Modeling controlled deposition of polydisperse aerosol in the 3D in-vitro exposure system

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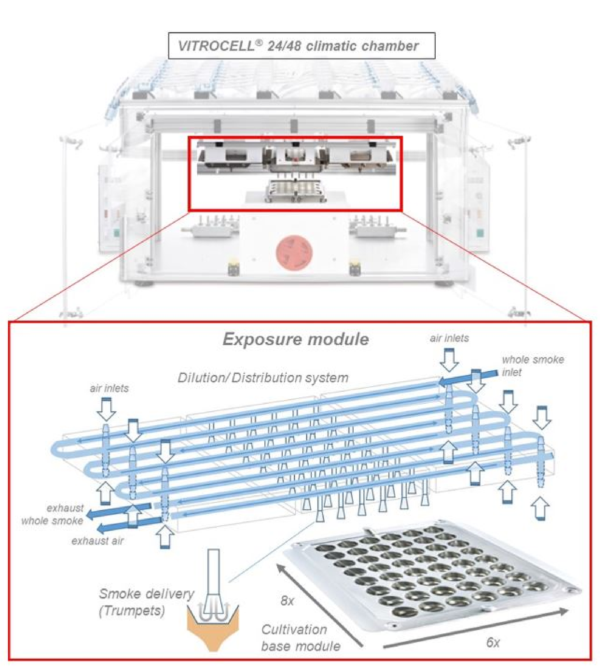
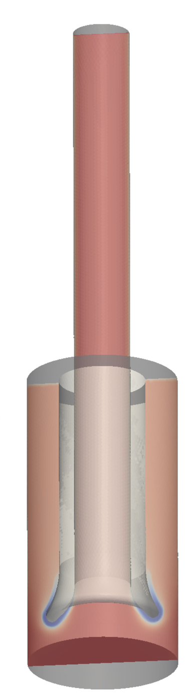
Introduction and motivation

Dosing of toxic substances in multi-well aerosol exposure systems is usually controlled via air dilution of the flowing aerosol, while the deposition of those substances on the biological inserts largely depends on the physical properties of the aerosol, i.e., droplet number, density and size of aerosol droplets. Consequently, both the design of the experimental exposure systems as the design of experimental studies/protocols using those systems become a challenging subject of the experimental and numerical investigations concerning reliability, repeatability and reproducibility of performed studies. The necessary system characterization can be performed both experimentally [1] and numerically [2]. In this context we present a multi-species aerosol model capable of capturing all major physical phenomena of the aerosol dynamics inside an in-vitro exposure system [3].

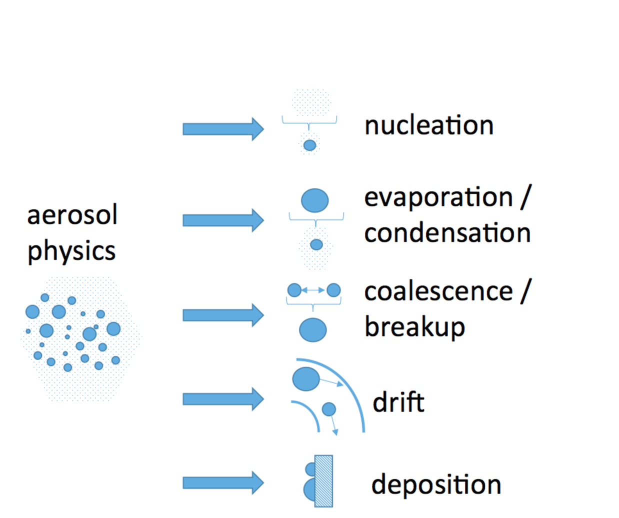


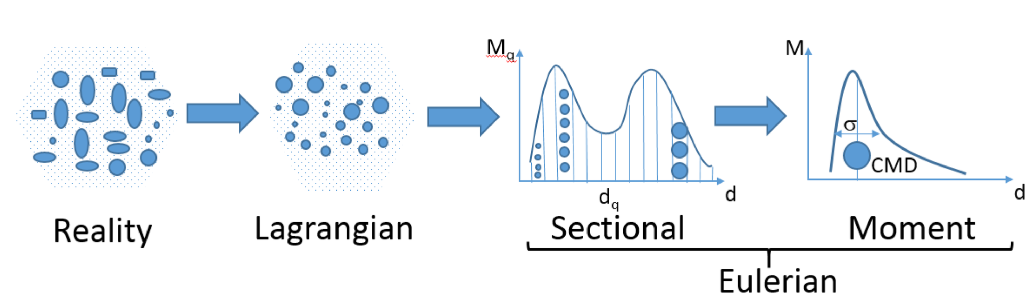
Modeling objectives:

- predict transport and evolution of multispecies polydisperse aerosols
- compute local aerosol deposition in complex geometries (dosimetry)
- support bridging *in-vivo* and *in-vitro* biological research



