

MODELING AEROSOL DEPOSITION IN A SINGLE BIFURCATION OF THE HUMAN RESPIRATORY TRACT

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Introduction. This work presents a computational tool for the study of the deposition of fine particles in a single bifurcation of the human tracheobronchial (TB) tree; it can be used to improve the understanding of how the properties of the aerosol and the characteristics of the airflow can cause or enhance particle deposition. By considering this simplest building block of the TB tree, one can evaluate the variability associated with different generations of the TB tree, different breathing conditions or individuals, as well as gender or age variations. Also, the properties of particles, flow and geometry that are crucial in building a larger (and simplified) full-scale deposition model for the lung can be identified, and the use of black-box approaches with (often uncontrollable) assumptions is avoided. This work is part of a new integrated Modeling Environment for TOrtal Risk studies (MENTOR), an evolving software system that is being developed extending the framework and features of EDMAS.¹

Method. The computational module discussed here consists of a prescribed laminar flow (slug or Poiseuille) in a geometry indicated by the solid lines of the left panel of Fig.1. The setup is in two spatial dimensions and the particles, except for the drag force, are subject to the main deposition mechanisms of impaction, sedimentation and diffusion. Furthermore, the effect of electrostatic precipitation has been incorporated in the model. The electrostatic forces consist of the so-called space charge forces (one charge seeing the Coulomb effect of all the other charges) as well as the image force stemming from the image charges (due to the tube walls, which are assumed to be grounded and conducting). In addition, the option of incorporating hygroscopic growth has been mathematically developed and encompassed in the formalism. Newton's equation is solved for the particles, providing their individual trajectories to monitor desposition. The equation of motion for a particle carried by the two-dimensional flow is

$$\frac{dm_i}{dt} \mathbf{v}_i + m_i \frac{d\mathbf{v}_i}{dt} = m_i \mathbf{g} - f(\mathbf{v}_i - \mathbf{V}_{flow}) + \mathbf{F}_{i,dif} + \mathbf{F}_{i,im} + \mathbf{F}_{i,sp} \quad (1)$$

where m_i is the mass of the i th particle, \mathbf{v}_i its velocity, \mathbf{g} the gravitational acceleration, f the viscous drag coefficient, \mathbf{F} denotes force and \mathbf{V}_{flow} is the flow velocity. Subscripts sp and im refer to the space charge and image electrostatic forces, respectively, while dif refers to diffusion.

The self-consistent, two-dimensional expression for the electrostatic force on the i -th particle from all the neighboring particles is

$$\mathbf{F}_{i,sp} = \sum_{j \neq i} \frac{q_i q_j}{2\pi \epsilon_0 ((x_i - x_j)^2 + (y_i - y_j)^2)} [(x_i - x_j) \hat{\mathbf{x}} + (y_i - y_j) \hat{\mathbf{y}}] \quad (2)$$

where the (x_j, y_j) indicate the position of the particle of charge q_j , hats denote unit vectors, and ϵ_0 is the dielectric constant of the vacuum. The image force from the summation of infinite charges induced by the two parallel lines q at $(2ih - y, -2ih + y)$ and $-q$ at $(-2ih + y, 2ih + y)$, where h is the width of the generation, y is the particle y -coordinate, and i takes positive integer values, is given by:

$$\mathbf{F}_{i,im} = \frac{q^2}{2\pi\epsilon_0} \left(-\frac{1}{2y_i} + \frac{\csc\left[\frac{\pi y_i}{h}\right] \left(-\pi y_i \cos\left[\frac{\pi y_i}{h}\right] + h \sin\left[\frac{\pi y_i}{h}\right] \right)}{2hy_i} \right) \hat{\mathbf{y}} \quad (3)$$

It should be noted that this Molecular Dynamics “particle following” methodology is ideal for the incorporation of hygroscopic growth. Hygroscopicity results in an increase of particle masses as they move in the humid environment of the TB airways. This is naturally incorporated in a mass variation term in the equation of motion (Eq.1). In the present formulation the mass variation can be calculated by using two-dimensional mass transport and heat transport equations. These equations, combined via the latent heat equation, yield an expression for the mass variation in terms of measurable quantities.

Results and Conclusions. A modular code entitled REBELS (REspiratory Bifurcation dEposition model Study) that solves the set of dynamical equations in the bifurcation geometry of Fig.1 has been developed. This code is modular in the input of the available flow profiles and in the properties (size, density, charge) of the particles, as well as those of the geometry (length, width of the airways, angle of gravity, angle of bifurcation). Particles of various sizes have been used for different generations, and the relative effect of different deposition mechanisms, as well as the local characteristics of deposition have been assessed and will be highlighted. A typical result for 1 μm particles is shown in Fig.1. The left panel shows the particle positions at the end of the exhalation period ($T_{inh} = T_{exh} = 2/3 T_{pause}$, where T denotes total time and *inh*, *exh* refer to inhalation and exhalation, respectively). The right panel indicates individual particle trajectories throughout the simulation.

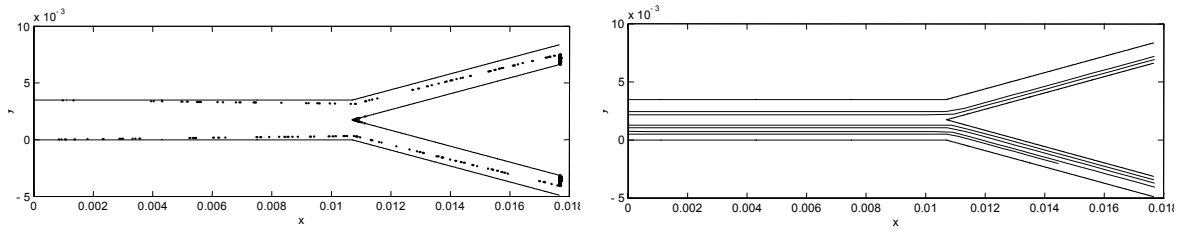


Figure 1. Particle Deposition and Individual Trajectories in the Bifurcation

Except for the evaluation of the relative strength of the main deposition mechanisms for different particle sizes, this elementary bifurcation setup provides a number of new insights. Contrary to what was previously reported, the space charge force is found to be of comparable effect to the image force (previously the former was assumed negligible). It, in fact, has stronger effect than the latter for smaller particle sizes whereas this trend is reversed for larger sizes. Also, in all the studies, the carinal ridge has been found to be a deposition hot-spot, an effect that can be attributed to the local geometry.

On-going extensions of this work involve the generalization (based on the most relevant factors) of the two-dimensional to a three-dimensional setup.

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References.

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