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Transport and deposition of nano-fibers in human upper tracheobronchial airways

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ABSTRACT

The elongated shape of the asbestos fibers makes them an extreme respiratory hazard as they can penetrate and deposit deep into the lung and could cause malignant pathological responses. Transport and deposition of these fibers are strongly affected by their diameter and aspect ratio, airflow condition, and the airway morphology. Compared to spherical particles, motions of elongated fibers are more complex due to the coupling between their translational and rotational movements. Very few prior works resolved the full motion of nano-scale fibers where the Brownian diffusion is dominant. In this work, the transport and deposition of nano-fibers were numerically simulated in a physiologically realistic lung bifurcation model. Detailed motion of the inhaled nano-fibers and their interactions with the surrounding environment were reproduced by solving a system of coupled nonlinear equations governing the translational and rotational motions. Hydrodynamic drag and torque, turbulence dispersion, gravitational sedimentation, and the Brownian diffusion were accounted for. Correlations of these forces with the fiber transport and deposition pattern, fiber characteristics, human breathing condition, and airway morphology were analyzed. The study uncovered the very important role of Brownian dynamics in the motion of the nano-fibers in human tracheobronchial airways, which can help explain many of the earlier experimental findings. The simulation results were compared with the experimental measurements, and the carcinogenicity of these fibers in human airways was discussed.

1. Introduction

Occupational exposure to asbestos fibers has been linked to the occurrence of malignant respiratory diseases such as mesothelioma and lung cancer. It is now widely accepted that the respiratory pathological response in living being is induced by the deposition and retention of inhaled asbestos fibers. Experimental data on fiber deposition in human patient tissues as well as in vivo animal studies were reported by several researchers, such as Lippmann (1988, 1990), Berman, Crump, Chatfield, Davis, and Jones (1995), and Suzuki, Yuen, and Ashley (2005). Based on the available data, EPA (2003) concluded that fibers with length shorter than 5 μm posed minimum risk, while the threshold for diameter needed further investigation. NIOSH (2008) concluded that fibers with length smaller than 1.5 μm or greater than 40 μm and diameter thinner than 0.25 μm or thicker than 3 μm, respectively, were at the highest risk to cause lung cancer.

While the carcinogenicity of the asbestos fiber could be estimated based on the direct pathological measurement, the physics of fiber transport and deposition is not fully understood. Compared to the spherical particles, far fewer studies have explored fiber transport and deposition due to the complex nature of the need to resolve the coupled rotational and translational motions. Jeffery (1922) evaluated the drag and torque acting on an elongated ellipsoidal fiber under creeping flow conditions, and studied the fiber rotational motion in a simple shear flow. Gallily and Eisner (1979) performed the

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Nomenclature

a	semi-minor axis of the ellipsoid
A	transformation matrix expressed in Euler's quaternion
C_i^t	translational slip-correction factors
C_i^r	rotational slip-correction factors
D	particle Brownian diffusivity
$d_{\hat{z}\hat{y}}, d_{\hat{x}\hat{z}}$	elements of fluid strain tensor
$\boldsymbol{f^B}$	Brownian diffusion force
$\boldsymbol{f^h}$	hydrodynamic drag
$\boldsymbol{f^L}$	shear induced lift force
$\boldsymbol{g}$	gravitational acceleration
$(I_{\hat{x}},I_{\hat{y}},I_{\hat{z}})$	momentum of inertia in the fiber coordinate
$\hat{\boldsymbol{K}}$	diagonal tensor in the fiber coordinate
$\hat{\hat{\boldsymbol{K}}}$	translational dyadic tensor in the co-moving coordinate
m^p	mass of the fiber
Pe	Peclet number
$R_{\hat{i}\hat{i}}^t$	resistant coefficient for an ellipsoidal translating along its principle axes in a quiescent fluid
$R_{\hat{i}\hat{i}}^r$	resistance coefficients for an ellipsoid rotating about its principle axes in a quiescent fluid
Re	Reynolds number
S	particle to fluid density ratio
Sc	Schmidt number
$\boldsymbol{S^r}$	spectral intensity tensors of the rotational Brownian motion
$\boldsymbol{S^t}$	spectral intensity tensors of the translational Brownian motion
t	time
$(T_{\hat{x}}^B, T_{\hat{y}}^B, T_{\hat{z}}^B)$	Brownian diffusion torque in the fiber coordinate
$(T_{\hat{x}}^h,T_{\hat{y}}^h,T_{\hat{z}}^h)$	hydrodynamic torque in the fiber coordinate
$\boldsymbol{U}$	fluid velocity vector
$\boldsymbol{V}$	fiber centroid velocity vector
$w_{\hat{z}\hat{y}}, w_{\hat{x}\hat{z}}, w_{\hat{y}\hat{x}}$	elements of fluid spin tensor
β	fiber aspect ratio
κ	Boltzmann constant
ρ	fluid density
$\delta(\ )$	Dirac Delta Function
ϑ	fiber absolute temperature
τ_{eq}	fiber equivalent relaxation time
$(\omega_{\hat{x}},\omega_{\hat{y}},\omega_{\hat{z}})$	fiber angular velocity vector in the fiber coordinate
μ	dynamic viscosity of the fluid
υ	kinematic viscosity of the fluid

