# Modeling of flow and evolving aerosol particles dynamics for computing local deposition in air-liquid interface experiments


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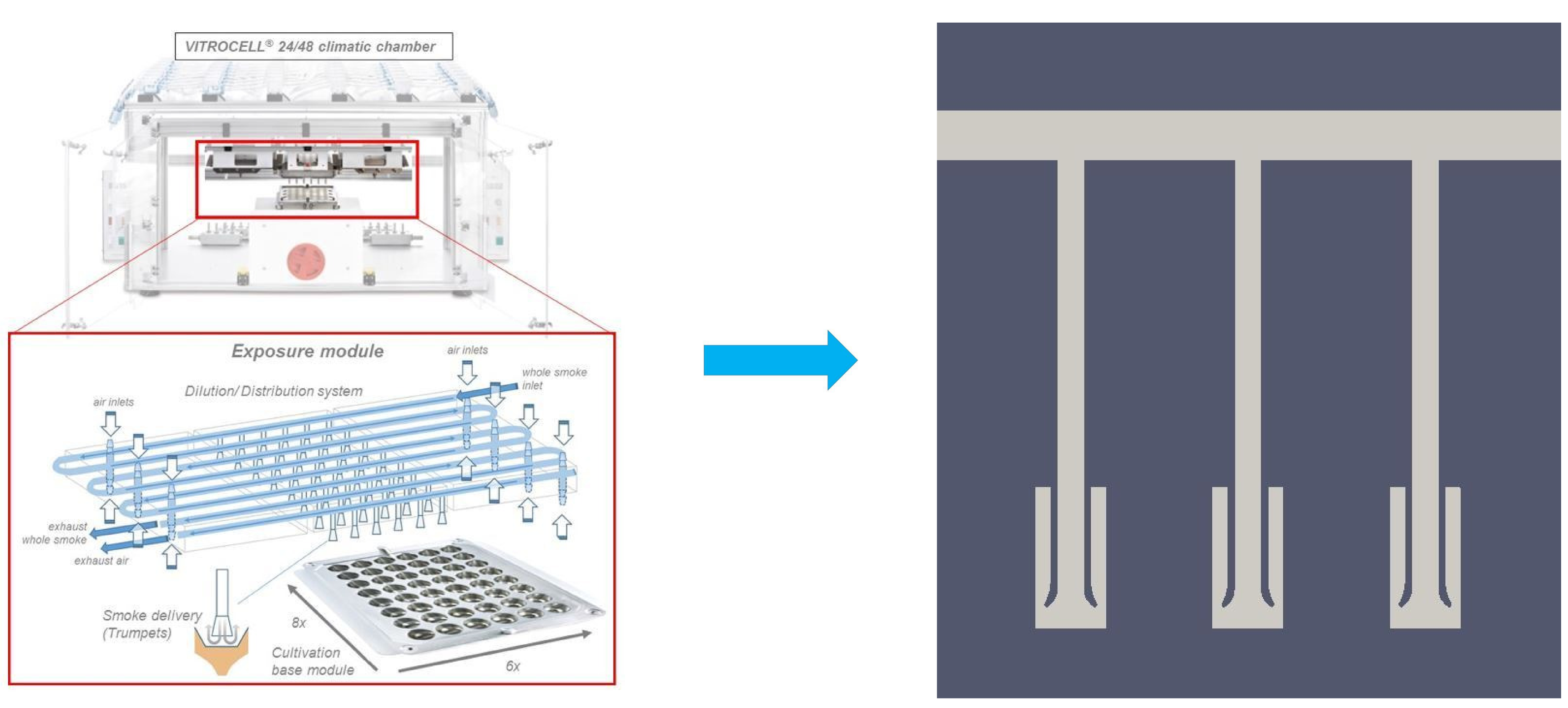
## Introduction

Understanding the physical conditions governing deposition of aerosol droplets and its influence on the cell functioning is a key step towards the ultimate goal to relate the exposure of inhaled and deposited aerosols to health outcomes. This is important two-fold, i.e., the same physical mechanisms are acting in much more complex geometries (e.g., human airways), and simultaneously acquired knowledge allows for improved in-vitro inhalation toxicology experiments. An approach to model the flow and evolving aerosol dynamics together with aerosol deposition in a simple trumpet-like geometry frequently used in in-vitro exposure systems is presented.




