European Journal of Mechanics B/Fluids 63 (2017) 73–89

Contents lists available at ScienceDirect

European Journal of Mechanics B/Fluids

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

Simulation of aerosol particle deposition in the upper human tracheobronchial tract

Andreas Lintermann [a,*], Wolfgang Schröder [a,b]

[a] Jülich Aachen Research Alliance, High Performance Computing (JARA-HPC), RWTH Aachen University, Kopernikusstr. 6, 52074 Aachen, Germany

[b] Institute of Aerodynamics, RWTH Aachen University, Wüllnerstr. 5a, 52062 Aachen, Germany

ARTICLE INFO

Article history:
Received 31 March 2016
Received in revised form
27 October 2016
Accepted 16 January 2017
Available online 20 January 2017

Keywords:
Euler–Lagrange Lattice-Boltzmann method
Particle deposition
Respiration
Small and large particles

ABSTRACT

The deposition of aerosol particles, e.g., fine dust particles, diesel aerosols, or wood dust, in the human lung is responsible for many respiratory diseases. Small respirable particles can cause inflammations of the bronchi, coughing, allergic reactions, and even lung cancer. The deposition of such aerosols in a realistic model of the upper human tracheobronchial tract is investigated by a one-way coupled *Euler–Lagrange* approach for the particle flow in the respiratory system. The flow is simulated by a *Lattice-Boltzmann Method* and the aerosols are tracked by a particle solver. Two cases are investigated. The first simulation considers heavy and large particles with a diameter of 100 μm representing situations with a reduced filtering function of the nasal cavity or air conditions found in coal mines and in carpenter's workshops. The second computation tracks a particle mixture with a diameter range of 2.5–10 μm including lighter and heavier aerosols in the human lung. The analysis of the particle deposition shows that 32% of the heavier and larger particles deposit deeper in the airways, while for the particle mixture only 6.9‰ deposit in the primary, lobar, and segmental bronchi. This investigation reveals that small and light particles penetrate into lung regions below the sixth generation where they can cause severe damage in the bronchi. Their distribution in the lung is mainly influenced by the flow and is independent of the particle diameter and density range that is used in this study. Large and heavy particles preferably deposit at bifurcations due to the carrier flow impinging on the tissue and due to particle inertia.

1. Introduction

Fine dust particles originate from natural and man-made processes, e.g., volcanic activity, fires, traffic, and industry, and are heavily found in urban environments. The inspiration of such particles may cause serious pathologies in the human lung [1]. Individuals living in municipal zones are endangered of contracting bronchitis, adenocarcinoma, and lung cancer due to air pollution. Despite the cleaning mechanism of the nasal cavity, small scale particles on the order of 10 μm, i.e., particulate matter (*PM*), may reach the human lung and deposit in the bronchi. Depending on the substances, the particles may induce free radicals which damage the cell structure and may hence lead to cancer. For example, Raaschou et al. [1] investigated the correlation of air pollution and lung cancer incidents in 17 cohorts in 9 European countries. Their findings show that PM_{10} and $PM_{2.5}$ with particle diameters smaller than 10 and 2.5 μm have an increased hazard risk. Such particle sizes not only appear in fine dust caused by traffic, but are also found in volcanic ash. Therefore, Pitz et al. [2] investigated the ash distribution caused from the eruption of the Eyjafjallajökull volcano in Iceland, which covered vast regions of Europe in 2010. The investigations at ground level were performed in Augsburg, Germany and showed a strong increase of PM_1 up to PM_4. Hence, even remote zones can be affected by such global incidents.

