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AEROSOL DEPOSITION CALCULATIONS WITH A STOCHASTIC LUNG MODEL

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Inhalation, deposition and exhalation of aerosol particles in the human respiratory tract are computed by the Monte Carlo code IDEAL.

The random selection of the diameters, lengths and branching angles of the tubes is based on statistical analysis of the largest data base available. Deposition probabilities are determined analytically.

Sensitivity of the deposited fraction to the variation of several geometrical parameters is studied.

Introduction

Earlier models [1, 2, 3] of inhaled particle deposition in the human lung make use of stylized forms which are approximations of the real anatomy of the respiratory tract. These models do not reflect variabilities of the components of the lung, thereby erroneously facilitate the aerosol deposition calculations.

Model

In our stochastic model, geometrical parameters of the pathways are randomly selected whereas deposition probabilities are calculated by the use of analytical formulae.

The mean values and deviations of the various geometrical data as well as the correlations between them are derived from an analysis of the morphometic data measured at the Lovelace Inhalation Toxicology Research Institute [4]. Details and results of this analysis are given elsewhere [5].

The deposition probabilities are calculated according to the formulae listed in [3] for the tube parts of the bifurcations, and an enhancement factor - dependent on the bifurcation number - is applied to inhalation.

In the IDEAL /Inhalation, Deposition and Exhalation of Aerosols in/from the Lung/ code the random walk of the particles is followed down to the acinus region from where they can start to be exhaled just at the beginning of the next exhalation period or stay there for longer times due to mixing. The acini themselves are represented by "effective diameters" for the deposition probability calculations.

Selection of parameters

Detailed results of an illustrative sample run have been presented in an earlier paper [6]. The main conditions applied there were the following:

- the breathing cycle was taken as given in Fig. 1,

- in accordance with the original comment of Raabe et al [4] we assumed that their data correspond to full inflation /$V_o = V_{in}$, $f_{in} = 1$/,
- a volume compression of 0.85 was assumed at the end of exhalation,
- a tidal volume of 500 cm^3 was selected, and thus from the relation

$$\frac{V_{tid}}{V_{tot}} = 1 - \frac{f_{ex}}{f_{in}}$$

a total lung volume of 3333 cm^3 resulted,
- a maximum enhancement factor of two was assumed for the second bifurcation; this factor decreased to one when reaching the sixth bifurcation,
- the effective acinus diameter was set to 0.7 mm,
- total mixing in the acini was assumed.

Deposited fractions of 0.1 μm diameter aerosols were presented for each lobe and each bifurcation number for the above conditions [6].

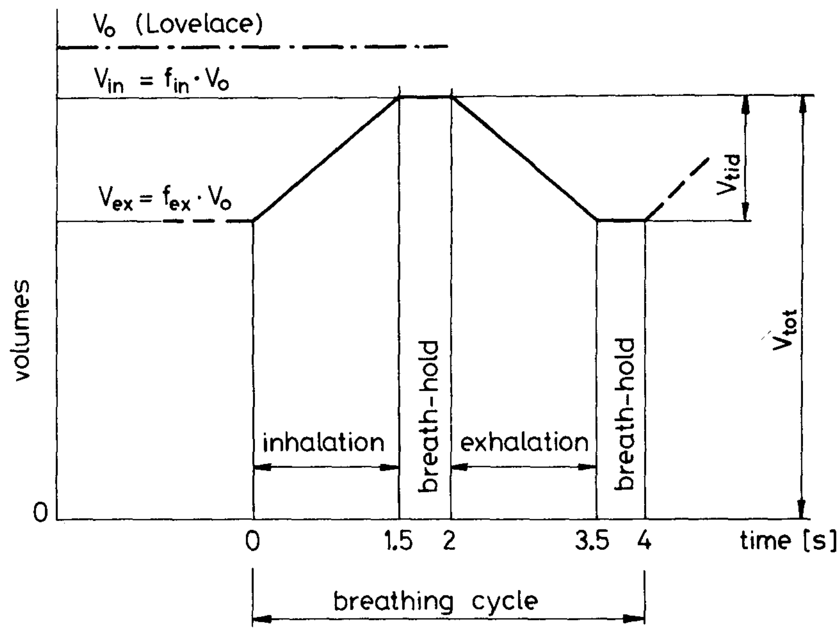

Fig. 1. Data of breathing cycle

Results by parameter variations

In the present work we aimed to study the effects of changing several of the parameters given above. Parameters not specifically mentioned remained unchanged.

