Elise Holmstedt

Division of Fluid and Experimental Mechanics,
Luleå University of Technology,
Luleå SE-97 187, Sweden
e-mail: eliseh@ltu.se

Hans O. Åkerstedt

Division of Fluid and Experimental Mechanics,
Luleå University of Technology,
Luleå SE-97 187, Sweden

T. Staffan Lundström

Division of Fluid and Experimental Mechanics,
Luleå University of Technology,
Luleå SE-97 187, Sweden

Sofie M. Högberg

Sandvik Materials Technology,
Storgatan 2,
Sandviken SE-811 81, Sweden

Modeling Transport and Deposition Efficiency of Oblate and Prolate Nano- and Micro-particles in a Virtual Model of the Human Airway

A model for the motion and deposition of oblate and prolate spheroids in the nano- and microscale was developed. The aim was to mimic the environment of the human lung, but the model is general and can be applied for different flows and geometries for small non-spherical particle Stokes and Reynolds numbers. A study of the motion and orientation of a single oblate and prolate particle has been done yielding that Brownian motion disturbs the Jeffery orbits for small particles. Prolate microparticles still display distinguishable orbits while oblate particles of the same size do not. A statistical study was done comparing the deposition efficiencies of oblate and prolate spheroids of different size and aspect ratio observing that smaller particles have higher deposition rate for lower aspect ratio while larger particles have higher deposition rates for large aspect ratio.

[DOI: 10.1115/1.4032934]

1 Introduction

Theories for the motion of oblate and prolate ellipsoids will be outlined and the models presented will be applied on particle deposition in the respiratory airways. The theory is important for a number of applications including particle deposition in the respiratory airway [1,2], the feeding of biofuels [3,4], the manufacturing of fiber-reinforced composites with added properties [5,6], and paper making [7,8]. Regarding particle deposition in the respiratory airways, the topic is significant both for evaluating health effects of inhaled toxic matter and for estimating the efficacy of drug delivery with pharmaceutical aerosols [9–11].

The development of new smart materials containing micro- and nano-particles, such as carbon nanotubes, is a very popular branch of material science nowadays. Such tiny and nonspherical particles are, however, potentially toxic and thus may pose a substantial health risk [12]. Carbon nanotubes are approximately 10–100 nm in diameter with lengths of around 150 μm and can be treated as prolate ellipsoids. Although usually smaller than asbestos fibers, there are concerns that they may cause similar adverse health effects upon inhalation. Nanoparticles may be given additional shapes like oblate spheroids [13]. This is a shape that also may describe wood chips and microparticles for drug delivery [14]. Hence, there are many reasons to do fundamental studies of the motion of prolate and oblate ellipsoids [15].

There are two main techniques for the analysis of the transport of particles and their deposition for a given flow and geometry. One method is to solve the particle equations of motion for a flow field given by the solution of the Navier–Stokes equations. To include effects of Brownian motion, a stochastic force is introduced. If launching a large number N of particles, particle deposition statistics can be disclosed. The error of the method when considering stochastic differential equations of this kind is of order $O(N^{-1/2})$ [16]. This method has been successfully applied to derive the deposition of prolate micro- and nano-particles for a fully developed pipe flow [17]. The second approach is to utilize

the Fokker–Planck equation to find solutions for the probability density function [16]. Statistical averages can then be found from moments of the probability density function. For spherical particles, this is equivalent to solving a steady convective–diffusion equation for the probability density function as a function of space. To find the deposition of particles, the diffusive flux is integrated over the boundary of the pipe. This method has, for instance, been used to study the deposition of spherical particles in a model airway with cartilaginous rings, representing the large conducting airways [18]. For nonspherical particles, the probability density function also depends on the orientation described by the Euler angles, and the deposition is found by averaging over the angles and integrating the probability diffusive flux over the pipe boundary [19]. Comparing the results between the two rather different approaches given in Refs. [17] and [19], a good agreement is found. The Fokker–Planck equation for nonspherical particles was considered for fully developed pipe flow by Asgharian and Graddon [20]. It should be pointed out that this method is a one-way coupling method between the continuous phase and the discrete phase. This means that the presence of the particles does not influence the flow of the continuous phase.

The present study is a continuation of the previous work [17] in which particle tracking of prolate spheroids in different generations of the human lung was considered. Here, using the same method, we consider the particle tracking of the other type of spheroids called oblate spheroids. We consider a single particle study comparing the Jeffery types of orbits for oblate and prolate particles, with and without the effects of Brownian motion. We also consider a comparison of the deposition statistics for the two types of particles for the application of the deposition in the different generations of the human lung.

2 Simulation Setup

We assume a flow speed corresponding to light physical activity for which the tracheal flow rate is 431 cm^3/s . The Reynolds number for the flow in trachea is then about 2000, and therefore in the transition region between laminar and turbulent flow. In generation 2, the Reynolds number is about 1100 and therefore laminar. In this study, we will consider laminar flow which means that this

Contributed by the Fluids Engineering Division of ASME for publication in the JOURNAL OF FLUIDS ENGINEERING. Manuscript received April 28, 2015; final manuscript received February 3, 2016; published online May 2, 2016. Assoc. Editor: Daniel Maynes.

study is limited to conditions from generation 2 and below. The maximum velocity for the flow to be laminar in generation 2 is about 3.5 m/s. We assume that the flow is in the y -direction with an inlet in the $y=0$ plane. A representation of the geometry can be seen in Fig. 1. In this figure, the initial positions of an oblate and prolate particle in a single particle simulation are also defined. Two types of geometries will be considered: a pipe with uniform cross section to study the evaluation of orientation of single particles and a larger-scale model where the deposition rates are calculated for a number of these pipes with a radius and length that goes from large to small corresponding to the size of the various bronchi. This information is then compiled to represent a model of the lung.

