Concentration of charged nano-particles in the human trachea; Effects of Cartilaginous Rings

Mathematics

KEYWORDS: Cartilaginous rings, Brownian diffusion, electrostatic parameter, convective, concentration, nano-particles.

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ABSTRACT

This paper presents an analytical study of the concentration of the charged nano-particles caused by convection, Brownian diffusion and electrostatics that are deposited in a human trachea. The upper airways are characterised by a certain wall structure called cartilaginous rings which modify the particle is compared to an airway with smooth wall and tube with cartilaginous rings with electrostatic parameter(α), and tube radius(r) and low Reynolds numbers(Re). The problem is defined by solving Navier-stokes equations in combination with a convective-diffusion equation and Gauss law for electrostatics. Three non-dimensional parameters describe the problem, the Pecklet number $P_e = 2\bar{U}a/D$, t he Reynolds number $R_e = 2\bar{U}a/\nu$ and an electrostatic parameter $\alpha = R^2 c_0 q^2/(4\varepsilon_0 KT)$. Here u is the mean velocity, R is the pipe radius and D is the diffusion co-efficient due to Brownian motion given by $D = kTCu/3\pi\mu d$, where Cu is the Cunnigham-factor $Cu = 1+\lambda/d(2.34+1.05\exp(-(\frac{0.39d}{\lambda}))$ Here we study the concentration of charged nano- particles of cartilaginous rings of wall structure, and airway with smooth wall for varying electrostatic parameters (α) and low Reynolds numbers in the trachea of deposition of charged particles in human airways.

INTRODUCTION

The airborne behaviour of inhaled particles would be anticipated to reflect the velocity distributions of air steams in which they are entrained and transported within the lung. However no systematic laboratory tests have been conducted to quantitate the effects of localized morphological features of the lung, such as cartilaginous rings of the wall structure, upon charged nano particles in the human trachea.

The analysis of particle deposition in the respiratory airways for the assessment of health effects of inhaled toxic matter and for the evaluation of the efficacy of drug delivery of pharmaceutical aerosols. The development of new superior materials containing nano-particles, such as carbon nano-tubes, is accelerating, and the area is a very important branch of material science nowadays. These tiny particles are, however, potentially toxic and pose a substantial health risk[1]. Carbon nano-tubes are about 10-100 nm in diameter with lengths of around 1-50 μm. Although the carbon nano-tubes are usually smaller than asbestos fibres, there are concerns that they may cause similar adverse health effects upon inhalation.

The cartilaginous rings present on the inner wall using data from standard medical textbooks (Putz and Pabst 2000; Kopf-Maier 2000) and dimensions proposed by Martonen et al. (1994), cartilaginous ring configurations are included as follows: the cross sectional shape of an individual cartilaginous ring is represented by a semicircle, the diameter of which is specified as 0.1 D_o Whear D_o is the diameter of the airways (16mm). Fourteen rings are spaced evenly along the inner wall of the trachea, which is similar to that seen in typical human anatomy textbooks (Putz and Pabst 2000; Kopf-Maier 2000). The dimensions proposed by Weibel (1963) are adopted for the bronchial tree.We also include a wall structure called cartilaginous rings, located in the upper airways of the human respiratory tract. The shapes of individual rings were semicircular. The spatial distributions along airway walls were either contiguous or regularly spaced. Smooth-walled tubes were considered as control cases. Here we study the concentration of charged nano particles of cartilaginous rings of wall structure, and airway with smooth wall for varying electrostatic parameter and low Reynolds number in the trachea of human airways.

MATHEMATICAL FORMULATION

Each generation of human airways is supposed to be described by a tube with a smooth surface or a tube with a cartilaginous ring structure. For the first generation of human airways is trachea we consider an axially symmetric concentration of charged nano-particles air with smooth wall and charged nano particle with cartilaginous rings with wall structure in human trachea. The governing set of equations with boundary conditions as follows,

$$(u.\nabla)u = -\nabla p + \frac{1}{R_e}\nabla^2 u \qquad (1)$$

$$\nabla.u = 0 \qquad (2)$$

$$(u.\nabla)c - \frac{1}{pe}\nabla\varphi.\nabla c + 4\alpha\frac{c^2}{pe} = \frac{1}{pe}\nabla^2 c \qquad (3)$$

$$\nabla^2\varphi = -4\alpha c \qquad (4)$$

Eq. (3) is an equation describing the evolution of the concentration c, which is an equation of convective diffusion type with an extra source-term including the effects from the electric field. Eq. (1) and (2) are the Navier-Stokes equations describing the evolution of the laminar fluid flow and Eq.(4) is Poisson's equation which gives the link between the charged particle and the electric field. The set of Eqs(1)-(4) needs to be solved analytically

