Journal of Aerosol Science 102 (2016) 105–127

Contents lists available at ScienceDirect

Journal of Aerosol Science

journal homepage: www.elsevier.com/locate/jaerosci

Characterization of aerosol Stokes number in 90° bends and idealized extrathoracic airways

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ARTICLE INFO

Keywords:
Particle deposition
Stokes number
Curved pipe
Respiratory airways
Direct numerical simulation (DNS)

ABSTRACT

Prediction of aerosol deposition in the respiratory system is important for improving the efficiency of inhaled drug delivery and for assessing the toxicity of airborne pollutants. Deposition is typically reported as a function of a global Stokes number which is based on a reference flow timescale, or the ratio of the characteristic flow length and velocity scales. In reality, however, particles experience varying flow timescales as they are advected through the airways, which motivates the use of an instantaneous Stokes number based on the local properties of the flow field. We then define the effective Stokes number as the time-average of the instantaneous value. This effective Stokes number thus encapsulates the flow history and geometric variability, and provides a more detailed account of the particle trajectory in the flow. Laminar and turbulent flows in a curved pipe are examined first and provide a simplified, or canonical, configuration of the flow in the upper airways. They are followed by a study of turbulent flow in an idealized mouth–throat geometry. Our results demonstrate that the effective Stokes number can deviate significantly from the traditional value based solely on the reference flow timescale. In addition, the effective Stokes number shows a clear correlation with deposition efficiency and can therefore be used to determine optimal aerosol release locations in order to minimize extrathoracic losses.

1. Introduction

Inhaled drug delivery is the main form of treatment for a number of respiratory diseases, such as asthma and chronic obstructive pulmonary disease (COPD). Knowledge of the aerosol deposition in the extrathoracic, or upper, airways is critical in the design of effective inhalation devices for optimum delivery to the lungs. The deposition is, however, highly dependent on the flow regime. In the upper airways, where the flow is turbulent or transitional, deposition occurs primarily via impaction as well as turbulent dispersion for the smaller particles. As the airways become smaller and the air velocity decreases, the flow laminarizes and deposition tends to occur due to sedimentation. For submicron particles in the small airways, Brownian diffusion becomes the dominant mechanism. The flow dynamics also vary significantly across subjects due to geometric variation of the airways, thereby resulting in large deviation in the deposition patterns and efficiencies (Grgic, Finlay, Burnell, & Heenan, 2004; Nicolaou & Zaki, 2013; Stahlhofen, Gebhart, & Heyder, 1981).

For efficient drug delivery to the target areas in the lung, the inhaled aerosol must first clear the mouth and throat. Often, however, large aerosol losses occur in this region. Therefore, in the optimization of inhaled drug delivery, many studies have focused

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http://dx.doi.org/10.1016/j.jaerosci.2016.09.003
Received 11 May 2016; Received in revised form 3 August 2016; Accepted 21 September 2016
Available online 25 September 2016
0021-8502/

on understanding and minimizing extrathoracic deposition. A number of *in vitro* experiments have examined the effects of particle size and flow rate on deposition in the mouth and throat (Cheng, Zhou, & Chen, 1999; Grgic, Finlay, & Heenan, 2004), as well as the effect of geometric variation (Grgic, Finlay, Burnell, et al., 2004; Heenan, Finlay, Grgic, Pollard, & Burnell, 2004). Advances in computing and numerical modelling techniques in the last decade have enabled increasingly more accurate simulations of the flow (Ball, Uddin, & Pollard, 2008; Heenan, Matida, Pollard, & Finlay, 2003; Lin, Tawhai, McLennan, & Hoffman, 2007; Nicolaou & Zaki, 2013) and aerosol deposition in the airways (Debhi, 2011; Jayaraju, Brouns, Verbanck, & Lacor, 2007; Kleinstreuer & Zhang, 2003; Li, Kleinstreuer, & Zhang, 2007; Matida, Finlay, Lange, & Grgic, 2004). The simulations can provide a detailed representation of the flow and the particle trajectories, compared to *in vitro* and *in vivo* studies. However, accurate and efficient prediction of the deposition remains challenging, due to the complexity of the airway geometries and of the flow. For this reason, many of the numerical studies on extrathoracic deposition have focused primarily on examining the suitability of various turbulence models and particle-tracking schemes (Debhi, 2011; Jayaraju et al., 2008; Matida et al., 2004; Stapleton et al., 2000).