2.1 Particle Geometry. The particles studied are oblate and prolate spheroids with two defining characteristics: β , aspect ratio, and d_f , geometric diameter. β is defined as radius of the major axis of the spheroids divided by the minor, so $\beta_{\text{prolate}} = a/b$ and $\beta_{\text{oblate}} = b/a$, where a is the polar semi-axis and b is the equatorial. The geometric diameter is based on the equatorial radius, so $d_f = 2b$. This is illustrated in Fig. 2.

2.2 Particle Equations of Motion. Two coordinate systems are defined to describe the movement of the particles. Global coordinates $[x, y, z]$ and local ones $[x', y', z']$ fixed to the particle with the polar axis along z' . The global coordinate system has the inlet of the airway on the $[x, z]$ plane with origin fixed in the center of the circular inlet and the flow field moving in the positive y -direction. As particles rotate, the angle between the local and global coordinates is described using Euler angles, as depicted in Fig. 3.

For this study, we assume that the Stokes number is small for the particles such that inertia may be neglected. To justify this approach, we start from the full set of equations of motion for the particles

$$m \frac{d^2 x_i}{dt^2} = F_i^h + F_i^g + f_i^{\text{Br}} \quad (1)$$

$$I_i \cdot \frac{d\omega_i}{dt} + \varepsilon_{ijk} \omega_j \omega_k I_k = T_i^h + T_i^{\text{Br}} \quad (2)$$

Here, I_i is the moment of inertia chosen with respect to the principal axes of the body and ω_i is the components of the angular velocity.

The forces affecting the particles are the hydrodynamic, gravitational, and Brownian, and the torques are hydrodynamic and Brownian. Before we consider the Stokes numbers and a discussion

Fig. 1 A representative sketch of the geometry used in the simulations with the initial position for an oblate and a prolate particle in the single particle runs

Fig. 2 Illustration of the spheroids used in the simulations: (a) oblate particle with polar semi-axis a and equatorial b and (b) prolate particle with polar semi-axis a and equatorial b

about the validity of neglecting inertia, we describe the different relevant forces in Secs. 2.3–2.5.

2.3 Hydrodynamic Force and Torque. The drag force on the particles considered in this study may be expressed as

$$\mathbf{F}^h = 3\pi\mu\mathbf{A}^T \begin{bmatrix} d_{\perp} & 0 & 0 \\ 0 & d_{\perp} & 0 \\ 0 & 0 & d_{\parallel} \end{bmatrix} \mathbf{A} \begin{bmatrix} u - \frac{dx}{dt} \\ v - \frac{dy}{dt} \\ w - \frac{dz}{dt} \end{bmatrix} \quad (3)$$

and is thus dependent on the orientation of the particle in the Stokes flow regime. In this equation, μ is the dynamic viscosity of the fluid, $[u, v, w]$ are the components of the fluid velocity, $[(dx/dt), (dy/dt), (dz/dt)]$ are the components of the particle velocities, and $\mathbf{A}$ is the rotation matrix between the local and global coordinates and defined as

$$\mathbf{A} = \begin{bmatrix} c\psi c\phi - c\theta s\phi s\psi & c\psi s\phi + c\theta c\phi s\psi & s\theta s\phi \\ -s\psi c\phi - c\theta s\phi c\psi & -s\psi s\phi + c\theta c\phi c\psi & s\theta c\phi \\ s\theta s\psi & -s\theta c\psi & c\theta \end{bmatrix} \quad (4)$$

where $c\phi = \cos \phi$, $s\phi = \sin \phi$, etc., and (ϕ, θ, ψ) are the Euler angles of the particles.

2.3.1 Translation. For a prolate spheroid, $d_{\perp}$ and $d_{\parallel}$ are the Stokes diameters oriented perpendicular and parallel to the direction of motion, respectively, and are given by [17]

Fig. 3 Euler angles connecting a particles local coordinates to the global ones [5]

$$\frac{d_{\perp}}{d_f} = \frac{\frac{8}{3}(\beta^2 - 1)}{C'_{\perp} \left[\frac{2\beta^2 - 3}{\sqrt{\beta^2 - 1}} \ln(\beta + \sqrt{\beta^2 - 1}) + \beta \right]} \quad (5)$$

$$\frac{d_{\parallel}}{d_f} = \frac{\frac{4}{3}(\beta^2 - 1)}{C'_{\parallel} \left[\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}} \ln(\beta + \sqrt{\beta^2 - 1}) - \beta \right]} \quad (6)$$

Here, β is the fiber aspect ratio, d_f is the geometric diameter, and $C'_{\parallel}$ and $C'_{\perp}$ are the slip correction factors for the fluid dynamic drag that are included to extend the validity of the drag force to include particles that are so small that their diameter is close to the mean free path of air molecules.

Equations (5) and (6) are valid for prolate as well as oblate spheroids if oblate spheroids are defined with $\beta < 1$. This means that the imaginary part of the logarithm and square root must be taken into account; hence, β is replaced with $1/\beta$ in Eqs. (7) and (8) so that the aspect ratio is defined as greater than unity for both prolate and oblate spheroids. The Stokes parameters for oblate spheroids are then given by

$$\frac{d_{\perp}}{d_f} = \frac{\frac{8}{3}(\beta^2 - 1)}{C'_{\perp} \left[\frac{\beta(3\beta^2 - 2)}{\sqrt{\beta^2 - 1}} \arctan(\sqrt{\beta^2 - 1}) - \beta \right]} \quad (7)$$

$$\frac{d_{\parallel}}{d_f} = \frac{\frac{4}{3}(\beta^2 - 1)}{C'_{\parallel} \left[\frac{\beta(\beta^2 - 2)}{\sqrt{\beta^2 - 1}} \arctan(\sqrt{\beta^2 - 1}) + \beta \right]} \quad (8)$$

This result is also given by Happel and Brennen [21].