Since the largest fraction of particles is deposited in the acinus region, first the effective acinus diameter was altered from 0.7 to 0.5 and 0.9 mm, respectively. The results given in Fig. 2 clearly demonstrate the strong influence of this parameter therefore a rigorous study is needed to

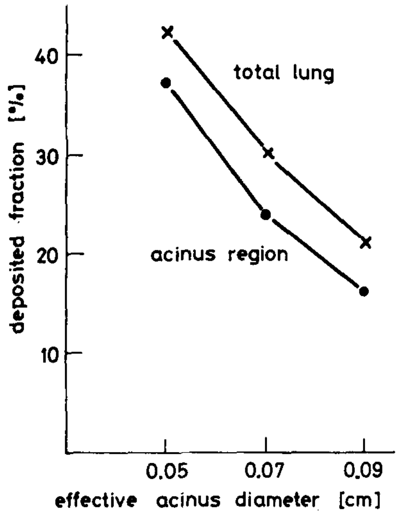

Fig. 2

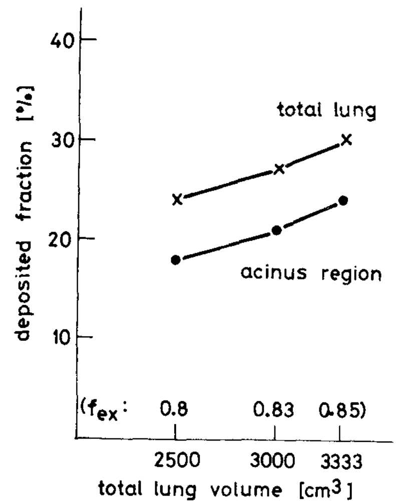

Fig. 3

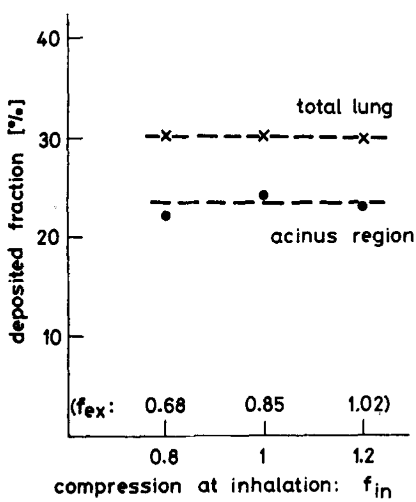

Fig. 4

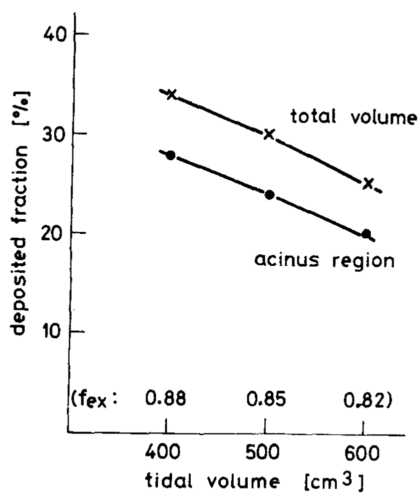

Fig. 5

Figs 2-5. Variation of the fractions of particles deposited in the lung on several parameters. The standard deviations are below 3 %

find the really correct value to be used in the future.

As one can see in Fig. 3, the increase of the total volume with fixed inhalation and tidal volumes slightly increases the deposition.

If the compression at inhalation /f_{in}/ is simultaneously changed with that at exhalation /f_{ex}/ in such a way that the in ratio remains unchanged /0.85/ then the deposition is practically constant /see Fig. 4/.

By increasing the tidal volume with decreasing exhalation compression and constant inhalation volume, the deposition decreases /Fig. 5/.

Conclusions

These preliminary studies clearly demonstrate that further research is needed for correctly modelling the acini, and that separate calculations are needed for people having different lung volumes.

Acknowledgments

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