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Effects of Chemical Exposure with Aerosol Particles through the Human Airways

Nirmala P. Ratchagar[1], **M. Chitra**[2]

[1]Professor, Department of Mathematics, Annamalai University,Chidambaram, Tamil Nadu, India

[2]Associate Professor, Department of Mathematics, Thiruvalluvar University, Vellore - 632 115, Tamil Nadu, India

Abstract: ***Inhalation is an important route of exposure to toxic chemicals especially in the work place. Chemicals absorbed by inhalation have specific properties which are gases such as carbon dioxide, vapour and aerosols. (i.e.) Small particles suspended in air.In this paper the effects of toxic chemicals is due to the inhalation of aerosol particles through the human respiratory tract have been studied Mathematical model is developed for steady laminar flow through the respiratory tract and solved analytically in the presence of first order chemical reaction with particals. The flow is assumed to be symmetrical flow of an Newtonian fluid flowing under constant pressure gradient .The effects of velocity profile, wall shear stress, flow rate, and both homogeneous and heterogeneous chemicals reactions on concentration of air are studied for different Reynolds number, slip parameter, and viscosity off air during light and heavy breathing under isothermal condition by using tylor's dispersion model. The solution is numerically computed and the results are depicted graphically***

Keywords: Chemical Reaction, Newtonian fluid, Homogeneous, Heterogeneous, Slip parmeter.

1. Introduction

Among the variety of factors influencing health of an individual, natural elements (the air we breathe, the water we drink, the radiation we are exposed to, etc) and man made environmental modifications (habitat, place of work, transport, industry and other development activities) play a crucial role. Chemical agents that are released into the environment from various anthropogenic activities have impact on human health seriously. The respiratory system is one major route whereby these chemicals and toxic agents enter the body and cause disorders, including mortality. On a global scale, millions suffer from respiratory ailments and other diseases attributed to the presence of toxic chemicals and biological agents in the air (see Fenger 1999). Although concentration of any pollutant in the environment is a quantitative expression of the presence of the pollutant, there is no exposure unless there is physical contact with human beings. Exposure denotes the event when a person comes into contact with a pollutant for a particular time. Airborne particulate matter (PM) is the recent focus of the world community as it penetrates the respiratory system of human beings and causes many disorders. It has also been shown through world wide studies that the urban population is at risk due to elevated levels of PM in the urban atmosphere. Several time series and Cohort studies (see Fenger 1999) have shown that children, elderly and asthmatic people are at higher risk due to air pollution.

A great deal of attention in recent years has been focused on the effects of chemical exposure on the workers health. Many chemicals, which were once regarded as safe, have been found to be associated with diseases ranging from milk skin rashes to chronic health impairment and fatal cancers. There are too many chemicals used in the work place whose harmful effects are still unknown. It is therefore essential to treat all chemicals with care.

The effects of both homogenous and heterogeneous reactions on the dispersion of a solute in a liquid flowing between two parallel plates in the presence of an irreversible first-order chemical reaction have been investigated by Gupta *et al.* (1972), Rudraiah (2001) and Shukla *et al.* (1979).

In this chapter an analytical solution for steady laminar flow through the respiratory tract is obtained in the presence of first order chemical reaction with aerosol particles. Here we consider the symmetrical flow of a Newtonian fluid flowing under the constant pressure gradient. The effects of velocity profile, wall shear stress, flow rate, and both homogeneous and heterogeneous chemical reactions on concentration of air are studied for different Reynolds number, slip parameter, and viscosity of air during light and heavy breathing, under isothermal condition by using Taylor's dispersion model. The solution is numerically computed and the results are depicted graphically, and some important conclusions are drawn in the final section.

