4th International Conference on Computational and Mathematical Biomedical Engineering - CMBE2015
29 June-1 July 2015, France
P. Nithiarasu and E. Budyn (Eds.)

ON THE STOKES NUMBER AND CHARACTERIZATION OF AEROSOL DEPOSITION IN THE RESPIRATORY AIRWAYS

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SUMMARY

Aerosol deposition in the respiratory airways has traditionally been examined in terms of the Stokes number based on the reference flow timescale. This choice leads to large scatter in deposition efficiency when plotted against the reference Stokes number because the velocity and length scales experienced by advected particles deviate considerably from the reference values. A time-average of the particle local Stokes number should be adopted instead. Our results demonstrate that this average, or effective, Stokes number can deviate significantly from the reference value, in particular in the intermediate Stokes number range where variation across subjects is largest.

Key words: *aerosol deposition, Stokes number, respiratory airways*

1 INTRODUCTION

Prediction of particle deposition in the respiratory airways is important for improving the efficiency of inhaled drug delivery and for assessing the toxicity of airborne pollutants. Studies have shown large inter-subject variation of aerosol deposition in the respiratory tract [1, 2]. Deposition efficiency in the extrathoracic airways was first described as a function of the inertial parameter, $\rho_p d_p^2 Q$, where ρ_p and d_p are the particle density and diameter respectively, and Q is the volumetric flow rate. However, large scatter was observed in the data, as the inertial parameter does not take into account the characteristics of the airway geometries.

Grgic et al. [3] claimed that the Stokes number, based on the mean diameter and mean flow velocity was a better parameter to describe deposition efficiency. Although deposition data showed better collapse when plotted against the Stokes number, scatter across subjects remained significant. This scatter arises due to the description of the Stokes number based on mean length and velocity scales. The diameter and velocity, however, differ considerably from the reference scales in many sections of the airways. Therefore, the effective Stokes number of a particle will vary appreciably as it is advected in the flow. Here we propose to adopt an effective Stokes number which is defined in terms of the local flow properties. We also demonstrate that the effective Stokes number of a particle does in fact deviate significantly from the reference value, in particular in the intermediate Stokes number range where inter-subject variability is most pronounced.

2 METHODOLOGY

2.1 Flow field

The flow equations are solved via an immersed boundary (IB) method developed for curvilinear grids [4]. A finite volume scheme is adopted, and time integration is performed via a second-order semi-implicit fractional step method (Crank-Nicolson for the diffusive terms and Adams-Bashforth for the convective terms). The discretized equations are given by

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

$$\nabla^2\phi^n=\frac{1}{\Delta t}\left(\nabla\cdot\hat{\boldsymbol{u}}-q^n\right) \quad (2)$$

$$\boldsymbol{u}^n=\hat{\boldsymbol{u}}-\Delta t\nabla\phi^n \quad (3)$$

$$p^n=p^{n-1}+\phi^n \quad (4)$$

where $\boldsymbol{f}$ is the momentum forcing vector added on the boundary and outside the fluid in order to satisfy no-slip at the immersed boundary, q is the mass source/sink applied to cells containing the immersed boundary in order to ensure mass conservation, $N(\boldsymbol{u})$ are the convective terms and $L(\boldsymbol{u})$ are the implicit diffusive terms.

2.2 Particle tracking

A Eulerian-Lagrangian approach is adopted to model particle transport and deposition. Particles are tracked through the flow field by solving their equation of motion,

$$m_p\frac{d\boldsymbol{u}_p}{dt}=\sum\boldsymbol{F}, \quad (5)$$

where m_p and $\boldsymbol{u}_p$ denote the particle mass and velocity respectively and $\sum\boldsymbol{F}$ represents all the forces acting on the particles. For particles in the micrometer range, the dominant forces are the aerodynamic drag and the gravitational force:

$$m_p\frac{d\boldsymbol{u}_p}{dt}=\frac{3}{4}\frac{\rho_f}{\rho_p}\frac{m_p}{d_p}C_D|\boldsymbol{u}-\boldsymbol{u}_p|\left(\boldsymbol{u}-\boldsymbol{u}_p\right)+m_p\boldsymbol{g}\frac{\rho_p-\rho_f}{\rho_p}, \quad (6)$$

where ρ_f is the fluid density and C_D is the drag coefficient. The correlation proposed by Schiller & Naumann [5] is adopted for the drag coefficient,

$$C_D=\frac{24}{Re_p}\left(1+0.15Re_p^{0.687}\right) \quad \text{with} \quad Re_p=\frac{\rho_f d_p|\boldsymbol{u}-\boldsymbol{u}_p|}{\mu_f}. \quad (7)$$