No exact expression for the slip correction factors exists for prolate and oblate spheroids, and an approximate method by Dahneke [22] is applied. This method will be outlined in Sec. 2.3.3.

2.3.2 Rotation. The equations for the fluid dynamic torque for an ellipsoid body in a viscous shear flow as derived by Jeffery [23] and simplified for the current case can be written in the following manner:

$$T_{x'}^h = \frac{1}{B_{\perp}} \left[(\zeta' - \omega_{x'}) - \left(\frac{\beta^2 - 1}{\beta^2 + 1} \right) \dot{\epsilon}_{y'z'} \right] \quad (9)$$

$$T_{y'}^h = \frac{1}{B_{\perp}} \left[(\eta' - \omega_{y'}) - \left(\frac{\beta^2 - 1}{\beta^2 + 1} \right) \dot{\epsilon}_{x'z'} \right] \quad (10)$$

Due to rotational symmetry rotation about the major axis does not affect the transport and is therefore omitted. The tensor ω_{ij} is the fiber angular velocity, $\dot{\epsilon}_{ij} = (1/2)((\partial u_i/\partial x_j) + (\partial u_j/\partial x_i))$ is the elements of the deformation rate, and $[\xi, \eta, \zeta]^T = (1/2)(\nabla \times \mathbf{u})$ is the spin tensor. The latter two tensors are derived from the global flow field and are translated to local equivalents by

$$\dot{\epsilon}_{i'j'} = \mathbf{A} \dot{\epsilon}_{ij} \mathbf{A}^T \quad (11)$$

$$[\xi', \eta', \zeta']^T = \mathbf{A} [\xi, \eta, \zeta]^T \quad (12)$$

The angular mobility for prolate spheroids may be expressed as [17]

$$B_{\perp, \text{prolate}}^r = \frac{3C'_{\perp} \left[\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}} \ln(\beta + \sqrt{\beta^2 - 1}) - \beta \right]}{2\pi\mu d_f^3 (\beta^4 - 1)} \quad (13)$$

For oblate spheroids, this mobility is given by the following relationship

$$B_{\perp, \text{oblate}}^r = \frac{3C'_{\perp} \left[\frac{(2 - \beta^2)\beta}{\sqrt{\beta^2 - 1}} \arctan(\sqrt{\beta^2 - 1}) - \beta \right]}{2\pi\mu d_f^3 \left(\frac{1}{\beta^2} - \beta^2 \right)} \quad (14)$$

2.3.3 Slip Corrections Factors. No exact expressions for the drag of prolate and oblate spheroids exist in the free molecular flow limit where $\text{Kn} = (2\lambda/d_f)$ approaches infinity, in which λ is the mean free path of the air molecules. For cylinders, however, expressions have been derived by Dahneke [24]. Therefore, in this limit, the drag of prolate and oblate spheroids is modeled by the results of a cylinder. To extend the validity for the drag force from small Knudsen numbers Kn to large Kn , the Cunningham factors are applied with an adjusted radii as suggested by Dahneke [24]. The Cunningham factors for prolate spheroids are given by Högberg et al. [17]. Using the replacement $\beta \rightarrow 1/\beta$ gives the following result for oblate spheroids:

$$C'_{\perp} = 1 + \frac{d_f}{2r'_{\perp}} \text{Kn} \left[1.257 + 0.4 \exp\left(\frac{-2.2r'_{\perp}}{d_f \text{Kn}}\right) \right] \quad (15)$$

The adjusted radii for translational motion parallel and perpendicular to the flow are then expressed as

$$r_1 = \frac{1.657d_f\beta}{16(\beta^2 - 1)} \quad (16)$$

$$\Lambda_1 = \frac{1}{\sqrt{\beta^2 - 1}} \quad (17)$$

$$\Lambda_3 = \Lambda_1 \log\left(\beta + \frac{1}{\Lambda_1}\right) \quad (18)$$

$$\Lambda_2 = \beta - \Lambda_3 \quad (19)$$

$$\begin{aligned} r'_{\perp} = & \frac{r_1}{2} \left[\frac{3\beta^2 + 4}{\sqrt{\beta^2 - 1}} \arctan\sqrt{\beta^2 - 1} - 1 \right] \\ & \times \left[\Lambda_1^2 \Lambda_2 \left\{ \frac{(6 - \pi)f}{4} - 2 \right\} + \Lambda_3 \left\{ 4 - \frac{4 - \pi}{2}f \right\} + \frac{f}{\beta} \right] \end{aligned} \quad (20)$$

$$\begin{aligned} r'_{\parallel} = & r_1 \left[\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}} \arctan\sqrt{\beta^2 - 1} + 1 \right] \\ & \times \left[\Lambda_1^2 \Lambda_2 \left\{ 4 - \frac{(6 - \pi)f}{2} \right\} \beta^{-2} + \Lambda_3 f + \frac{f}{\beta} \right] \end{aligned} \quad (21)$$

An adjusted radii for rotational movement of oblate spheroids around its axis is given by

$$r_{\perp}^r = \frac{1.675d_f}{\beta} \frac{3}{2} \left[\frac{(2-\beta^2) \times \beta \arctan(\sqrt{\beta^2-1}) - \beta}{\frac{1}{\beta^2 - \beta^2}} \right] \times \left[\frac{1}{4} + \frac{2\beta}{4} + \frac{(2\beta)^2}{4} + \frac{(2\beta)^3}{8} + f \left(\frac{\pi-6}{48} - \frac{2\beta}{8} - \frac{(2\beta)^2}{8} + \frac{(\pi-4)(2\beta)^3}{64} \right) \right] \quad (22)$$

2.4 Gravitational Settling. One deposition mechanism is gravitational settling or sedimentation. It comes into play for large particle masses for longer time periods and is most noticeable within horizontal small airways. Particle density is usually much greater than the surrounding air, and thus buoyancy can be neglected. The gravitational force is defined in the positive z -direction with magnitude

$$F_z^g = \pi \rho_f g d_f^3 \beta / 6 \quad (23)$$

for prolate spheroids and

$$F_z^g = \pi \rho_f g d_f^3 / 6\beta \quad (24)$$

for oblate spheroids, where ρ_f is the density of the particle and g is the gravitational acceleration.

