Numerical characterization of aerosol exposure systems: an analytical model to predict dose deposition

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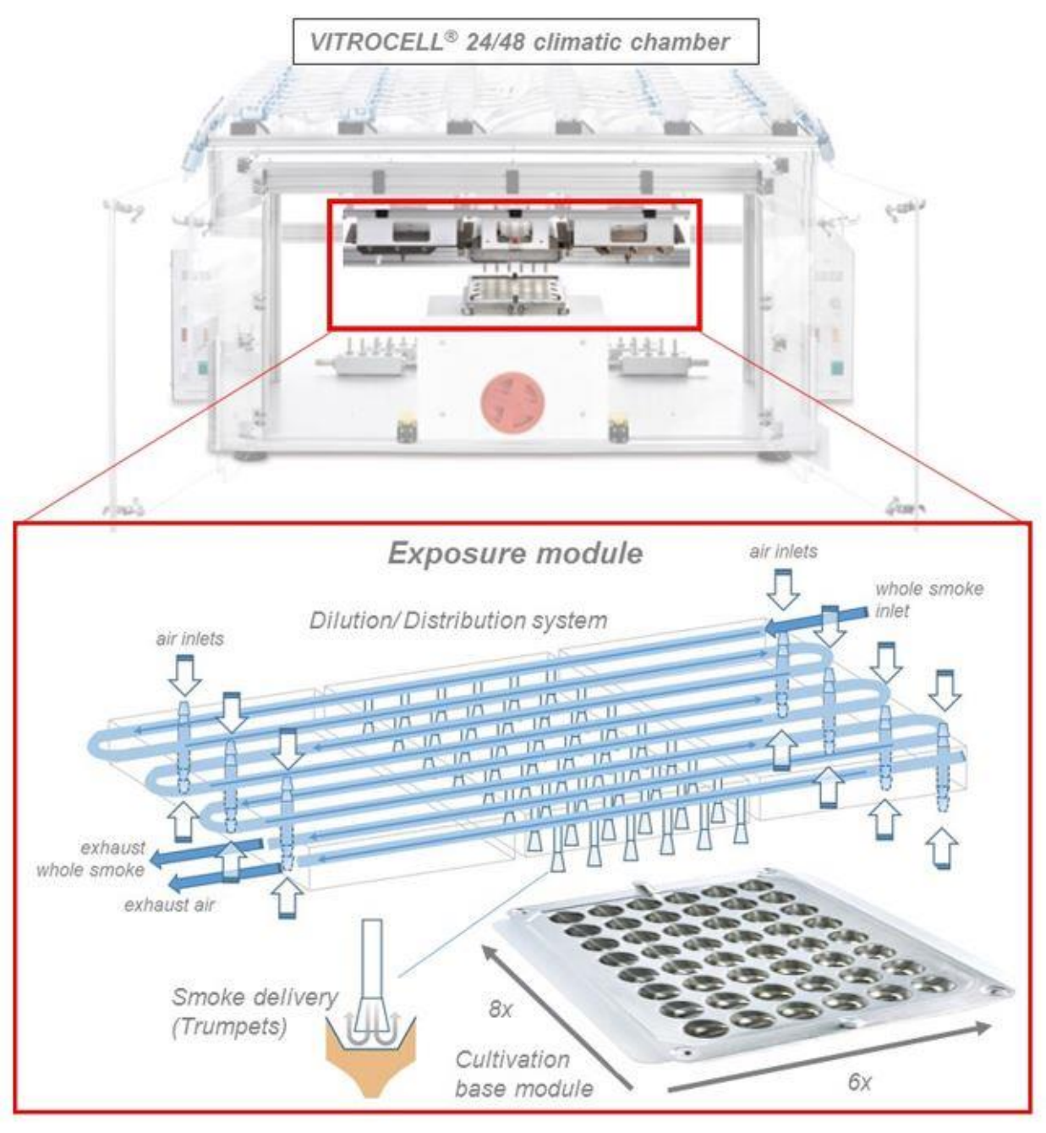
Introduction and Objectives

