MODELING OF NaCl AND H2SO4 AEROSOL HYDRATION AND RETENTION IN RESPIRATORY SYSTEMS

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ABSTRACT

The rehydration process is important to deposition and retention of soluble aerosols in the respiratory tract. In the very humid lung atmosphere, soluble aerosols become droplets of solution and grow rapidly in dimension. The phase transition and hydration rate of the common NaCl aerosols in transit through lung airways exhibit a completely different mode to that of presently the most environmentally hazardous H2SO4 aerosols. Previous aerosol retention models had shown significant discrepancies on dose-response relationships among human subjects and animal species. Recent experimental measurements indicate that aerosol residence time in the lung plays the most important role for biological effect estimation. In our present work, a time-dependent retention model is used to present aerosol growths and to compare the effects due to inhaled soluble NaCl versus H2SO4 aerosols. Results show good agreement with most of published experimental data.

AEROSOL GROWTH MODELS

The effect of particle hydration on the retention of inhaled soluble aerosols in the respiratory system has been studied in a broad manner. Results have indicated that only relative humidity (R.H.) plays an active role of influencing aerosol growth rate. Figure 1 shows that at any constant ambient temperature, behavior based on all four models exhibit the same trend for aerosol growth; that is, for R.H. greater than 98%, the four selected curves closely approximate each other. Since R.H. in the respiratory tract is believed to be within the range of 99-99.5% [1], it is reasonable to expect the four models to display similar retention patterns once the aerosol size has reached its terminal diameter prior to entering the trachea. Due to the deliquescence and hysteresis effects, variation in NaCl aerosol size is different from that of H2SO4 droplets.

In figure 2, the solid curve shows the effect of increasing R.H. on NaCl crystal, and the dashed curve represents the evaporation of NaCl. As R.H. is increased to above 75%, the NaCl crystal absorbs water and goes into solution; the droplet then continues to grow with increasing R.H. As R.H. decreases below 100%, the evaporation curve initially follows the condensation curve; however, at R.H. of 75%, the NaCl droplet does not crystallize, but remains supersaturated until a much lower R.H. [2]. For simplicity, both NaCl and H2SO4 aerosol final equilibrium sizes are determined by the modified ICRP Task Group's equation [3]:

$$d/d_o = [\rho_o/\rho\,(1 + (iM/M_o))\,H/(K - H)]^{1/3} \qquad (1)$$

where d and d_o are, respectively, final and initial diameters of the aerosol; ρ and ρ_o are initial and final mass densities; M and M_o are, respectively, molecular weight of water and that of the dry aerosol; H is the R.H.; i is the effective number of ions produced by dissociation of a solute molecule; and K is the Kelvin factor.

Equation (1) shows that the effect of hygroscopicity on retention will be less significant for aerosols of compounds having high molecular weight and large densities. For dry H2SO4, the density is 1.8 and molecular weight is about 98, both values being higher than those of NaCl which has a molecular

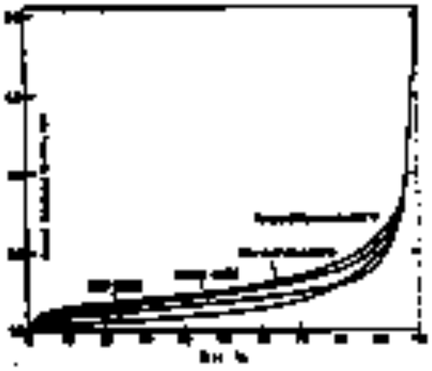

Fig 1. H2SO4 Hydration vs R.H.

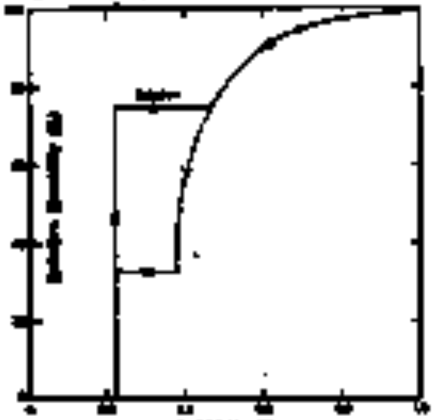

Figure 2. NaCl Size vs R.H.

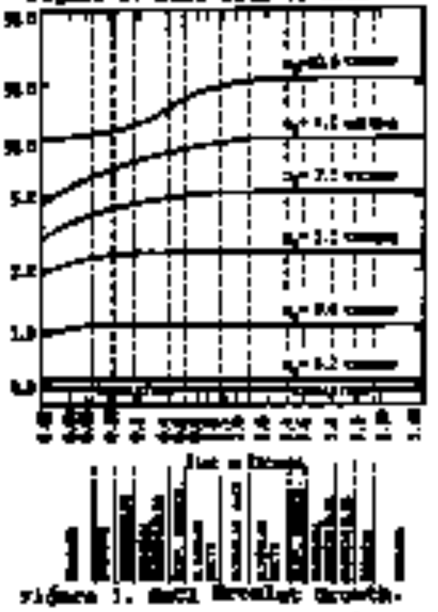

Figure 3. NaCl Droplet Growth.

