Modeling Mainstream Cigarette Smoke Inhalation and Deposition in the Human Lung
B. Asgharian1, O.T. Price1, C.U. Yurteri2, J. McAughey2
1Applied Research Associates, Inc., Raleigh, NC, USA
2British American Tobacco, Southampton, UK

Introduction

- Determination of dose to the lung of inhaled mainstream cigarette smoke (MCS) aids in determining vulnerable sites in the respiratory tract which experience enhanced deposition.
- A particle deposition model specific to cigarette smoke particles (CSP) was developed for oral cavities and the lung by extending existing models for environmental particles.
- The CSP deposition model included colligative and non-colligative effects. Colligative effects were due to particle-particle and particle-flow interactions. Non-colligative effects were single-particle aerodynamics.
- The colligative effects were treated by assuming the particles behave as a cloud. The non-colligative effects included the calculation of hydrodynamic drag on the particles when undergoing size change due to phase change and coagulation.

Modeling CSP Size Change

Conservation of mass:
The size and number evolution of CSP can be found from the application of the number or mass balance equation for airborne CSP at time t:

\[
\frac{dC}{dt} = \frac{\partial}{\partial x} \left( \frac{C v}{\rho} \right) + Q \delta C
\]

where C is CSP concentration, \( \delta C \) is the flux to the walls, and \( \beta C \) is the coagulation kernel.

Solution:
\[
C(t) = \frac{C_i e^{-\beta x}}{1 + \beta C_i} \left[ \int^t_0 \eta(t') \frac{d\eta}{dt} dt' \right]
\]
where \( C_i \) is the initial concentration and \( \eta \) is the deposition efficiency.

Size change by coagulation:

\[
\frac{dd_p}{dt} |_{\text{coag}} = \frac{1}{3} \frac{d_p}{dt} \left( \frac{C_i e^{-\beta x}}{1 + \beta C_i} \right) \left( \int^t_0 \eta(t') \frac{d\eta}{dt} dt' \right)
\]
where \( d_p \) is the CSP diameter and \( \eta \) is the deposition efficiency.

Size change by phase change:

\[
\frac{dd_p}{dt} |_{\text{phase}} = \frac{1}{\rho d_p} \left( \frac{\partial p}{\partial d_p} \right)_T \left( 1 + 1.3325 Kn + 1.71Kn \frac{M}{m_i} \right) e^{-\eta t}
\]

Modeling Lung Deposition of CSP Particles

The Multiple-Path, Particle Dosimetry model was modified to calculate losses of MCS particles in the lung. Modifications were made to the calculations of particle deposition in the oral cavity, the unique breathing pattern of smokers was included, and particle size change by phase change and coagulation was calculated. In addition, the cloud effect was accounted for in the calculations of MCS particle deposition throughout the respiratory tract. Furthermore, the lung deposition model was modified to allow inhalation of time-dependent concentrations of particles in the inhaled air.

Model Predictions

- CSP growth by various mechanisms appears to reach a plateau beyond which no further growth can occur. If one mechanism is altered, others compensate to ensure a final stable size.
- High deposition of particles occurs in the large airways of the lung due to impaction and the deep lung by sedimentation and diffusion.
- The deposition of CSP is directly related to the initial size of the freshly generated CSP. The smaller the size, the lower the deposition of particles in the lung airways will be.
- Model predictions indicate that particle deposition decreases with increasing mixture of the dilution air with the puff after the mouth-hold.

Nomenclature

- \( D_i \): Diffusion coefficient of component i
- \( M_i \): Molecular weight of component i
- \( \rho_i \): Density of component i
- \( R \): Gas constant
- \( T_\infty \): Surrounding temperature
- \( Kn \): Knudsen number
- \( S \): The colligative effects were treated by assuming the particles behave as a cloud.

Non-colligative effects included the calculation of hydrodynamic drag on the particles when undergoing size change due to phase change and coagulation.

Modeling CSP Deposition in Oral cavities

For a spherically-shaped oral cavity during a breath-hold, deposition efficiency at a constant settling velocity is given by:

\[
\eta = \frac{2}{3} \left( \frac{1}{1 + \frac{1}{Kn^3}} \right) \left[ \frac{1}{1 + \frac{1}{Kn^3}} \right] \left( \frac{1}{1 + \frac{1}{Kn^3}} \right)
\]

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Concluding Remarks

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