2. Mathematical Formulation

We consider following Taylor (1953) quasi-steady laminar flow through airways to understand the hydrodynamic dispersion with chemicals. The airways which is idealized by symmetrical cylindrical vertical tube is shown in Figure 1. We assume that the density ρ, acceleration due to gravity g^*, viscosity μ and slip parameter β^*, are all constants Following Taylor (1953) we assume (i) fully developed unidirectional flow driven by a constant pressure gradient in the axial direction. (ii) the velocity u^* in the axial direction is a function of r only. The momentum equation governing the axial flow of air is given by

$$0 = \frac{-dp^*}{dz^*} - \rho g^* + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(\mu r \frac{\partial u^*}{\partial r}\right)\right] \tag{1}$$

We assume that the suspended particle diffuse and simultaneously undergo a first order chemical reaction in the airways under isothermal conditions. The equation for the concentration C^* of air satisfies the equation.

$$\frac{\partial C^*}{\partial t^*}+u^*\frac{\partial C^*}{\partial z^*} = D^*\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C^*}{\partial t}\right)\right]+K_cC^* \qquad (2)$$

where D^* is the molecular diffusion coefficient (assumed constant) and K_c is the first-order reaction rate constant. In deriving, it is assumed that the suspended particles are present in a small concentration, the chemical reaction is first order and it occurs under such conditions that air film resistance is negligible. This means that the concentration profile is expected to vary slowly and uniformly and the reaction term K_cC^*/mole $cm^{-1}s^{-1}$ which represents the volume rate due to chemical reaction. To solve the above system of equations (1) and (2), we use the following boundary conditions.

The symmetry condition

$$\frac{\partial u^*}{\partial r} = 0 \text{ at } r = 0 \qquad (3)$$

the slip condition

$$-\beta^*\frac{\partial u^*}{\partial r} = u^* \text{ at } r = R_0 \qquad (4)$$

$$p^* = p_i \text{ at } z^* = 0 \qquad (5)$$

$$p^* = p_0 \text{ at } z^* = L \qquad (6)$$

Case (i) *In homogenous reaction*

The symmetry condition

$$\frac{\partial C^*}{\partial r} = 0 \text{ at } r = 0 \qquad (7)$$

$$\frac{\partial C^*}{\partial r} = 0 \text{ at } r = R_0 \qquad (8)$$

Case (ii) *In heterogeneous reaction*

The symmetry condition

$$\frac{\partial C^*}{\partial r} = 0 \text{ at } r = 0 \qquad (9)$$

$$\frac{\partial C^*}{\partial r} + f^* C^* = 0 \text{ at } r = R_0 \qquad (10)$$

We make the above equations dimensionless using the following quantities,

$$p = \frac{p^*}{\rho v_0^2},\ u = \frac{u^*}{v_0},\ z = \frac{z^*}{L}\ \tau = \frac{t^*}{\overline{t^*}}$$

$$g = \frac{g^*}{v_0^2/L},\ \bar{u} = \frac{u^*}{v_0},\ \beta = \frac{\beta^*}{R_0},\ \eta = \frac{r}{R_0}$$

$$\text{where } \overline{t^*} = \frac{L}{\bar{u}^*}$$

$$f = \frac{f^*}{R_0},\ D = \frac{D^*}{v_0R_0},\ C = \frac{C^*}{C_0},$$

$$\xi = \frac{z^*-\bar{u}^*t^*}{L},\ R_e = \frac{\rho v_0R_0}{\mu}$$

and obtain

$$\frac{1}{\eta}\left[\frac{\partial}{\partial\eta}\left(\eta\frac{\partial u}{\partial\eta}\right)\right] = \frac{\operatorname{Re}R_0}{L}\left[\frac{dp}{dz}+g\right] \qquad (11)$$

$$\frac{R_0}{DL}(u-\bar{u})\frac{\partial C}{\partial\xi} = \frac{\partial^2C}{\partial\eta^2}+\frac{1}{\eta}\frac{\partial C}{\partial\eta}+\alpha^2C \qquad (12)$$