2.3 The effective Stokes number

An important parameter which characterises the motion of particles is the non-dimensional Stokes number, defined as the ratio of the particle response time to the characteristic time scale of the flow,

$$Stk=\frac{\tau_p}{\tau_f} \quad \text{where} \quad \tau_p=\frac{\rho_p d_p^2}{18\mu_f}. \quad (8)$$

Typically, a reference Stokes number is defined, based on the characteristic flow velocity U and length scale D,

$$Stk_{ref}=\frac{\rho_p d_p^2}{18\mu_f}\frac{U}{D}. \quad (9)$$

In the extrathoracic airways, for example, U can be the mean flow velocity and D the mean airway diameter.

Here we propose the use of a Stokes number based on the local properties of the flow field, following the definition by Trujillo & Parkhill [6]. The authors compared inertial particle advection to passive fluid advection by examining the eigenvalues of both systems, and derived an expression for the local, or instantaneous, Stokes number,

$$Stk_{inst}=\frac{\rho_p d_p^2}{18\mu_f}|\Lambda_i|_{max} \qquad (i=1,2,3), \quad (10)$$

where Λ_i are the eigenvalues of the velocity gradient tensor, $\nabla \boldsymbol{u}$. We define the effective Stokes number as the time-average of the instantaneous value,

$$Stk_{eff} = \frac{1}{T} \int_0^T Stk_{inst} \; dt, \tag{11}$$

where T is the period during which a particle remains in the flow.

3 RESULTS AND CONCLUSIONS

Figure 1a shows the deposition efficiency versus Stokes number in the extrathoracic airways. The large variation in total deposition across subjects is evident, in particular in the intermediate Stokes number range. The deposition efficiency in a curved pipe is plotted in figure 1b, and it follows the same trend as the S-curve observed in the extrathoracic airways. The red line marks the deposition efficiency versus Stk_{ref} whilst the blue line corresponds to Stk_{eff}. A significant deviation between the reference and effective Stokes numbers results is observed in the intermediate Stokes number range.

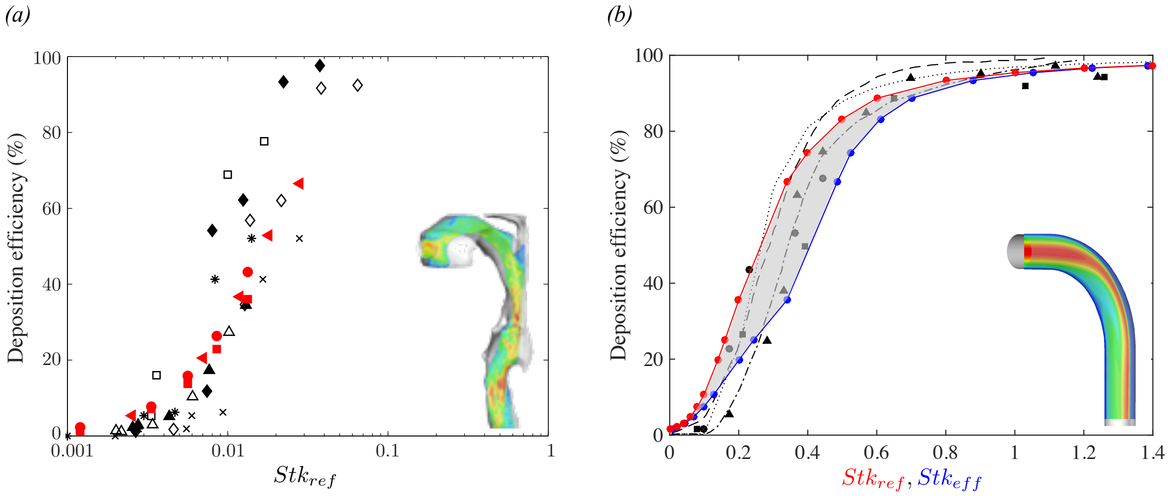

Figure 1: (a) Deposition efficiency versus Stokes number in (a) extrathoracic airways; (b) curved pipe at $Re_D = 1000$. Stk_{ref} in red and Stk_{eff} in blue. – – – [7]; ···· [8]; –·–· [9]; ▲; ■; ● [10].