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weight of 58.5 and particle density of 2.2 at 25°C. Thus, rehydration is more rapid for H_2SO_4 than in the case of NaCl. Shown in Figure 3 is the growth history of a NaCl aerosol in the human respiratory tract at various initial particle sizes calculated from equation (1). It is seen that aerosols of smaller initial sizes reach their equilibrium sizes quicker than do large aerosols. Ultrafine aerosols with initial diameters smaller than 0.2 micron seem to grow when they enter the trachea, while coarse aerosols do not reach their final sizes at all during the inhalation period. This suggests that the retention behavior of ultrafine hygroscopic aerosols in the human respiratory system may be treated in the same way as non-hygroscopic aerosols, provided that the appropriate terminal diameters of the hygroscopic aerosols are used as simulated non-hygroscopic aerosols [4].

RETENTION CALCULATION & RESULTS

According to our previously established time-dependent retention model [5], aerosol deposition in each airway generation and homogeneous aerosols from all succeeding generations can be described by Figure 4 and calculated as follows:

Inflow: $-[(t_{i+1}+t_c)/2 + (t - t_{i+1})]\,(q_{i+1}/t_c)$ (2)

Outflow: $-[(t_{i+1}+t_c)/2 + (t - t_i - t_{i+1})]\,(q_{i+1}/t_c)$ (3)

at $t_i + t_{i+1} < t \le t_c$, for i^{th} generation.

where q and t_c are, respectively, aerosol deposition fraction and clearance time in each generation; i is the generation number; and t is total aerosol exposure time. Assuming a R.H. value of 99.5% throughout the entire respiratory tract, the distribution of NaCl aerosols of both 0.1 and 1.0 microns is shown in Figure 5. Since the primary mechanism of 0.1-micron aerosol deposition is diffusion, retention for NaCl and non-hygroscopic aerosols exhibit similar patterns. For large aerosols with sizes greater than 0.2 micron, deposition mechanism may change from sedimentation to impaction due to hygroscopicity, thereby altering the retention pattern. Under various respiratory conditions, calculated NaCl aerosol retention agrees well with experimental data [6,7], as shown in Figure 6. Due to the inter-subject variability commonly observed in retention measurements, minor discrepancy exists for aerosol sizes below 0.1 micron. For one-hour exposure to H_2SO_4 aerosols, with three different concentrations on three different days, human airway clearance velocity changes can be described by Figure 7. It is observed that the higher the H_2SO_4 dose, the lower the velocity due to ciliastatic effect; and a turnaround exists at point t_c. In a comparable H_2SO_4 exposure experiment on rabbits [8], it was established that increasing exposure concentration first increases and then decreases the rate of mucociliary clearance.

Figure 4. Retention Simulation Model.

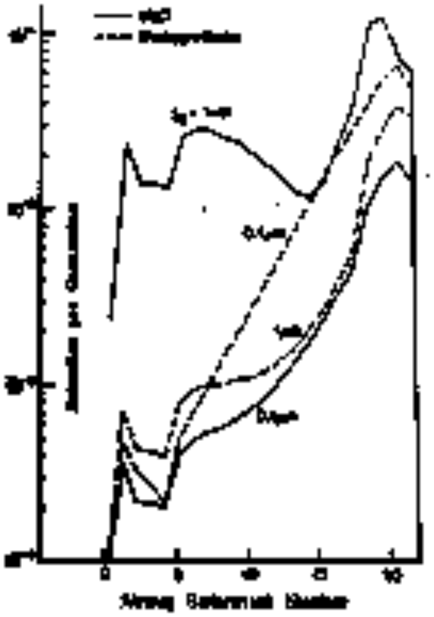

Figure 5. NaCl Retention in Airway.

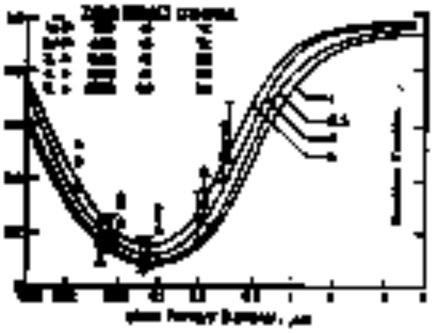

Figure 6. Calculation vs Data.

Figure 7. H_2SO_4 Dose-Response.

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