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INHALED AEROSOL TRANSPORT AND DEPOSITION CALCULATIONS FOR THE ICRP TASK GROUP

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Introduction

Important advances in understanding the fate of inhaled aerosols have been achieved since publication of the conclusions of the original ICRP Task Group on Lung Dynamics (TGLD, 1966). In particular, increasingly sophisticated experimental work with volunteer subjects has augmented the range of particle sizes and breathing conditions for which deposition data are now available. Meanwhile, there has been a similar expansion in the development of theoretical models to study inhaled aerosol behaviour. Such models can play an important part in efforts to assess the ultimate consequences of aerosol inhalation, both as aids in the interpretation of measurements and as tools for making predictions beyond the range covered by experimental data.

An ICRP Task Group is currently revising existing dosimetric models for the inhalation pathway. Part of this work includes the use of a theoretical model to estimate regional aerosol deposition under conditions where experimental measurements are sparse and where such knowledge is required in order to perform adequate assessments. Specifically, the model has been used: (i) to calculate deposition within a representative lung geometry for conditions chosen to simulate spontaneous breathing at different activity levels; and (ii) to estimate inhaled aerosol deposition for children of different ages.

Prior to performing the required simulations, a preparatory review was made of recent information related to the behaviour of inhaled aerosol, so bringing the theoretical framework of the model up to date. Subsequently, a number of controlled experimental inhalation studies were simulated, in order to validate the predictive capabilities of the model against data over as wide as possible a range of circumstances. Finally, aerosol deposition profiles in the lung have been predicted for each of the required inhalation conditions.

Aerosol Transport Model

The theoretical model used for the simulations has been developed from a mathematical framework originally derived for the study of pulmonary gas transport. A brief outline only of the basic methodology is possible here; however, details of the model have been described elsewhere (Nixon, 1977; Pack et al., 1977, Egan and Nixon, 1985, 1987).

Aerosol transport and deposition within the lung airways is represented by:

$$\frac{\partial}{\partial t} (A_T C) = - \frac{\partial}{\partial x} (A_A u C) + \frac{\partial}{\partial x} (A_A D \frac{\partial C}{\partial x}) - L \quad (1)$$

Within the model, A_A is the cross-sectional area for aerosol transport, summed over all airways at distance x from the origin of the trachea. A_T represents

the total cross-sectional area which, in the lung periphery, includes the additional volume associated with alveoli. The aerosol concentration, c , is governed by the mean convective flow velocity u , the effective axial diffusion coefficient, D , and the deposition rate per unit length, L . All variables are functions of time, t , and distance, x . Equation 1 is solved numerically for $c(x,t)$, adopting relevant initial and boundary conditions.

The model requires anatomical data, in order to define the geometry (A_A , A_T) of the transport component and to yield individual airway dimensions for evaluating the deposition term, L . For the initial calculations, performed to validate the model, and in some subsequent simulations, a "hybrid" anatomy has been used. This is assembled by combining the Task Group Composite Model (James *et al.*, 1989) for generations 0 to 15 of the adult male tracheobronchial tree with data from the reconstructed acinar model of Hansen and Ampaya (1975a, 1975b). Then, with the TB dimensions fixed, the alveolated region is scaled to achieve the necessary functional residual capacity. Modifications to this basic anatomy, required in order to study aerosol inhalation by women or children, are outlined below in the section describing model application.

Breathing is simulated by allowing the volumes associated with the alveolated region (as represented by A_A and A_T) to expand and contract about their mean values according to some predefined respiratory pattern. The mean flow velocity of aerosol at any depth in the lung airways, $u(x,t)$, is then evaluated by supposing these fluctuations to act upon an incompressible fluid.

The diffusion component of the transport model reflects the impact of bulk mixing between tidal and residual air, caused by the complex airflow patterns in the lung. Such mixing has been investigated experimentally by Scherer *et al.* (1975), whose measurements form the basis of the assumed axial diffusion coefficient, $D(x,t)$. The potential importance of axial mixing in determining equilibrium deposition levels for particles of low intrinsic mobility has been demonstrated in previous studies (e.g. Egan and Nixon, 1987).

Deposition is evaluated as being due to the combined effects of inertial impaction, gravitational settling and Brownian diffusion. The modelling for contributions to $L(x,t)$ from the various individual deposition processes is essentially the same as outlined previously (Egan and Nixon, 1985, 1987). One change to previous assumptions has, however, been made as a result of the reappraisal of experimental data relevant to inertial deposition (Gurman *et al.*, 1984). New expressions for the impaction efficiency, η_i , based on measured deposition in bronchial casts at relatively high Stokes number, Stk , have thus been derived, as follows:

For constant flow conditions, $\eta_i = 11.5 (Stk)^{1.82}$ in generations 1 to 3, and
 $\eta_i = 3.02 (Stk)^{1.68}$ in generation 4 and beyond;

while under cyclic flow conditions, with Stk based on the mean flow velocity, the corresponding terms are $\eta_i = 6.4 (Stk)^{1.45}$ in generations 1 to 3, and
 $\eta_i = 1.78 (Stk)^{1.25}$ beyond.

Model Validation

The principal motivation for adopting the above methodology in this study has been the desire for predictions of aerosol deposition under conditions where the experimental data base is particularly sparse. Confidence is lent to the calculations because, although certain individual processes (e.g. axial mixing and inertial deposition) are represented on the basis of empirical information, the overall model incorporates explicitly each of the important physical factors governing aerosol transport in the lungs. It was, however, considered that the predictive capabilities of the model needed first to be demonstrated by an appropriate validation procedure.

