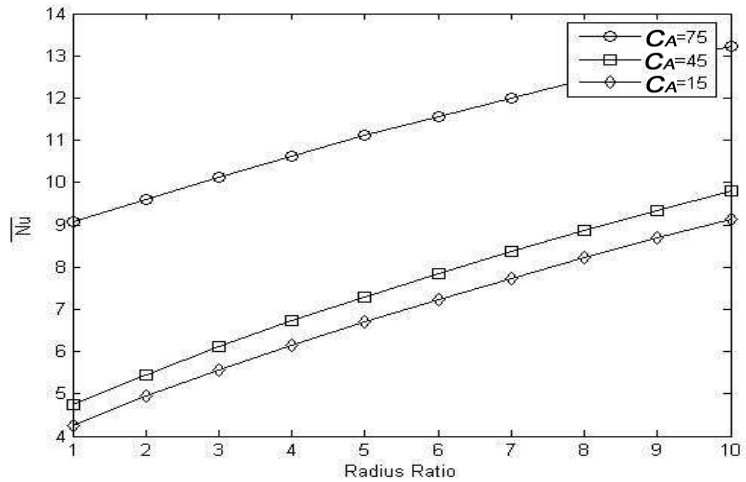
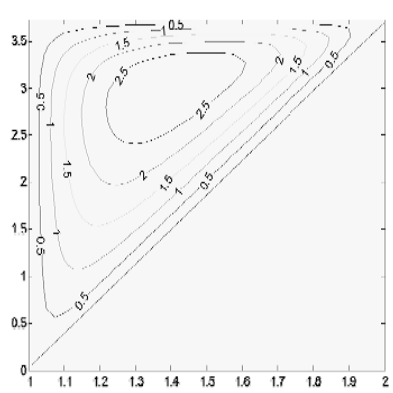


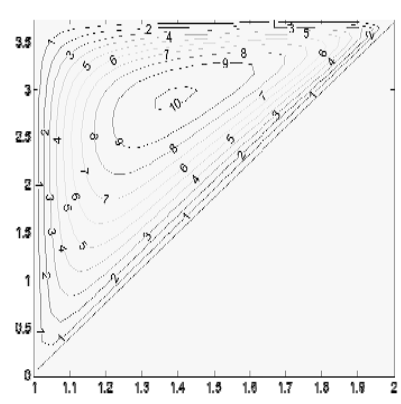
Figure 1.4.7 : $\bar{N}u$ variation with R_r at hot surface for different values of C_A at Ra = 100

Figure (1.4.7) illustrates the effect of Radius ratio (R_r) on average Nusselt number ($\bar{N}u$). This Figure corresponds to the value Ra = 50. It is seen that the average Nusselt number ($\bar{N}u$) at hot wall of the vertical annular cone increases with increase in Radius ratio (R_r). It is found that the average Nusselt number ($\bar{N}u$) at R_r = 1 increases by 9% when Cone angle (C_A) increased from 15 to 45. the corresponding increase in average Nusselt number ($\bar{N}u$) 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 ($\bar{N}u$) increases. The increase is marginal when the Cone angle (C_A) is increased from 15° to 45° when as we increases is substantial when we Cone angle (C_A) increases from 45° to 75°.

Figure (1.4.10) illustrates the effect of Radius ratio (R_r) on the average Nusselt number ($\bar{N}u$). This Figure corresponds to the value Ra = 100. It is seen that the average Nusselt number ($\bar{N}u$) at hot wall of the vertical annular cone increases with increase in Radius ratio (R_r). It is found that the average Nusselt number ($\bar{N}u$) 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 ($\bar{N}u$) at R_r = 10 is found to be 9.8%. This difference between the average Nusselt number ($\bar{N}u$) 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)





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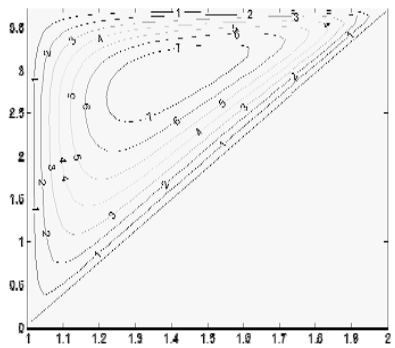

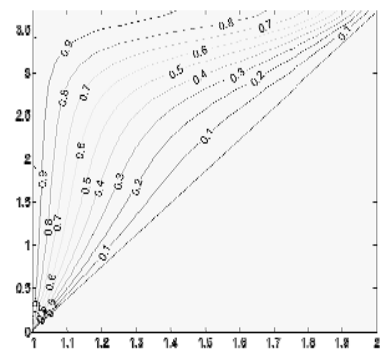

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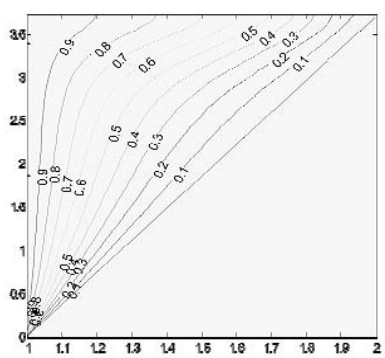

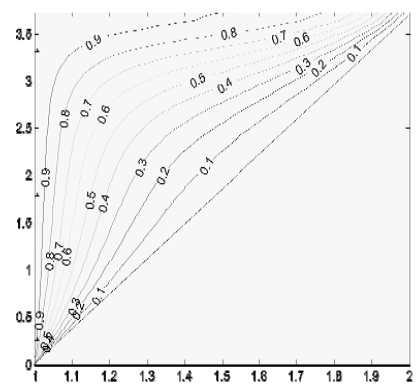

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Determination and Optimization of Bulk Total Energy for Gallium-Arsenide (Gaas) Atom using FHI98MD Input Variables

By J. A. Owolabi, M. Y. Onimisi & S. G. Abdu
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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 Stadele et al and -8.364 Rydberg/atom obtained 2003 by Franziska Gizegoizewski.

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GJSFR-A Classification : FOR Code: 091305

DETERMINATION AND OPTIMIZATION OF BULK TOTAL ENERGY FOR GALLIUM-ARSENIDE GAAS ATOM USING FHI98MD INPUT VARIABLES

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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).

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Keywords : optimization, bulk total energy calculations, local-density approximation, FHI98MD, GaAs.

I. 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.

$$H\Psi_i = E_i\Psi_i \tag{1}$$

where H is the many-body Hamiltonian, and Ψ is the many-body wave-function corresponding to the ith state which has energy E_i. The term Ψ 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) Theoritical Background

The approached used in this paper for the theory of electronic structure is that of DFT. In this approach, the electron density distribution $n(r)$ 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,

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

the density of the non-interacting system

$$n(r) = \sum_{i=1}^{N}\left|\psi_i(r)\right|^2 \tag{3}$$

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

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

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, $\varepsilon_{XC}(n)$. Thus the total exchange correlation energy functional is approximated as

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

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:

a. Convergence test by plotting parameter versus total energy;
b. Accuracy test by plotting parameter versus absolute difference between total energy and Harris energy
c. 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

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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

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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
Idyn	2
i_edyn	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

