International Journal of Heat and Fluid Flow 61 (2016) 677–710

Contents lists available at ScienceDirect

International Journal of Heat and Fluid Flow

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

Direct numerical simulation of particle laden flow in a human airway bifurcation model☆

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ARTICLE INFO

Article history:
Received 16 February 2016
Revised 24 May 2016
Accepted 21 July 2016
Available online 9 September 2016

Keywords:
Turbulent flow
Human airway
Bifurcation
Steady inspiration
Steady expiration
Aerosol lung deposition

ABSTRACT

During the delivery of inhaled medicines, and depending on the size distribution of the particles in the formulation, airway bifurcations are areas of preferential deposition. Previous studies of laminar flow through airway bifurcations point to an interplay of inertial and centrifugal forces that leads to rich flow phenomena and controls particle deposition patterns. However, recent computational studies have shown that the airflow in the upper human airways is turbulent during much of the respiratory cycle. The question of how the presence of turbulence modifies these effects remains open. In this study, we perform for the first time Direct Numerical Simulations (DNS) of fully developed turbulent flow through a single human airway bifurcation model, emulating steady prolonged inspiration and expiration. We use the rich information obtained from the DNS in order to identify key structures in the flow field and scrutinize their role in determining deposition patterns in the bifurcation. We find that the vortical structures present in the bifurcation during expiration differ from those identified during inspiration. While Dean vortices are present in both cases, a set of three dimensional “carinal vortices” are identified only during expiration. A set of laminar simulations in the same geometries, but at lower Reynolds numbers, allow us to identify key differences in aerosol deposition patterns between laminar and turbulent respiration. We also report deposition fractions for representative Stokes numbers for both laminar and turbulent conditions. Given the suspected role of external mechanical stress on the airway epithelium in determining mucus clearance and chronic disease development, here we report wall shear stress distributions for both the turbulent and laminar cases. Finally, we also perform Large Eddy Simulations (LES) and Reynolds-Averaged Navier-Stokes (RANS) simulations for the same configuration in order to asses their performance as compared to DNS. We find that LES and RANS perform well and that they are able to capture the key characteristics of the flow field. The agreement between DNS and RANS holds true only for the mean flow field, which is primarily influenced by curvature effects.

1. Introduction

Predicting regional deposition patterns of inhaled aerosols is important for the design and optimization of pharmaceutical formulation-device products and for understanding the health effects of inhaled pollutants. The geometry of the airways greatly influences the local airflow structures, which in turn affect aerosol deposition. Geometrical variabilities in the respiratory tracts of patients, for example due to disease-induced airway remodeling, complicate the efforts to understand patterns of regional deposition and point towards the need for airflow analysis that is customized for specific patient classes.

In this regard, computer simulations can be used to predict regional deposition, thus helping in the development of targeted inhalation therapies that are customized, if not to individuals, at least to classes of patients. Such computations need to be based on realistic airway geometries, often obtained from patient CT-scans. They must also be able to handle reliably the unsteadiness and laminar-turbulent-laminar transition as one moves from the upper to the lower conducting airways. Furthermore, they need to be affordable for use in routine medical evaluations of patients. DNS are computationally too demanding for routine use, while

☆ **Video clips and high resolution figures made available online:** http://dx.doi.org/10.1016/j.ijheatfluidflow.2016.07.013

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http://dx.doi.org/10.1016/j.ijheatfluidflow.2016.07.013

LES is now becoming barely affordable. Thus, for routine computations the emphasis remains on the use of simplified modeling approaches, such as RANS closures. Nevertheless, DNS and LES can be used to elucidate the regional flow characteristics in the conducting airways, thus helping to ensure that RANS computations are properly designed and tuned to capture the most important flow features.

The upper airways are composed of building blocks that can be represented by idealized geometries in benchmark studies, e.g. straight and bent pipes, tubular constrictions and expansions, and single bifurcations. For most of the aforementioned building blocks, RANS models can be validated, and if necessary tuned, using turbulent benchmark data in the scientific literature. The single bifurcation geometry is an exception.

To the best of our knowledge, turbulent flow through a bifurcation was never reported in the scientific literature. The aim of the present study is to use DNS and LES to characterize in detail the flow structures and particle deposition patterns in a human airway bifurcation model. RANS simulations are also performed and evaluated against the DNS and LES results, while Laminar simulations are carried out in an effort to identify turbulence-induced and laminar effects. In all cases, we compare and discuss the flow field and the deposition patterns. We note that our results may not be fully representative of those occurring in the lungs, where single isolated bifurcations do not occur.

2. Review of previous studies

The review papers by Hofmann (2011), Kleinstreuer and Zhang (2010) summarize the important studies related to the broader area of airflow and particle transport in the human lung. Here, we outline the main contributions in the literature that treat exclusively the case of particle laden flow in airway bifurcations under steady inhalation or exhalation conditions. For oscillatory flow the reader is referred to the experimental work of Jan et al. (1989), Lieber and Zhao (1998), Ramuzat and Riethmuller (2002), and the numerical work of Zhang et al. (2002c), Zhang and Kleinstreuer (2002), Zhang et al. (2002d), Choi et al. (2010).