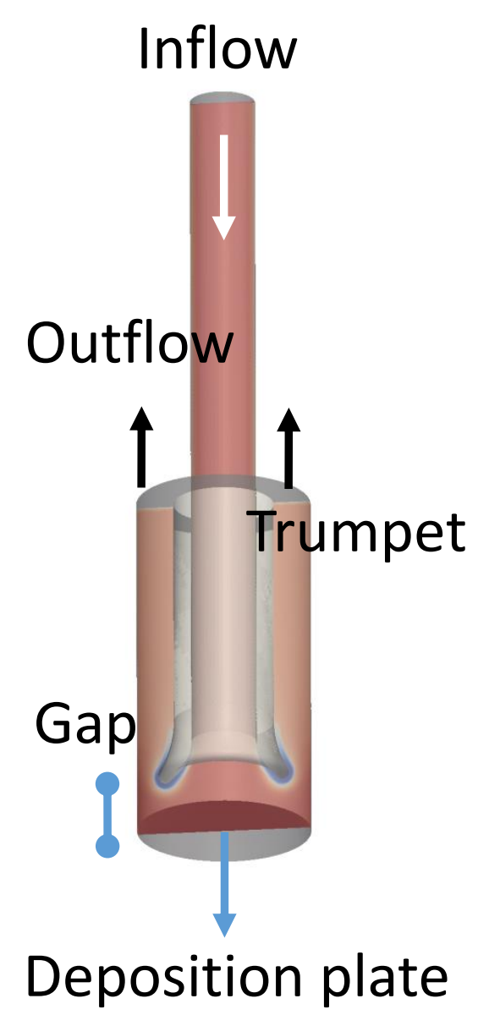
Multi-well aerosol exposure systems are used in modern toxicology assessment studies for simultaneous aerosol delivery to a large number of tissue/cell culture samples. Systems similar to those developed by Vitrocell® are designed to control experimental conditions and to deliver aerosol mixtures to a tissue culture through a trumpet-shaped pipes. The overall quality and reproducibility of the experiments, and the evaluation of the results, depend on control and prediction of the deposited dose. For this reason, it is important to understand which physical parameters influence the aerosol deposition in order to predict it. With limited experimental data in the available literature, applying computational modeling approaches is necessary to study and understand the fundamental mechanisms governing aerosol flow and deposition.