2.5 Brownian Motion. The Brownian force and torque are modeled as independent zero-mean Gaussian white noise processes [17], which for spheroids take the following form:

$$F_{i'}^{\text{Br}}(t) = \chi_{i'}^t \sqrt{\frac{\pi S_{i'}^t}{\delta t}} \quad (25)$$

$$T_{i'}^{\text{Br}}(t) = \chi_{i'}^r \sqrt{\frac{\pi S_{i'}^r}{\delta t}} \quad (26)$$

where $\chi_{i'}^t$ and $\chi_{i'}^r$ are standard normally distributed random numbers and δt is a Brownian time increment chosen as $\delta t = 10 \mu\text{s}$ after a numerical study where the results were compared to a theoretical value for diffusion velocity [25]. The spectral intensities $S_{i'}^t$ and $S_{i'}^r$ are given by

$$S_{i'}^t = \frac{2\sigma T}{\pi} \frac{1}{B_{i'}^t} \quad (27)$$

$$S_{i'}^r = \frac{2\sigma T}{\pi} \frac{1}{B_{i'}^r} \quad (28)$$

in which σ is the Boltzmann constant and T is the absolute temperature. $B_{i'}^t$ is given in Eqs. (13) and (14) and

$$B_{i'}^r = 1/3\pi\mu d_{i'} \quad (29)$$

The diffusion coefficients are given by

$$D_{i'}^t = \sigma T B_{i'}^t \quad (30)$$

$$D_{i'}^r = \sigma T B_{i'}^r \quad (31)$$

2.6 Stokes Numbers. To define the Stokes number, it is sufficient to consider the hydrodynamic forces and torques. Adding the inertia in Eq. (3), the equation of motion for the translational part is given by

$$m \begin{bmatrix} \frac{d^2x}{dt^2} \\ \frac{d^2y}{dt^2} \\ \frac{d^2z}{dt^2} \end{bmatrix} = 3\pi\mu \mathbf{A}^T \begin{bmatrix} d_{\perp} & 0 & 0 \\ 0 & d_{\perp} & 0 \\ 0 & 0 & d_{\parallel} \end{bmatrix} \mathbf{A} \begin{bmatrix} u - \frac{dx}{dt} \\ v - \frac{dy}{dt} \\ w - \frac{dz}{dt} \end{bmatrix} \quad (32)$$

An order of magnitude estimate of the terms in this equation gives for the perpendicular and the parallel part

$$\rho_p \frac{4}{24} \pi d_f^3 \beta \frac{U^2}{D} \approx 3\pi\mu d_f \frac{d_{\perp}}{d_f} U \quad (33)$$

$$\rho_p \frac{4}{24} \pi d_f^3 \beta \frac{U^2}{D} \approx 3\pi\mu d_f \frac{d_{\parallel}}{d_f} U \quad (34)$$

where U is a typical velocity of the flow and D is the typical length scale of the flow.

Defining the Stokes number as the ratio between the inertial force and the hydrodynamic force, we have for prolate spheroids

$$St_{\perp}^t = \frac{\rho_p d_f^2 \beta U d_f}{18\mu D d_{\perp}} \quad (35)$$

$$St_{\parallel}^t = \frac{\rho_p d_f^2 \beta U d_f}{18\mu D d_{\parallel}} \quad (36)$$

with the Stokes parameters given by Eqs. (5) and (6). For oblate spheroids, similar expressions for the Stokes numbers are given by letting $\beta \rightarrow 1/\beta$ and use the Stokes parameters (7) and (8).

The corresponding order of magnitude estimate for the rotational equation of motion gives the Stokes number as

$$St^r = \frac{I_{xx} B_{\perp}^r U}{D} \quad (37)$$

where $B_{\perp}^r$ is the angular mobility given by Eq. (13) for prolate spheroids and by Eq. (14) for oblate spheroids, and the relevant moment of inertia is given for prolate spheroids by

$$I_{xx} = I_{yy} = \frac{1}{120} \rho_p \pi \beta (1 + \beta^2) d_f^5 \quad (38)$$

and for oblate spheroids as

$$I_{xx} = I_{yy} = \frac{1}{120} \rho_p \pi \beta^{-1} (1 + \beta^{-2}) d_f^5 \quad (39)$$

For the neglect of the inertia terms, the Stokes number must be much smaller than one. In the cases that follow, this is more or less satisfied. A discussion of the Stokes number is thus provided in each particular case being studied.

2.7 Numerical Setup for Single Particle Study. To be able to properly observe the Jeffery orbits made by a single particle, it is necessary to follow the particle for a longer distance than for the airway model used in the multiparticle deposition simulations. In simulations of non-Brownian motion, that is, particles only affected by fluid shear, the nondimensional diameter of the airway has no large effect on the resulting Jeffery orbits since the flow shear rate U/R is similar between generations. When studying Brownian motion, a larger airway is preferable since it slows down the process and makes it easier to do observations, so for the following examples, generation 4 was chosen.

When keeping β constant, the geometric diameter of the particles has no impact on the Jeffery orbits of particles not affected

by Brownian motion, but has an inverse relationship with Brownian motion as it is, by its nature, a force that affects small particles. Therefore, a relatively large particle with $d_f = 1 \mu\text{m}$ was chosen, so the impact of Brownian motion can be observed on the rotational movement but it is not the dominating force acting on the particles and its translational contribution is minimal. All Stokes numbers for this case are very small so the inertia can be neglected.