Aerosols produced by inhalation devices are dilute dispersed flows which can be modelled using an Eulerian or a Lagrangian approach. The Eulerian, or two-fluid, approach treats the dispersed phase as a continuum, solving the conservation equations of particle mass and momentum. On the other hand, the Lagrangian approach treats the dispersed phase as a set of individual point-particles in a continuous carrier phase. The particles are tracked through the flow field by solving the equations of motion for each particle with the relevant forces acting on it. Description of turbulent dispersion and collision of particles with the airway walls is more natural with this approach. For this reason, the Lagrangian approach has featured prominently in studies of aerosol deposition in the airways (Debhi, 2011; Jayaraju et al., 2007; Kleinstreuer & Zhang, 2003; Li et al., 2007; Matida et al., 2004).

In order to characterize deposition in the extrathoracic airways a ‘lumped’ reference Stokes number, which is based on the mean diameter and mean flow velocity, is typically adopted in the literature. The deposition efficiency versus reference Stokes number, which follows an ‘S’ curve (Cheng et al., 1999; Grgic, Finlay, Burnell, et al., 2004), and deposition patterns for different particle sizes have been examined (Grgic, Finlay, Burnell, et al., 2004; Jayaraju et al., 2007; Zhang et al., 2002). Scatter in the deposition data can be observed when plotted against Stokes number, and is often attributed to the qualitative differences in the flow at different flow rates, and across subjects as a result of geometric variation. *In vitro* experiments performed by Grgic, Finlay, and Heenan (2004) in an idealized mouth–throat geometry showed that results at different flow rates appeared to lie on different curves, indicating a possible dependence on the Reynolds number. An empirical Reynolds number correction, $Re^{0.37}$, was applied to the Stokes number, collapsing their data onto one curve. Examination of the flow fields in a number of realistic mouth–throat geometries allowed Nicolaou and Zaki (2013) to explain the physical significance of this Reynolds number correction, which was attributed to at least two contributing factors: (1) the qualitative difference in the mean flow characteristics and (2) the difference in turbulence intensity. Using the viscous particle relaxation time, τ_p^+, they provided an explanation of the Reynolds number dependence.

The reference Stokes number, and even the Reynolds number correction, do not take into account the varying flow timescales that particles experience as they are advected through the flow. In order to better characterize the particle transport and deposition we therefore propose the use of an instantaneous Stokes number based on the local flow properties. We subsequently define the particle's effective Stokes number as the time-average of the instantaneous value. This effective Stokes number thus encapsulates the flow history and geometric variability, and is more representative of the particle trajectories. Laminar and turbulent flow cases in a curved pipe are considered first, followed by turbulent flow in an idealized mouth–throat geometry. In all cases, direct numerical simulations are performed and a Lagrangian–Eulerian approach is adopted for computing the particle trajectories.

The paper is organized as follows: In Section 2, the numerical method adopted for the solution of the flow equations and the particle tracking is described in detail, and the definitions of the instantaneous and effective Stokes numbers are introduced. In Section 3, results are presented for laminar and turbulent flow in a bent pipe, and for turbulent flow in an idealized mouth–throat geometry. Finally, Section 4 is a summary of the work and main findings.

2. Numerical method

2.1. Flow field

The Navier–Stokes equations are solved using a finite volume formulation, following the method by Rosenfeld, Kwak, and Vinokur (1991). Time integration is performed via a second-order semi-implicit fractional step method that uses Crank–Nicolson for the diffusive terms and Adams–Bashforth for the convective terms. The pressure Poisson equation is solved using a multi-grid algorithm with line-relaxation. Parallelism is achieved using message-passing interface (MPI). The algorithm has been adopted in a number of studies of transitional flows where accurately capturing the growth of flow instabilities is a primary consideration (Jung & Zaki, 2015; Zaki, 2013) and in direct numerical simulations of fully-turbulent flows where all the flow scales must be resolved (Jelly, Jung, & Zaki, 2014; Lee, Jung, Sung, & Zaki, 2013). Here too we perform direct numerical simulations which resolve all the flow scales, and therefore no turbulence modelling is necessary.

In order to model the complex airway geometries, a direct-forcing immersed boundary (IB) method developed for curvilinear grids is adopted (Nicolaou, Jung, & Zaki, 2015). The no-slip boundary condition at the airway walls is enforced via a momentum forcing term and mass conservation is satisfied via a mass source term in cells containing the immersed boundary. The discretized equations are given by

$$\frac{\hat{\boldsymbol{u}} - \boldsymbol{u}^{n-1}}{\Delta t} = -\left(\frac{1}{2}N(\boldsymbol{u}^{n-1}) + \frac{1}{2}N(\boldsymbol{u}^{n-2})\right) - \nabla p^{n-1} + \frac{1}{Re}\left(\frac{3}{2}L(\hat{\boldsymbol{u}}) - \frac{1}{2}L(\boldsymbol{u}^{n-1})\right) + \boldsymbol{f}^{n} \tag{1}$$