In-vivo investigations on particle depositions in the human lung as performed, e.g., in [3,4] often suffer from limited spatial and especially temporal resolution and do not account for the tracking of individual particles. In contrast, *Computational Fluid Dynamics (CFD)* methods can be used to determine the flow in the human lung [5–7] and to predict the corresponding deposition of individual *PM*s [8–15]. For such investigations different geometries of the human lung are used that are either based on artificial branching methods, 1D space-filling methods, or on the information obtained from *Computer Tomography* (*CT*) or *Magnet Resonance Imaging* (*MRI*). In Soni et al. [11,14] and Walters et al. [13] the models are based on a *Weibel* geometry [16], which

* Corresponding author. Fax: +49 241 80 92257.
E-mail addresses: Lintermann@jara.rwth-aachen.de (A. Lintermann), office@aia.rwth-aachen.de (W. Schröder).

http://dx.doi.org/10.1016/j.euromechflu.2017.01.008

successively branches in an artificial manner, i.e., circular pipes branch and successive generations are rotated by a previously defined angle. Soni et al. [11,14] use a hybrid *Finite-Element (FE)/Finite-Volume (FV)* solver to simulate the flow, while Walters et al. [13] use *ANSYS Fluent* for their computations. Both studies apply a Reynolds number of $Re = 319$ based on the diameter of the fourth generation inlet, the kinematic viscosity of air, and a volume flux of 20.83 ml/s. The resulting flow was analyzed by considering the pressure drop, velocity profiles, and the mass flux distribution. Furthermore, the transport of spherical particles with a diameter of 10 μm is performed in [11,14], while in [13] the deposition of 5, 15, and 20 μm particles is additionally investigated. Both studies reveal that PM_{10} have a low deposition likelihood in the first 11 generations, while particles of size 15 and 20 μm have an increased deposition likelihood. However, the *Weibel* model represents an idealized scenario and the results miss a transfer to realistic geometries.

Unlike in the aforementioned literature, the investigations in [8–10,15] use a bifurcation airway model [17] to simulate the flow and the particle dynamics. Worth Longest and Vinchurkar [8] investigate the effects of upstream transition and turbulence on the aerosol deposition for steady inspiration at 60 L/min, i.e., for heavy exertion, using 10 μm particles. They solve the *Reynolds-averaged Navier–Stokes (RANS)* equations with a k–ω and a *low-*Reynolds *number* (*LRN*) k–ω turbulence model [18,19] with *ANSYS Fluent 6.0* and show that the transitional flow influences the particle deposition behavior. Kleinstreuer and Zhang [9] and Zhang et al. [10] performed *RANS* computations of the flow with *ANSYS CFX* by using a *LRN* k–ω turbulence model. They simulated nano and micron non-interacting particles in a 16-generation lung model at a volume flux of 30 L/min [9] and 15 and 30 L/min [10]. They compare the deposition behavior to results obtained from a semi-analytical approach and found good agreement between the two methods w.r.t. to the whole respiratory tract. However, the findings concerning the local deposition behavior at bifurcations disagree due to the geometrical influence on the flow. Feng and Kleinstreuer [15] additionally model the particle–particle interaction using the *dense discrete model* with the *discrete element method* (*DDPM–DEM*) of *ANSYS Fluent 14.0* and compare the results to those obtained by different *computational fluid–particle dynamics*(*CF-PD*) models. Based on the investigations in [20], in which laminar flow was assumed, they chose a mesh consisting of approximately $0.65 \cdot 10^6$ cells for their computations. The simulations cover volume fluxes of 30 L/min and 60 L/min for which in [8–10] turbulent flow conditions were assumed. No mesh dependence study for transitional to turbulent flow is presented and hence it is not clear if unsteady secondary vortices are captured by the simulations in [15].