The placement of both oblate and prolate particles at the beginning of the simulations is such that the large surface of the particle is facing the flow as shown in Fig. 1. For prolate particles, this implies that the particle is directed perpendicular to the flow with $\theta = 90^\circ$ since its z' -axis is directed along the length of the particle. Oblate particles are placed parallel to the flow with $\theta = 0^\circ$ since its z' -axis is perpendicular to the surface of the particle. The angle ϕ describes the tilt of the particles z' -axis from the global z -axis (see Fig. 3). The particles initial position is such that $\phi = 0^\circ$, and thus, the pressure gradient over the particles on the horizontal plane is zero. The larger the distance between the center of the airway and the particles initial position, the slower the particle will move and thus experiences more Jeffery orbits. In this simulation, the initial position was at a distance of $0.7r$ from the center, where r is the radius of the airway.

2.8 Numerical Setup for Simulation of Deposition Efficiency in Human Airways. Lungs can be seen as pipes divided into smaller pipes that in turn are divided into even smaller pipes, etc. Each of these divisions is called a generation. The simulations are set up here to start at the second generation, where for light physical activity the flow is laminar. Using Weibel's model [26], it is furthermore assumed that pipes in this generation are 19 mm long and have a diameter of 4.15 mm. The simulations are performed down to the 16th generation where the radius of the pipes is assumed to be 0.2 mm and the length 1.65 mm [26]. The tracheal flow rate was $431 \text{ cm}^3/\text{s}$ corresponding to a tidal volume of 750 ml with an air temperature of 310 K and the particles have unit density. The model is currently setup and focused on the straight bronchi, not the intersections. Disturbances in the flow at the intersections are mainly driven by inertia and are therefore more important for higher Re than considered in this study. Secondary flow that can be induced in the interceptions and a partly developing flow at one side of the pipe after the intersection are therefore neglected in the current setup.

The purpose of the present work is to extend the methodology developed in Ref. [17] for prolates to oblates and to compare the behavior of these two shapes on the deposition rate in the human lung.

Simulations are thus run with 10,000 particles with a density of 1000 kg/m^3 for each combination of aspect ratio and geometric diameter, and the deposition rate is calculated by observing how many particles are deposited at the walls of the lungs as a ratio of the number of particles in the set. A study of the number of particles used in the simulation shows that 10,000 particles are enough to gather statistically accurate results. Larger number of particles produces the same results. This is also done in accordance to previously published work on the topic [17].

3 Results and Discussion

To elucidate the motion of oblate and prolate spheroids in human airways, it is necessary to both scrutinize the detailed motion of a single particle and the accumulated results of a large number of particles.

3.1 Following One Particle. Oblate and prolate spheroids are first studied for the case when they are only influenced by the flow field within the airways, discarding both Brownian motion and gravitational settling.

Oblate and prolate spheroids exhibit a similar behavior with Jeffery orbits appearing at the same interval, which can be seen in

Figs. 4(a) and 5(a). In Figs. 4(b) and 5(b), the particles Euler angles θ and ϕ can be seen. Since θ denotes the angle between the z' -axis of the particle and the z -axis of the flow, it changes 180° during a Jeffery orbit in a characteristic manner, quickly around positions perpendicular to the flow and slowly otherwise. The angle ϕ describes the rotational angle around the flow, i.e., if the particle is pointing up, down or to the sides, but since there are no horizontal forces acting on the particle, this angle is unchanged until halfway through a Jeffery orbit when it switches 180° instantaneously when the side that previously faced "up" now faces "down." Note that the size of the particles in the plots is greatly exaggerated for the sake of clarity.

When Brownian motion is included, the motion of the prolate and oblate particles becomes more irregular (see Figs. 6 and 7). For the prolate spheroids, although a randomized behavior is obvious, Jeffery orbits are still visible, but with a shorter and not as regular periodicity (see Fig. 7(a)). The behavior of the oblate spheroids is less regular without any Jeffery orbits (see Fig. 6(a)). It is also obvious that Brownian motion influences ϕ for both types of particles but much more for the oblate spheroids. This indicates that the motion of the oblate spheroids is much more sensitive to Brownian force disturbance. The reason for this is that the Brownian force is proportional to the square root of the rotational diffusion coefficient which is in general much larger for the oblate spheroids than for the prolate spheroids. The square root of the ratio between the two rotational diffusion coefficients is given by the square root of the ratio of the expressions for the corresponding angular mobilities (13) and (14). This ratio then becomes

$$q = \sqrt{\frac{B_{\perp, \text{oblate}}^r}{B_{\perp, \text{prolate}}^r}} = \sqrt{\frac{\left(\frac{2\beta^2 - 1}{\sqrt{\beta^2 - 1}} \ln\left(\beta + \sqrt{\beta^2 - 1}\right) - \beta\right)(\beta^4 - 1)}{\left(\frac{(2 - \beta^2)\beta}{\sqrt{\beta^2 - 1}} \arctan\left(\sqrt{\beta^2 - 1}\right) - \beta\right)\left(\frac{1}{\beta^2} - \beta^2\right)}} \quad (40)$$

This ratio which is only a function of β increases quickly with the β value, and for the β value 5, this ratio is about 7. Thus, the Brownian force is about seven times stronger for oblates when compared with the prolates.

3.2 Statistical Deposition Efficiency. During multiple particle simulations, 10,000 randomly distributed particles are launched and followed and their position of exit saved. Either the particles exited through the outlet or their mass center passed the wall. The deposition rate is then calculated as the number of particles deposited at the wall to the number of particles launched at the inlet. To get a clear picture on how the different parameters influence the deposition rate, two main cases were studied. First, the geometric diameter was changed and the aspect ratio was kept constant. In the second case, the influence of the aspect ratio β is in focus by varying it for a few different diameters of the particles. A gravitational force perpendicular to the flow is included in all the results presented here.

