COMPONENT-SPECIFIC MODELING OF CIGARETTE SMOKE PARTICLE DEPOSITION IN THE RESPIRATORY TRACT

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Introduction
- Despite significant attempts, a reliable, comprehensive cigarette smoke particle deposition model is still not available due to the lack of complete understanding of size change, transport, and deposition processes in respiratory tract. It is not clear which effects are major contributors to the observed enhanced deposition.
- Mainstream cigarette smoke (MCS) particles undergo a size change due to various processes during puff drawing, breath-hold, inhalation and exhalation. The size growth can occur by
  - Coagulation
  - Hygroscopic growth
  - Phase change
- A multi-component, mechanistic model for MCS particle transport and deposition has been developed which included cigarette-specific colligative and non-colligative effects on deposition.

Modeling MCS Particle Size Change

Conservation of mass:
The size and number evolution of MCS particles during smoking can be found from the application of the number or mass balance equation for airborne MCS particles at time t.

\[
\frac{dC}{dt} = \frac{\partial C}{\partial t} A + \frac{\partial}{\partial x} (\bar{C} \rho A) - \lambda C - \beta C^2 \rho \text{Coagulation}
\]

\[
\lambda C \text{ is the flux to the walls.}
\]

Solution:

\[
C = \frac{C e^{-\beta t}}{1 + \beta t}
\]

\[
\eta(t) = \int_0^t \lambda dt
\]

MCS size change by coagulation, water vapor exchange with the surrounding air, and phase change are found from the following relationships:

Size change by coagulation:

\[
\frac{dd}{dt} = \frac{1}{3} d_0 \psi^{2/3} \frac{dn}{dt} \psi + \beta C_0
\]

\[
\psi = 1 + \frac{\beta C_0}{e^{-\beta t}} \left(1 - \frac{1}{1 - \eta} \right)
\]

Size change by hygroscopic growth:

\[
\frac{dt}{dt} = \frac{d_0}{d_0 + p_0} \frac{1}{1 + 1.3325Ke + 1.77Ke} \left(1 - \frac{1}{1 - \eta} \right)
\]

MCS particle size change by phase change for nicotine:

\[
\frac{dn}{dt} = \frac{F_0}{F_0 + F_1} \frac{M_0}{M_1} \frac{1}{1 - \frac{1}{1 - \eta} \left(1 - \frac{1}{1 - \eta} \right)}
\]

Overall size change:

\[
\frac{dd}{dt} = \frac{\partial C}{\partial t} + \frac{\partial}{\partial x} (\bar{C} \rho A) - \lambda C - \beta C^2 \rho \text{Coagulation}
\]

Modeling MCS Particle Deposition in the Respiratory Tract

Losses in Oral Cavity:

\[
\eta = \frac{3}{2} \left(1 - \frac{1}{3} \left(t^*\right)^2\right)
\]

Lung deposition modeling:

Multiple-Path Particle Dosimetry (MPPD) model has been extended to cigarette smoking when MCS particles in the puff
- Undergo no, partial, or full mixing with the inhaled dilution air
- Behave as a bolus as they travel through lung airways
- Exert hydrodynamic forces on the neighboring particles (cloud effect)
- Are deposited by Brownian diffusion, gravitational settling and inertial impaction

Nomenclature

- \(D_n, D_x\): Water vapor and nicotine diffusion coefficient
- \(M_n, M_w, M_v\): Water vapor, nicotine, and semi-volatile molecular weights
- \(\rho_n, \rho_w, \rho_v, \rho_0\): Densities of water vapor, nicotine, particle, insoluble, and semi volatile components
- \(\beta\): Universal gas constant
- \(T_\text{a}, P_\text{a}\): Ambient temperature, pressure
- \(K_n\): Knudsen number
- \(S\): Saturation ratio
- \(\sigma_{v}, \sigma_{n}\): Water vapor and nicotine surface tension
- \(P_{\text{wv}}, P_{\text{sw}}\): Water vapor and nicotine saturation vapor pressure
- \(\bar{C}\): Deposition efficiency
- \(A\): Airway cross-sectional area
- \(Q\): Flow rate through an airway
- \(F_n, F_w, F_v\): mass fractions of nicotine, semi-volatile, insoluble, and water components
- \(\psi\): Deposition parameter for coagulation
- \(D_v\): MCS particle diameter
- \(C, C_i\): Concentration, initial concentration
- \(\eta\): Deposition efficiency
- \(B\): Coagulation kernel
- \(t^*\): Dimensionless time

Predicted Results

MCS particle size growth, coagulation, and phase change in the oral cavity for an initial 0.2 μm particle.

Deposition fractions of MCS particles in the Tracheobronchial, TB (C) and Pulmonary, PUL (D) regions of the human lung when the size of MCS particles is either constant or increasing (geometric diameter)

Deposition fraction of various size MCS particles in the oral cavities and the respiratory tract (E) Without mixing (bolus transport), and (F) With mixing (diluted smoke).

SUMMARY

A multi-component, mechanistic model forecasting MCS particle growth and deposition of inhaled particles during a smoking scenario has been implemented to MPPD. Future work will confirm the model with experimental measurements.

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