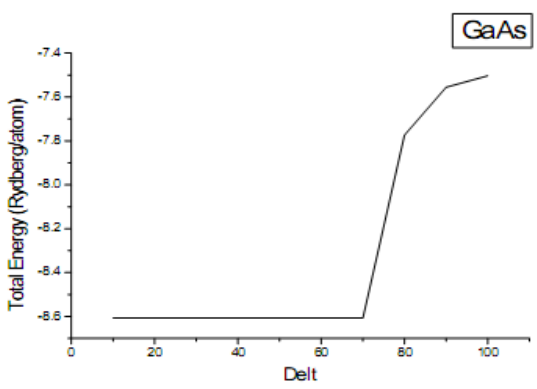

Figure 1 : Delt vs total energy (LDA) for GaAs

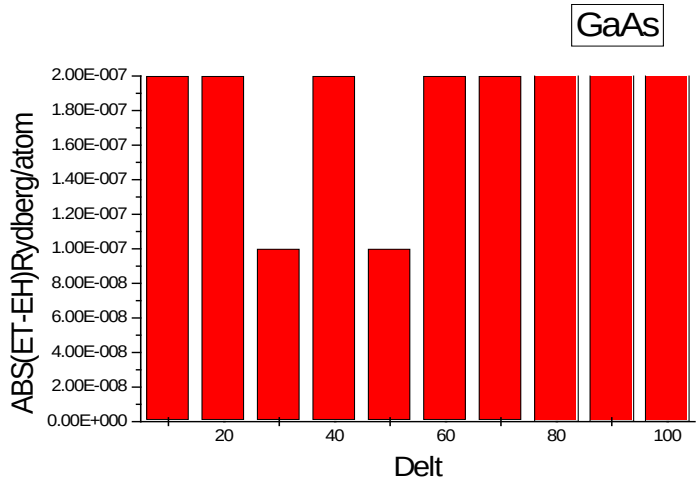

Figure 2 : Delt Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

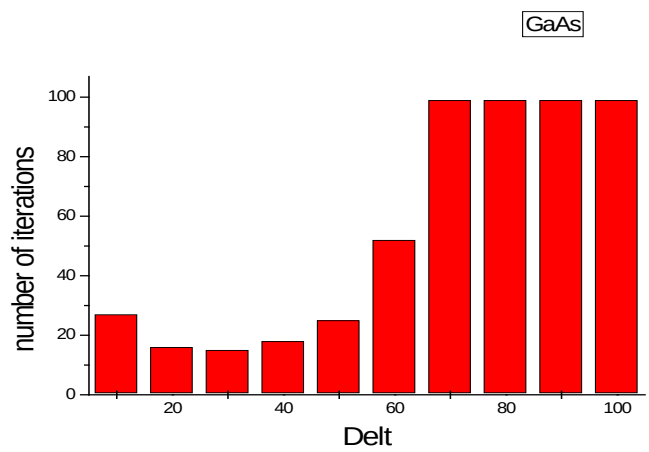

Figure 3 : Delt Vs number of iteration (LDA) for GaAs

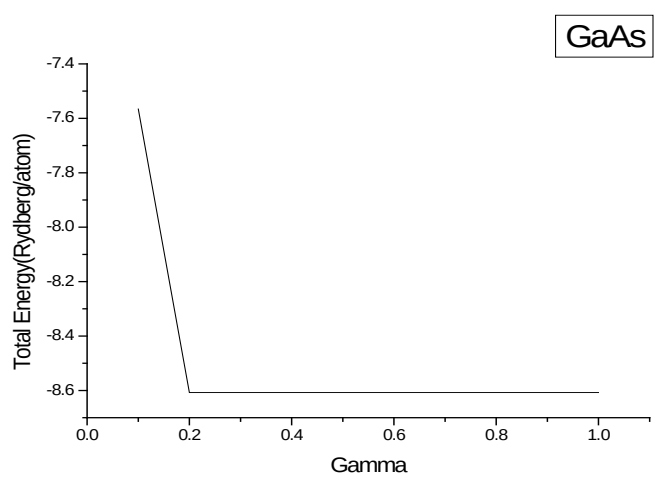

Figure 4 : Gamma vs. total energy (LDA) for GaAs

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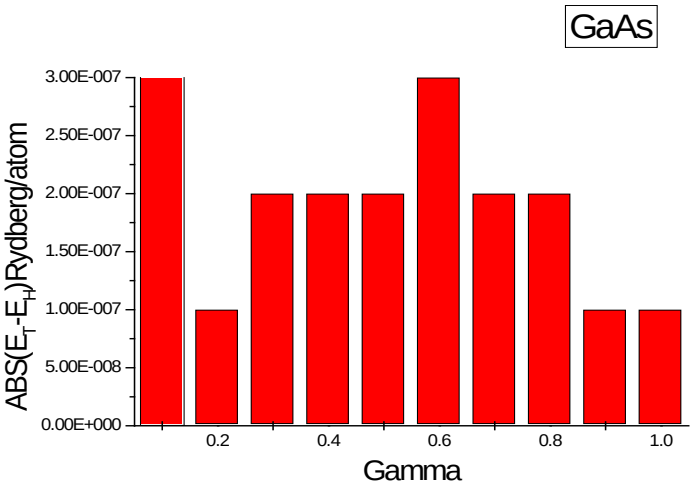

Figure 5 : Gamma Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

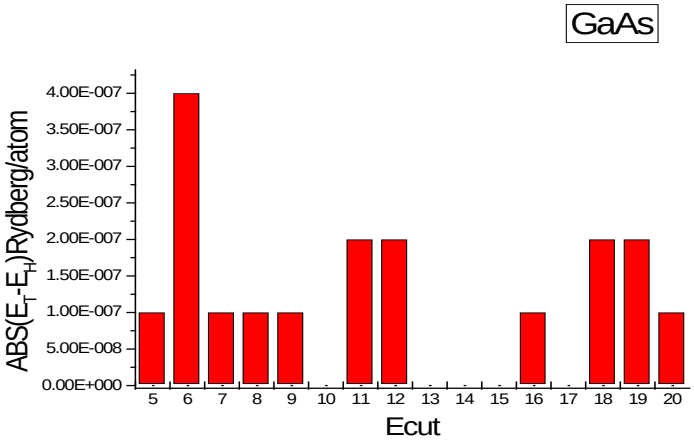

Figure 8 : Ecut Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

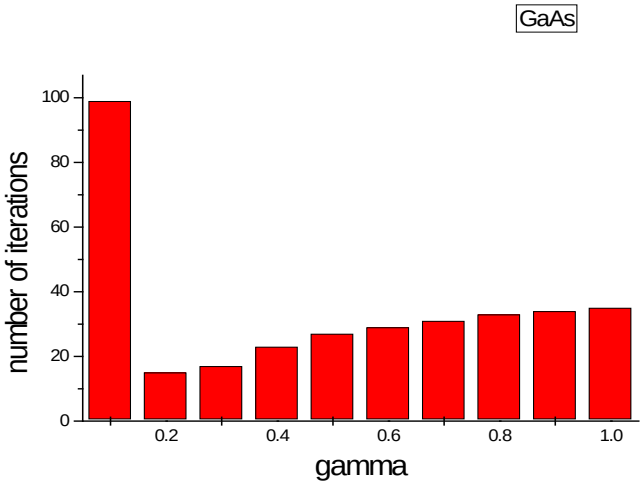

Figure 6 : Gamma Vs number of iterations (LDA) for GaAs

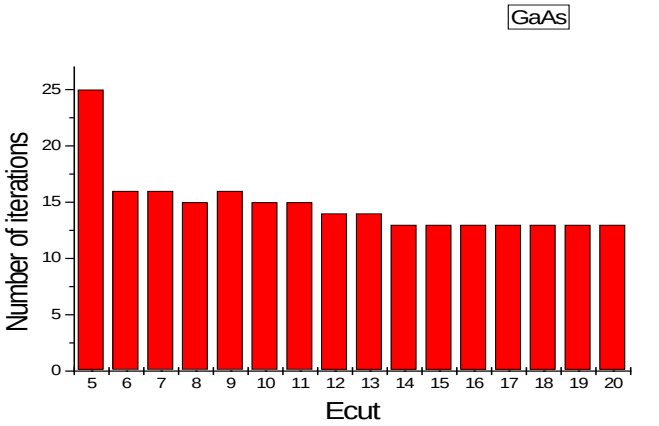

Figure 9 : Ecut Vs number of iterations (LDA) for GaAs

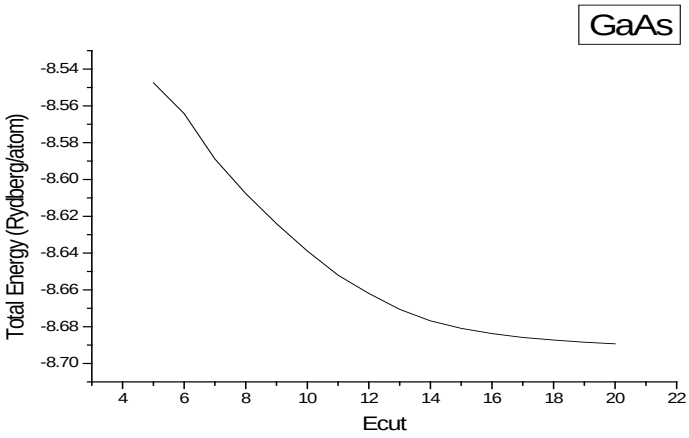

Figure 7 : Ecut Vs total energy (LDA) for GaAs

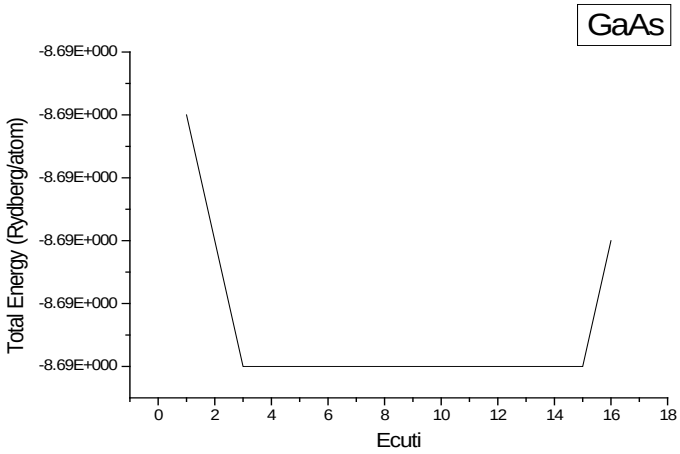

Figure 10 : Ecuti vs Total energy (LDA) for GaAs

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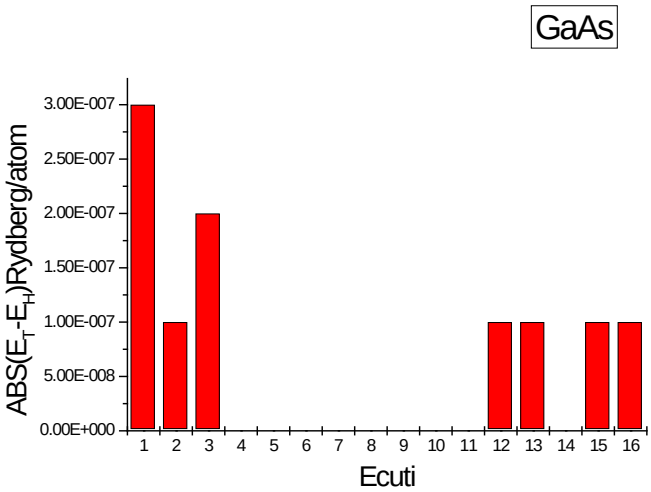

Figure 11 : Ecuti Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

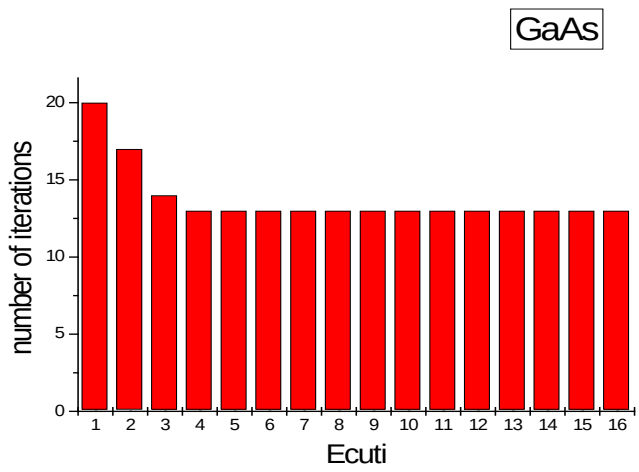

Figure 12 : Ecuti Vs number of iterations (LDA) for GaAs

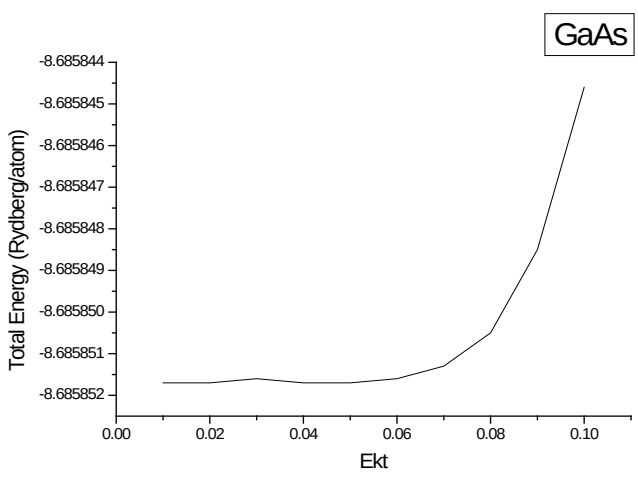

Figure 13 : EKT vs Total energy (LDA) for GaAs

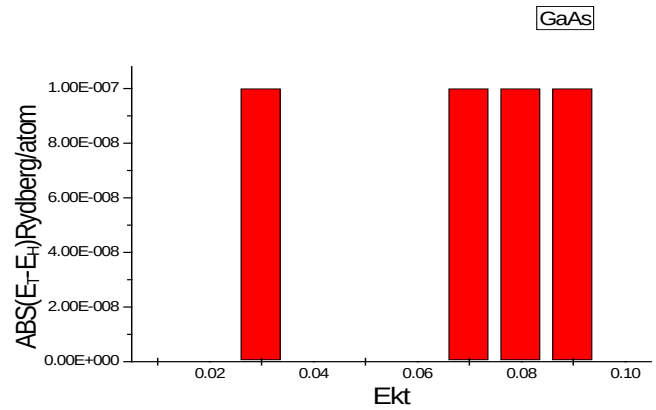

Figure 14 : EKT Vs Absolute difference between the Total energy and Harris Energy (LDA) for GaAs