We employed our recently developed Eulerian computational fluid dynamics (CFD) solver, AeroSolved (publicly available at www.aerosolved.com), for simulations of polydisperse multispecies aerosol transport and deposition. Various operating conditions were investigated, and the results were verified by comparisons with the available experimental data and other numerical simulations.



Modeling objectives:

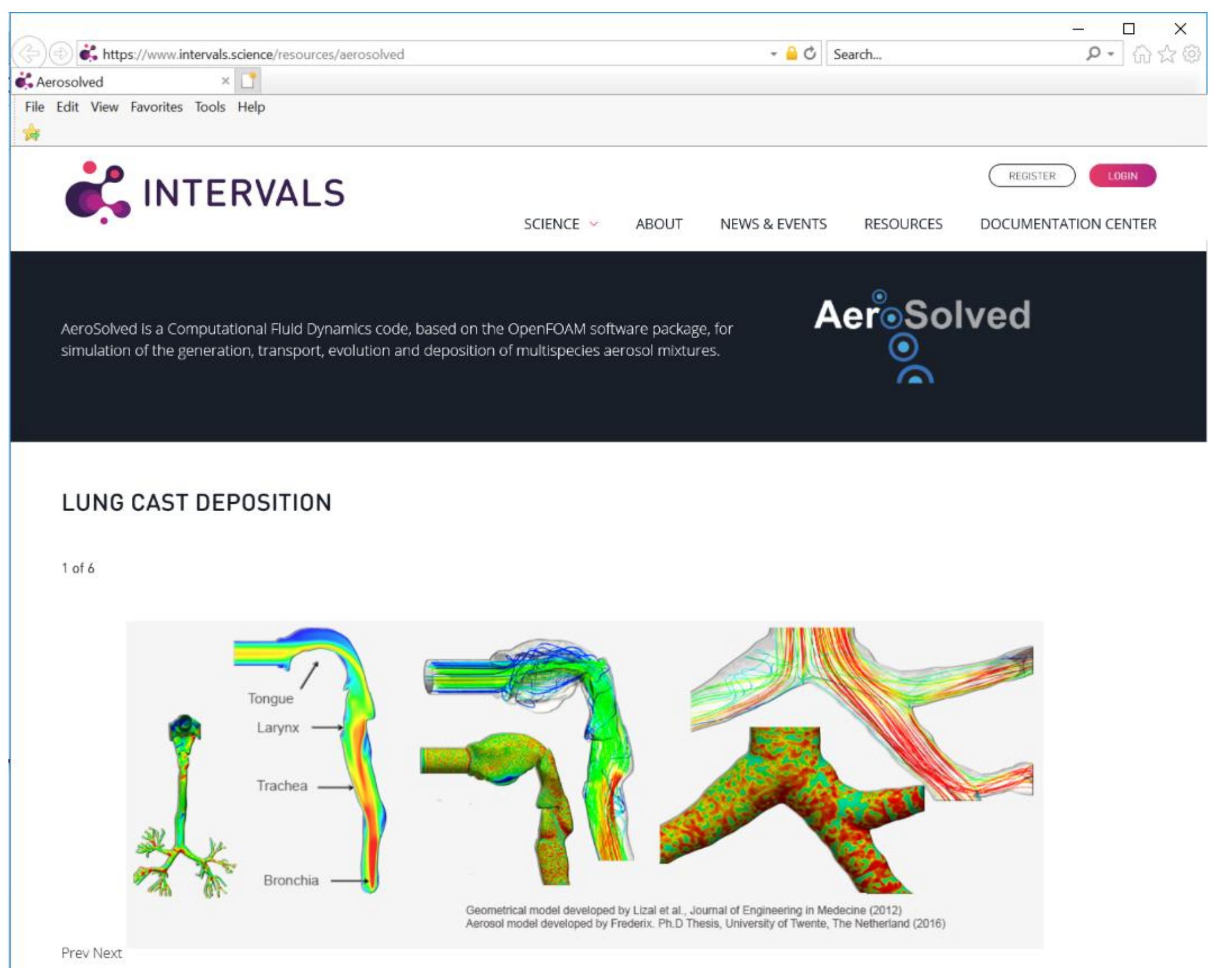
- Predict transport and evolution of multispecies polydisperse aerosols.
- Compute local aerosol deposition in complex geometries (dosimetry).
- Support bridging *in vivo* and *in vitro* biological research.



