ADVANCES IN AEROSOL DOSIMETRY MODELING

HEADSUP PM SYMPOSIUM
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D. M. Broday, P. Kevrekidis, and P. G. Georgopoulos
Exposure Measurement and Assessment Division
Environmental and Occupational Health Sciences Institute
170 Frelinghuysen Road, Piscataway, NJ 08854
Introduction

Rationale

– Changes in particle size and density due to condensation/evaporation process alter the aerodynamic and diffusive properties of inhaled matter, and therefore its deposition characteristics. This results in a modified deposition profile along the airways as compared to stable aerosol.

– Dosimetry models oftentimes used by regulatory agencies consider aerosols which consist of monodisperse particles having generic and constant composition. Such models may underpredict deposition of respirable particles from the intermediate size range \(0.1<\phi<1\text{mm}\) and overpredict deposition of fine and ultrafine particles \(\phi<0.1\text{mm}\).

– A dosimetry model that handles in a consistent way particles of both outdoor and indoor origin (i.e. with respect to chemical composition, size distribution, physicochemical properties) is required.
Introduction

Objective

– Develop computational tools for assessing exposure to respirable PM, having attributes of real airborne matter (as initial conditions):
  – polydispersity - multimodal lognormal distribution,
  – different aging times - mixture of crystalline and aqueous particles,
  – heterodispersity - particles of specific composition, not internally mixed aerosol.

– Relate inhaled concentrations of anthropogenic PM to the biological dose using a consistent mechanistic model compatible with the IAQ and urban scale aerosol models integrated in MENTOR-OPERAS (UAM-AERO, UAM-UDAERO, MAQSIP-UDAERO, etc.)

– Benefit from the extensive work done on the subject in the fields of inhalation toxicology and aerosol pharmacotherapy, using state-of-the-art science developed elsewhere as sub-modules (e.g. lung morphology & ventilation, macro and micro features of the air flow field, airway responsiveness, particle deposition and dispersion) within a consistent integrated dosimetry framework.
Introduction

Approach

Two complementary types of modeling approaches are used in the MENTOR-OPERAS framework for tracking the transport and fate of inhaled aerosols:

- **Micromodeling.** Trajectories of individual particles subjected to various simultaneous body and field forces are calculated in a single tracheobronchial airway bifurcation. The drag is calculated by a computational fluid dynamics (CFD) code for the case of a dilute aerosol.

- **Macromodeling.** The evolution of size distribution and composition of inhaled aerosol along successive airway generations of a human lung model is calculated using the aerosol general dynamic equation (GDE) with terms accounting for growth, transport, and deposition.

- The micromodeling is used to study the relative importance of different physical processes (deposition mechanisms, morphology–flow interactions, secondary effects due to finite charge and non-uniform temperature), whereas the macromodeling is used to study effects of particle chemical composition and physicochemical properties on the delivered dose.
Micromodeling

Methods

- Transport and deposition of aerosols in a single airway bifurcation of the human respiratory tract is predicted by solving Newton’s equations in 2D, and tracking individual particle trajectories,

\[
\frac{dm_i}{dt} \mathbf{v}_i + m_i \frac{d\mathbf{v}_i}{dt} = m_i \mathbf{g} - \mu \mathbf{k} (\mathbf{v}_i - \mathbf{U}) + \mathbf{F}_{\text{diff}} + \mathbf{F}_{\text{el}},
\]

where \( \mathbf{F}_{\text{el}} \) includes contributions of both space charge and image forces.

- Flow field: plug or Poiseuille flow.

- Dimensions (“morphology”) and simulation parameters (gravity angle, branching angle, airflow rate, airway lumen temperature) typical of the 5\textsuperscript{th}-6\textsuperscript{th} generation of the tracheobronchial airways.

- Interception is included; deposition of finite size particles.

- \( t_{\text{inspir.}} : t_{\text{pause}} : t_{\text{expir.}} = 1:2:3 \):
Particle Trajectories and Deposition Profile in a Single Airway Bifurcation

$\phi = 0.1\mu m$

$\phi = 1\mu m$
Particle Trajectories and Deposition Profile in a Single Airway Bifurcation

\[ \phi = 10\mu m \]
Micromodeling

Conclusions:

– In accordance with previous studies, diffusion is the most significant deposition mechanism for fine particles, whereas gravitational settling and inertial impaction are the important deposition mechanisms for large particles. Intermediate sized particles ($\phi=1\mu m$) are more persistent in the inspired air due to reduced deposition efficiency of the combined deposition mechanisms.

– The carinal ridge is a deposition “hot spot”. This result, which was demonstrated in studies accounting for secondary flow and flow splitting, is attributed here to the inertia (of large particles) and the slight decrease in Pe in daughter airways (for fine particles).