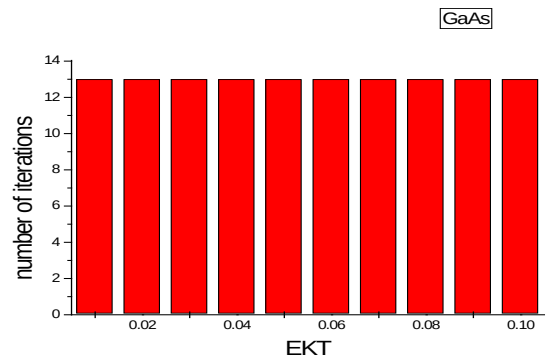

Figure 15 : EKT Vs number of iterations (LDA) for GaAs

i. *Total energy calculations for bulk GaAs*

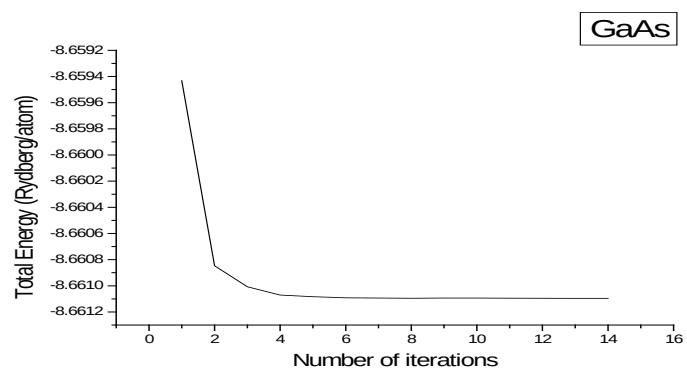

Figure 16 : Bulk Galliun-Asenide convergence test (LDA)

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

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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

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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

TEMPERATURE DEPENDENCE OF INVERSE DIELECTRIC SUSCEPTIBILITY IN KDP-TYPE CRYSTALS

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Temperature Dependence of Inverse Dielectric Susceptibility in KDP-Type Crystals

V. S. Bist [α] & N. S. Panwar [σ]

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 (KH_2PO_4), potassium dihydrogen arsenate (KH_2AsO_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 $(H_2PO_4^-)$ 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 selerites show a nearly two-fold increase (isotope effect) in transition temperature (T_c) on deuteration.

The KH_2PO_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[1]. 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[2]. The protons are self-trapped in one or the other of its equivalent positions according to recent neutron Compton scattering experiments[3]. While the tunneling model does not consider the hydrogen-bond geometry, the PO_4 tetrahedral distortion has theoretically been shown to give rise to a change in the ground state energy[4, 5].

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

In our previous works[20-21] we used the Blinc's Hamiltonian including the lattice anharmonicity upto fourth order, for the stochastic motion of $H_2PO_4^-$ 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*[8-9].

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II. Dielectric Susceptibility

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

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

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

$$G_{mn}(t-t') = << M_m(t); M_n(t') >>$$

$$= -j\theta(t-t') < [M_m(t); M_n(t')] >. \quad (2)$$

Where $\theta(t-t')$ is the Heaviside step function and the angular brackets $< -- >$ 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

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

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

$$G_{mn}(\omega + j\varepsilon) = << A_q(t); A_{q'}(t') >> = G'(\omega) - jG''(\omega). \quad (4)$$

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

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

wherte $\varepsilon'(\omega)$ 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[20]. The dielectric susceptibility for KDP - system can be obtained as

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

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

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

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

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

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

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

The imaginary part of which can be written as

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

and the real part as

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

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

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

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

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

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

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

The $\tilde{\tilde{\omega}}_{+}$ 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

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

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

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

III. Numerical Calculations

By using Blinc-de Gennes model parameters for KDP as given by Ganguli et al[28]. 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
$\Gamma_P(\omega)\times10^{-4}$ (cm^{-1})	2.87	2.31	1.76	1.88	1.90	1.92	20
$\tilde{\tilde{\omega}}$ (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
$\tilde{\tilde{\omega}}\times10^3$ (MHz)	1.3685	1.7104	1.7594	1.8898	1.9459	1.9476	*Present study*
$\chi_a^{-1}\times10^{-3}$	202.68	206	209.4	212.9	216.6	220.04	*Present study*
$\chi_c^{-1}\times10^{-4}$	3.518	20.45	54.99	143.78	259.13	408.49	*Present study*

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[8]. The solid lines are linear fits above Tc.

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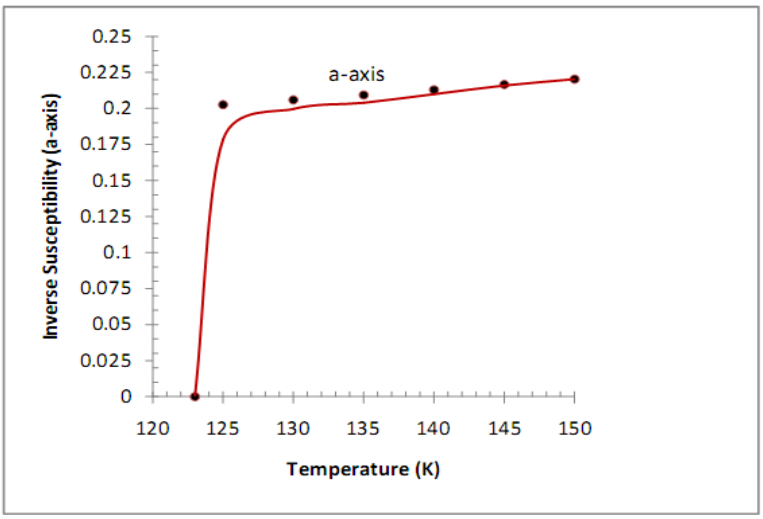

Figure 1 : Temperature dependence of inverse susceptibility in KDP crystal (a-axis)

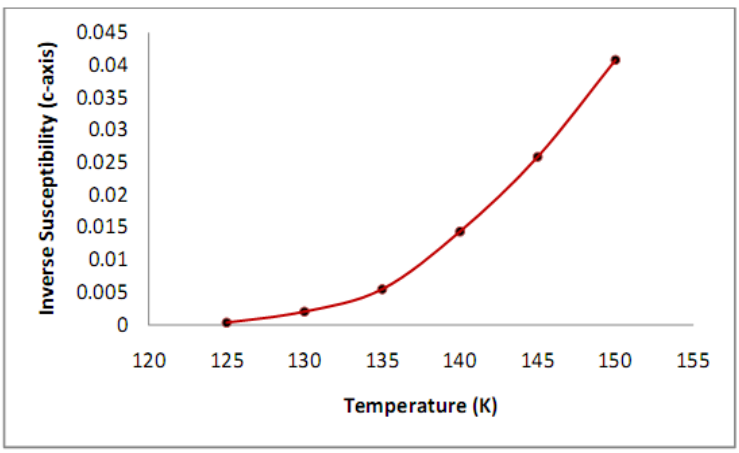

Figure 2 : Temperature dependence of inverse susceptibility in KDP crystal (c-axis)

V. Frequency Dependence of Dielectric Loss

Putting calculated value of $\Gamma_P(\omega)$, $\tilde{\tilde{\omega}}$, 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.

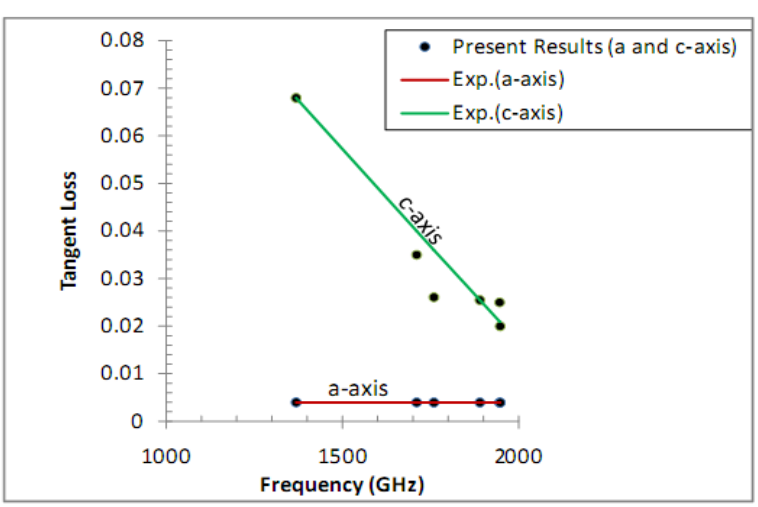

Figure 3 : Frequency dependence of dielectric loss in KDP crystal

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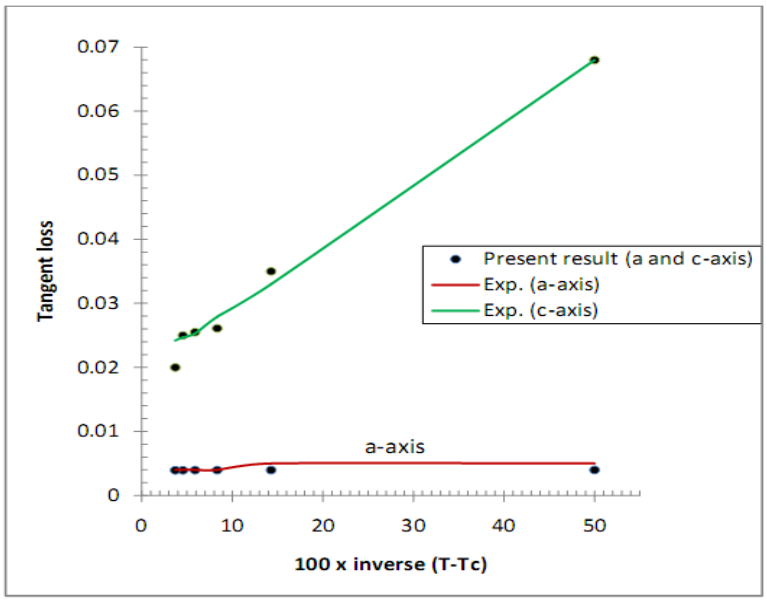

Figure 4 : Temperature dependence of dielectric loss in KDP crystal

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[28], 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[28] 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.