AeroSolved: Platform for Aerosol Numerical Modeling

AeroSolved is a CFD code based on the OpenFOAM software package for detailed simulation of aerosol dynamics. It is under continued development to improve its performance and extend its capabilities. In July 2017, it was released to the public domain under the free open-source GPLv3 license.

www.aerosolved.com



https://www.intervals.science/resources/aerosolved

Aerosolved

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AeroSolved is a Computational Fluid Dynamics code, based on the OpenFOAM software package, for simulation of the generation, transport, evolution and deposition of multispecies aerosol mixtures.

AeroSolved

LUNG CAST DEPOSITION

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Geometrical model developed by Lizal et al., Journal of Engineering in Medecine (2012)
Aerosol model developed by Frederix. Ph.D Thesis, University of Twente, The Netherland (2016)

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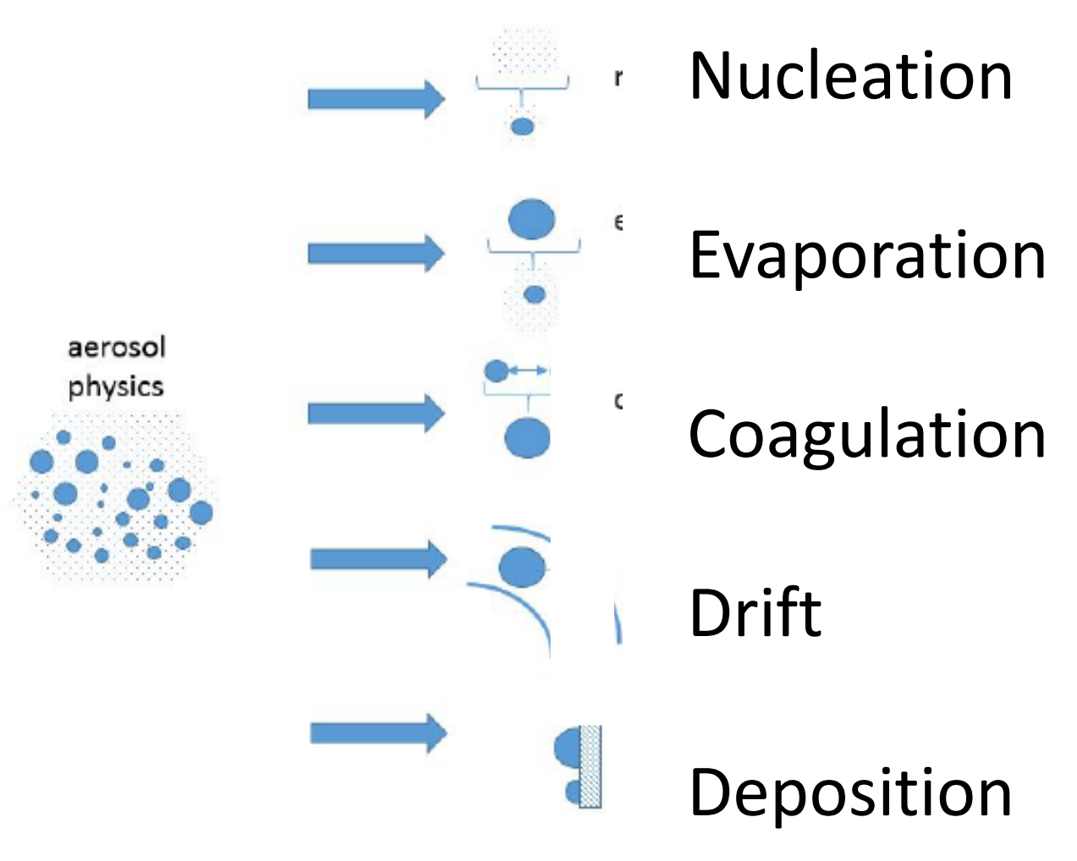
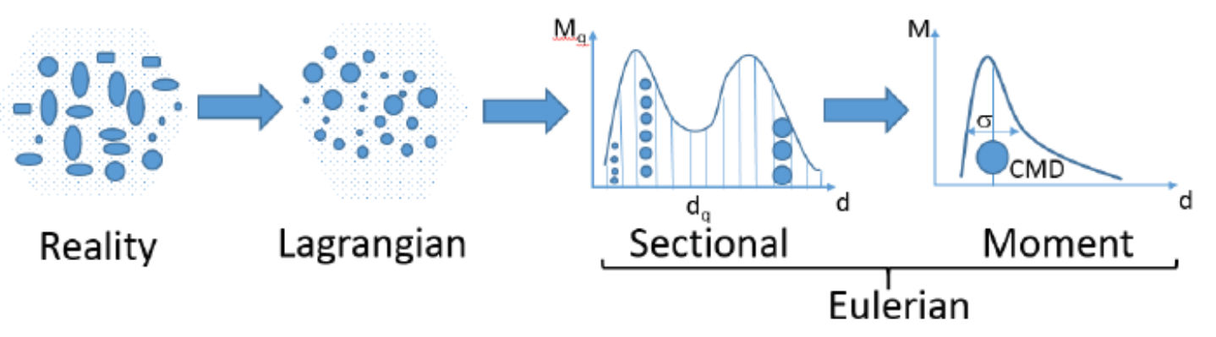
On GitHub :
pmpsa-cfd/aerosolved

AeroSolved.Contact@pmi.com



The aerosol is modeled within an Eulerian-Eulerian framework with the aerosol size distribution and aerosol dynamics represented by either a sectional or a two-moment method.



AeroSolved system of equations for *N* species and *Q* aerosol particle size sections:

Mass conservation
$$\partial_t\rho+\partial_j(\rho u_j)=-\partial_j[(1-\gamma)f_i],$$

Momentum conservation
$$\partial_t(\rho u_i)+\partial_j(\rho u_i u_j)=-\partial_i p+\partial_j(\mu\tau_{ij}),$$

Energy conservation
$$\rho c_p(\partial_t T+u_j\partial_j T)=\partial_j(k\partial_j T)+\partial_j(\mu u_k\tau_{kj})+\frac{DP}{Dt},$$

