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DDPM-DEM Simulations of Particulate Flows in Human Tracheobronchial Airways

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ABSTRACT

Dense particle-suspension flows in which particle-particle interactions are a dominant feature encompass a diverse range of industrial and geophysical contexts, e.g., slurry pipeline, fluidized beds, debris flows, sediment transport, etc. The one-way dispersed phase model (DPM), i.e., the conventional one-way coupling Euler-Lagrange method is not suitable for dense fluid-particle flows [1]. The reason is that such commercial CFD-software does not consider the contact between the fluid, particles and wall surfaces with respect to particle inertia and material properties. Hence, two-way coupling of the Dense Dispersed Phase Model (DDPM) combined with the Discrete Element Method (DEM) has been introduced into the commercial CFD software via in-house codes. As a result, more comprehensive and robust computational models based on the DDPM-DEM method have been developed, which can accurately predict the dynamics of dense particle suspensions.

Focusing on the interaction forces between particles and the combination of discrete and continuum phases, inhaled aerosol transport and deposition in the idealized tracheobronchial airways [2] was simulated and analyzed, generating more physical insight. In addition, it allows for comparisons between different numerical methods, i.e., the classical one-way Euler-Lagrange method, two-way Euler-Lagrange method, EL-ER method [3], and the present DDPM-DEM method, considering micron- and nano-particle transport and deposition in human lungs.

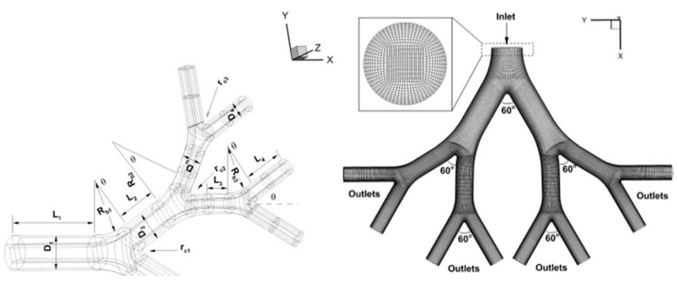
GEOMETRY AND MESH

A representative triple bifurcation bronchial airway model was selected to test the suitability of the DDPM-DEM method (see Fig. 1). The dimensions of the triple bifurcating geometry are for adults with a lung volume of 3500 mL. To represent bifurcating airways starting from different generations, the triple bifurcating airway geometry was scaled to duplicate the hydraulic diameter D_1 of the first bifurcation (see Fig. 1(a)) of different generations. For example, D_1=0.6cm represents the G3-G6 bifurcating lung airways, while D_1=0.026cm represents the G6-G9 bifurcating lung airways.

For the numerical simulation a structured, multi-block, body-fitted hexahedral mesh was developed (see Fig. 1(b)). Mesh independence tests have been successfully executed and presented in published papers [3]. The final mesh contained 628,712 cells, 655,822 nodes, and 1,912,466 faces.

DDPM-DEM GOVERNING EQUATIONS

For dense particle-suspension transport and particle deposition in lung airway bifurcations it is assumed that the airflow field is laminar and incompressible. The transient 3-D DDPM-DEM method is executed as follows.



(a) **(b)**

Fig. 1: (a) Configuration of Weibel's triple bifurcating airway geometry (b) Finite volume mesh of Weibel's triple bifurcating lung airway geometry

DDPM Governing Equations for Continuous Phase:

$$\frac{\partial\left(\alpha_f \rho_f\right)}{\partial t}+\nabla\cdot\left(\alpha_f \rho_f \vec{v}_f\right)=0 \quad (1)$$

$$\frac{\partial\left(\rho_f \alpha_f \vec{v}_f\right)}{\partial t}+\nabla\cdot\left(\alpha_f \rho_f \vec{v}_f \cdot \vec{v}_f\right)=-\alpha_f \nabla p+\nabla\cdot\left(\alpha_f \vec{\tau}_f\right)+\alpha_f \rho_f \vec{g}-\vec{R_{sl}} \quad (2)$$

Here, α_f is the porosity, $\vec{\tau}_f$ is the local stress tensor, and $\vec{R_{sl}}$ is the volumetric fluid-particle interaction force which can be expressed as:

$$\vec{R_{sl}}=\left(\sum_{i=1}^{k_V}\vec{F}_{D,i}\right)/\Delta V \quad (3)$$

where index k_v is the number of particles in the specific mesh cell, ΔV is the volume of the current mesh cell, and $F_{D,i}$ is the drag force.