Where $\alpha^2 = \dfrac{K_CR_0}{v_0DL}$

The boundary conditions are

$$\frac{\partial u}{\partial\eta} = 0 \text{ at } \eta = 0 \qquad (13)$$

$$-\beta\frac{\partial u}{\partial\eta} = u \text{ at } \eta = 1 \qquad (14)$$

$$p = p_i' \text{ at } z = 0 \qquad (15)$$

$$p = p_0' \text{ at } z = L \qquad (16)$$

$$\frac{\partial C}{\partial\eta} = 0 \text{ at } \eta = 0 \qquad (17)$$

$$\frac{\partial C}{\partial\eta} = 0 \text{ at } \eta = 1 \qquad (18)$$

$$\frac{\partial C}{\partial\eta} = 0 \text{ at } \eta = 0 \qquad (19)$$

$$\frac{\partial C}{\partial\eta}+fC = 0 \text{ at } \eta = 1 \qquad (20)$$

where v_0 is the characteristic velocity, '*L*' is the characteristic length; R_0 is the radius of the respiratory tract and $\bar{u}$ is the average velocity. f is the heterogeneous reaction rate parameter corresponding to catalytic reaction at the walls

3. Solutions

The velocity of air in the respiratory tract is obtained by solving equation (11) using boundary conditions (13), (14), (15) and (16) is

$$u = \frac{\operatorname{Re}R_0}{4L}\left(\frac{dp}{dz}+g\right)\left(\eta^2-1-2\beta\right)$$

$$= \frac{\operatorname{Re}R_0}{4L}\left(-\frac{dp}{dz}-g\right)\left(1-\eta^2+2\beta\right) \qquad (21)$$

The average velocity, defined by

$$\bar{u} = \frac{2v_0}{R_0}\int_0^1 u\,d\eta$$

$$= \frac{\operatorname{Re}R_0(1+4\beta)}{8L}\left(-\frac{dp}{dz}-g\right) \qquad (22)$$

If we now consider convection across a vertical tube moving with mean speed of flow, then relative to this the velocity of air is given by

$$u-\bar{u} = \frac{\operatorname{Re}R_0(1-2\eta^2)}{8L}\left(-\frac{dp}{dz}-g\right) \qquad (23)$$

The total flux Q has been obtained by

$$Q = \pi R_0^2 v_0 \bar{u}$$
$$= \frac{\pi R_0^3 v_0 \,\mathrm{Re}\,(1+4\beta)}{8\,L}\left(-\frac{dp}{dz}-g\right) \tag{24}$$

The resistance to flow of air is defined by

$$\lambda = \frac{8L}{\pi R_0^3\, v_0\, \mathrm{Re}\,(1+4\beta)} \tag{25}$$

Wall shearing stress distribution for air is defined by

$$\tau = \left[-\mu\frac{\partial u^*}{\partial r}\right]_{r=1}$$
$$= \left[\frac{-\mu\, v_0}{R_0}\frac{\partial u}{\partial \eta}\right]_{\eta=1}$$
$$= \frac{\mu\, v_0\,\mathrm{Re}}{2L}\left(-\frac{dp}{dz}-g\right)$$
$$= \frac{4\mu Q}{\pi R_0^3(1+4\beta)} \tag{26}$$

For the homogeneous chemical reaction, equation (12) is solved using the Hankel transform and the boundary conditions (17) and (18) and obtain the solution in this form

$$\mathrm{C} = \frac{\mathrm{Re}\, R_0^2}{4DL^2}\frac{\partial C}{\partial \xi}\left(-\frac{dp}{dz}-g\right)\sum_{n=1}^{\infty}\frac{1}{\alpha^2-\lambda_n^2}\left\{\left[\frac{-J_1(\lambda_n)}{\lambda_n}+\frac{8J_1(\lambda_n)}{\lambda_n^3}\right]\right.$$
$$\left. + J_1(\lambda_n)\lambda_n\left[\left(\sum_{n=1}^{\infty}\frac{1}{\alpha^2-\lambda_n^2}\left(1-\frac{8}{\lambda_n^2}\right)\right)\Big/\left(\sum_{n=1}^{\infty}\frac{\lambda_n^2}{\alpha^2-\lambda_n^2}\right)\right]\right\}\frac{J_0(\lambda_n\eta)}{J_1^2(\lambda_n)} \tag{27}$$

