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# MULTISCALE COMPUTATIONAL MODELS FOR RESPIRATORY AEROSOL DYNAMICS WITH MEDICAL APPLICATIONS

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## MINI-SYMPOSIUM PROPOSAL

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Inhalation of therapeutic drug aerosols is now becoming a novel way to administer micro/nanoparticles or vapors to treat lung and systemic diseases. Several attempts of such delivery have been made at least in experimental analyses on asthma, chronic obstructive pulmonary disease (COPD), lung hypoxia, edema, lung injury, lung transplantation fungal infection, pulmonary fibrosis, and lung cancer. However, due to certain design deficiencies, existing pulmonary drug delivery devices still have poor efficiencies for delivering drugs to designated sites. Significant portions of the aggressive medicine deposit on healthy tissues, which causes severe side effects and induces extra health care expenses. Therefore, there is an urgent need to understand the aerosol drug dynamics better and develop a revolutionary patient-specific pulmonary drug delivery method and device to improve therapeutic outcomes by significantly improving drug delivery efficacy significantly. Due to the invasive nature and imaging resolution limitations, clinical and animal studies are not able to provide the high-resolution data for the researcher to understand the particle dynamics in human lung airways. Compared to experimental investigations, an accurate and realistic computer simulation model, that is, a Computational Fluid-Particle Dynamics (CFPD) model governed by natural laws of physics, would significantly contribute to reducing the research time and cost and visualize drug-aerosol transport and deposition patterns with high resolution to advance the fundamental understanding of the underlying physics. To pave the way for the next-generation numerical model, challenges and potential breakthroughs may include (1) running simulations in human respiratory systems with entire conducting and respiratory zone configurations; (2) encompassing the complex airflow-particle-structure dynamics, for example, moving airway boundary, mucus clearance, and particle-particle interactions; and (3) coupling with PBPK/PD models and applications in drug inhaler design and formulation engineering to enhance the translocation efficiency to specific systemic regions.

The aim of this mini-symposium is to attract studies which provide the most advanced multiscale numerical modeling efforts for respiratory aerosol dynamics in pulmonary drug delivery device, human respiratory systems, and systemic regions. We would like to use this occasion to provide in-depth discussions of the whole range of progress and challenges related to the establishment of the numerical modeling framework to predict the transport, deposition, and translocation of inhaled drug aerosols. The ultimate goal is to find the most feasible way for the development of the next-generation multiscale model, which will bring the computational respiratory aerosol dynamics simulations to health endpoints with the details never undertaken before.

Potential topics include but are not limited to the following:

- Multiscale models (e.g., CFPD-PBPK, and CFD-DEM) for precise drug deliveries from drug inhalers to pulmonary or systemic regions
- Advanced numerical models for particle transport in deformable lung airways
- Complete airway tree reconstructions for CFPD simulations for full breathing cycles
- Intersubject variability effect on inhaled drug aerosol transport and deposition patterns, literally CFPD simulations with error bars
- In silico studies focusing on generalized pulmonary drug delivery and drug particulate matter dynamics related research areas, such as drug inhaler design optimizations and formulation engineering