

Numerical Simulation of Ozone Transport and Uptake in Asymmetrically-Branched Airways of the Respiratory Tract

Banafsheh Keshavarzi, James Ultman, and Ali Borhan

The Pennsylvania State University, Department of Chemical Engineering, University Park, PA 16802

The pattern of lung injury induced by the inhalation of reactive gases such as ozone (O_3), a ubiquitous air pollutant, is believed to depend on the dose delivered to different tissues in the respiratory tract. To test this hypothesis, we performed numerical simulations of ozone transport and uptake in anatomically-correct geometries of the conductive airways of a Rhesus monkey. The airway geometry was created using three-dimensional reconstruction of the tracheobronchial tree from MRI images of the lung, and an unstructured volume mesh was generated for the first few generations of the resulting branched structure. Three-dimensional numerical solutions of the Navier-Stokes, continuity, and species convection-diffusion equations subject to a surface reaction wall condition were subsequently obtained for steady inspiratory and expiratory flows at physiologically relevant Reynolds numbers ranging from 100 to 500. An effective rate constant for the surface reaction was formulated based on a quasi-steady diffusion-reaction analysis in the epithelial lining fluid. The total rate of O_3 uptake within each generation was determined, and hot spots of O_3 flux on the airway walls were identified. Spikes in O_3 flux appeared downstream of the first bifurcation, as was true for focal sites of epithelial damage previously observed in the Rhesus monkey [Postlethwait *et al.*, Am. J. Respir. Cell Molec. Biol. 22:191-199, 2000].

Results of the three-dimensional simulations for O_3 uptake along a single asymmetrically-branched airway path were also compared to the predictions of an axisymmetric single-path model (ASPM). The model consisted of a series of tubular airway branches of decreasing cross-sectional area connected through leakage zones that emulated the flow split at each bifurcation. The dimensions of this path were determined from 3-D reconstructions of MRI images. Single-path simulations of gas uptake were comparable to the predictions of the more realistic (but more computationally-intensive) three-dimensional simulations.