3.2.1 Changing the Geometric Diameter. With $\beta = 100$, there is a correlation between deposition efficiencies and particle size; when the particle size increases, so does the deposition rate independent of particle type, except for the case with the smallest particles with a geometric diameter of 10 nm, where the deposition efficiencies increase due to the greater influence of the Brownian diffusion (see Fig. 8).

In Fig. 8, the deposition rates are shown for a pair of one oblate particle and one prolate of the same volume such that the following relation holds:

Fig. 4 Description of the motion of an oblate spheroid with $d_f = 1 \mu\text{m}$, $\beta = 5$ and in an airway of generation 4: (a) the rotation of one oblate particle plotted at regular intervals as it moves through an airway and (b) the angles, q and f , describing the rotation of the oblate particle

Fig. 5 Description of the motion of a prolate spheroid with $d_f = 1 \mu\text{m}$, $\beta = 5$ and in an airway of generation 4: (a) the rotation of one prolate particle plotted at regular intervals as it moves through an airway and (b) the angles, q and f , describing the rotation of the prolate particle

$$d_{f,\text{oblate}} = \beta^{2/3} d_{f,\text{prolate}} \quad (41)$$

The largest oblate particle and the largest prolate particle should then be compared. It is seen that for the largest pair of particles, the oblates have a slightly higher deposition rate. This can be explained by the differences in the diffusion coefficients for the two particle types. As shown in Ref. [19], the effective diffusion coefficient after integration about the Euler angles becomes

$$D' = \frac{2}{3} D'_{\perp} + \frac{1}{3} D'_{\parallel} \quad (42)$$

Expanding the diffusion coefficients for large β , we then get for the oblate and prolate particles

$$D'_{\text{oblate}} \approx \frac{\kappa T (\pi\beta - 1)}{6\pi\mu d_{f,o}\beta} \quad (43)$$

$$D'_{\text{prolate}} \approx \frac{\kappa T \ln(2\beta)}{3\pi\mu d_{f,p}\beta} \quad (44)$$

The ratio between the diffusion coefficients using the relation (41) then follows

Fig. 6 Similar setup as in Fig. 4 but with Brownian motion included: (a) snapshots of an oblate particle as it moves through the airway and (b) the angular positions of an oblate particle

Fig. 7 Similar setup as in Fig. 5 but with Brownian motion included: (a) snapshots of a prolate particle as it moves through the airway and (b) the angular positions of a prolate particle

$$\frac{D'_{\perp, \text{oblate}}}{D'_{\perp, \text{prolate}}} \approx \frac{\pi\beta - 2}{2\beta^{2/3} \ln(2\beta)} \quad (45)$$

which is about 1.4 for $\beta = 100$, meaning that comparing oblates and prolates of the same volume, the deposition of oblates is slightly higher than the prolates in agreement with the results in Fig. 8.

The discussion above holds in the limit of small Knudsen number and for particles smaller than about 70 nm, so that if the Knudsen number is large, the diffusion coefficients must be modified by the Cunningham factors.

The Stokes number has been calculated for all the examples in Fig. 8 both the translational and rotational Stokes numbers. Some particle diameters are quite big, an oblate of diameter 107 μm and a prolate of diameter 5 μm . For these particles, the largest translational Stokes number is found: for the oblate 0.32 in generation 6 and for the prolate 0.25 in generation 4. The rotational Stokes number is for the largest oblate particle about 0.1 observed in generation 6, and for the largest rotational Stokes number for the largest prolates is also about 0.1. So, for the translational part, the Stokes number for the largest particles is smaller than unity but not by very much, and these larger particles can therefore be considered to be at the upper limit for which the theory is valid.

Fig. 8 Simulations of particles with a fixed aspect ratio of $\beta = 100$, but with a varied geometric diameter so that the oblate and prolate particle volumes are comparable

Another way to analyze the results is to look at the deposition rates as a number of particles travels through generations 2–16 and derive the probability that a particle ends up in a specific generation dependent on it traveling through the generations above it. If p_n is the deposition rate for generation n in accordance to the results presented in Fig. 8, we now focus on the deposition q_n in each generation where

$$q_2 = p_2 \quad (46)$$

$$q_n = (1 - q_{n-1})p_n \quad n > 2 \quad (47)$$

In this model, it is easy to distinguish in which generation most fibers are being deposited, as displayed in Figs. 9(a) and 9(b) where the deposition efficiencies for oblate and prolate spheroids have been plotted, respectively. Larger oblate spheroids are being deposited higher up in the airway while smaller particles have a quite even distribution. For prolate particles, it is clear that the majority of the particles are being deposited in the smallest bronchi.

3.2.2 Changing the Aspect Ratio. To make it easier to compare the results for oblate particles with those for prolate particles, the results from the simulations of the prolate particles deposition rate are plotted against the inverse of their β value on the x -axis on a logarithmic scale. Each line represents the deposition in each generation of bronchi with the prolate particles on the left-hand side, the oblate particles on the right-hand side, and a spherical particle with an aspect ratio of $\beta = 1$ in the middle. To compare the particles of similar size, particles with the same minor axis are chosen; to achieve this, the geometric diameter $d_{f, \text{oblate}}$ for the oblate particles is defined as $d_{f, \text{oblate}} = \beta d_{f, \text{prolate}}$.

To see the effect of the aspect ratio on the deposition efficiencies of particles, a number of simulations were carried out with a fixed diameter of the minor axis and an aspect ratio that goes from a prolate particle with $\beta_p = 100$ down to $\beta = 1$, and then up to $\beta_o = 100$ for oblate particles (see Fig. 10).