Aerosol physics and modeling approaches





Approach:

- two-moment model (fixed droplet size distribution width σ) [4]
- sectional model (resolved size distribution with discretized sections) [5]

Computational Fluid Dynamics with sectional aerosol modeling

Coupling of velocity $\mathbf{u}$, pressure p, density ρ and temperature T along with the equation of state (ideal gas law and incompressible liquid) and material properties: specific heat (c_p), conductivity (k), viscosity (μ), enthalpy of vaporization S_h and viscous stress tensor τ [6]:

$$\underbrace{\partial_t \rho + \partial_j(\rho u_j) = -\partial_j\left[(1-\gamma) f_j\right]}_{\text{mass conservation}}$$

$$\underbrace{\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = -\partial_i p + \partial_j(\mu \tau_{ij})}_{\text{momentum conservation}} \quad ; \quad i = 1,2,3$$

$$\underbrace{\rho c_p(\partial_t T + u_j \partial_j T) = \partial_j(k \partial_j T) + \partial_j(\mu u_k \tau_{kj}) + S_h + Dp/Dt}_{\text{energy conservation}}$$

Aerosol introduced by vapor Y_n and liquid Z_n mass fractions for N species and particle number densities ($\mathcal{N}_q = \rho M_q$) for Q sections accompanied by sources $\mathcal{J}_{Y_n}$, $\mathcal{J}_{Z_n}$ and $\mathcal{J}_{M_q}$ including aerosol processes (nucleation, condensation/evaporation and coagulation). The flux f_j accounts for the total mass transfer due to Stokes-Einstein droplet diffusion D_q and drift (Stokes drag and gravitation) driving deposition [3]:

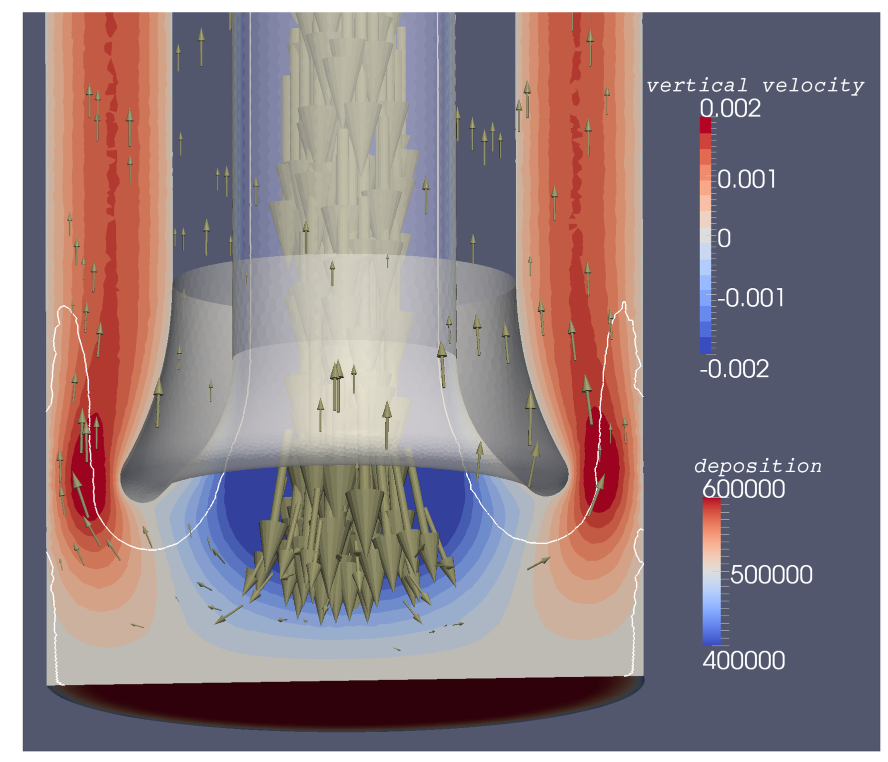
$$\underbrace{\partial_t(\rho Y_n) + \partial_j(\rho Y_n u_j) = \partial_j(Y^{-1}\gamma f_j Y_n) + \mathcal{J}_{Y_n}}_{n\text{-species vapor mass fraction transport}} \quad ; \quad n = 1, ..., \mathrm{N}$$

$$\underbrace{\partial_t(\rho Z_n) + \partial_j(\rho Z_n u_j) = -\partial_j(Z^{-1} f_j Z_n) + \mathcal{J}_{Z_n}}_{n\text{-species liquid mass fraction transport}}$$