DEM Translational Equation for Discrete Phase:

Due to the relatively small dimension of, say, micron particles, only the translational equation for the dense particulate discrete phase was considered, i.e.,

$$m_{p,i}\frac{d\vec{v}_{p,i}}{dt}=\sum_j\left(\vec{F}_{cn,ij}+\vec{F}_{dn,ij}+\vec{F}^t_{c,ij}\right)+\vec{F}_{D,i}+\vec{F}_{g,i} \quad (4)$$

The normal contact force $\vec{F}_{cn,ij}$, normal damping force $\vec{F}_{dn,ij}$, tangential contact force $\vec{F}^t_{c,ij}$, and Stokes drag force $\vec{F}_{D,i}$ are:

$$\vec{F}_{cn,ij}=-k_n\delta_{nij}^{3/2}\vec{n}_{ij} \quad (5)$$

$$\vec{F}_{dn,ij}=-\eta_{nij}\vec{v}_{pn,ij} \quad (6)$$

$$\vec{F}^{t}_{c,ij} = \mu_{friction} \left|\vec{F}^{n}_{c,ij}\right| \vec{v}_{pt,ij} / \left|\vec{v}_{pt,ij}\right| \quad (7)$$

$$\vec{F}_{D,i} = \left(\pi d_{p,i}^{2}/8\right) C_D \rho_f \left(\vec{v}_{p,i} - \vec{v}_f\right)\left|\vec{v}_{p,i} - \vec{v}_f\right| \quad (8)$$

The details for the force calculations are given in [3].

NUMERICAL SET-UP

The governing equations, subject to appropriate boundary conditions, were numerically solved using Fluent 14.0 enhanced by in-house user-defined functions (UDFs). To guarantee there is no inlet airflow effect, a fully-developed parabolic velocity profile was assumed. The averaged inlet Reynolds number was either 1000 or 2000. A random-parabolic distribution of micron particles at the inlet was invoked. Pressure outlet boundary conditions were employed.

RESULTS AND DISCUSSION

Comparison between DDPM-DEM and DPM:

As compared to experimental data, Figs. 2 (a) and (b) show that the combined DDPM-DEM accurately predicts the transport and deposition of dilute particle suspensions (here, less than 1.85%) in the G3-G6 bifurcating lung airways. Additionally, because the DDPM-DEM takes into account particle–particle interactions, it will be more accurate in simulating severe conditions, such as large pressure differentials, high velocity gradients, and intense particle collisions. It should be noted that the DPM results by Chen et al. [4] are somewhat off for various reasons, as discussed by Feng [3].

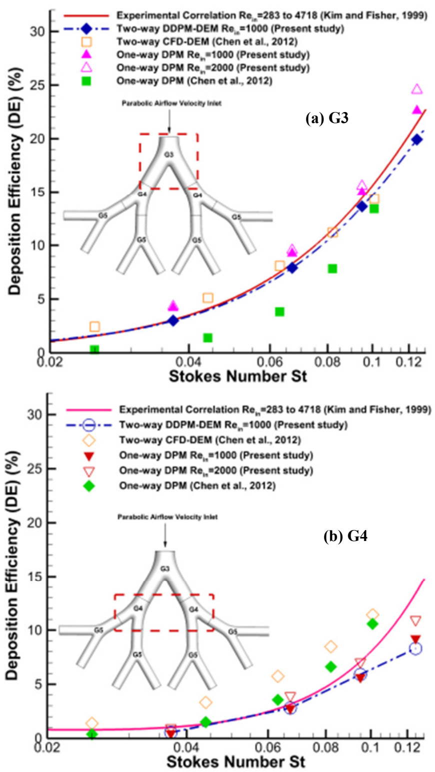


Fig. 2: Comparison between computational data using different numerical methods and measured particle deposition efficiency data correlation [1] for the first

