Deposition of Submicron Charged Particles in the Trachea of the Human Airways

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Introduction: The work addresses on the effect of charged particles and a cartilaginous ring wall structure on the deposition of submicron particles in the trachea of the human airways. It is an Eulerian description with a combination of turbulent flow, transport and migration of charged particles.

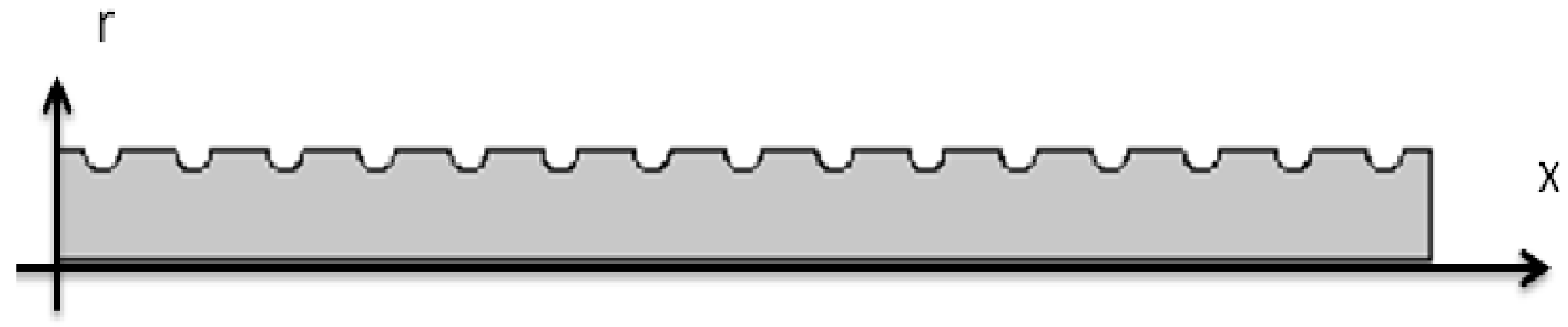


Figure 1. Axisymmetric pipe geometry with a cartilaginous ring wall structure. Radius of Trachea a=0.008[m] length 0.096[m]. Amplitude of rings 0.0008[m]. Inlet at x=0.

Computational Methods: The problem is solved by Comsol Multiphysics using the interfaces, low-Reynolds number k-ε model for turbulent flow, transport of diluted species, and electrostatics. The following equations are solved

$$\rho(\bar{\mathbf{u}}\cdot\nabla)\bar{\mathbf{u}} = \nabla\cdot(-\bar{p}\mathbf{I} + (\mu+\mu_t)(\nabla\bar{\mathbf{u}} + (\nabla\bar{\mathbf{u}})^T) - \frac{2}{3}\rho k\mathbf{I})$$

$$\nabla\cdot\bar{\mathbf{u}} = 0$$

$$\rho(\bar{\mathbf{u}}\cdot\nabla)k = 2\mu_t\nabla\bar{\mathbf{u}}\cdot\nabla\bar{\mathbf{u}} - \mu\nabla\bar{\mathbf{u}}\cdot(\nabla\bar{\mathbf{u}})^T + \nabla\cdot((\mu + \frac{\mu_t}{\sigma_k})\nabla k)$$

$$\rho(\bar{\mathbf{u}}\cdot\nabla)\varepsilon = C_{\varepsilon 1}\frac{\varepsilon}{k}2\mu_t\nabla\bar{\mathbf{u}}\cdot\nabla\bar{\mathbf{u}} - C_{\varepsilon 2}\frac{\varepsilon}{k}\rho\nu\nabla\bar{\mathbf{u}}\cdot(\nabla\bar{\mathbf{u}})^T +$$