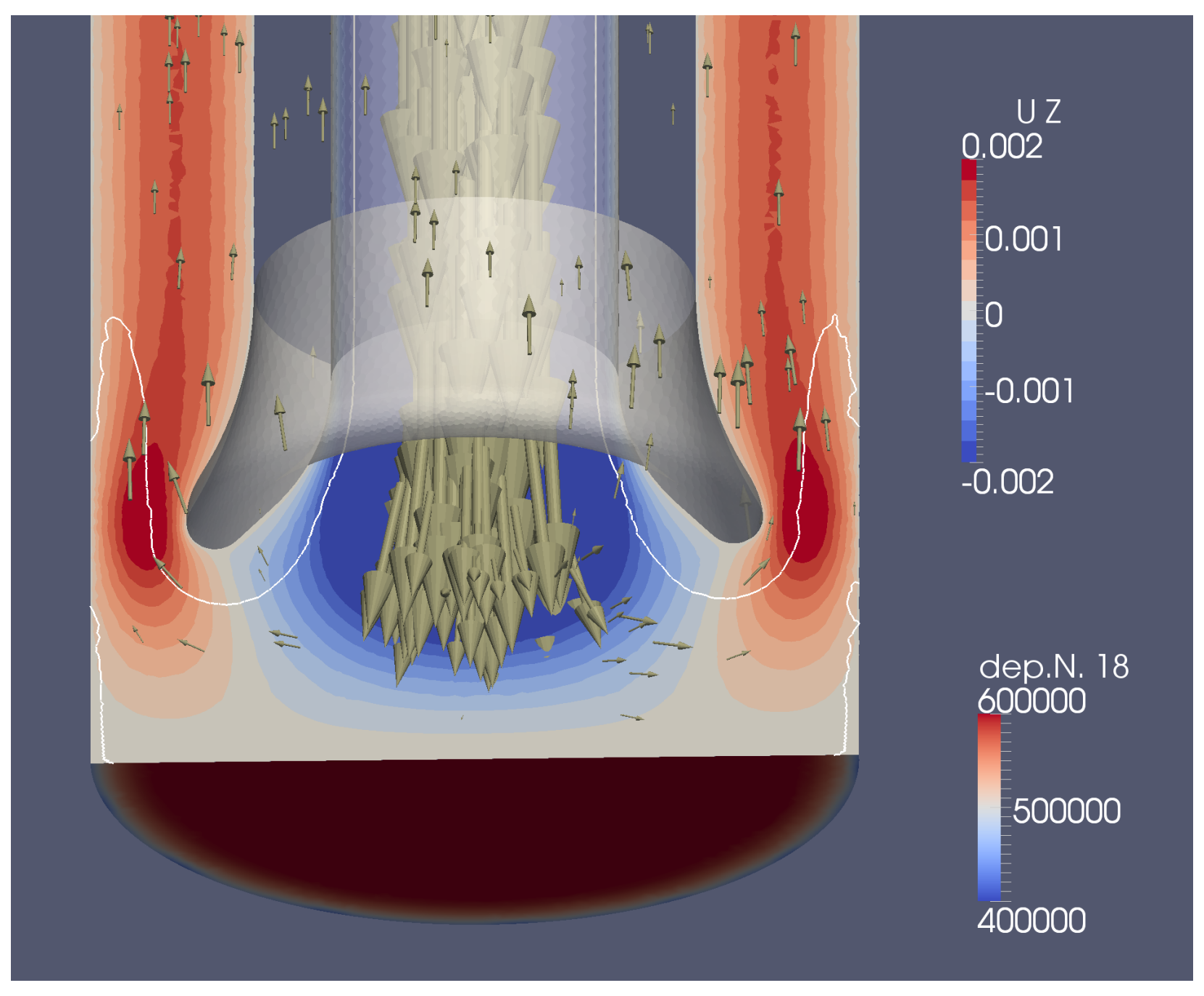
gas phases
$$\partial_t(\rho Y_n)+\partial_j(\rho Y_n u_j)=\partial_j(Y^{-1}\gamma f_j Y_n)+S_{Y_n}, \qquad n=1,\dots,N$$

liquid phases
$$\partial_t(\rho Z_n)+\partial_j(\rho Z_n u_j)=-\partial_j(Z^{-1}f_j Z_n)+S_{Z_n}, \qquad n=1,\dots,N$$