For the heterogeneous chemical reaction, the solution of (12), using the boundary conditions (19) and (20), is

$$\mathrm{C} = \frac{\mathrm{Re}\, R_0^2}{4DL^2}\frac{\partial C}{\partial \xi}\left(-\frac{dp}{dz}-g\right)\sum_{n=1}^{\infty}\frac{1}{\alpha^2-\lambda_n^2}\left\{\left[\frac{-J_1(\lambda_n)}{\lambda_n}+\frac{8J_1(\lambda_n)}{\lambda_n^3}\right]\right.$$
$$\left. + J_1(\lambda_n)\lambda_n\left[\left(2\sum_{n=1}^{\infty}\frac{1}{\alpha^2-\lambda_n^2}\left(1-\frac{8}{\lambda_n^2}\right)\right)\Big/\left(R_0^2 f + 2\sum_{n=1}^{\infty}\frac{\lambda_n^2}{\alpha^2-\lambda_n^2}\right)\right]\right\}\frac{J_0(\lambda_n\eta)}{J_1^2(\lambda_n)} \tag{28}$$

4. Conclusions

In this chapter, we have investigated the effects of homogeneous and heterogeneous chemical reaction on dispersion of suspended particles in the laminar flow of a Newtonian fluid in the vertical tube following Taylor's model. The expressions for axial velocity, resistance, wall shear stress and concentration with homogeneous and heterogeneous chemical reactions are numerically computed for different value of parameters and the results are discussed here.

The axial velocity has been computed using equation (21) and the results are depicted in Figure 2 . Figure 2 is concerned with axial velocity for different values of the slip parameter and Reynolds number. From which we conclude that an increase in the slip parameter decreases the velocity for different Reynolds number during heavy and light breathing. Also from this figure we conclude that the axial velocity is less during heavy breathing for Reynolds number 2800 than during light breathing for Reynolds number 1700, (see Gemci 2000).

The resistance to flow and wall shear stress has been computed using equation (25) & (26) and the results are depicted in Figure 3 and Figure 4 respectively. From Figure 3 we conclude that by increasing slip parameter β decreases the resistance for different Reynolds number during heavy and light breathing. Also from Figure 2 we conclude that the resistance is higher during heavy breathing for Reynolds number 2800 than during light breathing for Reynolds number 1700.

From Figure 4 we conclude that by increasing the viscosity of air μ increases the wall shear stress for fixed slip parameter β and increasing slip parameter β decreases the wall shear stress for fixed viscosity of air μ.. The concentration of homogeneous chemical reaction has been computed using equation (27) and the results are depicted in Figure 5. From which we conclude that an increase in chemical reaction coefficient α, decreases the concentration of homogeneous chemical reaction for different Reynolds numbers during heavy and light breathing. Also from this figure we conclude that the concentration of homogeneous chemical reaction is higher during heavy breathing for Reynolds number 2800 than during light breathing for Reynolds number 1700 for a fixed α. The concentration of heterogeneous chemical reaction has been computed using equation 28 and the results are depicted in Figure 6. From which we conclude that an increase in chemical reaction coefficient α decreases the concentration of heterogeneous chemical reaction for fixed heterogeneous reaction rate parameter f and as heterogeneous reaction rate parameter f increases the concentration of heterogeneous chemical reaction decreases for fixed chemical reaction coefficient α for different Reynolds numbers during heavy and light breathing. Also from this we conclude that concentration of heterogeneous chemical reaction is higher during heavy breathing for Reynolds number 2800 than during light breathing for Reynolds number 1700.

From the above results we can conclude that the effects of chemicals can be either acute or chronic, depending on the concentration and duration of the exposure.

