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STOCHASTIC SIMULATION OF PARTICLE DEPOSITION IN HUMAN AIRWAYS

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The statistical nature of the structure of the human airway system and its asymmetric branching pattern suggest the application of stochastic modeling techniques, such as the Monte Carlo method. From a modeling point of view, only stochastic models are capable of describing properly the structure of the respiratory tract, for variability, asymmetry and non-linearity are inherent features of all biological systems.

A stochastic simulation model of particle behavior in the human respiratory tract has been developed to study aerosol deposition in realistic, i. e., asymmetric and irregularly-branching, airway structures. While the random tracheobronchial structure, reflecting intra-subject variability, is based on a statistical analysis of measured morphometric data (Koblinger and Hofmann, 1985), the pulmonary region of the lung is simulated by a randomized structure of a human respiratory acinus. Intersuject variability, which is most effective in upper bronchial airways, is considered by using actually measured dimensions in the human test subjects investigated in the gamma camera and SPECT (single photon emission computed tomography) studies. The statistical nature of the airway model, characterized by parameter distributions and correlations among various parameters, requires a random pathway model for the computation of particle deposition patterns, utilizing Monte Carlo techniques. The developed computer code combines this random geometry selection with an analytical deposition algorithm, using sets of equations simulating various deposition mechanisms and bifurcation enhancement factors to allow for the heterogeneous dispersion pattern among airway surfaces.

A unique feature of this stochastic deposition model is its capability to predict three-dimensional deposition distributions of inhaled aerosols within the human lung. At each step of the random pathway selection, the exact positions of the identified bifurcation units and the corresponding deposition fractions in prespecified volume elements are stored, thus allowing reconstruction of the spatial aerosol distribution. Quantitative images of such deposition patterns can be obtained experimentally by two-dimensional gamma camera measurements (projection on a plane outside the lung) or three-dimensional SPECT investigations (projection on planes through the lung). Comparisons of theoretical predictions with these experimental data are sensitive tests of the computed regio-

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nal deposition patterns within the human lung. Preliminary results with patients demonstrate the applicability of this method for model validation, through the agreement between theory and experiment is still more qualitative than quantitative (Hofmann et al., 1988). Because of the wealth of data describing the spatial distributions in both measurement and theoretical prediction, we plan to use cluster analysis techniques to quantify the comparison between the two data sets.

The laboratory rat is often used as a surrogate to estimate hazard to human health following inhalation exposure to ambient aerosols. Extrapolation of rat deposition data to humans depends, however, on the similarities and differences between the morphometric structures of the two airway systems. The main structural difference between the lungs of the two species, aside from dimensions per se, is their respective airway branching pattern: while the human lung is a rather symmetrically, dichotomously dividing system, the rat network is a more monopodial branching structure (Koblinger and Hofmann, 1988). Because of the strong correlation between diameter and generation number of a given airway in the human lung, diameters and generations can be used interchangably. A statistical analysis of the rat morphometry reveals, however, that such a correlation does not exist in the rat lung and only diameters correctly describe the location and physiological function of an airway in the lung.

We, therefore, recommend to classify a given airway in the rat lung by its diameter and not by a theoretically assigned generation number (Hofmann et al., in press). A comparison of the two concepts for the rat lung shows that there is fair agreement between the two ordering schemes from generations 9 through 15 (or 0,95–0,35 mm) suggesting that airways in this diameter range branch more symmetrically. Proximal to generation 9, the characteristic monopodial branching pattern rules out any correlation, and distal to generation 15, where the termination probability (the probability to reach an acinus) essentially determines particle deposition, no comparison can be made as termination is independent of the generation number. Thus, to accomplish an interspecies comparison of regional deposition patterns, which would be facilitated by applying the same concept to both morphometries, one possible strategy would be to convert the generations in the human lung to airway diameter classes.

Experimentally observed heterogeneous deposition patterns within airway branching sites suggest that the airway system of the lung may be more properly described as a sequence of Y-shaped bifurcation units than as a series of tube-like airways. Theoretical evaluation of deposition in a single bifurcation is usually simulated by deposition in a bend tube, considering inertial impaction only. Here, particle deposition in a threedimensional bifurcation model has been computed for the simultaneous effects of inertial impaction, gravitational settling and interception (Balashazy et al., 1988). In the present approach, a bifurcation is characterized as a contiguous system of two bends and three straight tubes, with a defined curvature radius of the bend tubes and an effective branching angle between them. We assumed idealized flow profiles of uniform velo-

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city in the straight segments and rotational velocity in the bend parts of the bifurcation model, the latter being corrected for physiologically realistic flow conditions.

This model allows us to calculate the integral as well as the differential distribution of the deposition efficiency within a bifurcation, which may be of great significance in microdosimetry computations. Compared to single bend tube models, our bifurcation model predicts a smaller deposition efficiency at low Stokes numbers, but higher deposition at larger Stokes numbers, consistent with experimental results. Since the real structure of the human lung is stochastic and asymmetric in nature, this model can also be used to study the effect of airway asymmetry and variability on deposition in stochastic lung models. It is interesting to note that asymmetry in branching angle has virtually no effect upon particle deposition, while asymmetry in daughter diameter and flow rate exert a small influence.

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