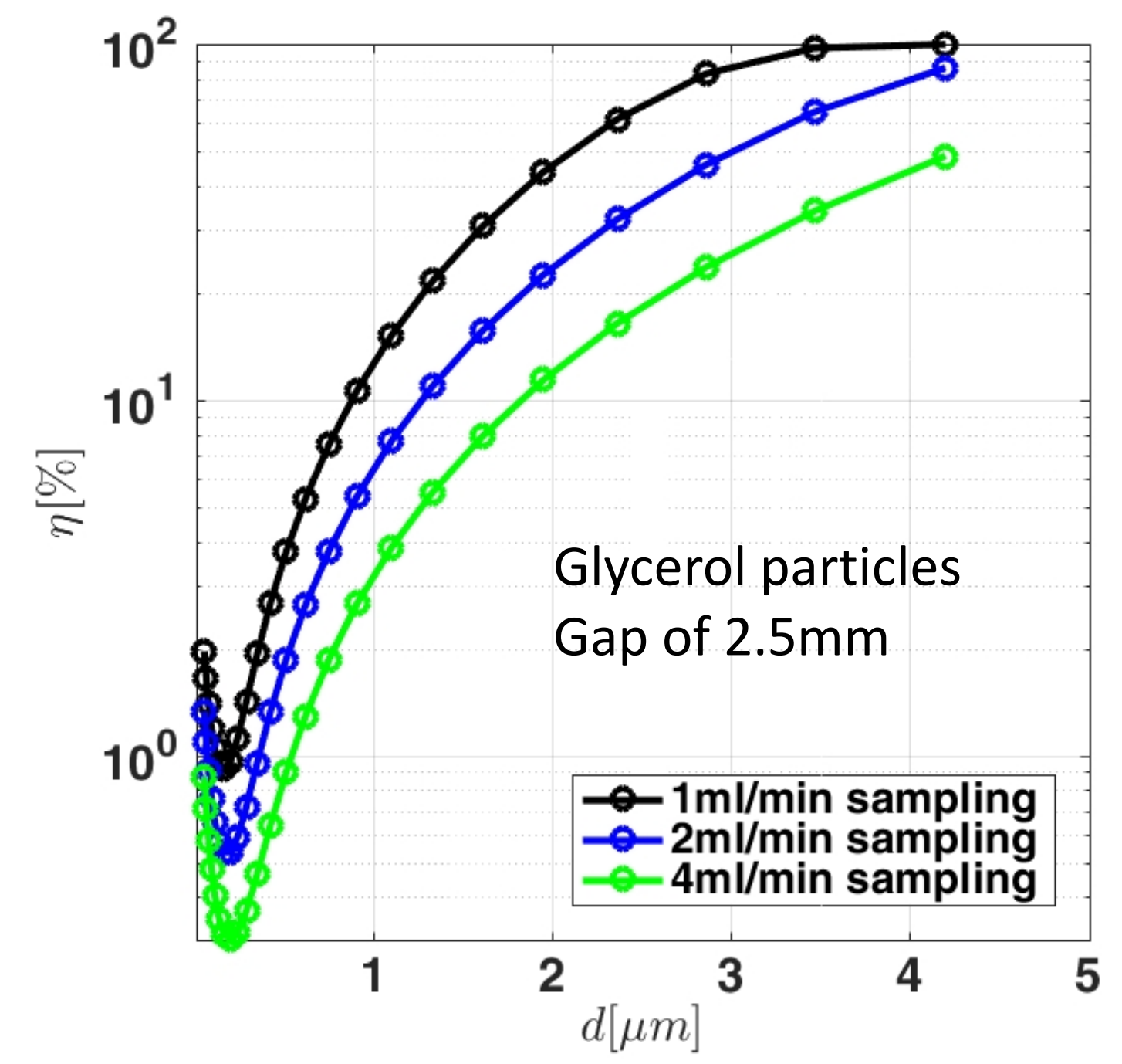
particle number densities
$$\partial_t(\rho M_q)+\partial_j(\rho M_q u_j)=-\partial_j(\rho M_q u^l_{j,q})+\partial_j(\rho D_q\sigma_j M_q)+S_{M_q}, \qquad q=1,\dots,Q$$

Mass conservation constrains
$$\textstyle\sum_{n=1}^{N}(Y_n+Z_n)=1 \qquad Z=\sum_{q=1}^{Q}s_q M_q$$