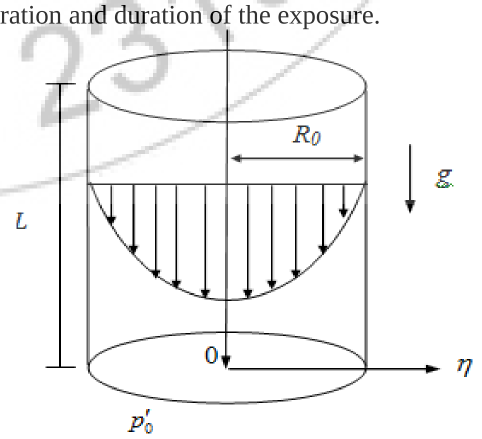

Figure 1: Geometry of respiratory tract

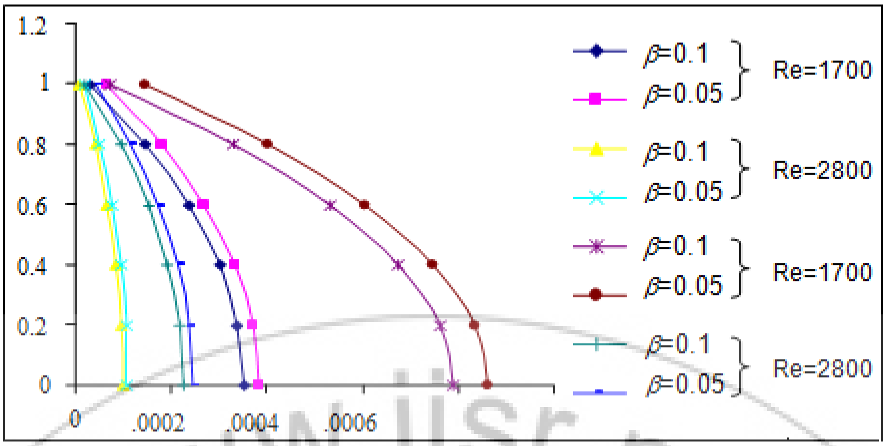

Figure 2: Variation of axial velocity profile ***u*** with radial position ***η*** (light breathing: Re = 1700, heavy breathing: Re=2800)

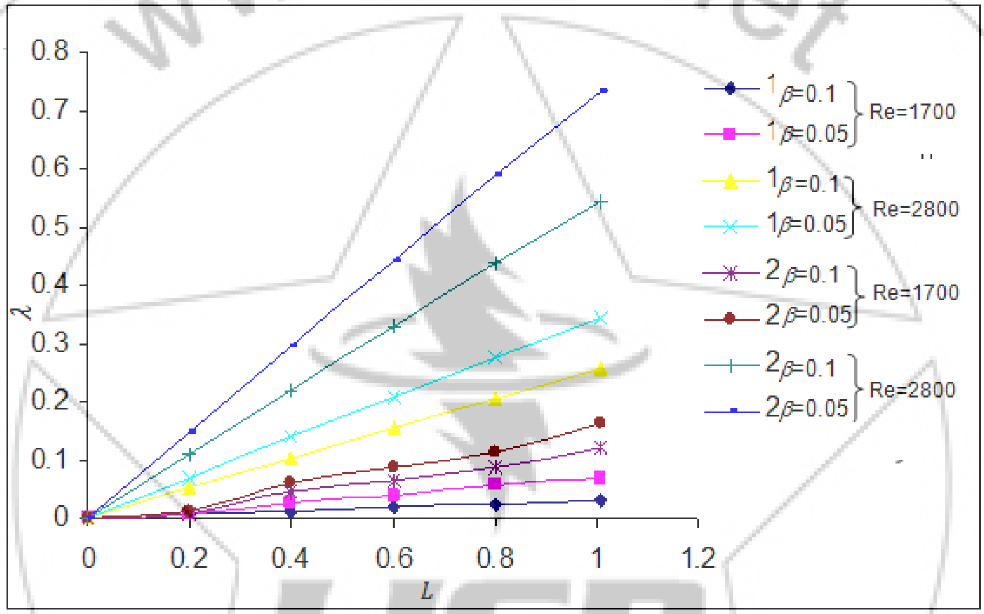

Figure 3: Variation of resistance *λ* with ***L*** (light breathing: Re = 1700, heavy breathing: Re=2800)