As shown in Figs. 10(a) and 10(b), for smaller particles, the maximum deposition rates occur for spherical particles while particles with a higher aspect ratio have a lower deposition rate. For smaller particles, the Brownian force has the largest influence on the movements of particles; therefore, it is natural that a smaller particle, such as the sphere, has a larger deposition rate.

Once the particles get larger, this behavior can be observed to change. Studying Fig. 10(c), the deposition efficiencies for particles with a minor axis diameter of $d_f = 460$ nm start increasing for oblate spheroids with a large β compared to prolate spheroids. Oblate spheroids with a small β can still be seen to be following the earlier pattern which gives a minimum deposition rate for oblate spheroids somewhere around $\beta = 3$. At particle size of

Fig. 9 Deposition efficiencies for each generation as particles pass through the complete model of the lung: (a) deposition of oblate spheroids in a multigenerational model of a lung and (b) deposition of prolate spheroids in a multigenerational model of a lung

Fig. 10 Simulations of depositions of particles with changed aspect ratio. Plotted on a logarithmic scale with the inverse of β for the prolate particles: (a) minor axis of 46 nm, (b) minor axis of 100 nm, (c) minor axis of 460 nm, and (d) minor axis of 1 μm.

$d_f = 1 \mu\text{m}$, the behavior of the oblate spheroids is constant with increasing deposition rates as β increases, as shown in Fig. 10(d). A similar pattern for prolate particles is also starting to appear. This behavior arises from the increasing influence gravity has on the heavier particles. The relative magnitude of the gravitational effect for the different particles can be gathered by comparing the particle volumes

$$\frac{V_o}{V_p} = \frac{\frac{1}{\beta} d_{fo}^3}{\beta d_{fp}^3} \quad (48)$$

where $d_{fo} = \beta d_{fp}$. So

$$\frac{V_o}{V_p} = \beta \quad (49)$$

Since the particles are quite small in the particular cases mentioned above, all Stokes numbers are quite small for all β so the inertia can safely be neglected.

4 Conclusions

A semi-analytical model describing the motion of oblate and prolate spheroids on the nano- and micro-scales has been developed, and simulations enabling both single particle tracking and aggregation of multiple particle deposition were carried out. In this work, the focus was on particle movement and deposition in bronchi, but the model can be applied to a variety of cases with small particle Reynolds and Stokes numbers including more advanced models of the geometry of the human lung [27].

It is clear from the simulations that the shape of the particles greatly influences the deposition of said particles. It is well known that reduced particle size reduces the gravitational sedimentation but increases the Brownian diffusion, which corresponds to the results from this model. What the model has shown is how great each of those effects has on the particles and also how different shapes are affected differently. There is a clear connection between a reduction in deposition rate and a reduced particle diameter meaning a reduction of the effect of gravitational sedimentation. There is also an increase in deposition for the very small particles, where the Brownian diffusion starts to have a noticeable effect which leads to a deposition minimum for a certain geometric diameter for each aspect ratio. There is also a higher deposition rate for the larger oblate spheroids as compared to prolate spheroids. This behavior can be traced back to the greater influence the Brownian forces have on them. There was also a noticeable influence on the results from changing the aspect ratios of the particles. The deposition efficiencies for the smallest particles were the lowest for both the oblate and prolate spheroids with the highest aspect ratio, with spherical particles having the highest deposition rates. For particles in the microscale, this behavior was inverse and the highest deposition was found with the highest aspect ratios. By running simulations without gravitational forces acting on the particles, this behavior is concluded to be influenced by sedimentation effects. Thus, smaller prolate spheroids will get the deepest into the lungs while oblate spheroids will be intercepted in the larger bronchi.

The stability of the path of the particle is shown to be greatly dependent on particle shape and size. Particles that are only influenced by the flow field will display clear Jeffery orbits, whose frequency is only set by the particle aspect ratio and where in the flow field the particle is moving. When the particles are under the influence of Brownian forces, this behavior is changed and particle type and size become important. Prolate microparticles still display distinguishable Jeffery orbits while oblate particles of the same size do not, indicating that their rotational position is much

less stable. Nanoparticles of both types did not have distinguishable Jeffery orbits since the Brownian forces acting on them were too great.

In these simulations, we have neglected the inertia. This can be done if the Stokes number is much less than one. This is not always the case for the larger particles included but since the bifurcation zones, where inertia plays a significant role, are not included in the study, this may still be a valid assumption. It might also be so that the larger particles studied do not make it into the lungs in a large amount. To exemplify, it has been numerically shown that when the size of the particles increases from 5 to 10 μm , the deposition in the higher airways, including bifurcations, increases substantially [28].

Acknowledgment

The authors would like to thank the Swedish Research Council for funding this work.