Ramakrishan and Tanaka[29], using the fermions Green's function, showed that with Tyablikov-type decoupling[30] the transverse susceptibility of KDP reproduces, the result of Havlin, Litov and Uehling[6]. 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[32]. 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_2PO_4, RbH_2PO_4, PbH_2PO_4, TlH_2PO_4[8-11].

The observed dielectric susceptibility may be expressed as a linear combination of the susceptibility originating due to the two relaxation times $(\tau_1, \text{and}\, \tau_2)$: τ_1 corresponding to $\tilde{\tilde{\omega}}_-$, tends to infinity as $T \to T_c$ and the other τ_2, corresponding to a $\tilde{\tilde{\omega}}_+$, is weakly temperature dependent.

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

χ_1 and χ_2 represent the contribution of the static susceptibility (χ_0) from the two relaxation

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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 χ_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[27], because of the fact that $\chi_1 \to \infty$, as $\tau_1 \to \infty$ at $T \to T_c$. (iii) The contribution to $\mathrm{Re}\,\chi(\omega)$ 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

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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, lacers, 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;

$$\frac{\partial^2\Theta}{\partial x^2}+\frac{\partial^2\Theta}{\partial y^2}=\rho(r),. \qquad (1a)$$

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

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

The boundary fixed temperatures are as follows:,

$$\Theta(1,1)=750K, \Theta(1,6)=700K,\ \Theta\,(1,12)=700K,\ \Theta\,(1,19)=700K, \qquad (2a)$$
$$\Theta\,(2,6)=700K, \Theta(1,11)=700K, \Theta\,(2,1)=800K, \Theta\,(3,1)=800K,$$
$$\Theta\,(4,1)=800K, \Theta\,(5,1)=800K, \Theta\,(2,33)=500K, \Theta\,(3,34)=500K,$$
$$\Theta\,(4,35)=500K,\ \Theta\,(5,36)=500, \Theta\ (11,37)=600K$$

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

$$\frac{\partial\Theta}{\partial n}=\begin{cases}\frac{-M\Theta+S}{\kappa}, \\ 4E\sigma\Theta_r^3(\Theta-\Theta_r), \\ \frac{-h\Theta}{b}\ln(1+\frac{bg}{K_o\Theta_o})\end{cases} \qquad (2b)$$

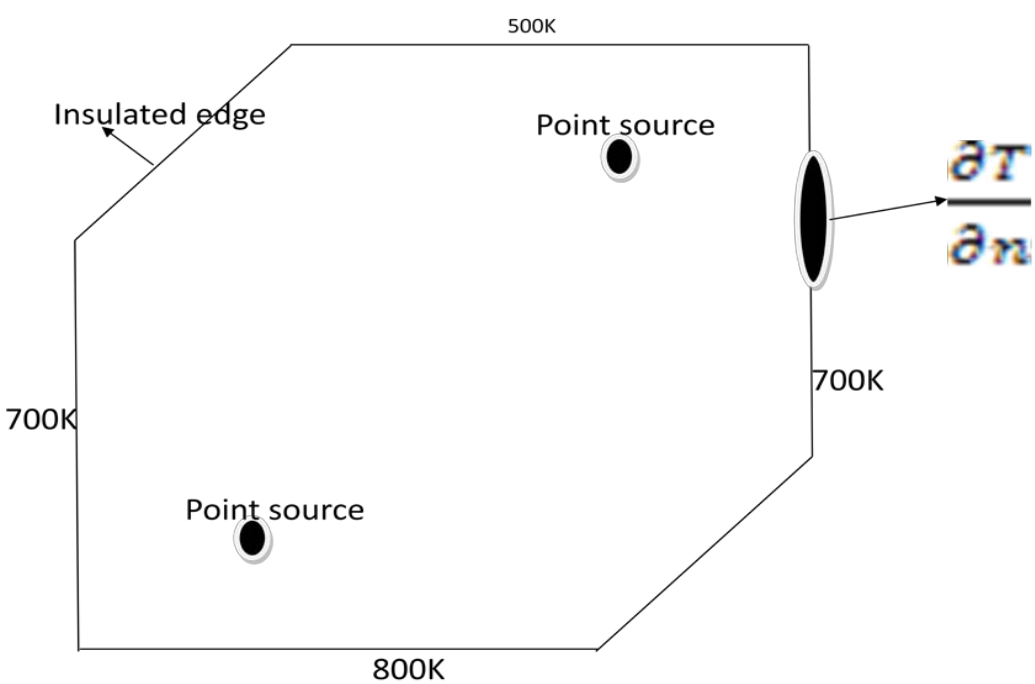

Figure 1 : The physical hexagonal pure metal for the simulation of heat flow

From equation (2a) above we have as follows: E is surface emissivity, h is thermal conductivity, σ is Stefan-Boltzmann constant, Θ_r is the temperature of external radiation source, Θ_o assumed lower limit temperature and M, S, b, g, K_0 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

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

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

where Θ is the temperature field, Θ' 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,

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

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;

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

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

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

for some edge S over which the plate losses heat to the surrounding, A is the plate area, γ is some constant coefficient, ∇^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.

$$[\mathrm{h}\iint \begin{pmatrix} \frac{\partial h_1}{\partial x} & 0 & \frac{\partial h_2}{\partial x} & 0 \\ 0 & \frac{\partial h_1}{\partial y} & 0 & \frac{\partial h_2}{\partial y} \\ \frac{\partial h_1}{\partial y} & \frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial y} & \frac{\partial h_2}{\partial x} \end{pmatrix}^T \begin{pmatrix} \kappa & 0 & 0 \\ 0 & \kappa & 0 \\ 0 & 0 & \kappa \end{pmatrix} \begin{pmatrix} \frac{\partial h_1}{\partial x} & 0 & \frac{\partial h_2}{\partial x} & 0 \\ 0 & \frac{\partial h_1}{\partial y} & 0 & \frac{\partial h_2}{\partial y} \\ \frac{\partial h_1}{\partial y} & \frac{\partial h_1}{\partial x} & \frac{\partial h_2}{\partial y} & \frac{\partial h_2}{\partial x} \end{pmatrix} \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} dxdy] \begin{pmatrix} \Theta_i \\ \Theta_j \\ \Theta_k \end{pmatrix} =$$

$$\mathrm{h}\iint \begin{pmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{pmatrix}^T Q \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} dxdy +$$

$$\int_S \begin{pmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{pmatrix}^T \frac{\partial \Theta}{\partial n} \begin{vmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \end{vmatrix} ds +$$

$$\sum_i \begin{pmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{pmatrix}^T Q_p \frac{\Theta_p}{k}\,. \qquad (7)$$

The above equilibrium equation can be written in compact form as

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

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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

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

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 4th 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

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deviations can pose overheating of the material surface which in turn pose the tendency of formation of surface bumps or deformation on cooling. Cad well 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, lacers, 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].

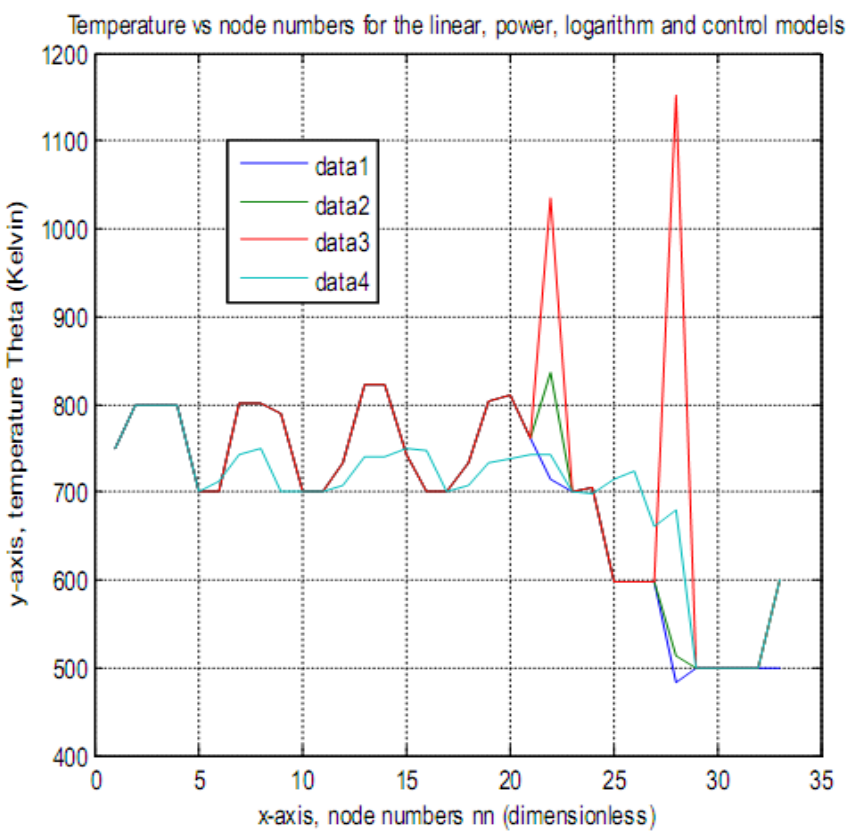

Figure 3 : MATLAB simulation results of the temperature Vs node numbers. Data 1 is the graph for the linear potential; Data 2 is the graph for the radiation potential; Data 3 is the graph for the logarithmic potential; Data 4 is the graph for the control model

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Rotating Light House Effect

By R. Rajamohan (Retd.) & A. Satya Narayanan
Indian Institute of Astrophysics, India

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 anamolies 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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Rotating Light House Effect

R. Rajamohan (Retd.) [α] & A. Satya Narayanan [σ]

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 anamolies 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 Nth pulse to meet the receiver will be NCP_e.

$$D_0 = NCP_e = Ct_0 \tag{1}$$

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

$$P_e = \frac{d_0}{NC} = \frac{t_0}{N} \tag{2}$$

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

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

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

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

$$= NP_e + \frac{\bar{V}P_e}{C - \bar{V}}N \tag{5}$$

Thus for uniform motion

$$P = P_e + \frac{P_e}{N} \tag{6}$$

Also

$$P_{Observed} = P_e + \triangle P_e = P_e + \frac{P_e}{N} \tag{7}$$

For an accelerating observer, we can write

$$P = P_e + \frac{1}{2}\frac{2P_e}{N} \tag{8}$$

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.

$$\dot{P} = \frac{2P_e}{N} \tag{9}$$

$$= \frac{2P_e^2}{t_0} = \frac{2CP_e^2}{D_0} \tag{10}$$

Thus

$$\frac{\dot{P}}{P_e} = \frac{2}{t_0} \tag{11}$$

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

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

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

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

Therefore the period derivative is

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

As $V \to 0$

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

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 $t_e \to 0$. 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 $\triangle\theta$ given by

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

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

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

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

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

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

$$\approx 41 \ \ arcsec/century \quad (23)$$

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 paramaters 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

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

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

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

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

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

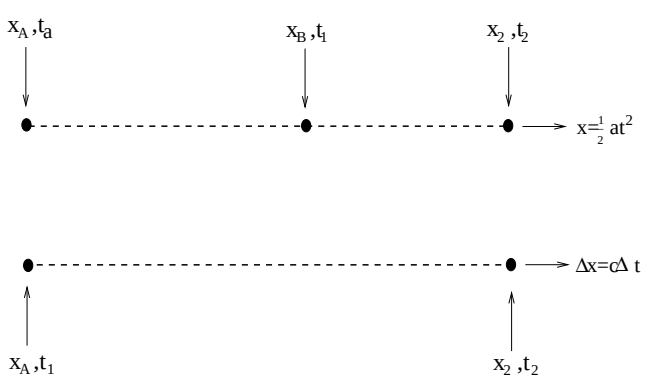

Figure 1 : The relative positions of the two signals

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

as

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

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

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

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

as

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

Therefore

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

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

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).