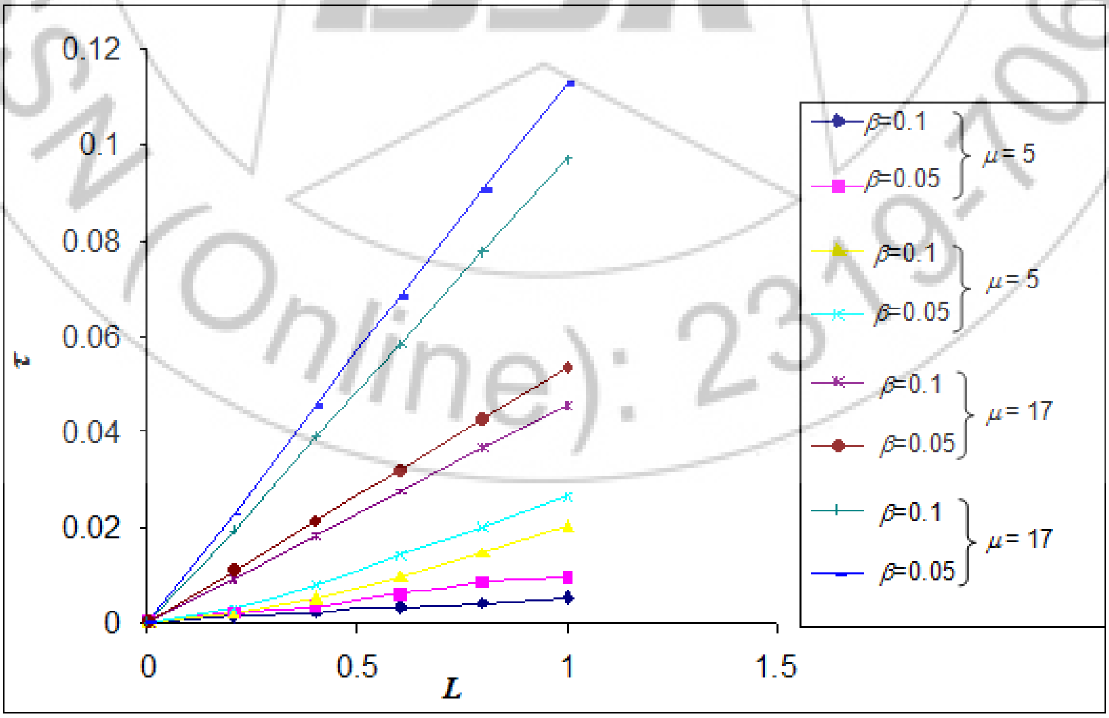

Figure 4: Variation of wall shear stress *τ* with ***L***

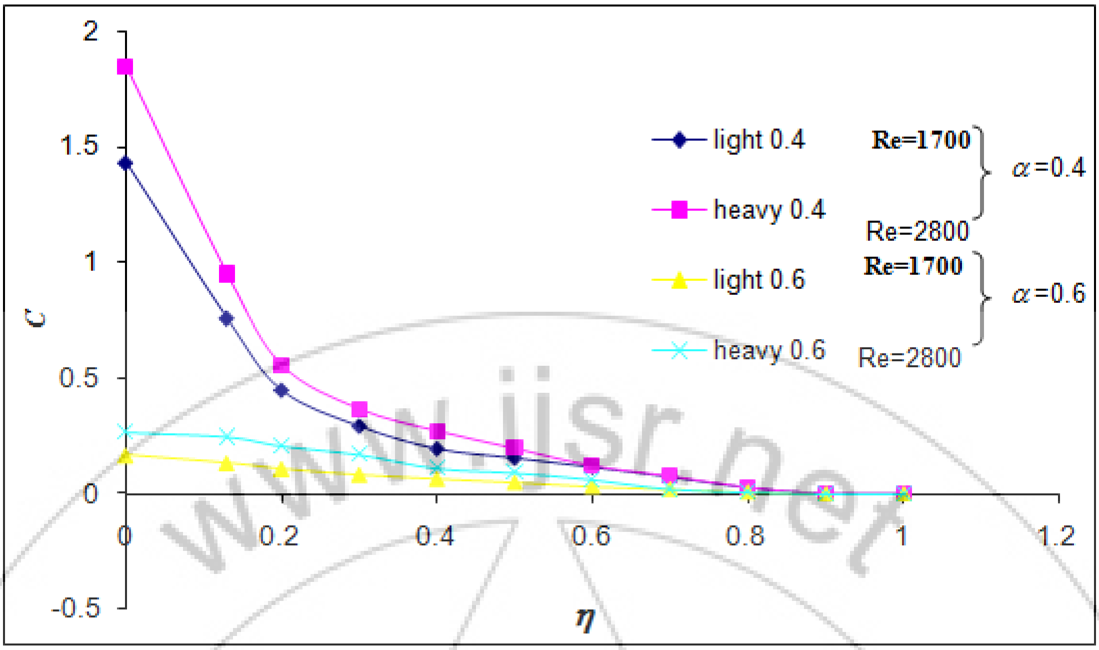

Figure 5: Variation of Concentration ***C*** (homogeneous reaction) with radial position η for different coefficient of chemical reaction are α (light breathing: Re = 1700, heavy breathing: Re=2800)