– Space charge and image electrostatic forces seem to have comparable effects on particle deposition. The space charge force appear to be slightly more significant for fine particles while image forces are somewhat more important for deposition of large particles.
Macromodeling

Methods

- Transport and deposition of aerosols in the human airways is predicted using a variant of the aerosol general dynamic equation (GDE),

\[
\frac{dn_k}{dt} = \frac{dn_k}{dt} \bigg|_{\text{process}} - s_{k,j} n_k
\]

- Condensation/evaporation resulted from vapor convective–diffusive flux,

\[
\phi \frac{d\phi}{dt} = \frac{4D_v^* M_w \rho_s(T_a)}{R \rho_d} \left( \frac{RH}{T_a} - \frac{a_w}{T_d} \exp \left[ \frac{4M_w \sigma}{R \rho_w \phi T_d} + \frac{h_{fg} M_w}{R} \left( \frac{1}{T_a} - \frac{1}{T_d} \right) \right] \right)
\]

\[
\frac{dT_d}{dt} = \frac{3}{\phi^2 c_{p,w}} \left[ \frac{4k_v^*}{\rho_d} (T_a - T_d) + h_{fg} \phi \frac{d\phi}{dt} \right]
\]

- Initial conditions: (multimodal) lognormal shape, distinct modal physicochemical and thermodynamic properties.
Lung model

- Lung model: Weibel’s idealized dichotomous scheme (Weibel, 1963) scaled allometrically to reflect a functional reserve capacity (FRC) of 3000cm$^3$.

- Airway bifurcations represented by branching angles from Yeh and Schum's typical lung pathway model (Yeh and Schum, 1980).

- Generation-dependent thermodynamic conditions (temperature and relative humidity) in the airway lumen. Default profiles along the thoracic airways are taken constant at $T=37^\circ C$ and $RH=99.5\%$, respectively, corresponding to nasal breathing (Martonen, 1989; Hiller, 1991).

- Ventilation parameters: the air flow corresponds to lung ventilation at sedentary breathing conditions (tidal volume $V_T=500ml$, breathing frequency $f=12min^{-1}$) and during intensive exercise ($V_T=2000ml$, $f=30min^{-1}$).
Particle Deposition

Particle deposition due to the three major deposition mechanisms (diffusion, gravitational settling, and inertial impaction) is considered in terms of deposition probability of individual particles from a cloud of non-interacting particles. Default expressions apply for a unidirectional air flow with a uniform profile,

\[ s_{k,j} = \frac{p_{k,j}}{t_{res,j}} \]

\[ p_{k,j} = p_{k,j}^{*} \prod_{i=1}^{j-1} (1 - p_{k,i}^{*}) \left( 1 - \sum_{i=1}^{j-1} t_{res,i}/T_{spir.} \right) \]

\[ p_{k,j}^{*} = 1 - \left( 1 - p_{d}\right)\left(1 - \sqrt{p_i^2 + p_s^2}\right) \]

\[ p_d = 3.46\Delta^{1/2} Sc^{-1/6} \]

\[ p_i = \frac{4 \sin \theta_b}{\pi d/d_p} St \frac{l}{d_p} \]

\[ p_s = \frac{2}{\pi} \left( \beta \sqrt{1 - \beta^2} + \arcsin \beta \right) \]

\[ \Delta = \frac{D_p}{d^2} t_{res} \] diffusion

\[ St = \frac{\phi^2}{18 \mu} \frac{D_p t_{res}}{t_{res}} \] inertial impaction

\[ \beta = \frac{v_{set} \cos \theta_g}{d \mu} t_{res} \] gravitational settling

\[ \rho \]
Evolution of Particle size in the Lungs

Initial conditions:
- Coarse fraction: (NH₄)₂SO₄, CMD 0.1µm, GSD 1.5, aqueous state
- Fine fraction: Na₂SO₄, CMD 1µm, GSD 1.8, crystalline state

Lung conditions:
- T=37°C, RH=99.5%
Deposition of Hygroscopic Particles in the Lungs

Persistent Particles

Deposition Fraction
Total Deposition by Number

Stable Aerosol

Hygroscopic Aerosol
Conclusions:

- Fine hygroscopic particles grow into intermediate-sized particles ($0.1 < f < 1 \text{mm}$). Such particles tend to deposit to a lesser extent, due to decreased diffusivity, than non-hygroscopic fine particles of the same initial size distribution.

- Particles that are initially in the intermediate size range, and which otherwise tend to persist in the inspired air, experience enhanced deposition resulting from the increase in size.

- Therefore, hygroscopic effects alter the size and composition characteristics of the dose, can potentially augment human exposure to particles of intermediate size, and may reduce the biological dose of ultrafine particles.

- Conditioning of the airway air due to condensation/evaporation is negligible for normal residential, occupational, or ambient aerosol concentrations.
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