References

- [1] Zhang, Z., Kleinstreuer, C., and Kim, J. C. S., 2001, "Flow Structure and Particle Transport in a Triple Bifurcation Airway Model," *ASME J. Fluids Eng.*, **123**(2), pp. 320–330.
- [2] Högberg, S., Åkerstedt, H., Holmstedt, E., Lundström, T., and Sandström, T., 2012, "Time-Dependent Deposition of Micro- and Nanofibers in Straight Model Airways," *ASME J. Fluids Eng.*, **134**(5), p. 051208.
- [3] Svoboda, K., Pohorelý, M., Hartman, M., and Martinec, J., 2009, "Pretreatment and Feeding of Biomass for Pressurized Entrained Flow Gasification," *Fuel Process. Technol.*, **90**(5), pp. 629–635.
- [4] Teaters, L. C., and Battaglia, F., 2014, "On the Computational Modeling of Unfluidized and Fluidized Bed Dynamics," *ASME J. Fluids Eng.*, **136**(10), p. 104501.
- [5] Högberg, S., and Lundström, T., 2011, "Motion of Dispersed Carbon Nanotubes During Impregnation of Fabrics," *Plast., Rubber Compos.*, **40**(2), pp. 70–79.
- [6] Lundström, T., and Frishfelds, V., 2013, "Modeling Filtration of Particulate Flow During Impregnation of Dual-Scale Fabrics," *J. Compos. Mater.*, **47**(15), pp. 1907–1915.
- [7] Carlsson, A., Lundell, F., and Söderberg, L. D., 2006, "Fiber Orientation Control Related to Papermaking," *ASME J. Fluids Eng.*, **129**(4), pp. 457–465.
- [8] Vakil, A., and Green, S. I., 2013, "Numerical Study of Two-Dimensional Circular Cylinders in Tandem at Moderate Reynolds Numbers," *ASME J. Fluids Eng.*, **135**(7), p. 071204.
- [9] Feng, Y., and Kleinstreuer, C., 2013, "Analysis of Non-Spherical Particle Transport in Complex Internal Shear Flows," *Phys. Fluids*, **25**(9), p. 091904.
- [10] Kleinstreuer, C., and Feng, Y., 2013, "Computational Analysis of Non-Spherical Particle Transport and Deposition in Shear Flow With Application to Lung Aerosol Dynamics—A Review," *ASME J. Biochem. Eng.*, **135**(2), p. 021008.
- [11] Dastan, A., Abouali, O., and Ahmadi, G., 2014, "CFD Simulation of Total and Regional Fiber Deposition in Human Nasal Cavities," *J. Aerosol Sci.*, **69**, pp. 132–149.
- [12] Poland, C. A., Duffin, R., Kinloch, I., Maynard, A., Wallace, W. A. H., Seaton, A., Stone, V., Brown, S., MacNee, W., and Donaldson, K., 2008, "Carbon Nanotubes Introduced Into the Abdominal Cavity of Mice Show Asbestos-Like Pathogenicity in a Pilot Study," *Nat. Nanotechnol.*, **3**(7), pp. 423–438.
- [13] Cauchois, O., Segura-Sanchez, F., and Ponchela, G., 2013, "Molecular Weight Controls the Elongation of Oblate-Shaped Degradable Poly(γ -Benzyl-L-Glutamate) Nanoparticles," *Int. J. Pharm.*, **452**(1–2), pp. 292–299.
- [14] Champion, J. A., Katare, Y. K., and Mitragotri, S., 2007, "Particle Shape: A New Design Parameter for Micro- and Nanoscale Drug Delivery Carriers," *J. Controlled Release*, **121**(1–2), pp. 3–9.
- [15] Verrelli, D. I., 2014, "Convenient Formulae for the Drag on a Prolate Ellipsoid Moving Along Its Axis of Symmetry Perpendicular to a Plane Surface," *Int. J. Multiphase Flow*, **65**, pp. 138–142.
- [16] Risken, H., 1996, *The Fokker-Planck Equation*, Springer, Berlin.
- [17] Högberg, S. M., Åkerstedt, H. O., Lundström, T. S., and Freund, J. F., 2010, "Respiratory Deposition of Fibers in the Non-Inertial Regime: Development and Application of a Semi-Analytical Model," *Aerosol Sci. Technol.*, **44**(10), pp. 847–860.
- [18] Åkerstedt, H. O., Högberg, S. M., Lundström, T. S., and Sandström, T., 2010, "The Effect of Cartilaginous Rings on Particle Deposition by Convection and Brownian Diffusion," *Nat. Sci.*, **2**(7), pp. 769–779.
- [19] Åkerstedt, H. O., Högberg, S. M., and Lundström, T. S., 2013, "An Asymptotic Approach of Brownian Deposition of Nanofibres in Pipe Flow," *Theory Comput. Fluid Dyn.*, **27**(5), pp. 561–575.
- [20] Asgharian, B., Yu, C. P., and Gradon, L., 1988, "Diffusion of Fibers in Tubular Flow," *Aerosol Sci. Technol.*, **9**(3), pp. 213–219.
- [21] Happel, J., and Brenner, H., 1983, *Low Reynolds Number Hydrodynamics*, Springer, The Netherlands.

- [22] Dahneke, B. E., 1973, "Slip Correction Factors for Nonspherical Bodies—I. Introduction and Continuum Flow," *J. Aerosol Sci.*, **4**(2), pp. 139–145.
- [23] Jeffery, G. B., 1922, "The Motion of Ellipsoidal Particles Immersed in a Viscous Fluid," *Proc. R. Soc. London*, **102**(175), pp. 161–179.
- [24] Dahneke, B. E., 1973, "Slip Correction Factors for Nonspherical Flow—II. Free Molecule Flow," *J. Aerosol Sci.*, **4**(2), pp. 147–161.
- [25] Grassia, P. S., Hinch, E. J., and Nitsche, L. C., 1995, "Computer Simulations of Brownian Motion of Complex Systems," *J. Fluid Mech.*, **282**, pp. 373–403.
- [26] Weibel, E. R., 1963, *Morphometry of the Human Lung*, Springer, Berlin.
- [27] Walters, D. K., Burgreen, G. W., Hester, R. L., Thompson, D. S., Lavalley, D. M., Pruett, W. A., and Wang, X., 2014, "Cyclic Breathing Simulations in Large-Scale Models of the Lung Airway From the Oronasal Opening to the Terminal Bronchioles," *ASME J. Fluids Eng.*, **136**(10), p. 101101.
- [28] Högberg, S. M., Åkerstedt, H. O., and Lundström, T., 2007, "Nanoparticle Transport and Deposition in Human Lung," *Interdisciplinary Transport Phenomena V: Fluid, Thermal, Biological Materials and Space Sciences*, Bansko, Bulgaria Paper No: ITP-07-17.