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

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

Setting $t_A = 0$, we get

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

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

$$P = \frac{P_e}{(1 - \frac{(1/2)at_2)}{C})} + \frac{PP_e}{(1 - \frac{(1/2)a(t_2 + t_A)}{C})t_1} \tag{32}$$

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

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$P_e/(1-V/C)$, 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) $\triangle T = CP_e$ where V is the average velocity in the time interval $\triangle T$.

$$\frac{1}{\triangle T} = \frac{V}{CP_e}; -\frac{\triangle \dot{T}}{\triangle T^2} = \frac{\dot{V}}{CP_e} or -\frac{\triangle \dot{T}}{\triangle T} = \frac{\dot{V}}{CP_e}\triangle T = \frac{\dot{V}}{V} \tag{34}$$

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.

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

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

$$d_0 = (1/2)aT_0^2 \tag{36}$$

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

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

and

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

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

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

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

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 $NP = P_iN + (1/2)\dot{P}P_iN^2$ where N is the number of cycles and is the initial period

$$\frac{\dot{P}}{P_e} = \frac{2}{T_0} \tag{40}$$

Note that the change in the velocity by 'aP_e' occurs for every '$V P_e$' 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

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

where R_A and R_B are the radius vectors.

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

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

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

$$= (GM)^{1/2}\{\frac{1}{R_A^{1/2}} - \frac{1}{R_A^{1/2}(1 - d/R_A)^{1/2}}\}$$

$$= (GM)^{1/2}\{\frac{1}{R_A^{1/2}} - \frac{1}{R_A^{1/2}}\{1 + \frac{d}{2R_A} + \frac{3d^2}{8R_A^2}\}\}$$

$$= (GM)^{1/2}\{\frac{1}{R_A^{1/2}} \cdot \frac{d}{R_A} + \frac{1}{R_A^{1/2}}\frac{3d^2}{8R_A^2}\}$$

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

$$\frac{1}{2}\sqrt{2}\frac{V_{rel}}{d} = \frac{1}{\sqrt{2}}[(\frac{GM}{R_A})^{1/2} - (\frac{GM}{R_B})^{1/2}]/|R_A - R_B|$$

$$\approx \frac{1}{\sqrt{2}}\frac{(GM)^{1/2}}{R_A^{3/2}} + \frac{1}{\sqrt{2}} \cdot \frac{3}{8}\frac{(GM)^{1/2}}{R_A^{3/2}} \cdot \frac{d}{R_A}$$

$\frac{(GM)^{1/2}}{R^{3/2}}$ 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.

$$d_0 = (1/2)aT_0^2 \tag{41}$$

Therefore

$$\frac{2}{T_0} = \sqrt{2}\frac{v_\tau}{d_0} \tag{42}$$

$\sqrt{2}$ 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 anamolies 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 be-tween 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 Stocastic 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.

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A STOCASTIC SEMI-EMPIRICAL MODEL FOR FIRST ORDER DECAY PHARMACOKINETICS

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

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 exciting 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:

$$C(t) = C_0 + C(nI), \tag{1}$$

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:

$$P_r + P_p = 1 \tag{2}$$

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

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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

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

$$C(0) = C_0, \quad (3b)$$

where k is the elimation 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;

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

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

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

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

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

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

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

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

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

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

The level increases to

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

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

$$C(NI) = C_0(1 + e^{-kt} + e^{-2kI} + \cdots + e^{-NkI}). \quad (9)$$

This is the general solution popularly found in the literatures.

Equ.(9) can be written in compact form as

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

By partial fraction decomposition, this equation can be expressed as

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

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

$$C_s = \frac{C_0}{1-e^{-Ik}} \quad (12)$$

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

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

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

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

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;

$$e^{nx} \cong 1 + nx \quad (14)$$

This transformation reduces Equ.(13) into

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

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

$$C(t) = \alpha C(nI) + \beta, \quad (16)$$

Where the slope α coincides with $\ln C_0$ and β is the intercept.

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

$$\Psi(t)_l, = E(e^{tC}) = e^{\beta In}\Psi(\alpha In) \quad (17a)$$

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

$$\Psi(t)_C = E(e^{\gamma}), \quad (17b)$$

where γ is a complex number given as;

$$\gamma = inIC(nI) \quad (17c)$$

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

$$\Psi(t)_C = 1, t \geq 0 \ (but\ zero\ else\ where) \quad (18)$$

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

$$\dot{C_r} = -\sum_{n=1}^{N} \frac{C_0}{(1+nkI)(kI)}\Psi(t)_C \quad (19)$$

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

$$\dot{C}_r = -\sum_{n=1}^{N} \frac{C_0}{(Ik)^2(n+\frac{1}{Ik})} \Psi(nI)_C \qquad (20)$$

Here the convergence is achieved such that $\frac{1}{Ik}$ 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 $n = \left|\frac{-1}{Ik}\right|$ with a pole of order 1. Following the well-known standard complex variable theory, we can calculate the residue, R, by the formula;

$$R = \lim_{n \to \left|\frac{-1}{Ik}\right|} \left\{ \frac{d^{p-1}}{dn^{p-1}} \left[n + \frac{1}{Ik} \dot{C}_r(nI) \right] \right\}^P, \qquad (21)$$

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;

$$C_r(\dot{nI}) = \frac{C_0}{(Ik)^2}; t \geq 0 \qquad (22)$$

ii. *The Probability Density Functions*

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

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

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

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

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 flunctuation $\sigma = 1$, can be written as;

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

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

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

iii. *The Stochastic Model*

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

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

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;

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

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:

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

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 spurious 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).

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Table 1 : Summary of simulation data

I(hr)	label	$T_{\frac{1}{2}}(hr)$	$C_0(\frac{mg}{kg})$	$C_s(\frac{mg}{kg})$	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

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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

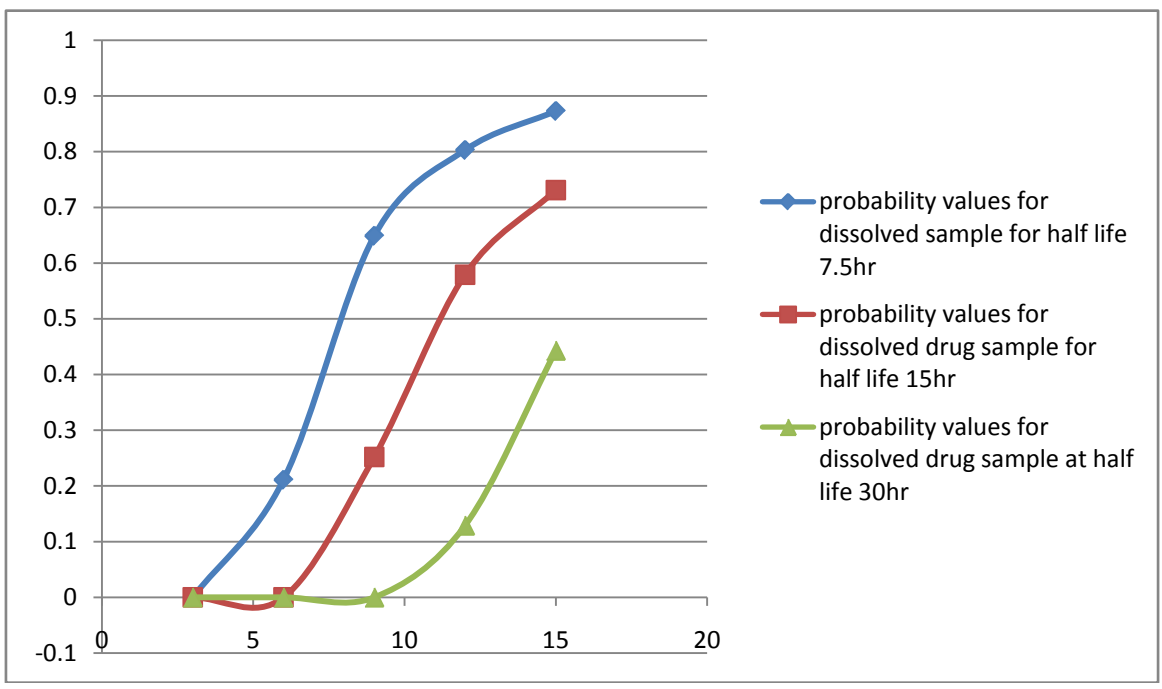

Figure 2 : Probability densities for real drug concentration profiles against time for ingestion time interval of 3hr

