Calculating Particle Deposition in Human Lungs for Particles of Unknown Shape: Implications for Soot Agglomerates

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Introduction

Reliable determination of particle deposition in the respiratory tract is an important aspect of human health risk assessment and air quality control. Recent regulatory interest in irregularly shaped particles such as soot agglomerates or custom-engineered nanoparticles has created a need for deposition models for non-spherical particle shapes.

There are several numerical deposition models that allow the prediction of particle lung deposition for variable particle size and density (e.g. ICRP, 1994). However, the effect of non-spherical (unknown) particle shape is usually not accounted for in these models.

Objectives

1) Derive a method to adapt standard deposition models for spherical particles to particles of non-spherical or even unkown shape.

2) Apply this method to soot agglomerates.

Method

Background

Respiratory particle deposition mainly depends on diffusion, impaction and sedimentation (Hinds, 1982).

		For spheres (χ=1)	For arbitrary particle shape
Diffusion coefficient:	$D \sim C(d_B)/d_B$	$\sim C(d_v)/d_v$	$\sim C(d_v)/(\chi d_v)$
Stokes number:	$Stk \sim \rho_0 d_a^2 C(d_a)$	$\sim \rho_p d_v^2 C(d_v)$	$\sim \rho_p d_v^2 C(d_v)/\chi$
Settling velocity:	$v_{TS} \sim \rho_0 d_a^2 C(d_a)$	$\sim \rho_p d_v^2 C(d_v)$	$\sim \rho_p d_v^2 C(d_v)/\chi$

d_B: equivalent mobility (thermodynamic) diameter
d_a: aerodynamic diameter
d_v: equivalent volume diameter
C: Cunningham slip correction
ρ_p, ρ_0: particle and unit density (1000 kg/m^3)
χ: dynamic shape factor

Problem Particle density ρ_p and/or shape factor χ are frequently not known.

Solution Use the effective mobility density ρ_B: $\rho_0 d_a^2 C(d_a) = \rho_B d_B^2 C(d_B)$

ρ_B can easily be determined from online measurements of d_B and m_p: $\rho_B = \frac{6 m_p}{\pi d_B^3} = \frac{\rho_p}{\chi^3}\left(\frac{C(d_v)}{C(d_B)}\right)^3$

Diffusion, impaction and sedimentation can now be expressed as:	Spheres (χ=1)		Arbitrary particle shape (χ unkown)
	$D \sim C(d_v)/d_v$	$\Leftrightarrow$	$C(d_B)/d_B$
	$Stk \sim v_{TS} \sim \rho_p d_v^2 C(d_v)$	$\Leftrightarrow$	$\rho_B d_B^2 C(d_B)$

Summary $\rho_p, d_v \Leftrightarrow \rho_B, d_B$

Exchange of input parameters

Results

Influence of effective mobility density ρ_B

Total and alveolar human lung deposition for varying ρ_B was assessed by applying this method to a human lung deposition model (Ferron et al., 1988).

Assumed respiration conditions:
tidal volume of 750 cm^3; equal in- and exhalation times of 2.5 s (sitting male, ICRP, 1994).

Findings:

1) For d_B>0.2µm: ρ_B (↓) → deposition (↓)
(inertial and gravitational deposition scale with ρ_B)

2) For d_B<0.2µm: Deposition is independent of ρ_B
(diffusion-dominated regime)

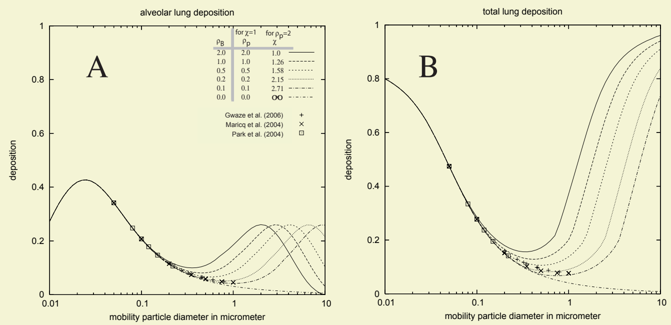

Fig. 1A and 1B: Alveolar (A) and total (B) lung deposition (relative to inhaled concentration) for particles with 0 < ρ_B < 2 g cm^{-3} based on an adapted standard deposition model (ICRP, 1994). The symbols represent the calculated deposition of soot agglomerates (from Diesel and biomass combustion) based on literature data.

Application to soot agglomerates

For soot, ρ_B correlates nagatively with d_B due to particle shape effects. Here we used $\rho_B(d_B)$ values for Diesel soot (Park et al., 2004; Maricq et al., (2004) extrapolated to 1µm) and biomass burning soot (Gwaze et al., 2006) with 0.1<ρ_B< 1.1 g cm^{-3} to calculate lung deposition of soot particles.

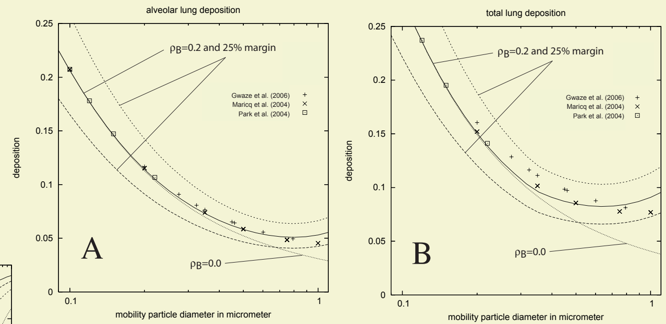

Fig. 2a and 2B: Alveolar (A) and total (B) lung deposition of Diesel and bio-mass burning soot based on ρ_B values reported in the literature. For comparison, we also plot particle deposition for spherical particles (χ=1) with constant ρ_p = 0.2 g cm^{-3} and the +/-25% margins. Finally, the ρ_p = 0 g cm^{-3} line illustrates particle deposition due to diffusion only.

As seen from Fig. 1A and 1B the deposition of soot particles with sizes >0.2µm (<0.2µm) is poorly (well) approximated by the deposition curves for spherical particles with ρ_B = 2 g cm^{-3} (material density of soot). On the other hand (Fig. 2), the deposition curves for ρ_B = 0.2 g cm^{-3} approximate soot deposition well (< 25% for alveolar and total deposition, respectively) over the entire submicron size range (<1.0µm).

Conclusions

- Transformation of deposition models for spherical particles to particles with irregular or unknown shape is possible by a simple transformation of the input parameters: ρ_p, d_v (volume-) → ρ_B d_B, (mobility-based parameters)
- Total and alveolar lung deposition of submicron soot particles can be approximated well (+/-25%) by assuming spherical particles with a constant ρ_B of 0.2 g cm^{-3}.

Literature

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