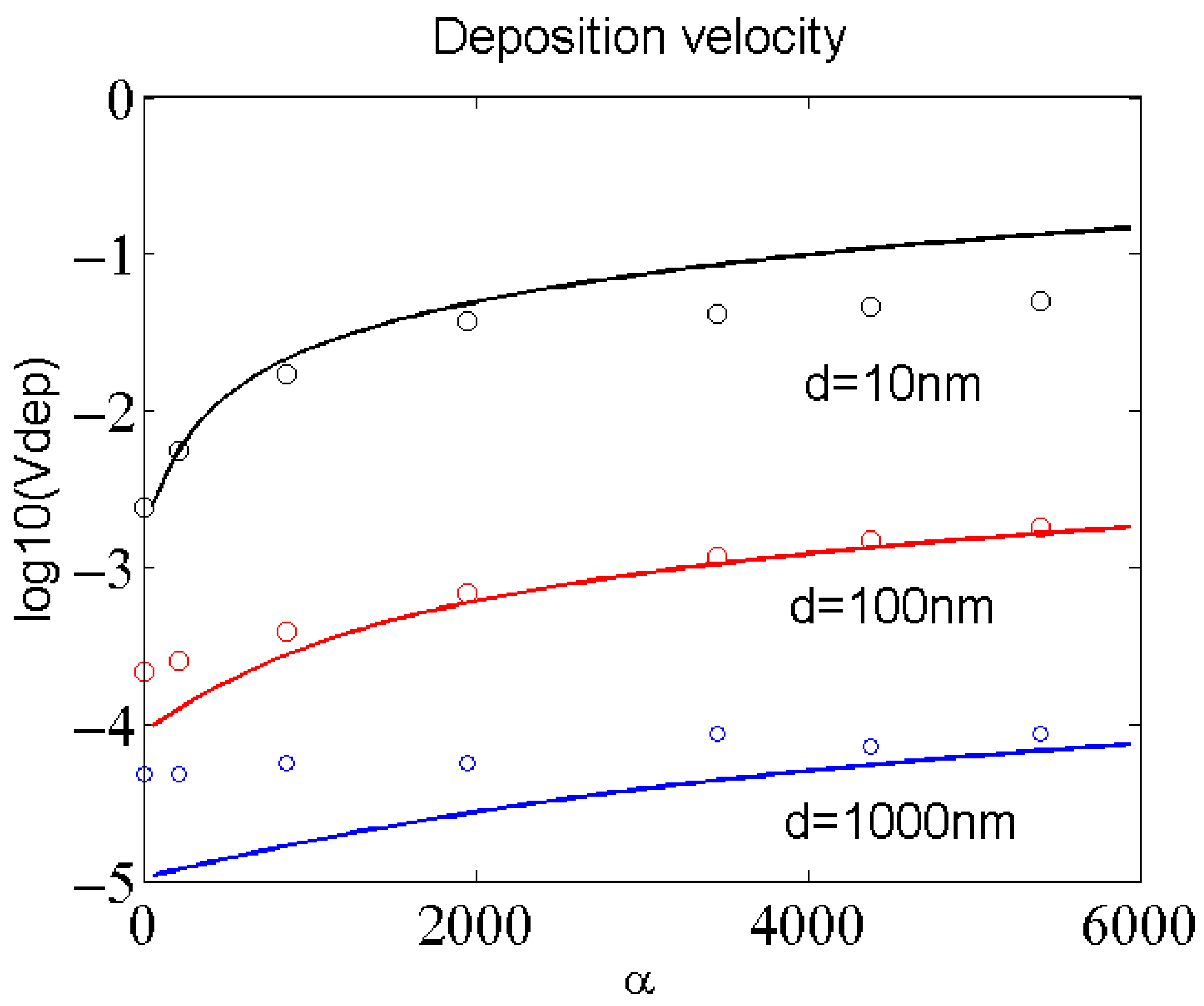
$$+\nabla\cdot((\mu + \frac{\mu_t}{\sigma_\varepsilon})\nabla\varepsilon) - f_\varepsilon C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k}$$

$$\mu_t = \rho f_\mu C_\mu \frac{k^2}{\varepsilon}$$

$$(\bar{\mathbf{u}}\cdot\nabla)c - \frac{qD}{\kappa T}(\nabla c\cdot\nabla\phi) + \frac{q^2 D}{\varepsilon_0\kappa T}c^2 - \nabla\cdot((D + D_t)\nabla c) = 0$$

$$\nabla^2\phi = -\frac{qc}{\varepsilon_0}$$

Results: The results using Comsol are first validated with theory for the case of a fully developed pipe flow with smooth walls. In **figure 2** deposition velocity calculated by theory and Comsol are compared for three different particle sizes d=10nm,100nm and 1000nm and for different values of the electrostatic parameter α. For large particles the disagreement is large which can be deduced from an incorrect prediction of the eddy diffusivity in the near wall region using the Comsol model.



$$\alpha = \frac{1}{4}\frac{c_0 q^2 a^2}{\varepsilon_0 \kappa T}$$

Figure 2. Deposition velocity as a function of α.