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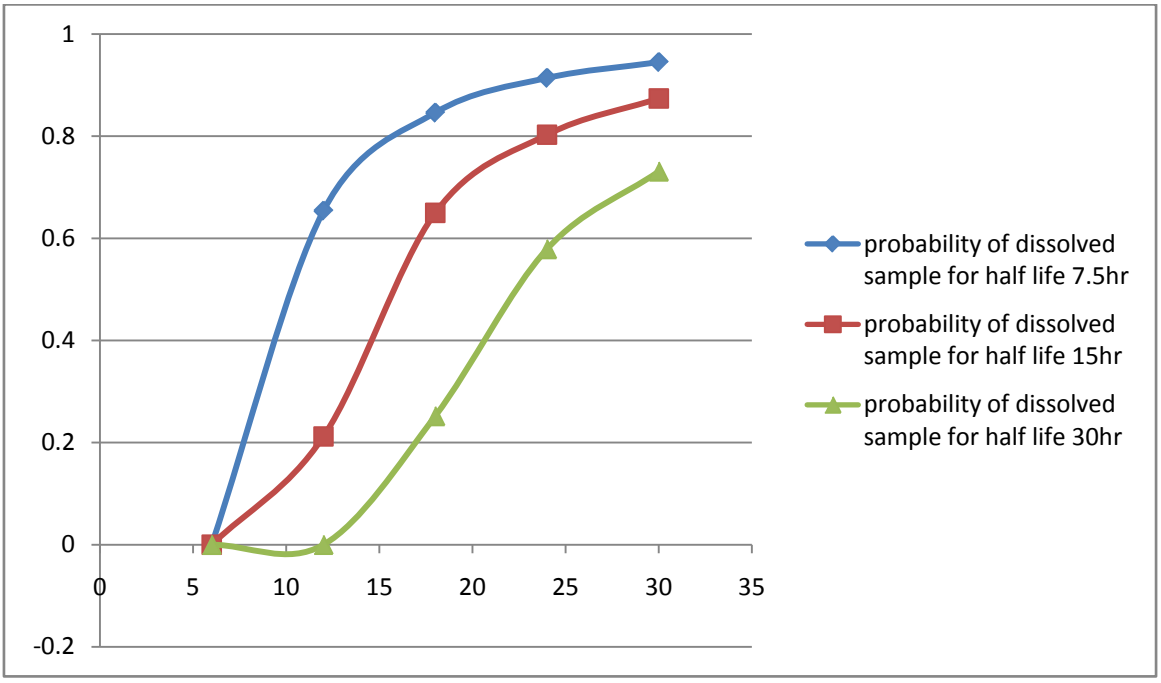

Figure 3 : Probability densities for real drug concentration profiles against time for ingestion time interval of 6hr

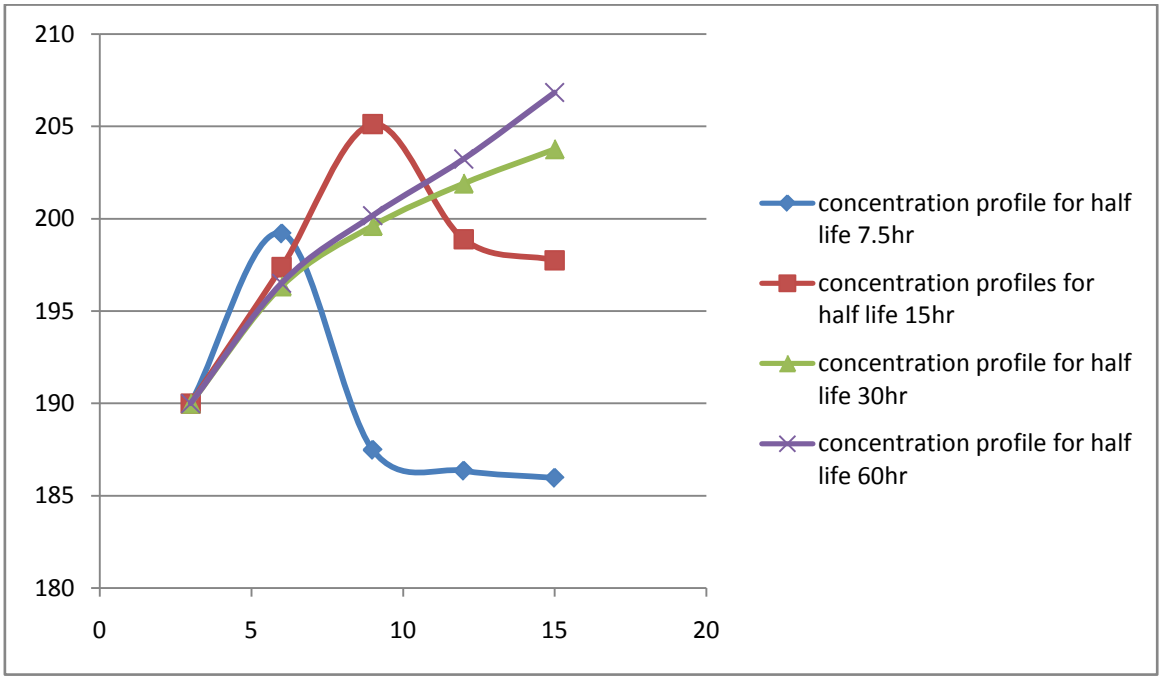

Figure 4 : Real drug concentration (mg/kg) profiles against ingestion time for ingestion time interval of 3hr

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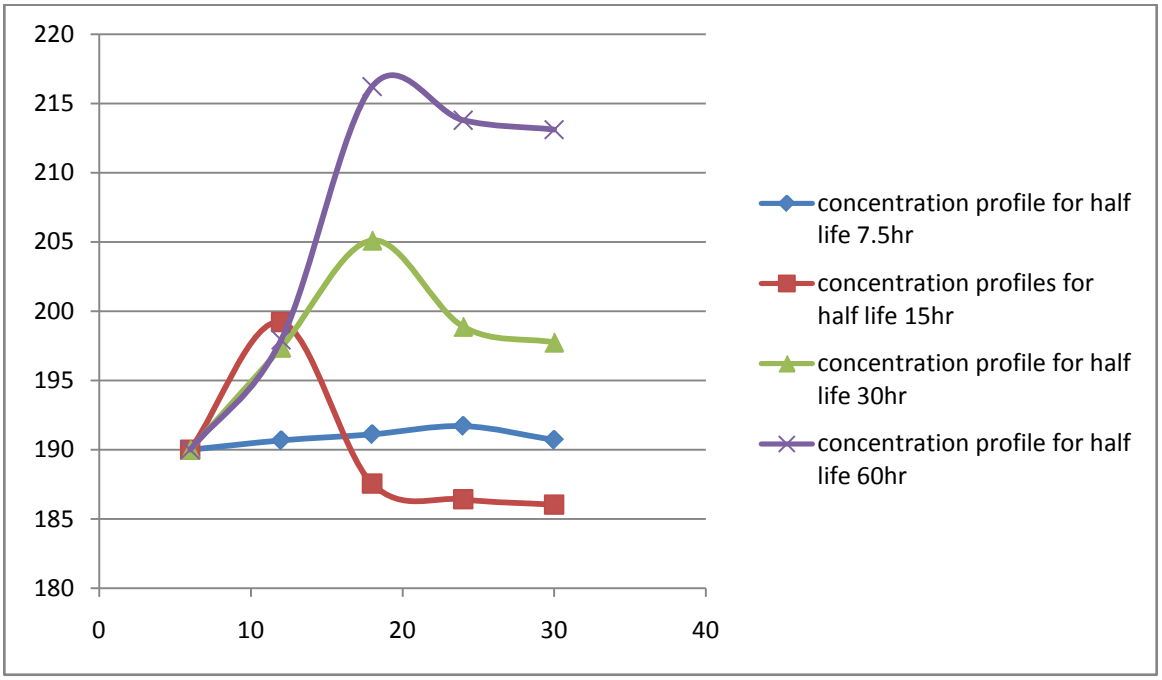

Figure 5 : Real concentration of drug (mg/kg) against ingestion time (hr) for ingestion time interval of 6hr

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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1. General,

2. Ethical Guidelines,

3. Submission of Manuscripts,

4. Manuscript's Category,

5. Structure and Format of Manuscript,

6. After Acceptance.

1. GENERAL

Before submitting your research paper, one is advised to go through the details as mentioned in following heads. It will be beneficial, while peer reviewer justify your paper for publication.

Scope

The Global Journals Inc. (US) welcome the submission of original paper, review paper, survey article relevant to the all the streams of Philosophy and knowledge. The Global Journals Inc. (US) is parental platform for Global Journal of Computer Science and Technology, Researches in Engineering, Medical Research, Science Frontier Research, Human Social Science, Management, and Business organization. The choice of specific field can be done otherwise as following in Abstracting and Indexing Page on this Website. As the all Global

Journals Inc. (US) are being abstracted and indexed (in process) by most of the reputed organizations. Topics of only narrow interest will not be accepted unless they have wider potential or consequences.

2. ETHICAL GUIDELINES

Authors should follow the ethical guidelines as mentioned below for publication of research paper and research activities.

Papers are accepted on strict understanding that the material in whole or in part has not been, nor is being, considered for publication elsewhere. If the paper once accepted by Global Journals Inc. (US) and Editorial Board, will become the copyright of the Global Journals Inc. (US).

Authorship: The authors and coauthors should have active contribution to conception design, analysis and interpretation of findings. They should critically review the contents and drafting of the paper. All should approve the final version of the paper before submission

The Global Journals Inc. (US) follows the definition of authorship set up by the Global Academy of Research and Development. According to the Global Academy of R&D authorship, criteria must be based on:

1) Substantial contributions to conception and acquisition of data, analysis and interpretation of the findings.

2) Drafting the paper and revising it critically regarding important academic content.

3) Final approval of the version of the paper to be published.

All authors should have been credited according to their appropriate contribution in research activity and preparing paper. Contributors who do not match the criteria as authors may be mentioned under Acknowledgement.

Acknowledgements: Contributors to the research other than authors credited should be mentioned under acknowledgement. The specifications of the source of funding for the research if appropriate can be included. Suppliers of resources may be mentioned along with address.

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3. SUBMISSION OF MANUSCRIPTS

Manuscripts should be uploaded via this online submission page. The online submission is most efficient method for submission of papers, as it enables rapid distribution of manuscripts and consequently speeds up the review procedure. It also enables authors to know the status of their own manuscripts by emailing us. Complete instructions for submitting a paper is available below.

Manuscript submission is a systematic procedure and little preparation is required beyond having all parts of your manuscript in a given format and a computer with an Internet connection and a Web browser. Full help and instructions are provided on-screen. As an author, you will be prompted for login and manuscript details as Field of Paper and then to upload your manuscript file(s) according to the instructions.

To avoid postal delays, all transaction is preferred by e-mail. A finished manuscript submission is confirmed by e-mail immediately and your paper enters the editorial process with no postal delays. When a conclusion is made about the publication of your paper by our Editorial Board, revisions can be submitted online with the same procedure, with an occasion to view and respond to all comments.

Complete support for both authors and co-author is provided.

4. MANUSCRIPT'S CATEGORY

Based on potential and nature, the manuscript can be categorized under the following heads:

Original research paper: Such papers are reports of high-level significant original research work.

Review papers: These are concise, significant but helpful and decisive topics for young researchers.

Research articles: These are handled with small investigation and applications

Research letters: The letters are small and concise comments on previously published matters.

