

Computational study of aerosol flow in bifurcations

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INTRODUCTION

Aerosol flows within the respiratory system are of great importance in order to assess the risk of airborne micro- and nano- particles deposition in the system and the benefit of pharmaceutical drugs inhalation. The former is related to the toxicity of the particles and possible lesions in the deposition sites and the latter to the efficiency and optimization of inhalation devices and pharmacologic aerosol therapy. In order to identify the aerosol mechanisms, which are most important for these flows, many researchers studied aerosol flows in bifurcations, since the shape of the bronchial trees can be approximated by successive bifurcations up to the alveolus. Thus, there are experimental (Myojo, 1987), theoretical (Gradon & Orlicki, 1990) and computational studies (Balásházy & Hofmann, 1993; Farkas & Balásházy, 2008; Zhang et al., 2009) of aerosol flows in a bifurcation. In the majority of the latter studies commercial Computational Fluid Dynamics (CFD) software are used to obtain the fluid flow field combined with user defined equations in the same codes (Nowak et al, 2003), Monte Carlo techniques (Balásházy & Hofmann, 1993) or Lagrangian formulation (Longest & Xi, 2007; Farkas & Balásházy, 2008) to solve for particle dynamics.

In the present work, a parametric study of aerosol flow in bifurcations is performed. In particular, the flow of monodisperse aerosol populations in a bifurcation is simulated using non-commercial CFD codes for the continuous and the particulate phase, where both particle diffusion and inertial effects are taken into account, using an Eulerian formulation of the particle General Dynamic Equation (GDE).

METHODS

The effect of inertia on Brownian diffusional transport, in isothermal aerosol flows, under steady state conditions, is explicitly considered through the low Stokes number expansion of the average momentum equation (Fernandez De La Mora & Rosner, 1982). As a result, a first-order correction to the particle velocity field due to particle inertia is obtained:

$$\vec{v}_p = \vec{v} - D\nabla \ln c - \tau_p (\vec{v} \cdot \nabla) \vec{v} + O(\tau_p^2), \quad (1)$$

where \vec{v} is the carrier gas velocity, c the particle concentration, D the Brownian diffusion coefficient and τ_p the particle relaxation time. In this case the GDE that describes the particle concentration c and its variation in space and time takes the form:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\vec{v}) - \tau_p \nabla \cdot [c(\vec{v} \cdot \nabla)\vec{v}] = \nabla \cdot D\nabla c, \quad (2)$$

that incorporates effects due to particle inertia to first order in the particle relaxation time, in an Eulerian description.

The non-commercial CFD code developed by Neofytou, 2005, which is used in the current study, utilises the finite volume method and is applied to the solution of the velocity and pressure fields of the carrier gas and subsequently the GDE (eq.(2)) for the particle size distribution. High order upwind discretisation schemes are used for the second and third term on the left hand side of eq.(2), whereas for the term on the right hand side central difference schemes are preferred.

With the use of the aforementioned computational tools, a parametric study of the aerosol flow in the bifurcation is performed. Inlet fluid and concentration profiles, fluid Reynolds number, bifurcation geometry and size and shape of the particles serve as parameters of our study. The numerical results of the present study are compared with solutions available in literature.

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