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A multiscale simulation method for aerosol transport in a mouth-to-lobar bronchi model

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Prediction of aerosol deposition in the respiratory tract has become a major focus for inhaled drug delivery and air pollution prevention. Computational fluid-particle dynamics (CFPD) provides the most accurate local prediction results, but the computational cost is unbearable for the CFPD simulation of the whole respiratory tract. This challenge arises due to the multiscale nature of the respiratory tract and numerous bronchioles [1]. A common practice is to truncate the bronchial tree and simulate on the truncated model using CFPD. In this study, a novel boundary condition for the truncated respiratory tract model based on multiscale simulation is proposed, named extended-bronchus-network (EBN) boundary condition. The truncated model is extended to the terminal bronchial and the air flow in the extended part is simulated using local hydraulic resistance equivalence pore network model (PNM) [2]. The pressure and flow rate at the outlet of truncated model is consistent with PNM, which provides the outlet boundary condition for CFPD of truncated model. A comparison against EBN with the widely used uniform pressure outlet boundary condition [3] is made. It reveals that EBN boundary condition in this study is more physiologically and closely to the clinical data. The maximum relative disparity of nano-micro aerosol penetration fraction of the right middle lobe and right lower lobe between these two methods is 93% and the maximum relative disparity of aerosol deposition fraction within the trachea-lobar bronchi is 30%. EBN boundary condition is implemented for the simulation of nano-micro particles transport in the mouth-to-lobar bronchi (MLB) model at the inspiration volume rate of 15, 60, 90 L/min, respectively. Result shows that for particles equal to or less than 1 μm in size, over 90% penetrate deeper into the pulmonary lobes, with inspiration volume rate and particle size having minimal impact on penetration fraction. However, micro particles more probably deposit in the MLB with larger inspiration volume rate. Notably, when particles larger than 6 μm are inhaled at 15 L/min or particles larger than 3 μm are inhaled at 60 L/min, over 40% of them deposit in the MLB. Particle deposition hotspots forming reason is qualitatively analyzed. This work provides a reference for the optimization of drug delivery, targeted therapy, the prevention and control of pollutants. It also lays a foundation for the simulation of aerosol transport in whole lung.

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