After validation the model is applied to 10nm particles for a pipe with cartilaginous rings. In **figure 3** the flow, the concentration and electric field are presented in the region before and after the first ring. In **figure 4** the total particle deposition in trachea is shown.

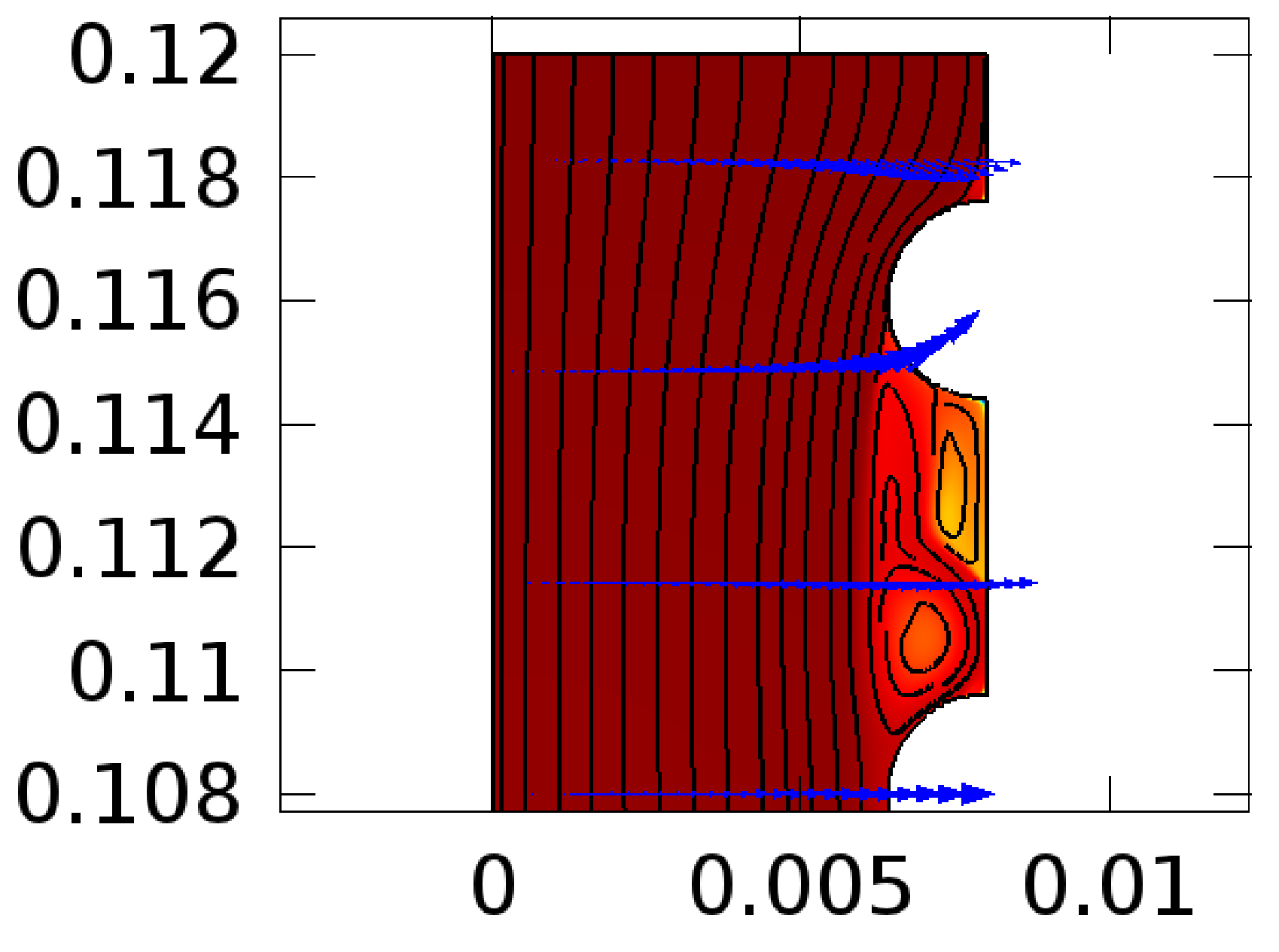


Figure 3 Streamlines, concentration, electric field