Deposition Patterns:

Figures 3(a) and 3(b) depict deposited micron particles (d_p=10μm) at G3 to G6 for different Stokes numbers. Particle deposition occurs at the stagnation points due to direct impaction and gravitational sedimentation. The asymmetric particle deposition patterns are due to the particle-particle contact interaction, and random particle inlet distribution. Clearly, higher Stokes numbers induce a stronger impaction effect on particle deposition.

Transport Characteristics:

Particle transport patterns at different time steps are shown in Figs. 4(a) to 4(f). The particles obtained similar velocity distributions during the air-solid coupling process. The impaction and particle splash near the first bifurcation can be observed clearly from Figs. 4(c) and 4(d).

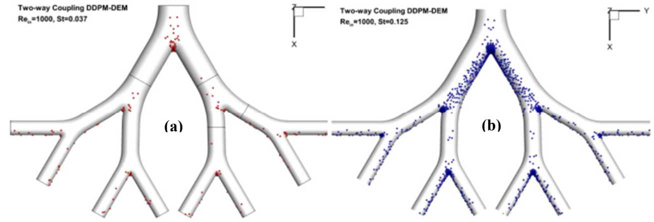


Fig. 3: Particle (d_p=10 μm) deposition comparisons in bifurcating airway model G3-G6 using two-way coupling DDPM-DEM (a) St=0.037 (b) St=0.125

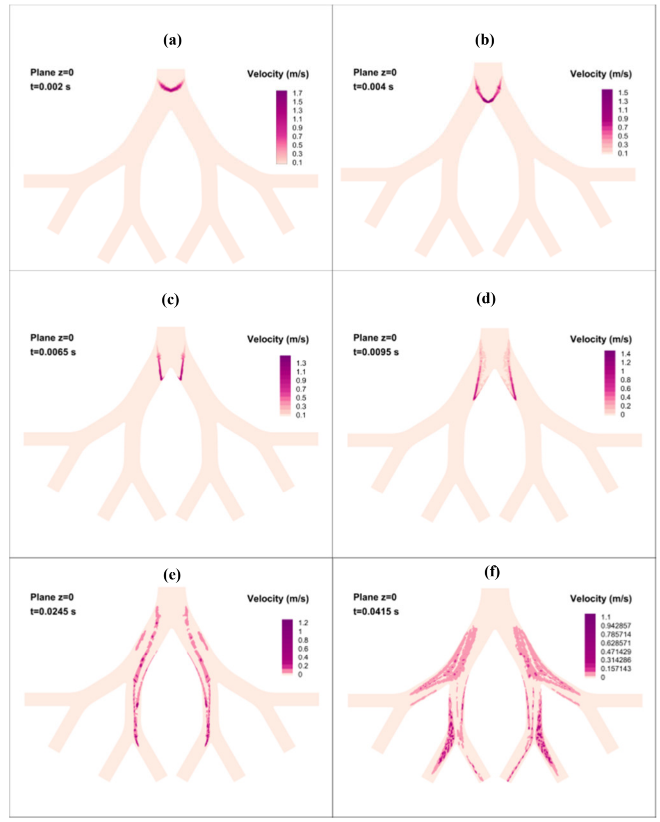


Fig. 4: Transient particle transport patterns in bifurcating airways for Re_{in}=1000, St=0.125, d_p=10 μm (a) t=0.002s (b) t=0.004s (c) t=0.0065s (d) t=0.0095s (e) t=0.0245s (f) t=0.0415s.

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