Results from the bent pipe simulation with $Stk_{ref} = 0.2$ are shown in figure 2. The contours show the effective Stokes number of the particles visualized at their initial location. The spread in Stk_{eff} is evident. In figure 2b, only the particles that deposit are shown, and there is clear correlation with the higher Stk_{eff}. The probability density function of Stk_{eff} is plotted in figure 3, and is separated into two classes: particles that deposit which have a mean effective Stokes number, $\overline{Stk^d_{eff}} = 0.57$; and particles that remain in the flow whose mean effective Stokes number is $\overline{Stk^f_{eff}} = 0.21$.

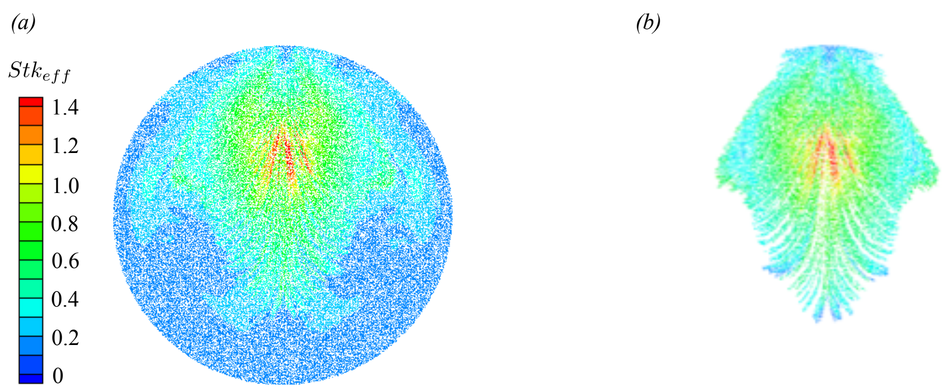

Figure 2: Particles at inlet coloured by the effective Stokes number for $Stk_{ref} = 0.2$. (a) All particles; (b) only deposited particles.

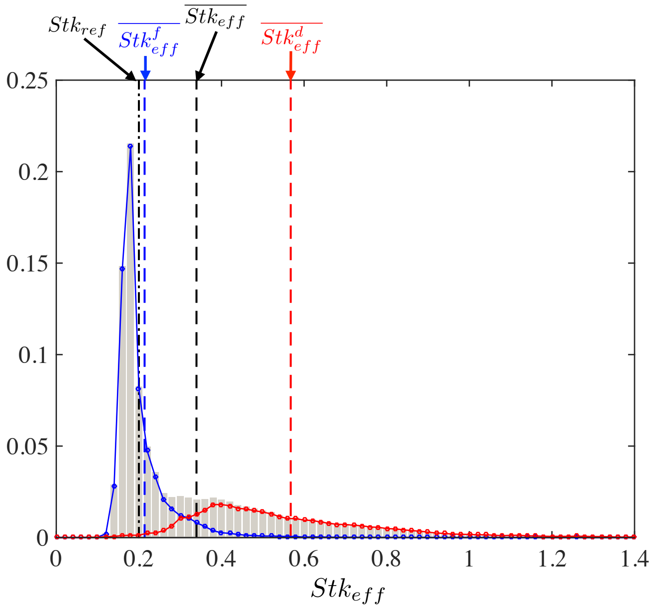

Figure 3: Pdf of effective Stokes number for $Stk_{ref} = 0.2$. ■ All particles; — particles not deposited; — deposited particles.

Based on the present results, part of the scatter observed in the extrathoracic deposition across subjects could be attributed to the use of a reference Stokes number as the deposition parameter. The reference Stokes number is based on a global characterisation of the flow field, while the local flow conditions experienced by the aerosol vary significantly from this reference value. The effective Stokes number, which is computed based on the local velocity gradient tensor, is the appropriate parameter to describe aerosol transport and deposition efficiency. We are currently adopting the definition of Stk_{eff} in an ongoing effort to better characterize aerosol deposition in the extrathoracic airways, and in particular intra- and inter-subject variations of deposition efficiency.

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