5.STRUCTURE AND FORMAT OF MANUSCRIPT

The recommended size of original research paper is less than seven thousand words, review papers fewer than seven thousands words also.Preparation of research paper or how to write research paper, are major hurdle, while writing manuscript. The research articles and research letters should be fewer than three thousand words, the structure original research paper; sometime review paper should be as follows:

Papers: These are reports of significant research (typically less than 7000 words equivalent, including tables, figures, references), and comprise:

(a)Title should be relevant and commensurate with the theme of the paper.

(b) A brief Summary, "Abstract" (less than 150 words) containing the major results and conclusions.

(c) Up to ten keywords, that precisely identifies the paper's subject, purpose, and focus.

(d) An Introduction, giving necessary background excluding subheadings; objectives must be clearly declared.

(e) Resources and techniques with sufficient complete experimental details (wherever possible by reference) to permit repetition; sources of information must be given and numerical methods must be specified by reference, unless non-standard.

(f) Results should be presented concisely, by well-designed tables and/or figures; the same data may not be used in both; suitable statistical data should be given. All data must be obtained with attention to numerical detail in the planning stage. As reproduced design has been recognized to be important to experiments for a considerable time, the Editor has decided that any paper that appears not to have adequate numerical treatments of the data will be returned un-refereed;

(g) Discussion should cover the implications and consequences, not just recapitulating the results; conclusions should be summarizing.

(h) Brief Acknowledgements.

(i) References in the proper form.

Authors should very cautiously consider the preparation of papers to ensure that they communicate efficiently. Papers are much more likely to be accepted, if they are cautiously designed and laid out, contain few or no errors, are summarizing, and be conventional to the approach and instructions. They will in addition, be published with much less delays than those that require much technical and editorial correction.

The Editorial Board reserves the right to make literary corrections and to make suggestions to improve briefness.

It is vital, that authors take care in submitting a manuscript that is written in simple language and adheres to published guidelines.

Format

Language: The language of publication is UK English. Authors, for whom English is a second language, must have their manuscript efficiently edited by an English-speaking person before submission to make sure that, the English is of high excellence. It is preferable, that manuscripts should be professionally edited.

Standard Usage, Abbreviations, and Units: Spelling and hyphenation should be conventional to The Concise Oxford English Dictionary. Statistics and measurements should at all times be given in figures, e.g. 16 min, except for when the number begins a sentence. When the number does not refer to a unit of measurement it should be spelt in full unless, it is 160 or greater.

Abbreviations supposed to be used carefully. The abbreviated name or expression is supposed to be cited in full at first usage, followed by the conventional abbreviation in parentheses.

Metric SI units are supposed to generally be used excluding where they conflict with current practice or are confusing. For illustration, 1.4 l rather than 1.4 × 10-3 m3, or 4 mm somewhat than 4 × 10-3 m. Chemical formula and solutions must identify the form used, e.g. anhydrous or hydrated, and the concentration must be in clearly defined units. Common species names should be followed by underlines at the first mention. For following use the generic name should be constricted to a single letter, if it is clear.

Structure

All manuscripts submitted to Global Journals Inc. (US), ought to include:

Title: The title page must carry an instructive title that reflects the content, a running title (less than 45 characters together with spaces), names of the authors and co-authors, and the place(s) wherever the work was carried out. The full postal address in addition with the e-mail address of related author must be given. Up to eleven keywords or very brief phrases have to be given to help data retrieval, mining and indexing.

Abstract, used in Original Papers and Reviews:

Optimizing Abstract for Search Engines

Many researchers searching for information online will use search engines such as Google, Yahoo or similar. By optimizing your paper for search engines, you will amplify the chance of someone finding it. This in turn will make it more likely to be viewed and/or cited in a further work. Global Journals Inc. (US) have compiled these guidelines to facilitate you to maximize the web-friendliness of the most public part of your paper.

Key Words

A major linchpin in research work for the writing research paper is the keyword search, which one will employ to find both library and Internet resources.

One must be persistent and creative in using keywords. An effective keyword search requires a strategy and planning a list of possible keywords and phrases to try.

Search engines for most searches, use Boolean searching, which is somewhat different from Internet searches. The Boolean search uses "operators," words (and, or, not, and near) that enable you to expand or narrow your affords. Tips for research paper while preparing research paper are very helpful guideline of research paper.

Choice of key words is first tool of tips to write research paper. Research paper writing is an art.A few tips for deciding as strategically as possible about keyword search:

- One should start brainstorming lists of possible keywords before even begin searching. Think about the most important concepts related to research work. Ask, "What words would a source have to include to be truly valuable in research paper?" Then consider synonyms for the important words.
- It may take the discovery of only one relevant paper to let steer in the right keyword direction because in most databases, the keywords under which a research paper is abstracted are listed with the paper.
- One should avoid outdated words.

Keywords are the key that opens a door to research work sources. Keyword searching is an art in which researcher's skills are bound to improve with experience and time.

Numerical Methods: Numerical methods used should be clear and, where appropriate, supported by references.

Acknowledgements: Please make these as concise as possible.

References

References follow the Harvard scheme of referencing. References in the text should cite the authors' names followed by the time of their publication, unless there are three or more authors when simply the first author's name is quoted followed by et al. unpublished work has to only be cited where necessary, and only in the text. Copies of references in press in other journals have to be supplied with submitted typescripts. It is necessary that all citations and references be carefully checked before submission, as mistakes or omissions will cause delays.

References to information on the World Wide Web can be given, but only if the information is available without charge to readers on an official site. Wikipedia and Similar websites are not allowed where anyone can change the information. Authors will be asked to make available electronic copies of the cited information for inclusion on the Global Journals Inc. (US) homepage at the judgment of the Editorial Board.

The Editorial Board and Global Journals Inc. (US) recommend that, citation of online-published papers and other material should be done via a DOI (digital object identifier). If an author cites anything, which does not have a DOI, they run the risk of the cited material not being noticeable.

The Editorial Board and Global Journals Inc. (US) recommend the use of a tool such as Reference Manager for reference management and formatting.

Tables, Figures and Figure Legends

Tables: Tables should be few in number, cautiously designed, uncrowned, and include only essential data. Each must have an Arabic number, e.g. Table 4, a self-explanatory caption and be on a separate sheet. Vertical lines should not be used.

Figures: Figures are supposed to be submitted as separate files. Always take in a citation in the text for each figure using Arabic numbers, e.g. Fig. 4. Artwork must be submitted online in electronic form by e-mailing them.

Preparation of Electronic Figures for Publication

Even though low quality images are sufficient for review purposes, print publication requires high quality images to prevent the final product being blurred or fuzzy. Submit (or e-mail) EPS (line art) or TIFF (halftone/photographs) files only. MS PowerPoint and Word Graphics are unsuitable for printed pictures. Do not use pixel-oriented software. Scans (TIFF only) should have a resolution of at least 350 dpi (halftone) or 700 to 1100 dpi (line drawings) in relation to the imitation size. Please give the data for figures in black and white or submit a Color Work Agreement Form. EPS files must be saved with fonts embedded (and with a TIFF preview, if possible).

For scanned images, the scanning resolution (at final image size) ought to be as follows to ensure good reproduction: line art: >650 dpi; halftones (including gel photographs) : >350 dpi; figures containing both halftone and line images: >650 dpi.

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Figure Legends: Self-explanatory legends of all figures should be incorporated separately under the heading 'Legends to Figures'. In the full-text online edition of the journal, figure legends may possibly be truncated in abbreviated links to the full screen version. Therefore, the first 100 characters of any legend should notify the reader, about the key aspects of the figure.

6. AFTER ACCEPTANCE

Upon approval of a paper for publication, the manuscript will be forwarded to the dean, who is responsible for the publication of the Global Journals Inc. (US).

6.1 Proof Corrections

The corresponding author will receive an e-mail alert containing a link to a website or will be attached. A working e-mail address must therefore be provided for the related author.

Acrobat Reader will be required in order to read this file. This software can be downloaded

(Free of charge) from the following website:

www.adobe.com/products/acrobat/readstep2.html. This will facilitate the file to be opened, read on screen, and printed out in order for any corrections to be added. Further instructions will be sent with the proof.

Proofs must be returned to the dean at dean@globaljournals.org within three days of receipt.

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6.4 Author Material Archive Policy

Please note that if not specifically requested, publisher will dispose off hardcopy & electronic information submitted, after the two months of publication. If you require the return of any information submitted, please inform the Editorial Board or dean as soon as possible.

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Before start writing a good quality Computer Science Research Paper, let us first understand what is Computer Science Research Paper? So, Computer Science Research Paper is the paper which is written by professionals or scientists who are associated to Computer Science and Information Technology, or doing research study in these areas. If you are novel to this field then you can consult about this field from your supervisor or guide.

TECHNIQUES FOR WRITING A GOOD QUALITY RESEARCH PAPER:

1. Choosing the topic: In most cases, the topic is searched by the interest of author but it can be also suggested by the guides. You can have several topics and then you can judge that in which topic or subject you are finding yourself most comfortable. This can be done by asking several questions to yourself, like Will I be able to carry our search in this area? Will I find all necessary recourses to accomplish the search? Will I be able to find all information in this field area? If the answer of these types of questions will be "Yes" then you can choose that topic. In most of the cases, you may have to conduct the surveys and have to visit several places because this field is related to Computer Science and Information Technology. Also, you may have to do a lot of work to find all rise and falls regarding the various data of that subject. Sometimes, detailed information plays a vital role, instead of short information.

2. Evaluators are human: First thing to remember that evaluators are also human being. They are not only meant for rejecting a paper. They are here to evaluate your paper. So, present your Best.

3. Think Like Evaluators: If you are in a confusion or getting demotivated that your paper will be accepted by evaluators or not, then think and try to evaluate your paper like an Evaluator. Try to understand that what an evaluator wants in your research paper and automatically you will have your answer.

4. Make blueprints of paper: The outline is the plan or framework that will help you to arrange your thoughts. It will make your paper logical. But remember that all points of your outline must be related to the topic you have chosen.

5. Ask your Guides: If you are having any difficulty in your research, then do not hesitate to share your difficulty to your guide (if you have any). They will surely help you out and resolve your doubts. If you can't clarify what exactly you require for your work then ask the supervisor to help you with the alternative. He might also provide you the list of essential readings.

6. Use of computer is recommended: As you are doing research in the field of Computer Science, then this point is quite obvious.

7. Use right software: Always use good quality software packages. If you are not capable to judge good software then you can lose quality of your paper unknowingly. There are various software programs available to help you, which you can get through Internet.

8. Use the Internet for help: An excellent start for your paper can be by using the Google. It is an excellent search engine, where you can have your doubts resolved. You may also read some answers for the frequent question how to write my research paper or find model research paper. From the internet library you can download books. If you have all required books make important reading selecting and analyzing the specified information. Then put together research paper sketch out.