The boundary conditions for the fluid flow are no slip on the tube r=R. At the inlet z=0 a uniform velocity is chosen and at z=L outlet conditions are applied. For the application of the diffusion-convection mode, the concentration at the inlet is uniform c =c0 .The boundary condition of the absorbing wall is c=0 and at the outlet convective flux is chosen. For the electrostatics mode, zero chare/symmetry is chosen at the inlet and outlet, Since the wall at r=R of the respiratory airways consists of a so called mucus-layer including mainly saline water, the wall is treated as a good conductor and therefore the electric potential is taken as zero.

Boundary conditions

(i) $u = 0$, $r = R$, No slip on the wall

(ii) $\frac{\partial u}{\partial r} = 0$ at $r = 0$

(iii) $c = c_0$ at $r = R$

(iii) $\frac{\partial c}{\partial r} = 0$ at $r = 0$

(iv) $c = 0$, $z = 0$,

(v) $\frac{\partial c}{\partial z} = 0$ at $z = L$

Using dimensionless quantities,

$$\eta = \frac{r}{R}; Z^* = \frac{Z}{L};$$

$$P_e = 2\overline{U}a/D, \quad R_e = 2\overline{U}a/v,$$

$$\propto = a^2 C_0 q^2/(4\varepsilon_0 KT).$$

$$D = KTCu/3\pi\mu d,$$

$$Cu = 1 + \lambda/d(2.34 + 1.05\exp(-\frac{0.39d}{\lambda}))$$

Boundary conditions

(i) $u = 0, \eta = 1,$

(ii) $\frac{\partial u}{\partial \eta} = 0, at\ \eta = 0$

(iii) $\frac{\partial \psi}{\partial \eta} = 0, at\ \eta = 0$

(iv) c=0, at z=0

(v) $\frac{\partial c}{\partial z} = 0$ at z = 1

Using dimensionless

$$(2) => \frac{1}{\eta}\frac{\partial}{\partial \eta}\left(\eta \frac{\partial u}{\partial \eta}\right) = R_e R\left(\frac{\partial p}{\partial z}\right)$$

Solving the equation and using boundary conditions(ii) &(i) we get

$$u = \frac{RR_e}{4}[\eta^2 - 1]\frac{\partial p}{\partial z} \quad (5)$$

$$(3) => (u.\nabla)c - \frac{1}{pe}\nabla\varphi.\nabla c + 4\alpha\frac{c^2}{pe} = \frac{1}{pe}\nabla^2 c$$

$$u\frac{\partial c}{\partial z} - \frac{1}{pe}\frac{\partial \varphi}{\partial r}\frac{\partial c}{\partial z} + \frac{4\alpha}{pe}c^2 = \frac{1}{pe}\left(\frac{1}{r}\frac{\partial c}{\partial r}\left(r\frac{\partial c}{\partial r}\right)\right)$$

Using (5) we get

$$(\eta^2 - 1)\left(\frac{c_0 R_e pe R^3}{4}\right)\left(\frac{\partial p}{\partial z}\right)\left(\frac{\partial c}{\partial z}\right) - \left(\frac{q c_0{}^2 R^3}{\varepsilon_0}\right)\left(\frac{\partial \psi}{\partial \eta}\right)K1 + (4\alpha c_0^2 R^2)c^2 = \left[\frac{1}{\eta}\frac{\partial}{\partial \eta}\left(\eta\frac{\partial c}{\partial \eta}\right)\right] \quad (6)$$

$$(4) => \nabla^2\varphi = -4\alpha c$$

$$\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial \varphi}{\partial r}) = -4\alpha c$$

$$\frac{1}{\eta}\frac{\partial}{\partial \eta}\left(\eta\frac{\partial \psi}{\partial \eta}\right) = -Q_4 c$$

Solving the equation and using the boundary condition (iv) we get

$$\frac{\partial \psi}{\partial \eta} = \frac{-Q_4 c\eta}{2} \quad (7)$$

$$where\ Q_4 = \frac{qa^2}{kT}$$

$$(6) => (\eta^2 - 1)Q_1\left(\frac{\partial p}{\partial z}\right)\left(\frac{\partial c}{\partial z}\right) - Q_2\left(\frac{\partial c}{\partial \eta}\right)K_1 + Q_3 c^2 = \left[\frac{1}{\eta}\frac{\partial}{\partial \eta}\left(\eta\frac{\partial c}{\partial \eta}\right)\right]$$

We solve these equations using Hankel transform of the form

$\bar{C} = \int_0^1 cJ_0(\varepsilon_n \eta)\, d\eta$ Where the Kernel $J_0(\varepsilon_n \eta)$ is the Bessel function of order zero.