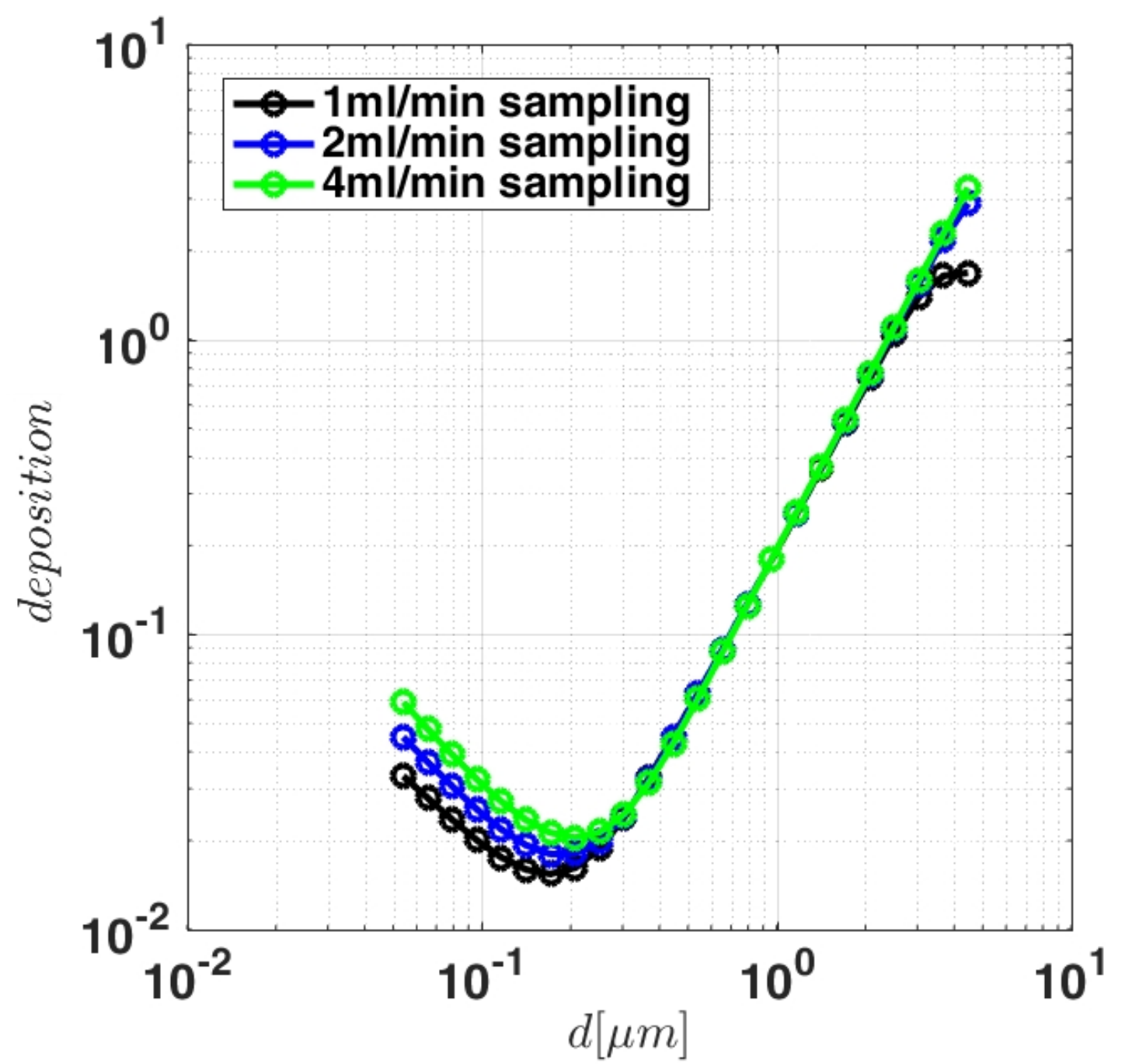
Simulations of Exposure System



Detailed CFD simulations were performed to analyze the aerosol deposition in air-liquid interface exposure systems. All relevant system parameters were varied within the operationally relevant ranges. The illustration to the left shows the flow and 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 transports the aerosol smoothly. Thus, no deposition by impaction has been observed.



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



Aerosol deposition flux versus particle diameter for three sampling flow rates (1ml/min; 2ml/min; 4ml/min). Deposition for larger particles is dominated by gravity and independent of the low sampling rate.