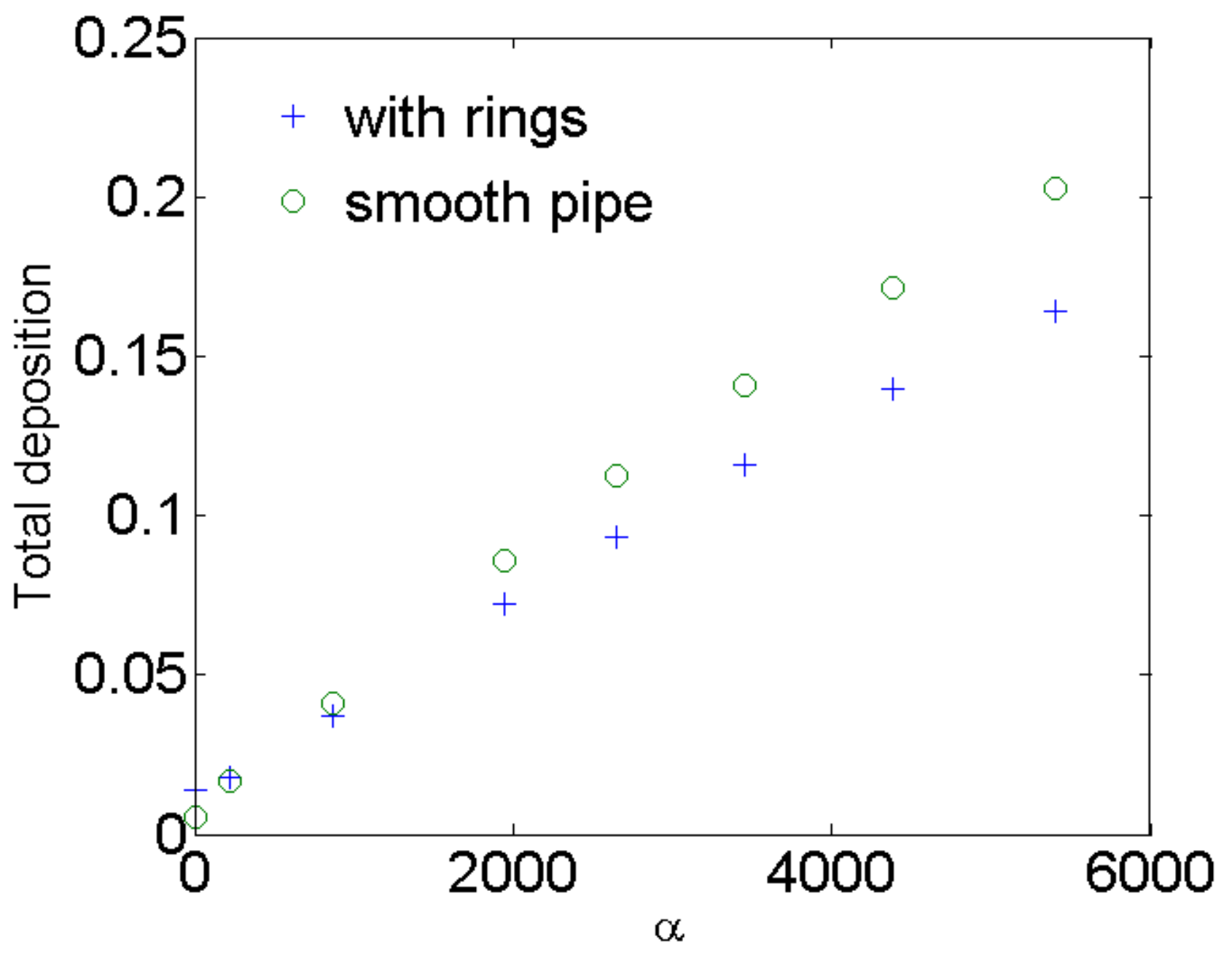


Figure 4 Fraction of deposited particles

Conclusions: Charged particles give a substantial increase in deposition from 1% for uncharged particles up to about 20% for charged particles. Cartilaginous rings reduce deposition. The results should be of importance in an optimal design of therapeutic aerosols.

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