Applying Hankel Transform,on equation (6)

$$Q_1\left(\frac{\partial p}{\partial z}\right)\int_0^1 \frac{\partial c}{\partial z}(\eta^2 - 1)\eta J_0(p\eta)d\eta - Q_2 k_1\left(\frac{\partial \psi}{\partial \eta}\right)\int_0^1 \eta J_0(p\eta)d\eta + Q_3\int_0^1 c^2\eta J_0(p\eta)d\eta = \int_0^1 \frac{\partial^2 c}{\partial \eta^2}\eta J_0(p\eta)d\eta + \int_0^1 \frac{1}{\eta}\frac{\partial c}{\partial \eta}\eta J_0(p\eta)d\eta$$

$$-\frac{4}{p^3}Q_1 J_1(p)\left(\frac{\partial p}{\partial z}\right)\frac{\partial c}{\partial z} + Q_2 k_1 Q_4 c\left[\frac{1}{p} - \frac{4}{p^3}J_1(p)\right] + Q_3 c^2\frac{J_1(p)}{p} = -p^2\tilde{c}$$

On simplifying we get

$$Q_5\left(\frac{\partial p}{\partial z}\right)\left(\frac{\partial c}{\partial z}\right) + Q_6 = -p^2\tilde{c} \quad (8)$$

Where

$$Q_1 = \frac{R^3 c_0 R_e pe}{4};\ Q_2 = \frac{q c_0^2 R^3}{\varepsilon_0}$$

$$Q_3 = 4\alpha c_0^2 R^2;\ \ Q_4 = \frac{qa^2}{kT}$$

$$Q_5 = -\frac{4}{p^3}Q_1 J_1(p);$$

$$Q_6 = Q_2 k_1 Q_4 c\left[\frac{1}{p} - \frac{4}{p^3}J_1(p)\right] + Q_3 c^2\frac{J_1(p)}{p}$$

Solving the equation (8)we get

$$\tilde{c} = -\frac{1}{p^2}\left[Q_5\left(\frac{\partial p}{\partial z}\right)\left(\frac{\partial c}{\partial z}\right) + Q_6\right] \quad (9)$$

Applying Inverse Hankel Transform, we get

$$c = 2\left\{\sum_{p=1}^{\infty} -\frac{1}{p^2}\left[Q_5\left(\frac{\partial p}{\partial z}\right)\left(\frac{\partial c}{\partial z}\right) + Q_6\right]\frac{J_0(p\eta)}{(J_1(p))^2}\right\}$$

$$c = B_1\sum_{p=1}^{\infty} -\frac{J_0(p\eta)}{p^3 J_1(p)} - B_2\sum_{p=1}^{\infty}\left[\frac{1}{p} - \frac{4}{p^3}J_1(p)\right]\frac{J_0(p\eta)}{p^2(J_1(p))^2} + B_3\sum_{p=1}^{\infty}\left(\frac{\partial c}{\partial z}\right)\frac{J_0(p\eta)}{p^5 J_1(p)} \quad (10)$$

Where $B_1 = 8\alpha R^2 c_0^2$

$$B_2 = \left(\frac{2R^3 c_0^2 q^2 a^2}{\varepsilon_0 kT}\right)c\left(\frac{\partial c}{\partial \eta}\right)$$

$$B_3 = (2R^3 c_0 R_e pe)\frac{\partial p}{\partial z}$$

$$\therefore C = E + F\frac{\partial c}{\partial z} \quad (11)$$

Solving the equation (11) and using the boundary condition (v) we get

$$C = E\left(1 - e^{\frac{1}{F}z}\right) \quad (12)$$

where

$$E = B_1\sum_{p=1}^{\infty} -\frac{J_0(p\eta)}{p^3 J_1(p)} - B_2\sum_{p=1}^{\infty}\left[\frac{1}{p} - \frac{4}{p^3}J_1(p)\right]\frac{J_0(p\eta)}{p^2(J_1(p))^2}$$

$$F = B_3\sum_{p=1}^{\infty}\frac{J_0(p\eta)}{p^5 J_1(p)}$$

C represents the concentration of smooth wall structure of trachea.