The results of previous studies using the same basic model (Egan and Nixon, 1985, 1987) have compared well with published experimental data, indicating the general validity of the approach. From the viewpoint of making reliable predictions, it is significant to note that such agreement was not achieved at the expense of "tuning" model parameters. Nevertheless, it was considered that the use of new anatomical data, together with revisions to the deposition model, warranted a renewed comparison between model prediction and experiment.

Simulations undertaken to validate the model's capabilities cover a range of unit density particle diameters from 5 nm to 14 μm , for four different combinations of constant volumetric flow rate, Q , and tidal volume, V_T :

- | | |
|--|---|
| (i) $Q = 250 \text{ cm}^3\text{s}^{-1}$, $V_T = 1000 \text{ cm}^3$ | (ii) $Q = 750 \text{ cm}^3\text{s}^{-1}$, $V_T = 1500 \text{ cm}^3$ |
| (iii) $Q = 250 \text{ cm}^3\text{s}^{-1}$, $V_T = 500 \text{ cm}^3$ | (iv) $Q = 250 \text{ cm}^3\text{s}^{-1}$, $V_T = 250 \text{ cm}^3$. |

The results of the calculations have been compared with experimental data obtained over several years for the same range of particle sizes and breathing conditions (Heyder et al, 1986). As a general rule, for diameters less than around 5 μm , the predicted deposition in the alveolated airways tends to underestimate slightly that fraction of the thoracic deposit which is observed to be cleared slowly. The model results therefore suggest impaired clearance from certain regions of the conducting airways, perhaps the more distal generations, may be taking place. Nevertheless, it is worth noting that a significant result of all the simulations is that the whole of the predicted tracheobronchial deposit is necessary to explain the fast-cleared fraction at larger (>5 μm) sizes. These and other issues related to a comparison between model predictions and data are more fully discussed by Nixon and Egan (1987).

As a consequence of the validation studies, the agreement between model and experimental results was judged to be good enough to justify extrapolation to study deposition under spontaneous breathing and for age-dependent anatomies.

Application

Spontaneous breathing is simulated by assuming a sinusoidal variation in flow rate over the breathing cycle, rather than the constant flow conditions used in the validation studies. Calculations were initially performed for an adult male, using the "hybrid" lung anatomy described above under four different combinations of mean flow rate and tidal volume, representing: sleep, sitting, light exercise and heavy exercise.

Deposition estimates for an adult woman are derived using a smaller lung anatomy, after making appropriate changes to the respiratory parameters. The relevant airway dimensions in the woman's lung are obtained by scaling all generations of the basic "hybrid" model according to the difference in functional residual capacity (FRC). In the present work, this leads to a uniform reduction of each airway until the volume is approximately 81% of that previously assumed for the adult male.

Calculations are also performed to assess age-dependence of inhaled aerosol deposition. At ages over 2 years, it is assumed that the child's lung has a full complement of airways and alveoli (Gehr, 1987). Dimensions of the proximal airways (generations 0 - 8) as a function of age are derived from the Task Group Composite Model, using scaling factors based on the regressions with body height given by Phalen et al. (1985) for each generation. The dimensions of alveolated airways (i.e. beyond generation 15) are obtained by scaling the data of Hansen and Ampaya (1975b), according to the change in lung volume compared with the adult, after first removing the contribution to FRC made by the dead-space. Finally, intermediate airway dimensions are defined by semi-logarithmic interpolation along the bronchial tree between the estimated diameters and lengths obtained for generations 8 and 16.

At the time of writing, some of these calculations are still being performed and a full set of results is therefore not yet available. The results of all simulations will be published together at a later date.

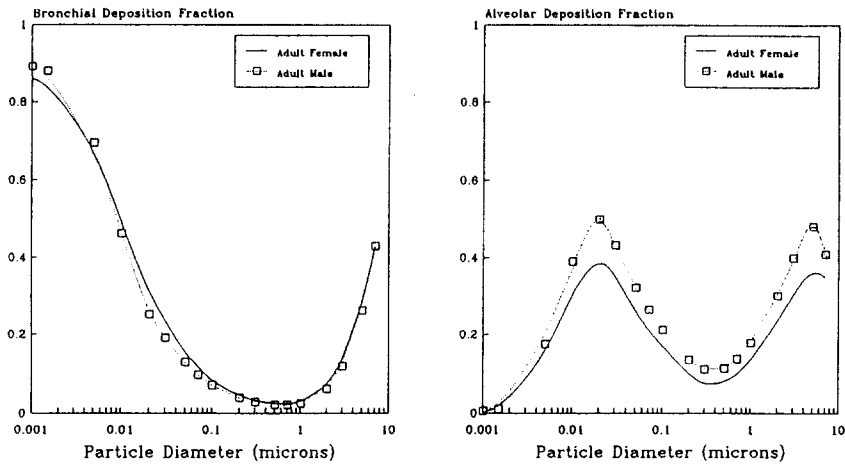


Figure 1. Comparison of regional deposition estimates for adult male and female; breathing at rest.

For illustration, Figure 1 compares the predicted regional deposition within adult male and female lungs for breathing at rest (neglecting extrathoracic deposition). The fraction of the tidal volume which is convected to the alveolated airways is larger for the man (81%) than for the woman (74%), so increasing deposition in this region. Transit times through the conducting airways are shorter in the man's lung, however, tending to decrease the deposition efficiency for diffusion and sedimentation in the bronchial tree.

Investigations are also continuing with the aim of defining a model for growth in the peripheral airways, consistent with the latest data for children up to the age of 2 years. At this stage, deposition calculations therefore remain to be fully defined for infant lungs. The final complete set of predictions, based on the methods outlined here, will enable the ICRP Task Group to assess the potential radiological significance of age-dependent and sex-dependent factors associated with the inhalation of radioactive aerosols.

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