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Computationally Efficient Analysis of Particle Transport and Deposition in a Human Whole-Lung-Airway Model. Part I: Theory and Model Validation

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Abstract

Computational predictions of aerosol transport and deposition in the human respiratory tract can assist in evaluating detrimental or therapeutic health effects when inhaling toxic particles or administering drugs. However, the sheer complexity of the human lung, featuring a total of 16 million tubular airways, prohibits detailed computer simulations of the fluid-particle dynamics for the entire respiratory system. Thus, in order to obtain useful and efficient particle deposition results, an alternative modeling approach is necessary where the whole-lung geometry is approximated and physiological boundary conditions are implemented to simulate breathing. In Part I, the present new whole-lung-airway model (WLAM) represents the actual lung geometry via a basic 3-D mouth-to-trachea configuration while all subsequent airways are lumped together, i.e., reduced to an exponentially expanding 1-D conduit. The diameter for each generation of the 1-D extension can be obtained on a subject-specific basis from the calculated total volume which represents each generation of the individual. The alveolar volume was added based on the approximate number of alveoli per generation. A wall-displacement boundary condition was applied at the bottom surface of the first-generation WLAM, so that any breathing pattern due to the negative alveolar pressure can be reproduced. Specifically, different inhalation/exhalation scenarios (rest, exercise, etc.) were implemented by controlling the wall/mesh displacements to simulate realistic breathing cycles in the WLAM. Total and regional particle deposition results agree with experimental lung deposition results. The outcomes provide critical insight to and quantitative results of aerosol deposition in human whole-lung airways with modest computational resources. Hence, the WLAM can be used in analyzing human exposure to toxic particulate matter or it can assist in estimating pharmacological effects of administered drug-aerosols. As a practical WLAM application, the transport and deposition of asthma drugs from a commercial dry-powder inhaler is discussed in Part II.