Unlike the investigations in [7–11,13–15], Taherian et al. [12] use a realistic 5-generation lung geometry. The model is obtained from *MRI* and *CT*. They apply an implicit *unsteady RANS* (*URANS*) solver with a k–ω turbulence model integrated into the *STAR CCM+ CFD* software environment. They assume a turbulence intensity of 1% for flow rates of 62.5, 125, and 250 ml/s and consider the transport of heavy particles with diameters of 1 μm, 5 μm, and 10 μm. The flow analysis is based on the turbulent kinetic energy, the mean velocity, and the velocity vectors. The particle deposition is characterized by the ratio of the released to deposited particles under a varying Stokes number for the different volume fluxes. Unfortunately, the investigations in [12] lack a detailed discussion of the results. Corley et al. [21,22] also use realistic geometries that stem from *CT* data. They simulate the flow in the human respiratory tract using the *OpenFOAM* software on $0.52 \cdot 10^6$ and $1.1 \cdot 10^6$ cells. In both investigations the transport of small scale molecules are modeled by additionally solving a scalar transport equation. That is, the distribution of the ingredients of cigarette smoke, i.e., acrolein, acetaldehyde, and formaldehyde are simulated in the respiratory tract. Since such molecules are smaller compared to particles sizes found in fine dust, tracking of individual particles and including the effects of particle drag is not necessary. However, when considering $PM_{2.5}$–PM_{10}, as done in the current study, this effect should not be neglected. Since *RANS* computations only yield time-averaged solutions, unsteady flow features cannot be captured by this method. Furthermore, it has to be stated that the solutions depend on the constants for the k–ϵ and k–ω turbulence models. Therefore, Choi et al. [23] and Zhang and Kleinstreuer [24] used *Large-Eddy Simulations* (*LES*) to simulate respiratory flows with the Smagorinsky [25] and the wall-adapted local eddy-viscosity (WALE) [26] subgrid-scale models. In [23] the flow in the upper respiratory and tracheobronchial tract up to the 4th lung generation is considered. The geometry is obtained from *CT* data and the investigations mainly focus on an analysis of the laryngeal jet and do not consider the fate of inhaled particles. Zhang and Kleinstreuer [24] use *LES* computations to evaluate the applicability of *RANS* models for the computation of the flow in an artificial model of the upper human airway. By comparing the results to experimental findings they show that *RANS* computations using the standard k–ω turbulence model cannot compete with *LES* computations. For time-averaged flow computations, however, the results for the *LRN* k–ω and the *Shear–Stress Transport* (*SST*) transition model were comparable to those of the *LES*. In addition, they also simulated nano-scale particles by solving a convection–diffusion mass transfer equation, i.e., like in [21,22] no individual particles are tracked.

To get a more detailed insight into the impact of the intricate flow structure on the general deposition behavior of *PM* within a diameter range of 2.5–100 μm in realistic geometries, highly resolved simulations are performed by a *Lattice-Boltzmann Method* (*LBM*). To avoid any kind of impact that is due to eddy viscosity or subgrid-scale modeling no turbulence models as used in *RANS* or *LES* approaches are considered in the formulation of the problem. The current approach is to spatially and temporally highly resolve the flow field by the *LBM* such that the flow structures that are determined by the discrete form of the conservation equations of a viscous fluid are directly captured. The *LBM* is also well known to have good scalability properties, i.e., simulations can be performed very efficiently [27], and the implementation of boundary conditions is straightforward unlike, e.g., in *FV* methods, where complex cut-cell methods [28] are necessary to accurately prescribe wall-boundary conditions. The simulations presented in this paper can be considered an immediate multiphase flow extension of the analysis in [5,6]. In contrast, Trunk et al. [29] who use an *Euler–Euler* approach for the *LBM*-particle simulation in bifurcating pipe geometries the present approach is similar to that of [30], which also uses an *Euler–Lagrange* approach for the analysis of particle depositions in the human nose. That is, the present algorithm also uses the communication-optimal strategy for parallelization that has been shown to be more efficient for complex geometries [30]. Particles are tracked by coupling a particle solver to the *LBM* and by releasing $15 \cdot 10^3$ particles at the trachea inlet into a converged steady solution of the flow in the human lung that was computed on $22.35 \cdot 10^6$ cells. The simulations are performed for two different particle sizes. The first simulation considers particles with a diameter range of 2.5–10 μm, i.e., respirable fine dust particles found in traffic exhaust gases. The second simulation tracks large particles with a diameter of 100 μm in the human lung and represents cases in which the filtering function of the nasal cavity is reduced or the inhaled air is highly loaded by such particles, e.g., as found in the ambient air in coal mines or in carpenter's workshops [31].

This paper is organized as follows. The numerical method for the simulation of the flow, the boundary conditions, the method to