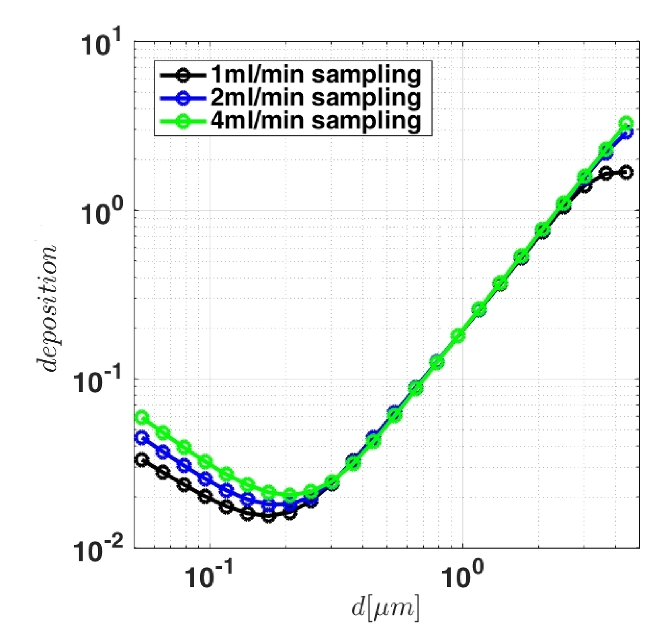
$$\underbrace{\partial_t(\rho M_q) + \partial_j(\rho M_q u_j) = -\partial_j(\rho M_q u_{j,q}) + \partial_j(\rho D_q \partial_j M_q) + \mathcal{J}_{M_q}}_{q\text{-section particle number density transport}} \; ; \; q = 1, ..., \mathrm{Q}$$

Consistency is guaranteed by computations of the local mean vapor to liquid density ratio $\gamma = \rho_v/\rho_l$ and total local vapor $Y = \sum_n Y_n$ and liquid $Z = \sum_n Z_n$ mass. Vapor diffusion (Hirschfelder-Curtiss approximation) is included in $\mathcal{J}_{Y_n}$.

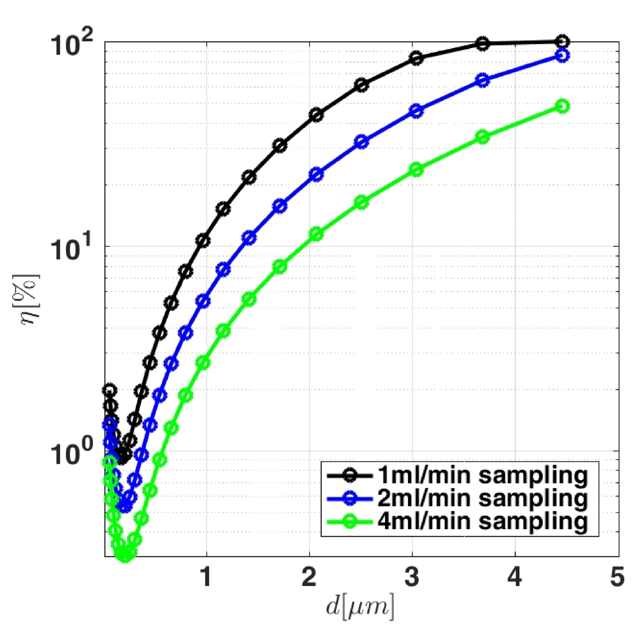
Application: aerosol deposition in 3D geometry



The figure shows the flow and the deposition of aerosol in a Vitrocell 24/48 trumpet. At the exit of the trumpet, the flow slows down and creates a region of null velocity and uniform aerosol concentration over the deposition plate. The gentle flow around the trumpet smoothly transports the aerosol. Thus no deposition by impaction has been observed.



Aerosol deposition flux versus droplet diameter for three sampling flow rates ($1ml/min$, $2ml/min$, $4ml/min$). Deposition for larger droplets is dominated by gravity ($\propto \mathcal{N}_q * \rho_l * d_q^2$) and independent on the sampling rate.



Aerosol deposition efficiency η versus droplet diameter for the three sampling flow rates. Efficiency decreases with increasing flow rate. Full deposition can be reached for large droplets and low sampling rates.

Concluding remarks

- A computational platform for CFD simulations of multispecies evolving aerosols including drift and deposition has been developed [3, 4, 5, 6].
- Aerosol deposition in a Vitrocell® 24/48 system was analyzed for different droplet sizes and trumpet sampling rates.
- Deposition varies significantly with the aerosol droplet size, and reaches a minimum for droplets of about $0.2\mu m$.
- Large droplets ($>0.4\mu m$) deposit in the Vitrocell® 24/48 trumpet only due to a settling/gravitational mechanism which is independent on the sampling rate and increases with the droplet size. As a consequence the deposition efficiency, or the fraction of the sampled aerosol that deposits on the plate, decreases with increasing sampling rates.
- On-going work: investigations of non-isokinetic sampling and deposition for evolving multispecies aerosols [2].
- Future work: further validation, extension and refinements of aerosol physics models.

References

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