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www.elsevier.com/locate/jaerosci

PII: S0021-8502(17)30222-7

DOI: https://doi.org/10.1016/j.jaerosci.2017.10.001

Reference: AS5200

To appear in: Journal of Aerosol Science

Received date: 19 June 2017

Revised date: 28 September 2017 Accepted date: 2 October 2017

Cite this article as: Arun V Kolanjiyil and Clement Kleinstreuer, Computational Analysis of Aerosol-Dynamics in a Human Whole-Lung Airway Model, *Journal of Aerosol Science*, https://doi.org/10.1016/j.jaerosci.2017.10.001

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ACCEPTED MANUSCRIPT

Computational Analysis of Aerosol-Dynamics in a Human Whole-Lung Airway Model

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Abstract

Prediction of the air-particle dynamics in human lungs can reveal critical deposition sites of toxins or can determine best physical parameters for direct drug delivery and associated inhaler devices. However, the sheer complexity of the human lung, featuring a total of 16 million airways, prohibits a full-scale study. So, as an alternative, a physiologically realistic and computationally efficient computer simulation model has been developed. The configuration of the new whole-lung airway model (WLAM) consists of subject-specific upper airways from nose/mouth to, say, generation 3, which are then connected to adjustable triple bifurcation units (TBUs). These TBUs are in series and parallel to cover the remaining generations, based on morphometric measurements of human lung casts. Actual transient airflow, fluid-particle dynamics and alveolar tissue dynamics have been implemented to evaluate the impact of all respiratory airways under realistic inlet conditions. Specifically, the expanding and contracting motion of the alveoli mimic inhalation and exhalation in the alveolar region. Particle transport and deposition depend on the lung-airway geometry, particle characteristics, and inhalation flow frequency. Considering inhalation/exhalation in form of a square-wave breathing profile at 15L/min with different tidal volumes and 3µm-size microspheres as a WLAM test case, significantly higher deposition was observed in the alveolar region than in the upper airways. For short and light breathing conditions, multiple breathing cycles are required to exhale all the suspended particles. Particle deposition patterns differ for inhalation vs. exhalation, as well as in subsequent breathing cycles. During later cycles, the suspended particles tend to travel to distal airways. The model predictions agree well with in vivo results. The new WLAM can be used for local, segmental and total deposition predictions of inhaled toxic or therapeutic aerosols, and for providing inhaler-design guidelines to improve drug-aerosol targeting.

Keywords: Whole-lung Airway Model, Particle Deposition, Lung Air-particle Dynamics, Local and Total Lung Depositions, Actual Breathing Modes, Alveolar Region.

1. Introduction

Inhaled drug therapy has become an intriguing treatment option for obstructive lung diseases, such as asthma and COPD as well as other systemic pathogenic conditions. In contrast, exposure to atmospheric pollutants has resulted in higher incidences of obstructive lung diseases (Geiser &

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