## Flow modeling: multispecies low-Mach approach

Coupling of the mass, momentum and energy conservation is done via the Navier-Stokes and temperature equations [1]:

$$\partial_t \rho + \partial_j(\rho u_j) = 0 \qquad (1)$$

$$\partial_t(\rho u_i) + \partial_j(\rho u_j u_i) = -\partial_i p + \partial_j(\tau_{ij}) \quad ; \quad i = 1, ..., 3 \qquad (2)$$

$$\rho c_p(\partial_t T + u_j \partial_j T) = -\partial_j q_j - \tau_{ij}\partial_i u_j + (\partial_{\ln T}(\ln \hat{V}))_{p,\chi_\alpha}(\partial_t p + u_j \partial_j p) + S_h \qquad (3)$$

where $t$ is time, $\rho$ is the total mass density of the mixture, $u_i$ is the velocity, $p$ is the pressure, and $\tau_{ij}$ is the rate of the strain tensor. In the fluid temperature equation, $c_p$ is the specific heat of the mixture at constant pressure, $T$ is the temperature, and $q_j$ is the heat flux, $\hat{V}$ is the volume per unit mass and $\chi_\alpha$ is the molar fraction of constituent $\alpha$. The energy source term $S_h$ is related to the enthalpy of the phase change transition. The operator $\partial_t$ is the temporal partial derivative and $\partial_j$ is the partial derivative with respect to the spatial coordinate $j$. The Einstein summation convention is assumed.

## Aerosol modeling: Eulerian-Eulerian drift-flux

The multispecies characteristics of the gas-liquid mixture is guaranteed by decomposition of the mass via the mass fractions equations for the gas phase ($Y$) and liquid phase ($Z$) linked with the the physical characterization of the aerosol by the general dynamic equation (GDE) for the aerosol particle number concentration $N_\beta$:

$$\partial_t(\rho Y_\alpha) + \partial_j(\rho Y_\alpha(u_j + v_{s,j}^{(g)})) = -\partial_j j_{j,\alpha} + S_\alpha \quad ; \quad \alpha = 1, ..., n \qquad (4)$$

$$\partial_t(\rho Z_\beta) + \partial_j(\rho Z_\beta(u_j + v_{s,j}^{(\beta)})) = -\partial_j j_{j,\beta} + S_\beta \quad ; \quad \beta = 1, ..., m \qquad (5)$$

$$\partial_t(m_{p,\beta} N_\beta) + \partial_j(m_{p,\beta} N_\beta(u_j + v_{s,j}^{(\beta)})) = -\partial_j j_{j,\beta}^* + S_\beta \quad ; \quad \beta = 1, ..., m \qquad (6)$$

where $Y_\alpha$ is the mass fraction of the component $\alpha \in \{1, ..., n\}$ in the gas phase, and the total mass fraction of particles of size $\beta$ is denoted as $Z_\beta$, $\beta \in \{1, ..., m\}$. The diffusion mass fluxes are denoted by $j_{j,\alpha}$, $j_{j,\beta}$, and $j_{j,\beta}^*$ and the mass of an individual particle of size $\beta$ is $m_{p,\beta}$. The velocities $v_{s,j}^{(g)}$ and $v_{s,j}^{(\beta)}$ are the slip velocities of the gas phase and particles of size $\beta$, respectively. The phase change mass transfer source terms are $S_\alpha$ and $S_\beta$.

## Aerosol transport and evolution

Transport and evolution of the multispecies aerosol follows:

- Condensation/evaporation including Kelvin effect and Knudsen correction [2]
- Coalescence for polydisperse droplet distributions [3]
- Drift-flux velocities based on inertial and gravitational forces with Cunninghan correction [4]
- Assumption on the same species composition for the gas and liquid phases: $Z_\beta = \sum_{\alpha=1}^{n} Z_{\beta,\alpha}$, where $Z_{\beta,\alpha}$ is the mass fraction of component $\alpha$ in the $n$-components mixture constituting the particles of size $\beta$
- Assumption on log-normal distribution of the particle size with given geometric standard deviation ($\beta \equiv 1$)