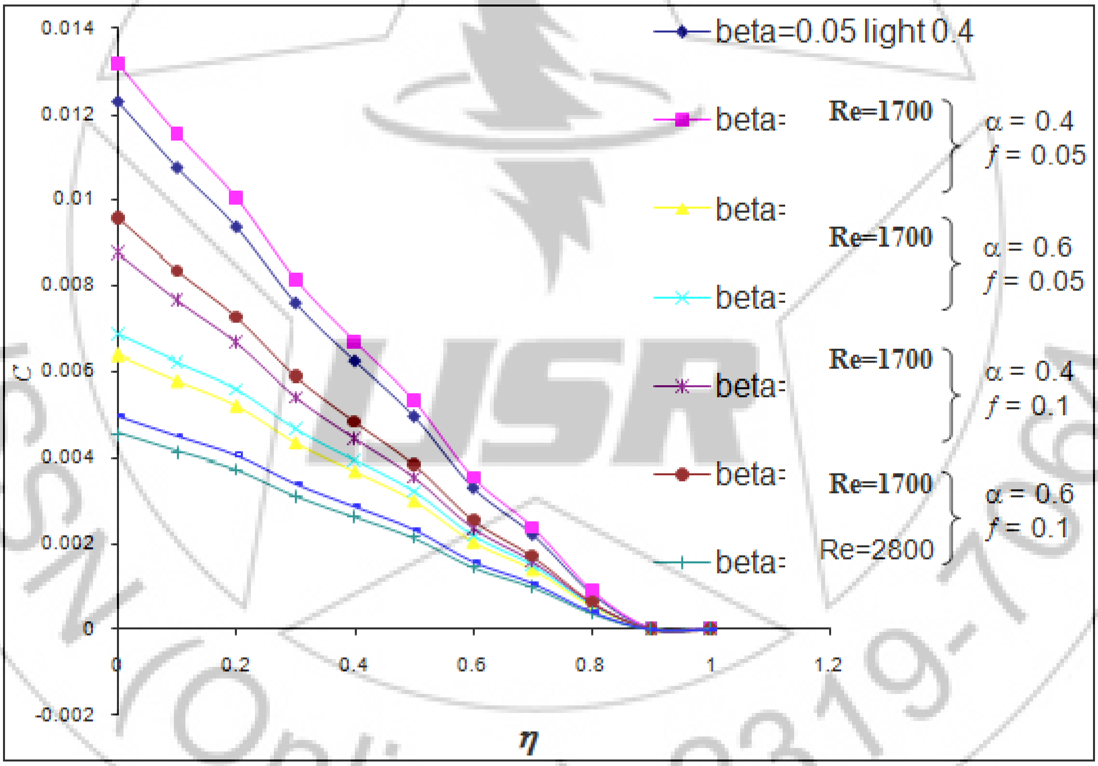

Figure 6: Variation of Concentration C (heterogeneous reaction) with radial position η for different coefficient of chemical reaction rate α and different heterogeneous reaction rate parameter f (light breathing: Re = 1700, heavy breathing: Re=2800)

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