9. Use and get big pictures: Always use encyclopedias, Wikipedia to get pictures so that you can go into the depth.

10. Bookmarks are useful: When you read any book or magazine, you generally use bookmarks, right! It is a good habit, which helps to not to lose your continuity. You should always use bookmarks while searching on Internet also, which will make your search easier.

11. Revise what you wrote: When you write anything, always read it, summarize it and then finalize it.

12. Make all efforts: Make all efforts to mention what you are going to write in your paper. That means always have a good start. Try to mention everything in introduction, that what is the need of a particular research paper. Polish your work by good skill of writing and always give an evaluator, what he wants.

13. Have backups: When you are going to do any important thing like making research paper, you should always have backup copies of it either in your computer or in paper. This will help you to not to lose any of your important.

14. Produce good diagrams of your own: Always try to include good charts or diagrams in your paper to improve quality. Using several and unnecessary diagrams will degrade the quality of your paper by creating "hotchpotch." So always, try to make and include those diagrams, which are made by your own to improve readability and understandability of your paper.

15. Use of direct quotes: When you do research relevant to literature, history or current affairs then use of quotes become essential but if study is relevant to science then use of quotes is not preferable.

16. Use proper verb tense: Use proper verb tenses in your paper. Use past tense, to present those events that happened. Use present tense to indicate events that are going on. Use future tense to indicate future happening events. Use of improper and wrong tenses will confuse the evaluator. Avoid the sentences that are incomplete.

17. Never use online paper: If you are getting any paper on Internet, then never use it as your research paper because it might be possible that evaluator has already seen it or maybe it is outdated version.

18. Pick a good study spot: To do your research studies always try to pick a spot, which is quiet. Every spot is not for studies. Spot that suits you choose it and proceed further.

19. Know what you know: Always try to know, what you know by making objectives. Else, you will be confused and cannot achieve your target.

20. Use good quality grammar: Always use a good quality grammar and use words that will throw positive impact on evaluator. Use of good quality grammar does not mean to use tough words, that for each word the evaluator has to go through dictionary. Do not start sentence with a conjunction. Do not fragment sentences. Eliminate one-word sentences. Ignore passive voice. Do not ever use a big word when a diminutive one would suffice. Verbs have to be in agreement with their subjects. Prepositions are not expressions to finish sentences with. It is incorrect to ever divide an infinitive. Avoid clichés like the disease. Also, always shun irritating alliteration. Use language that is simple and straight forward. put together a neat summary.

21. Arrangement of information: Each section of the main body should start with an opening sentence and there should be a changeover at the end of the section. Give only valid and powerful arguments to your topic. You may also maintain your arguments with records.

22. Never start in last minute: Always start at right time and give enough time to research work. Leaving everything to the last minute will degrade your paper and spoil your work.

23. Multitasking in research is not good: Doing several things at the same time proves bad habit in case of research activity. Research is an area, where everything has a particular time slot. Divide your research work in parts and do particular part in particular time slot.

24. Never copy others' work: Never copy others' work and give it your name because if evaluator has seen it anywhere you will be in trouble.

25. Take proper rest and food: No matter how many hours you spend for your research activity, if you are not taking care of your health then all your efforts will be in vain. For a quality research, study is must, and this can be done by taking proper rest and food.

26. Go for seminars: Attend seminars if the topic is relevant to your research area. Utilize all your resources.

27. Refresh your mind after intervals: Try to give rest to your mind by listening to soft music or by sleeping in intervals. This will also improve your memory.

28. Make colleagues: Always try to make colleagues. No matter how sharper or intelligent you are, if you make colleagues you can have several ideas, which will be helpful for your research.

29. Think technically: Always think technically. If anything happens, then search its reasons, its benefits, and demerits.

30. Think and then print: When you will go to print your paper, notice that tables are not be split, headings are not detached from their descriptions, and page sequence is maintained.

31. Adding unnecessary information: Do not add unnecessary information, like, I have used MS Excel to draw graph. Do not add irrelevant and inappropriate material. These all will create superfluous. Foreign terminology and phrases are not apropos. One should NEVER take a broad view. Analogy in script is like feathers on a snake. Not at all use a large word when a very small one would be sufficient. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Amplification is a billion times of inferior quality than sarcasm.

32. Never oversimplify everything: To add material in your research paper, never go for oversimplification. This will definitely irritate the evaluator. Be more or less specific. Also too, by no means, ever use rhythmic redundancies. Contractions aren't essential and shouldn't be there used. Comparisons are as terrible as clichés. Give up ampersands and abbreviations, and so on. Remove commas, that are, not necessary. Parenthetical words however should be together with this in commas. Understatement is all the time the complete best way to put onward earth-shaking thoughts. Give a detailed literary review.

33. Report concluded results: Use concluded results. From raw data, filter the results and then conclude your studies based on measurements and observations taken. Significant figures and appropriate number of decimal places should be used. Parenthetical remarks are prohibitive. Proofread carefully at final stage. In the end give outline to your arguments. Spot out perspectives of further study of this subject. Justify your conclusion by at the bottom of them with sufficient justifications and examples.

34. After conclusion: Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium though which your research is going to be in print to the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects in your research.

Informal Guidelines of Research Paper Writing

Key points to remember:

- Submit all work in its final form.
- Write your paper in the form, which is presented in the guidelines using the template.
- Please note the criterion for grading the final paper by peer-reviewers.

Final Points:

A purpose of organizing a research paper is to let people to interpret your effort selectively. The journal requires the following sections, submitted in the order listed, each section to start on a new page.

The introduction will be compiled from reference matter and will reflect the design processes or outline of basis that direct you to make study. As you will carry out the process of study, the method and process section will be constructed as like that. The result segment will show related statistics in nearly sequential order and will direct the reviewers next to the similar intellectual paths throughout the data that you took to carry out your study. The discussion section will provide understanding of the data and projections as to the implication of the results. The use of good quality references all through the paper will give the effort trustworthiness by representing an alertness of prior workings.

Writing a research paper is not an easy job no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record keeping are the only means to make straightforward the progression.

General style:

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

To make a paper clear

· Adhere to recommended page limits

Mistakes to evade

- Insertion a title at the foot of a page with the subsequent text on the next page
- Separating a table/chart or figure - impound each figure/table to a single page
- Submitting a manuscript with pages out of sequence

In every sections of your document

· Use standard writing style including articles ("a", "the," etc.)

· Keep on paying attention on the research topic of the paper

· Use paragraphs to split each significant point (excluding for the abstract)

· Align the primary line of each section

· Present your points in sound order

· Use present tense to report well accepted

· Use past tense to describe specific results

· Shun familiar wording, don't address the reviewer directly, and don't use slang, slang language, or superlatives

· Shun use of extra pictures - include only those figures essential to presenting results

Title Page:

Choose a revealing title. It should be short. It should not have non-standard acronyms or abbreviations. It should not exceed two printed lines. It should include the name(s) and address (es) of all authors.

Abstract:

The summary should be two hundred words or less. It should briefly and clearly explain the key findings reported in the manuscript--must have precise statistics. It should not have abnormal acronyms or abbreviations. It should be logical in itself. Shun citing references at this point.

An abstract is a brief distinct paragraph summary of finished work or work in development. In a minute or less a reviewer can be taught the foundation behind the study, common approach to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Yet, use comprehensive sentences and do not let go readability for briefness. You can maintain it succinct by phrasing sentences so that they provide more than lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study, with the subsequent elements in any summary. Try to maintain the initial two items to no more than one ruling each.

- Reason of the study - theory, overall issue, purpose
- Fundamental goal
- To the point depiction of the research
- Consequences, including definite statistics - if the consequences are quantitative in nature, account quantitative data; results of any numerical analysis should be reported
- Significant conclusions or questions that track from the research(es)

Approach:

- Single section, and succinct
- As a outline of job done, it is always written in past tense
- A conceptual should situate on its own, and not submit to any other part of the paper such as a form or table
- Center on shortening results - bound background information to a verdict or two, if completely necessary
- What you account in an conceptual must be regular with what you reported in the manuscript
- Exact spelling, clearness of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else

Introduction:

The **Introduction** should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable to comprehend and calculate the purpose of your study without having to submit to other works. The basis for the study should be offered. Give most important references but shun difficult to make a comprehensive appraisal of the topic. In the introduction, describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will have no attention in your result. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here. Following approach can create a valuable beginning:

- Explain the value (significance) of the study
- Shield the model - why did you employ this particular system or method? What is its compensation? You strength remark on its appropriateness from a abstract point of vision as well as point out sensible reasons for using it.
- Present a justification. Status your particular theory (es) or aim(s), and describe the logic that led you to choose them.
- Very for a short time explain the tentative propose and how it skilled the declared objectives.

Approach:

- Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done.
- Sort out your thoughts; manufacture one key point with every section. If you make the four points listed above, you will need a least of four paragraphs.

- Present surroundings information only as desirable in order hold up a situation. The reviewer does not desire to read the whole thing you know about a topic.
- Shape the theory/purpose specifically - do not take a broad view.
- As always, give awareness to spelling, simplicity and correctness of sentences and phrases.

Procedures (Methods and Materials):

This part is supposed to be the easiest to carve if you have good skills. A sound written Procedures segment allows a capable scientist to replacement your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt for the least amount of information that would permit another capable scientist to spare your outcome but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section. When a technique is used that has been well described in another object, mention the specific item describing a way but draw the basic principle while stating the situation. The purpose is to text all particular resources and broad procedures, so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step by step report of the whole thing you did, nor is a methods section a set of orders.

Materials:

- Explain materials individually only if the study is so complex that it saves liberty this way.
- Embrace particular materials, and any tools or provisions that are not frequently found in laboratories.
- Do not take in frequently found.
- If use of a definite type of tools.
- Materials may be reported in a part section or else they may be recognized along with your measures.

Methods:

- Report the method (not particulars of each process that engaged the same methodology)
- Describe the method entirely
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures
- Simplify - details how procedures were completed not how they were exclusively performed on a particular day.
- If well known procedures were used, account the procedure by name, possibly with reference, and that's all.

Approach:

- It is embarrassed or not possible to use vigorous voice when documenting methods with no using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result when script up the methods most authors use third person passive voice.
- Use standard style in this and in every other part of the paper - avoid familiar lists, and use full sentences.

What to keep away from

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings - save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part a entirely objective details of the outcome, and save all understanding for the discussion.

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.
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- 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

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- 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
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- All figure and table must be adequately complete that it could situate on its own, divide from text

Discussion:

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- 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:

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- 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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References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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