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Micron-particle transport, interactions and deposition in triple lung-airway bifurcations using a novel modeling approach

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ABSTRACT

Particulate suspensions inhaled by humans are typically dilute and hence interactions between particles can be neglected. In such cases conventional Euler–Lagrange or Euler–Euler methods are suitable to simulate micron- or nano-particle transport and deposition in human respiratory systems. However, when challenging conditions, such as large pressure differentials, high velocity gradients and/or intense particle collisions, exist, alternative approaches for numerical analysis are required to capture fluid–particle, particle–particle, and particle–wall interactions. In the present study, the dense discrete phase model (DDPM) in conjunction with the discrete element method (DEM) have been employed to simulate micron–particle transport, interaction and deposition dynamics in different triple bifurcations (i.e., G3–G6, G6–G9, and G9–G12), using ANSYS Fluent 14.0 enhanced by user-defined functions (UDFs). In light of the relatively high computational cost when employing DDPM–DEM for such simulations throughout the human respiratory system, it may be necessary to combine different computational fluid–particle dynamics (CF–PD) models based on the *local intensity* of particle–particle interactions. Thus, the validity and necessity of the DDPM–DEM approach for different lung airway generations were numerically investigated, considering new parametric criteria for the use of most suitable numerical models. Specifically, the relative intensities of three major particle deposition mechanisms (i.e., inertial impaction, secondary-flow effect, and particle–particle-interaction impact) in idealized lung-airway segments were investigated. As a result, a new criterion for CF–PD model combination in terms of a relationship between inlet-particle stacking-volume fraction, ϕ, and percentage-of-fate changing particles, $\Delta\beta_p$, is proposed. Visualizations of the fluid–particle dynamics in bifurcating airways have been provided as well. Results of this study pave the way for accurate and cost-effective CF–PD simulations of lung-aerosol dynamics, aiming at the improvement of respiratory dose estimation for health risk assessment in case of toxic particles and for treatment options in case of therapeutic particles.

1. Introduction

Accurate simulation of airflow structures and related aerosol deposition in realistic models of the human respiratory system, using computational fluid–particle dynamics (CF–PD), are of fundamental importance (Kleinstreuer & Feng, 2013).

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Nomenclature

$d_{p,eq}$	equivalent particle diameter
d_p	particle diameter
D_{in}	inlet diameter
DE	deposition efficiency
E_{eq}	equivalent Young's modulus
$\vec{F}_{c,ij}$	inter-particle contact force between particle i and particle j
$\vec{F}^{n}_{c,ij}$	normal contact force between particle i and particle j
$\vec{F}^{t}_{c,ij}$	tangential contact force between particle i and particle j
$\vec{F}_{D,i}$	drag force acting on particle i
$\vec{F}_{pf,i}$	fluid–particle interaction forces acting on particle i
$\vec{F}_{g,i}$	the gravity of particle i
G	the particle's shear modulus
k_n	normal stiffness
k_v	the number of particles in the specific mesh cell
M_{layer}	initial stacking-layer number of particles
N_{in}	the total number of particles released at the inlet
$\vec{R_{sl}}$	volumetric fluid–particle interaction force
Re_{in}	inlet Reynolds number
St	Stokes number
Δt_p	discrete-phase time step
$\vec{v}_{pn,ij}$	normal component of the relative velocity $\vec{v}_{p,ij}$ between particle i and particle j
$\vec{v}_{pt,ij}$	tangential component of the relative velocity vector between particle i and particle j

Greeks

α_f	fluid volume fraction
$\Delta\beta_p$	percentage of fate changing particles
δ	unit tensor
δ_{nij}	normal overlap distance between contacting particle i and particle j
ε	the coefficient of restitution
η_{nij}	normal damping coefficient
σ	Poisson's ratio
$\vec{\tau}_f$	local stress tensor
ϕ	inlet particle stacking volume fraction

Subscripts and superscripts

c	contact force
f	fluid phase
i	particle index i
in	inlet
j	particle index j
n	normal direction
p	particulate phase
t	tangential direction

For the inhalation of micron particles, most will typically deposit before passing through the trachea due to inertial impaction and strong turbulent dispersion in the oral region and nasal cavities. The remaining particle suspension is dilute when entering the tracheobronchial airways so that particle–particle interacting mechanisms can be neglected. In such cases conventional Euler–Lagrange methods are accurate for the prediction of particle transport and deposition in lung airways. However, when high concentrations of air pollutants are inhaled or dense drug particle suspensions are delivered for lung or systemic disease targeting, particle–particle and particle–wall interactions are the dominant features which strongly influence particle transport and deposition in lung airways (Aljuri et al., 2012; Kleinstreuer et al., 2008; Tong et al., 2010). Conventional Euler–Lagrange methods (i.e., discrete phase models (DPMs)) are not suitable for dense fluid–particle flows because of the restriction on the volume fraction of the discrete phase. Such numerical DPMs do not consider explicitly the contact between the fluid, particles and wall surfaces with respect to particle inertial and material properties. Additionally, two-way coupling is necessary for dense particle-suspension flows in complex conduits. The use of the discrete element method (DEM) will ensure realistic particle flow. It was first proposed by Cundall & Strack (1979), based on molecular dynamics. The most attractive feature of DEMs is the highly efficient algorithms of the contact detection and contact force calculation between arbitrary shaped particles (Wang et al., 2010). The dense discrete phase model (DDPM) combined with DEM is one of the CF–PD modeling approaches discussed by Tsuji et al. (1992, 1993). Specifically, with CFD–DEM which is similar to DDPM–DEM, the motion of translating and interacting particles is described by DEM, based on Newton's second law, while the DDPM describes the fluid flow field, determined by a solution of the local averaged Navier–Stokes equations. The coupling between the discrete and continuous phases can be achieved via an interphase interaction term in the Navier–Stokes equation (Kafui et al., 2002). Thus, in DDPM–DEM the motion of each particle is analyzed by incorporating the contact forces and the moments due to the neighboring particles. This method has gained a prominent application in the modeling of fluidized beds (Alobaid et al., 2012; Li et al., 2012; Neuwirth et al., 2012), as well as multi-scale strategy achievement which combines different numerical models that describe gas–solid flows at different levels of detail (e.g., DNS, DEM, and DPM) (Di Renzo et al., 2011; Van der Hoef et al., 2008). The coupling algorithm of DDPM–DEM is presented by Fig. 1. More recent applications include the investigation of dense powder dispersion in drug-aerosol inhalers (Tong et al., 2010, 2012), as well as pulmonary drug delivery, as discussed by Chen et al. (2012). Specifically, its application to inhaler development has largely been focused on investigating pharmaceutical agglomerate break-up in dry powder inhalers (Wong et al., 2012). For example, Tong et al. (2010, 2012) recently employed ANSYS Fluent with in-house user-defined functions (UDFs) to powder dispersion in a commercial Aerolizer® Inhaler model. Chen et al. (2012) employed the one-way and two-way DDPM–DEM methods for particle transport and deposition in a pulmonary airway bifurcation. They