theoretical and experimental analysis of the motion of non-spherical aerosol particles in a 2D Poiseuille flow. Chen and Yu (1991) reported the sedimentation of fibers in laminar flows in a horizontal circular duct assuming a constant shear field. Fan and Ahmadi (1995) studied the wall deposition of ellipsoidal fibers in a turbulent channel flow using the sublayer model. More recently, Tian, Ahmadi, Wang, and Hopke (2012) investigated the aerodynamic characteristics of the ellipsoidal fibers in low Reynolds number flows. Among few practical applications, Asgharian and Yu (1989), and Asgharian and Anijilvel (1995) analyzed the deposition of fibers in pseudo human and rat airways via a mathematical model, and also suggested some empirical equations for estimating the fiber deposition rate.

More recently, Tian and Ahmadi (2013) provided a detailed study of the coupled translational and rotational motion of micro-fibers in the human tracheobronchial airways. They used a diameter of 3.66 μm, with aspect ratio from 3 to 80, for which the fiber inertia is important. Their study revealed that the fiber orientation during their transport and the occurrence of fiber rotation are strongly correlated with the fiber aspect ratio and the strength of the shear flow. The study also provided considerable insight into the parameters that affect the fiber deposition in airway passages, and especially on the effect of fiber rotation that is difficult to infer from experimental studies.

In this study, the work of Tian and Ahmadi (2013) is extended to nano-fibers. In particular, the transport and deposition of nano-fibers with diameter of 1–1000 nm in a physiologically realistic human airway bifurcation model were studied using a series of computer simulations. This group of fibers has been identified to have the highest risk to cause lung cancer (NIOSH, 2008) and mesothelioma (Lippmann, 1988, 1990); however, no detailed study that could explain the high carcinogenicity has been reported. In addition to all the hydrodynamic forces acting on the inertial fibers, the Brownian diffusion forces are significant for the nano-fibers. The focus of the present study was to explore the effect of Brownian diffusion on the movements of ultra-thin fibers, and how it affects the transport and deposition of these ultra-fine fibers in the human airway passages. The system of equations governing the fiber's coupled translational and rotational motions, including the drag and torque, turbulence dispersion, gravitational sedimentation, and the Brownian diffusion, were used in the analysis. For a dilute suspension, the one-way coupling assumption was used, and an in-house C++ code was developed as post processing for the ANSYS-FLUENT code (FLUENT, 1998), for analyzing the inhaled fiber movements. Results of the present simulations were compared with the limited available experimental data, and reasonable agreement was found.

2. Governing equations

2.1. Fiber equation of motion

The nano-fiber is modeled as a slender elongated ellipsoid characterized by its aspect ratio β, and the diameter d or the semi-minor axis a. Details of the fiber kinematics could be found in the work of Tian and Ahmadi (2013). Accordingly, the