## Geometry & outcome

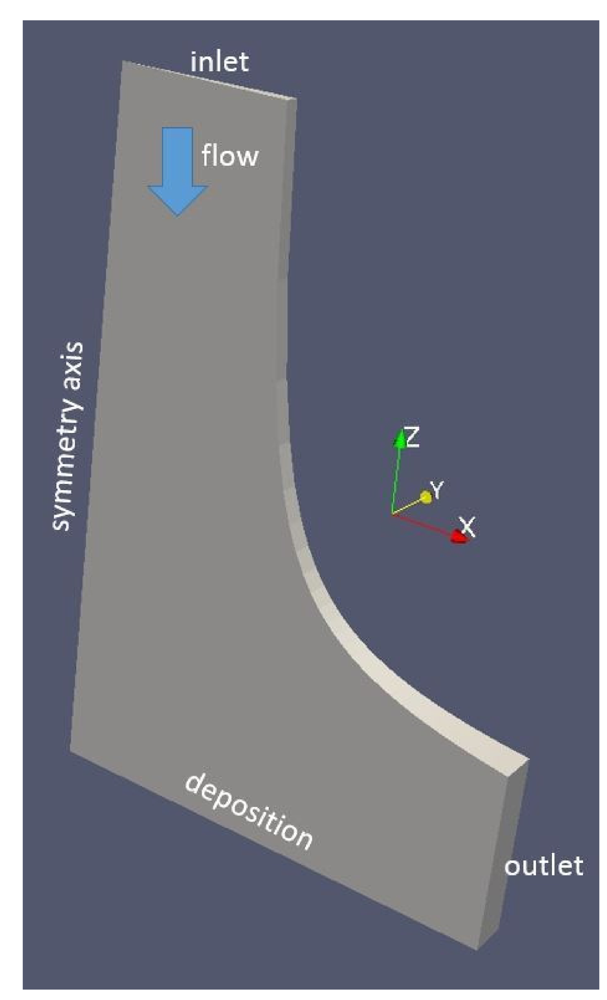



Figure 1: Axi-symmetric representation of trumpet geometry

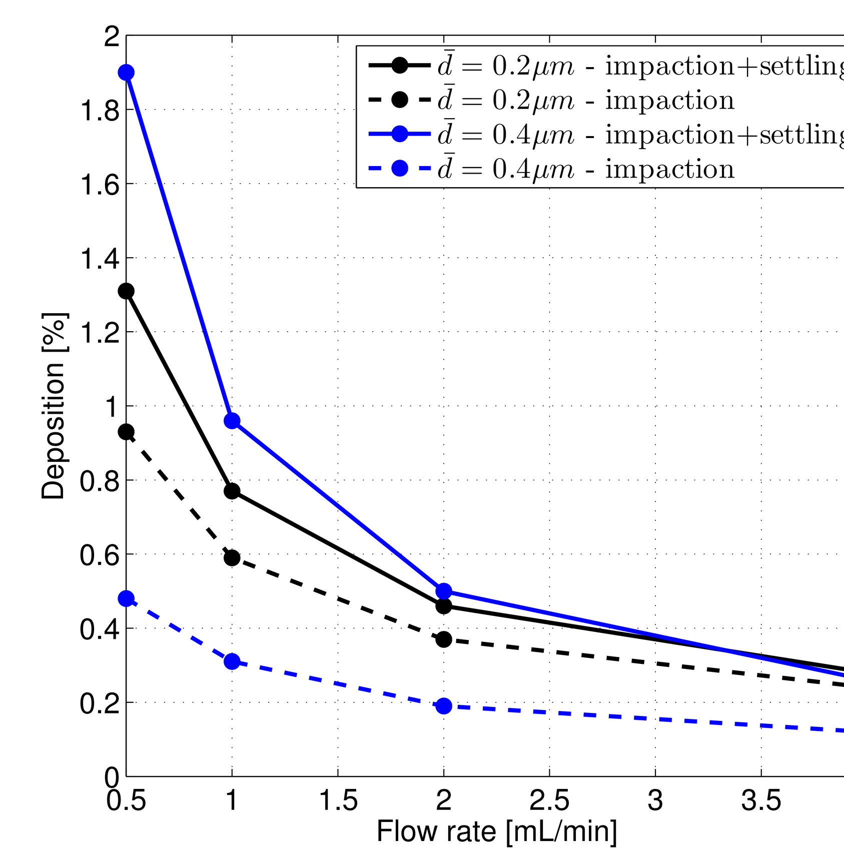



Figure 2: Deposition of two mean-size $\bar{d}$ aerosol distributions taking into account impaction and gravitational settling for four various flow rates

## Conclusions

- Computational framework for Eulerian-Eulerian multi-species aerosol flow developed - relevant for accurate computations of deposition rates in exposure systems
- Comprehensive aerosol dynamics encountering evolution of polydisperse droplets included - crucial for capturing liquid aerosol aging affecting tissue exposure rates
- On-going: model validation for deposition and evolving size distribution (multi-bin approach) model development ($\beta > 1$)
- Application: in-vitro exposure simulations for precise dosimetry assessment

## References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