The early experimental studies of Kim, Iglesias, and Garcia were the first to report Deposition Efficiencies (DE) and Deposition Patterns (DP) of micron-size particles in Y-shaped glass tube models. Under steady inspiration Kim and Iglesias (1989) found that particle deposition occurred mainly near the bifurcation and increased with increasing Stokes number. Branching asymmetry and flow distribution patterns did not affect the DE. Furthermore, only for large branching angles did the DE increase. Under steady expiration, Kim et al. (1989) found that particle deposition occurred principally in a short section of the parent tube immediately proximal to the bifurcation and increased with increasing flow rate, particle size, or branching angle. In addition, Kim et al. (1994) found that particle deposition took place mainly on and in the immediate vicinity of the bifurcation ridge. DE in the bifurcation region increased with increasing *St*, while the daughter to parent diameter ratio showed only a minor effect on DE. They concluded that *St* may be the single most important factor for particle deposition in the bifurcating airways in the inertial regime.

Zhao and Lieber were the first to analyze the flow field in a symmetric bifurcation model with constant cross sectional area, under laminar steady inspiration (Zhao and Lieber, 1994b) and steady expiration (Zhao and Lieber, 1994a) conditions. Fresconi et al. (2003) focused on the characteristics of the secondary flow in a Y-shaped bifurcation, also during expiration. Their results (at Reynolds number falling in the transitional regime) illustrate unsteadiness, associated with a hairpin vortex, and symmetry-breaking of the flow field.

Considering steady inspiration in the laminar and transitional flow regimes, Kim and Fisher (1999) investigated the local DE and DP of aerosol particles in sequential double bifurcation tube models. They examined two different branching geometries for the second bifurcation (in-plane and off-plane) and they found the DE in the second bifurcation to be comparable to those in the first bifurcation; the Stokes number *St* was again found to be the strongest determinant of DP.

At the same time, a number of numerical studies have also contributed to our overall understanding of the flow and deposition phenomena taking place in human airway bifurcations, mostly under laminar conditions. For inspiratory flow, Balásházy and Hofmann (1993b) reported particle deposition hot spots at carinal ridges, while in the case of expiratory flow (Balásházy and Hofmann, 1993a) reported particle deposition hot spots downstream of the central bifurcation zone. Subsequently, Balásházy et al. (1996) discussed the effects of different airway bifurcation geometries (narrow vs smooth central zone) on the resulting airflow fields and particle DP. Comparing the results of narrow and smooth bifurcation models they found reduced skewness of the inspiratory flow in the daughter branches, smaller secondary velocity components, and regions of reverse flow in the vicinity of the carina in the smooth model. Under inspiratory breathing conditions Balásházy et al. (1999) computed the local deposition enhancement factors (ratio of local to average deposition densities) and identified regions of highly localized depositions.

At about the same time, a series of numerical studies were performed in multi-level bifurcations. For example, Heistracher and Hofmann (1997) examined the flow and particle deposition sites in a symmetric double bifurcation. They observed distinct asymmetries in air mass transport and DP between the branches of the second bifurcation. Subsequently, Hofmann et al. (2001) analyzed the relationship between localized fluid dynamics and localized particle DP within bronchial airway bifurcations upon inspiration and expiration, for different bifurcation geometries, flow conditions, and particle sizes. They observed a distinct relationship between secondary flow patterns and deposition density plots, demonstrating that particle DP in airway bifurcations are not only determined by physical forces acting upon individual particles, but also by convective transport processes of the carrier fluid.

Comer et al. (2001b) analyzed extensively the airflow in double bifurcation models, under planar and non-planar configurations, with rounded and sharp carinal ridges. In the same geometries, Comer et al. (2001a) reported particle trajectories and DP. At low Reynolds numbers, the particles followed the axial airflow, while at higher Reynolds numbers, the secondary and vortical flows became important, causing the formation of particle-free zones near the tube centers and subsequently elevated particle concentrations near the walls.

Liu et al. (2002) examined the inspiratory flow characteristics in symmetric double bifurcations with in-plane and off-plane geometrical configurations. Particular attention was paid in establishing relations between the Reynolds number and the overall flow characteristics, including flow patterns and pressure drop. Afterwards, Liu et al. (2003) carried out a similar investigation for asymmetric bifurcations.

Zhang et al. (2002a), Zhang et al. (2002b) examined particle DP and efficiencies in a triple bifurcation under cyclic as well as steady state inhalation conditions. The resulting particle DP were analyzed and then summarized in terms of DE. In addition, they developed particle maps that show the release positions of deposited aerosols.

Balásházy et al. (2003) computed particle DP in lobar-segmental airway bifurcations and quantified the resulting inhomogeneous DP in terms of deposition enhancement factors. Their results revealed that a small fraction of epithelial cells located at carinal