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Comparison of analytical and CFD models with regard to micron particle deposition in a human 16-generation tracheobronchial airway model

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ABSTRACT

A representative human tracheobronchial tree has been geometrically represented with adjustable triple-bifurcation units (TBUs) in order to effectively simulate local and global micron particle depositions. It is the first comprehensive attempt to compute micron-particle transport in a (Weibel Type A) 16-generation model with realistic inlet conditions. The CFD modeling predictions are compared to experimental observations as well as analytical modeling results. Based on the findings with the validated computer simulation model, the following conclusions can be drawn:

(i) Surprisingly, simulated inspiratory deposition fractions for the *entire* tracheobronchial region (say, G0–G15) with repeated TBUs in parallel and in series agree rather well with those calculated using analytical/semi-empirical expressions. However, the predicted particle-deposition fractions based on such analytical formulas differ greatly from the present simulation results for most *local* bifurcations, due to the effects of local geometry and resulting local flow features and particle distributions. Clearly, the effects of realistic geometries, flow structures and particle distributions in different individual bifurcations accidentally cancel each other so that the simulated deposition efficiencies during inspiration in a relatively large airway region may agree quite well with those obtained from analytical expressions. Furthermore, with the lack of local resolution, analytical models do not provide any physical insight to the air–particle dynamics in the tracheobronchial region.

(ii) The maximum deposition enhancement factors (DEF) may be in the order of 10^2 to 10^3 for micron particles in the tracheobronchial airways, implying potential health effects when the inhaled particles are toxic.

(iii) The presence of sedimentation for micron particles in lower bronchial airways may change the local impaction-based deposition patterns seen for larger airways and hence reduces the maximum DEF values.

(iv) Rotation of an airway bifurcation cause a significant impact on distal bifurcations rather than on the proximal ones. Such geometric effects are minor when compared to the effects of airflow and particle transport/deposition history, i.e., upstream effects.

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1. Introduction

Micron particle deposition in the tracheobronchial (TB) airways under normal inhalation conditions (say, inspiratory flow rate $Q = 15$–30 L/min), is of interest to toxicologists and regulators in case of toxic particulate matter as well as to health-care providers in case of bio-aerosols, radioactive and therapeutic particles (see review by Kleinstreuer, Zhang, & Donohue, 2008). While experimental deposition data sets are most valuable for gaining new physical insight and validating computer simulation models, it is the latter which allow for more realistic, detailed and less costly particle-deposition studies. Nevertheless, there are three challenging aspects when determining particle deposition in the human respiratory tract, i.e., the complex airway geometry, two- or three-phase flow simulation, and fluid–structure interaction. Computer modeling of the entire TB region, let alone the respiratory system, is still prohibitive. For example, considering the idealized lung model of Weibel (1963), there are 2^{15} branches for the 16th generation alone.

As a radically alternative approach, one-dimensional global airway systems have been constructed covering major respiratory zones or the entire lung. Classic examples are single- or multi-path models with analytical equations based on deposition calculations (Asgharian, Hofman, & Bergmann, 2001; Choi & Kim, 2007; Koblinger & Hofmann, 1990; NCRP, 1997; RIVM, 2002), and empirical correlations for total or regional depositions (ICRP, 1994; Kim & Hu, 2006; Kim & Jaques, 2004). While such greatly simplified systems can predict total micron particle depositions in the lung quite well, they also can be off by several factors at individual bifurcations (see Kleinstreuer, Zhang, & Kim, 2007).

A compromise solution to this complex problem in terms of computationally efficacy and realism has been proposed by Kleinstreuer and Zhang (2008). They divided the conducting zone, i.e., trachea (G0) to generation G15 into five intricately connected segments via adjustable triple-bifurcation units (TBUs). These TBUs extend "in series" as well as "parallel" after appropriate flow rate and geometry scaling, including out-of-plane branch orientation and branch asymmetry, in order to capture actual lung morphologies. Previous computational studies focused on specific TB segments, say, two or at most six bifurcations (for the most recent contributions see Li, Kleinstreuer, & Zhang, 2007; Longest & Xi, 2007; Zhang, Kleinstreuer, Donohue, & Kim, 2005; among others). The paper by Nowak, Kakade, and Annapragada (2003) gives the impression that they have already solved the problem of particle transport and deposition in the (entire) human lung. Specifically, their methodology of "3.5 generation subunit" used is quite different from what is presented in this paper. Their subunits are isolated, i.e., not interconnected for particle transport, assuming uniform particle distributions and averaged velocity profiles at the inlet of each subunit. Some other shortcomings of their paper include a lack of model validation, assumption of laminar flow, and ignoring the impact of head airways.

In this paper, the validated TBU model was employed to simulate in detail airflow as well as micron-particle transport and deposition in the TB airways. Deposition correlations for the entire TB tree are discussed as well.

2. Theory

2.1. Multi-level airway geometries

The TB region of 16 generations (i.e., G0–G15) is segmented into five levels, each represented by a TBU. These scaled TBUs extend in series and parallel in order to accommodate the TB tree (Fig. 1). Level by level, the TBUs can be adjusted to represent patient-specific lung morphologies with unique geometric features, such as asymmetric bifurcations, branches with partial occlusions and out-of-plane configurations to capture "subject variability", if so desired. In any case, air–particle outflow conditions of a representative oral airway model (Zhang et al., 2005) are taken as inlet conditions for G0, which at the G3 outlets are adjusted to become inlet conditions for G3–G6, etc. (see Fig. 1). Thus, multi-level adjustments include scaled geometric configurations and local flow field quantities, such as velocities, pressures and, if appropriate, turbulence parameters, as well as particle distributions and velocity profiles. The TBU dimensions are similar to the Weibel Type A geometries, assuming a lung volume of 3.5 L. The aerosol dynamics in the first TBU, i.e., G0–G3, compared well with simulation results obtained for a more realistic triple bifurcation (see Li et al., 2007). Uniform pressures were assumed at the outlets of the bifurcation units. But, the outlet tubes were extended to eliminate/reduce any outlet and downstream effects.

2.2. Airflow equations

For inhalation flow rates above 12 L/min turbulent flow may occur in the trachea and the first few bifurcations due to the laryngeal jet (Kleinstreuer & Zhang, 2003; Zhang & Kleinstreuer, 2004; among others). Various low-Reynolds number (LRN) turbulence models have been proposed (see Tian & Ahmadi, 2007; Zhang & Kleinstreuer, 2003a); however, as confirmed by Varghese and Frankel (2003) an adapted form of the LRN k–ω turbulence model of Wilcox (1998) is most appropriate for such internal laminar-to-turbulent flows. It does not require extra wall-layer functions, captures both flow regimes automatically, and produces sufficiently accurate results (Zhang & Kleinstreuer, 2003a).

All airflow equations as well as the necessary initial and boundary conditions are outlined in Zhang and Kleinstreuer (2003a, 2003b). For the assumed inhalation flow rate of 30 L/min, the flow field after bifurcation B6 for the present configuration is fully laminar (Kleinstreuer & Zhang, 2008).