Introduction

To assess the potential health effects associated with smoking, the doses and sites of uptake and deposition in the lung for various constituents of smoke following inhalation of a cigarette single puff are required.

Constituents in the cigarette single puff may exist in particle phase, gas phase, or a mixture of both depending on the vapor pressure of the constituent.

Model predictions indicate a faster release of nicotine than those observed experimentally. The time difference is attributed primarily to partitioning of nicotine from the particle to the vapor phase.

The amount of nicotine changing from particle to vapor is dependent on smoke temperature, relative humidity, and particle chemical properties such as its pH.

A semi-empirical equation to correct for particle-vapor partitioning was derived based on numerical calculations of nicotine uptake fraction in a denuder study.

The new particle size change model was then used in the deposition model for cigarette smoke particles (CSP) to predict particle deposition and nicotine uptake fraction in the lung. The new model is potentially capable of predicting the amount and site of nicotine absorption into the lung tissues.

Modeling Particles Deposition

\[
\frac{\partial C_{pj}}{\partial t} + \frac{Q_j}{A_j} \frac{\partial C_{pj}}{\partial z} = D_{pj} \frac{\partial^2 C_{pj}}{\partial z^2} - \Delta \lambda_{pj} C_{pj} + \Delta \eta_{pj} \frac{C_{pj}}{Q_j} \eta_{pj,i,j} - \eta_{pj,i,j} + 1 - \eta_{pj,i,j}
\]

Deposition fraction (DF) of particles:

\[
DF_j = \frac{Q_j}{V_{l,j}} \sum_{i=0}^{\infty} \frac{m_{pi,j} \cdot m_{p,j,i}}{4p_{pi} \cdot m_{p,j}^{1/2}} \cdot C_{pi,j} + C_{pi+j,j,i} \frac{\eta_{pj,i,j} - \eta_{pj,i,j}}{1 - \eta_{pj,i,j}}
\]

where nicotine mass is calculated from particle size change by phase change:

\[
\text{Deposited mass of nicotine} = DF \times C_p \times V_j \times \text{Nicotine mass}
\]

Model Predictions

Deposition fraction of particles in a denuder study with measurements as given below.

\[
\xi = 0.174 - 0.03 \times RH/100 - 0.15556 \times \left( \frac{RH}{100} \right)^2
\]

where RH is the relative humidity. The particle size change model was used in Multiple Path Particle Dosimetry (MPPD, ARA, Raleigh NC) to calculate particle deposition fraction in lung airways.

Commercial

\[
\text{Particle flux/time/volume} = \frac{m_{pj,i,j}}{V_{l,j} \cdot \Delta \eta_{pj,i,j}}
\]

Airway j:

An elemental segment in a lung airway used to calculate local deposition fraction of particles

\[
\Delta Z_i = Z_i - Z_i - 1
\]

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