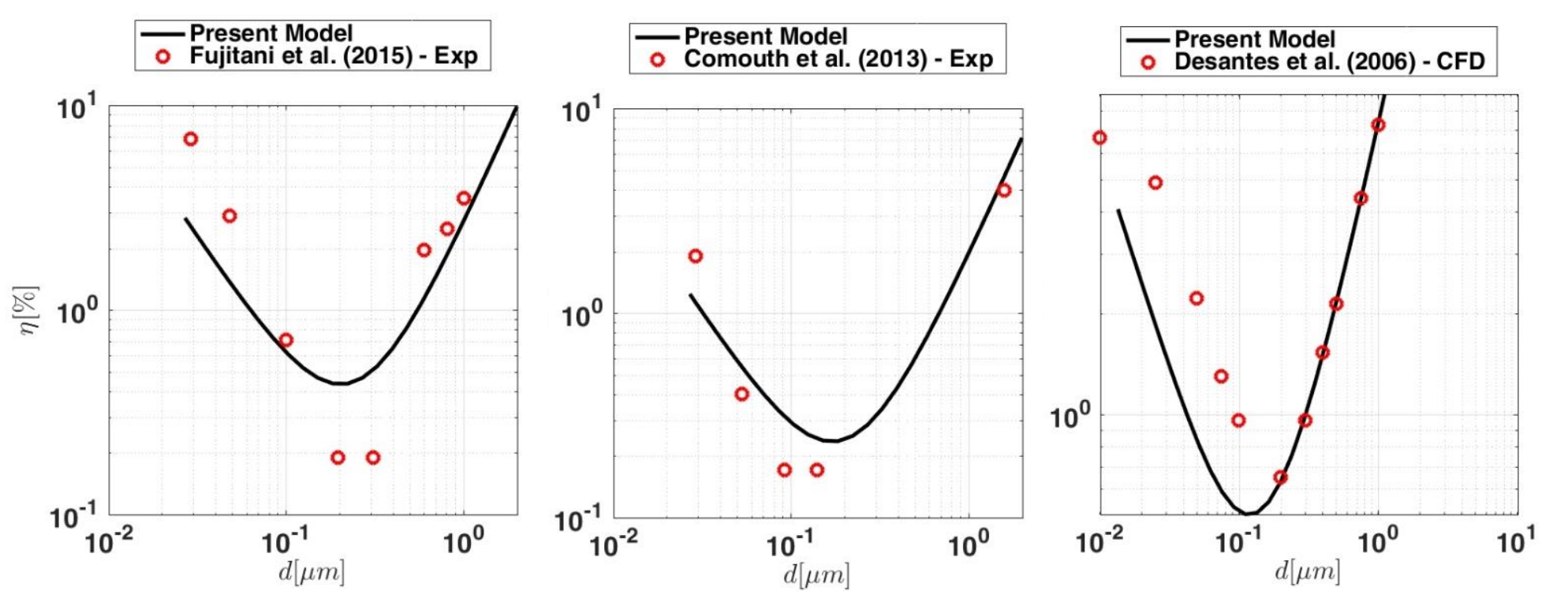
Analytical Model

The insight gained into the physical mechanisms allowed us to build an analytical model for the aerosol deposition:

$$\eta(\%)=\min\left(1\ ,\frac{A}{q_v}\left(v_s+\frac{D}{\delta}\right)\right)$$

The model is based only on the exposure plate area, A; sampling flow rate, q_v; aerosol settling velocity, v_s; Diffusion, D; and boundary layer thickness, δ. The model was validated against data available in the literature.

		Cell	Rp [mm]	Qv [ml/min]	P [g/cm3]	Hgap [mm]
Fujitani et al. (2015)	Exp.	Vitrocell	5.5	7.8	1.06	1.0
Comouth et al. (2013)	Exp.	Vitrocell PT-CF	12.5	100	2.0	2.0
Desantes et al. (2006)	CFD	Perfusion cell	17.5	33	1.2	7.0



Analytical model (solid line) vs. literature data (symbols) for various in vitro exposure systems.

Concluding Remarks

- A computational platform has been developed for CFD simulations of multispecies evolving aerosols including drift and deposition. Aerosol deposition in a Vitrocell® 24/48 system was analyzed for different particle sizes and trumpet sampling flow rates.
- Deposition varies significantly with the aerosol particle size and reaches a minimum for particles of about 0.2 µm in diameter.
- Large particles (>0.4 µm) deposit in the Vitrocell® 24/48 only due to a settling/gravitational mechanism, which is independent of the sampling rate and increases with the particle size. As a consequence, deposition efficiency, or the fraction of the sampled aerosol that deposits on the plate, decreases with increasing sampling rates.
- Deposition of small particles (<0.1 µm) is governed by diffusion mechanism and is dependent on the main flow and geometry parameters.
- The effect of the trumpet gap and liquid density on deposition has been analyzed, showing that the gap between the trumpet and the deposition plate has an effect on the deposition of small diffusion-dominated particles, while liquid density affects the sedimentation of large particles.
- A general physical-based model for deposition efficiency has been proposed and validated for computing deposition efficiency. The model uses only geometry and physical parameters and does not require any fitting parameters.

For more details: F. Lucci, N. D. Castro, A. A. Rostami, M. J. Oldham, J. Hoeng, Y. B. Pithawalla, A. K. Kuczaj, *Characterization and modeling of aerosol deposition in Vitrocell® exposure systems - exposure well chamber deposition efficiency*, Journal of Aerosol Science, Volume 123, 2018, Pages 141-160

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Competing Financial Interest

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