ANALYTICAL MODEL OF HYGROSCOPIC PARTICLE BEHAVIOR IN HUMAN AIRWAYS

T. B. MARTONEN
Pulmonary Division,
Department of Medicine,
University of California,
Irvine, CA 92717, U.S.A.

A model is developed to calculate the deposition of hygroscopic aerosols in the human tracheobronchial (TB) tree. The TB airflow pattern assumed is consistent with experimental observations and accounts for anatomical features such as the larynx and cartilaginous rings in large airways. Some original deposition efficiency formulae are presented for laminar and turbulent airstreams. Stepwise growth is simulated by changes in particle size and density at each TB generation. The dose distribution of NaCl aerosols is studied as a function of inhaled particle size and flow rate. Two NaCl growth rate curves are used which differ in the mode of aerosol–air mixing in the trachea. The initial rate of aerosol mixing in the human due to the laryngeal jet is shown to be an important factor affecting the deposition of hygroscopic aerosols. Total TB deposition of NaCl exceeds that for nonhygroscopic particles of the same inhaled aerodynamic size. Hygroscopic growth can also influence the regional TB distribution of dose when submicron NaCl particles grow rapidly enough to deposit by impaction and sedimentation.

1. Introduction. Hygroscopic aerosol particles may absorb water vapor or evaporate while traveling through humid passages of the human tracheobronchial (TB) tree until an equilibrium size distribution is reached. The aerodynamic diameter of an inspired hygroscopic particle may vary with location within the TB tree due to changes in its shape, dimensions and density. Since rate of clearance from the lung can be related to site of initial deposition the influence of hygroscopic growth upon particle dynamics and efficiency of deposition is of importance in the hazard evaluation of airborne contaminants. Furthermore, the importance of being able to accurately predict the distribution of deposited particles within the TB tree in aerosol therapy to optimize the therapeutic effect of medicinal aerosols has been discussed by Lourenco (1973).

Attempts to calculate the deposition efficiency of hygroscopic particles in the human respiratory tract have either assumed a fixed aerodynamic particle size throughout the whole TB tree, or used theoretically calculated particle growth rate curves (Milburn et al., 1957; Task Group on Lung Dynamics, 1966; Ferron, 1977). Also, simplified airstream patterns often assumed were not compatible with published observations. To more accurately understand the behavior and predict the deposition of
hygroscopic aerosols a new analytical model has been developed. Some original theoretical deposition formulae are derived for both laminar and turbulent air flow patterns to account for the glottis and airway surface irregularities which are significant contributors to flow instabilities. A significant improvement over other models is that hygroscopic particles are allowed to have changing aerodynamic size with passage through the entire TB tree. A particle’s parameters are changed in a stepwise manner so that a new diameter and density are used in deposition efficiency calculations for each bronchial generation. The model calculates the total dose delivered to, and the regional distribution within, the TB tree of inhaled particulate matter as a function of aerodynamic size and inspiratory flow rate.

The model is used to study the influence of hygroscopic particle growth upon the deposition of NaCl aerosols during inspiration. Results for NaCl may apply to medicinal aerosols containing hygroscopic salts. The human TB morphology is described by the findings of Weibel (1963) and Horsfield et al. (1971). Use of an experimental growth rate curve measured in a simulated upper TB environment permits the effect of the laryngeal jet upon hygroscopic aerosol behavior to be quantitated. It is shown to be a most significant factor affecting the fate of inhaled particles.

2. Development of an Analytical Particle Deposition Model. Theoretical formulae for calculating particle deposition efficiencies in straight or curved, smooth-walled tubes of circular cross-section have been derived with attention paid for application to branching networks such as the human TB tree. Deposition at branching sites, or bifurcations, is assumed to be caused by inertial impaction, while that occurring in cylindrical airway segments is assumed to be due to sedimentation and diffusion. Therefore, inertial impaction will be modeled using a curved tube, and sedimentation and diffusion using a straight-tube geometry. The deposition efficiencies of the impaction, sedimentation and diffusion mechanisms will be denoted as $P(I)$, $P(S)$ and $P(D)$ respectively. Total deposition efficiency, $P(T)$, will be calculated from the superposition equation

$$P(T) = P(S) + P(D) + P(I) - P(S)P(I) - P(S)P(D) - P(D)P(I) + P(D)P(S)P(I)$$

used by Landahl (1950) to account for the fact that particles deposited by one mechanism are not available for deposition by another.

In an inclined airway, relative motion between a particle and air may