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 unknown shape.
2) Apply this method to soot agglomerates.

Method

Background

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

\[ \frac{dC}{dX} = \frac{C}{C(0)} \quad \text{(X=1)} \]

**For spheres**

**For arbitrary particle shape**

Diffusion coefficient: \( D \sim C(d_x) d_s \sim C(d_y) d_s \sim C(d_y)(X d_y) \)

Stokes number: \( Stk \sim \rho_d d_i^2 C(d_x) \sim \rho_d d_i^2 C(d_y) \sim \rho_d d_i^2 C(d_x)/X \)

Settling velocity: \( v_{ts} \sim \rho_d d_i^2 C(d_x) \sim \rho_d d_i^2 C(d_y) \sim \rho_d d_i^2 C(d_x)/X \)

\( d_c \): equivalent mobility (thermodynamic) diameter
\( C \): Cunningham slip correction
\( \rho_a, \rho_d \): particle and unit density (1000 kg/m³)

Problem

Particle density \( \rho_p \) and/or shape factor \( X \) are frequently not known.

Solution

Use the effective mobility density \( \rho_B \): \( \rho_B \) can easily be determined from online measurements of \( d_g \) and \( m_p \):

\[ \rho_B = \frac{6 \rho_d}{\pi d_s^2} \quad \rho_p \approx \frac{\rho_a}{1 + \frac{d_c}{d_s}} \]

\( Spheres \quad (X=1) \)

Arbitrary particle shape (\( X \) unknown)

\[ \frac{dC}{dX} \sim C(d_x) d_s \iff C(d_y) d_s \]

\[ Stk \sim v_{ts} \sim \rho_p d_i^2 C(d_x) \iff \rho_p d_i^2 C(d_y) \]

Summary

\[ \rho_p, d_c \iff \rho_p, d_s \]

Exchange of input parameters

Results

Influence of effective mobility density \( \rho_B \)

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

Assumed respiration conditions:
- tidal volume of 750 cm³;
- equal in- and exhalation times of 2.5 s (sitting male, ICRP, 1994).

Findings:

1) For \( d_g > 0.2 \mu m \): \( \rho_B \) (\( \rho \) ) → deposition (\( \rho_B \))
   (inertial and gravitational deposition scale with \( \rho_B \))

2) For \( d_g < 0.2 \mu m \): Deposition is independent of \( \rho_B \)
   (diffusion-dominated regime)

Application to soot agglomerates

For soot, \( \rho_B \) correlates negatively with \( d_g \) due to particle shape effects. Here we used \( \rho_B(\delta_g) \) 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\( \rho_B \) < 1.1 g cm⁻³ to calculate lung deposition of soot particles.

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 \( \rho_B = 2 \) g cm⁻³ (material density of soot). On the other hand (Fig. 2), the deposition curves for \( \rho_B = 0.2 \) 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:
  \[ \rho_p, d_v \text{ (volume)} \rightarrow \rho_B d_g, \text{ (mobility-based parameters)} \]

- Total and alveolar lung deposition of submicron soot particles can be approximated well (+/-25%) by assuming spherical particles with a constant \( \rho_B \) of 0.2 g cm⁻³.

Literature