Concentration of cartilaginous rings of wall structure trachea is derived by equation (10) using the boundary condition(v) we get

$$C' = B_1 \sum_{p=1}^{5} -\frac{J_0(p\eta)}{p^3 J_1(p)} + B_3 \sum_{p=1}^{5} \left(\frac{\partial c}{\partial z}\right) \frac{J_0(p\eta)}{p^5 J_1(p)}$$

$$\therefore \quad C' = G + F\frac{\partial c}{\partial z} \qquad (12)$$

Solving the equation (11) and using the boundary condition (v) we get

$$C' = G\left(1 - e^{\frac{1}{p^2}z}\right) \qquad (13)$$

Equation (13) represents the Concentration of cartilaginous rings of wall structure in human trachea

where

$$G = B_1 \sum_{p=1}^{\infty} -\frac{J_0(p\eta)}{p^3 J_1(p)}$$

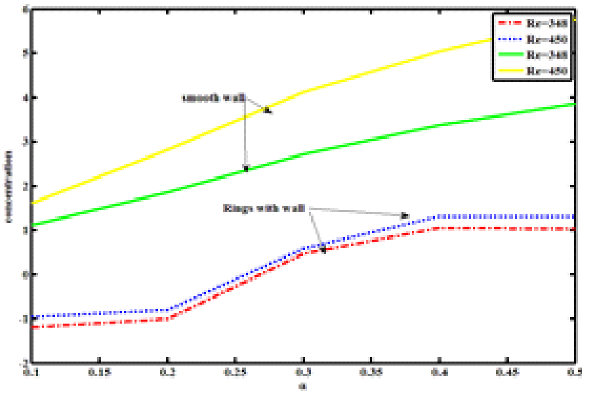

Figure 1: Variation of concentration with electrostatic parameter α for different values of Low Reynolds number(with smooth wall and cartilaginous rings with wall structure) Re=348,Re=450

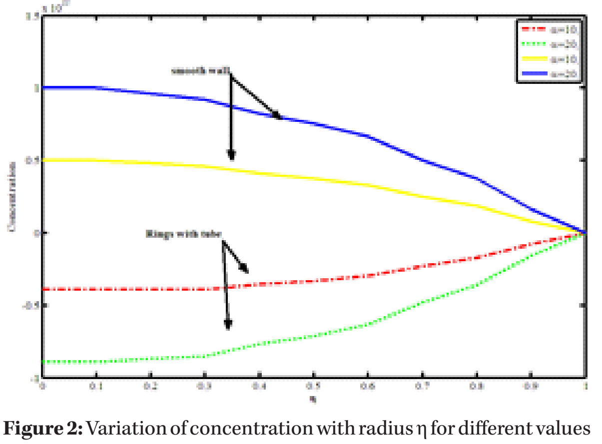

Figure 2: Variation of concentration with radius η for different values electrostatic parameter α (with smooth wall and cartilaginous ring with wall structure)

RESULTS AND CONCLUSIONS:

The concentration of charged nano- particles that are deposited on the walls of cylindrical tube with periodically spaced cartilaginous rings with wall structure and smooth wall pipe in human trachea are investigated. The model includes convective and Brownian diffusion transport as well as effects from the electric field created by charged particles. The effects of the cartilaginous rings of wall structure is introduced with amplitude of the rings equal to 0.1 diameters.

In Figure 1 The comparison of concentration of charged nano-particles of smooth wall pipe and cartilaginous rings with wall structure is graphically varying with the electrostatic parameter(α) for different values of low Reynolds numbers(Re).The result shows that the concentration increases with increasing low Reynolds number in both smooth wall and cartilaginous rings with wall structure in human trachea. Also the concentration higher in smooth wall when compare to the cartilaginous rings with wall structure in human trachea.

In Figure 2 The comparison of concentration of charged nano-particles of smooth wall pipe and cartilaginous rings of wall structure is ploted verses the the Radial position of the tube(r) with varying electrostatic parameter(α) The result shows that the concentration increases with increasing low electrostatic parameter(α) in both smooth wall and cartilaginous ring wall structure in human trachea. Also the concentration higher in smooth wall when compare the cartilaginous ring structure of wall.

The presence of the cartilaginous rings alters the airflow field, especially the flow pattern of the laryngeal jet, which is the dominant factor determining particle in the trachea. Although this study is conducted in an idealized airway model that could claim only to characterize a set of typical respiratory tract conditions and not all possible conditions, the results are instructive. Our study shows that the presence of cartilaginous rings significantly enhance concentration of charged nano particle in trachea. This implies that the current approach to model human airways by using smooth walled tubes could underestimate concentration of charged nano – particle that are deposited within trachea. Detailed morphological features of the respiratory tract(e.g. cartilaginous rings) could also play an unexpected role in intersubject variability, because surface irregularities could be expected to vary from individual to individual.

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