Hygroscopic growth modelling for hygroscopic nanometric aerosols in the human respiratory tract

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The understanding of these really small particles is a crucial issue for our society, through the environmental pollution or the aerosol therapy. Moreover, nanometric particles of aerosols require to take into account in the models used for bigger particles the possible growth of particles due to the humidity, which cannot be neglected any more. Indeed, several studies (Longest, 2011) have shown that the size of initially small particles in a dry air can become significantly bigger in the pulmonary conditions. Thus, even if the deposition area is well known in the nonhygroscopic case, it is not the case in the hygroscopic one. In our situation, these deposition areas depend not only on the initial size of the particles, but also on the initial composition of the particles and the characterisitics of the inspired air (temperature and humidity).

Local hygroscopic particle and lung trumpet models

A purely local model is first investigated, in which we try to improve our understanding of the physical processes involved in the hygroscopic growth. The local area of the airways is considered as a tube of diameter D_{tube} in which the air remains static and has a uniform temperature T_{air} and a uniform water vapor mass fraction $Y_{v;air}$. The wall has constant temperature T_{wall} and relative humidity RH_{wall}, which results in a constant water vapor mass fraction $Y_{v;wall}$ on the wall. Similarly as the droplet, both conditions on the wall and in the air imply two fluxes: q_{wall}, the heat flux due to the difference of temperature ($T_{air} - T_{wall}$), and n_{wall}, the evaporating/ condensating mass flux of water vapor due to the difference of water vapor mass fraction ($Y_{v;air} - Y_{v;wall}$). We place a density n_{part} of identical particles. We obtain then four fluxes which can be summarized in Fig. 1.

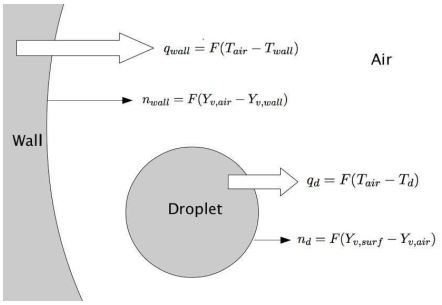

Figure1: Temperature and mass water vapor fluxes.

Second, we use the trumpet model of the lung geometry described in (Martin *et al*, 2013) to let particles move in the respiratory tract, with the human conditions T_{wall} = 37°C and RH_{wall} = 99:5%, and the following respiration parameters: time of a cycle T = 5 s with 1.75 s of inspiration and 3:25 s of expiration. The composition of all the droplets is the one from (Longest, 2011): initial radius r_{d0} and the massic fraction of component (NaCl) denoted mfs.

Numerical observations from the models

The influence of the injection time on the particle size is quite clear on Fig. 2. We can al the time when a particle reaches its maximum humidity is reached when the particle is in the last generations of the upper airways.

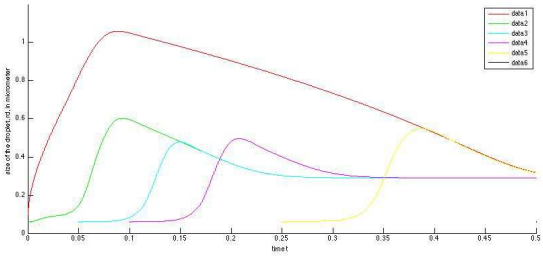

Figure 2: Time variation of particle size: T_{air} (t=0) = 15°C, RH_{air}(t=0) = 50%, r_{d0} = 60 nm, and mfs = 0.5. In each test, data 1 to 6 correspond to several injection times of the nanoparticles (0 s; 2.5 ms, 50 ms, 0.1 s, 0.25 s, 0.5 s, respectively).

Next, when we do not have over-humidity, the droplets size smoothly increases towards its equilibrium value, whereas, whenever over-humidity occurs, the particles can grow significantly bigger than their equilibrium size before reaching it again.

Eventually, it is important to note that the mfs of course has an effect on the equilibrium size of the particles. For instance, with the same experimental data otherwise, taking mfs = 0.5 and 0.8, the equilibrium values are respectively approximately 300 or 400 nm.

Longest, P.W. and Hindle, M. (2011) *Numerical model to characterize the size increase of combination drug and hygroscopic excipient nanoparticle aerosols*, Aerosol Sci. Technol. 45(7):884-899.

Martin, S. and Maury, B. (2013) *Modeling of the oxygen transfer in the respiratory process*, ESAIM: Mathematical Modelling and Numerical Analysis, 47:935-960.