Modeling transport and evolution of aerosols for accurate predictions of local deposition in an in-vitro exposure system

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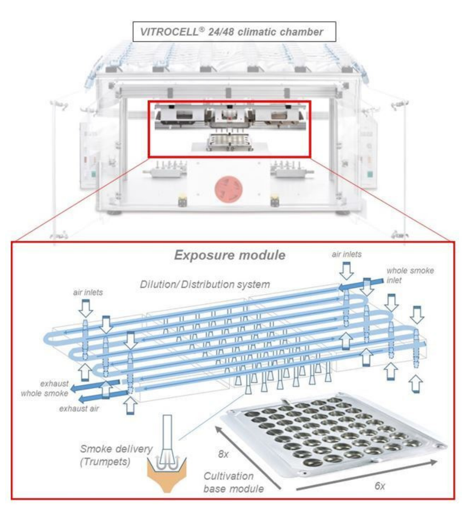
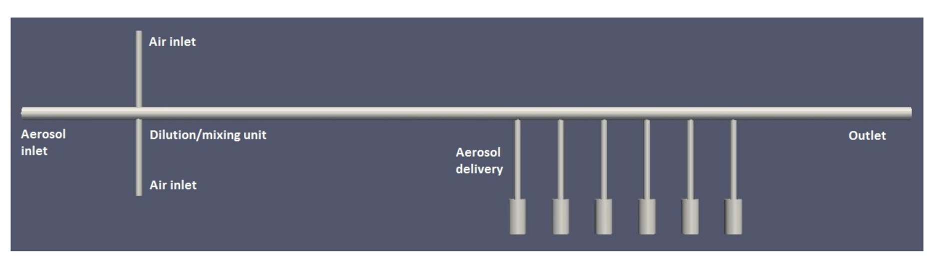
Introduction

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. Evaluation of flow and aerosol dynamics together with aerosol deposition in the in-vitro exposure system is presented here.



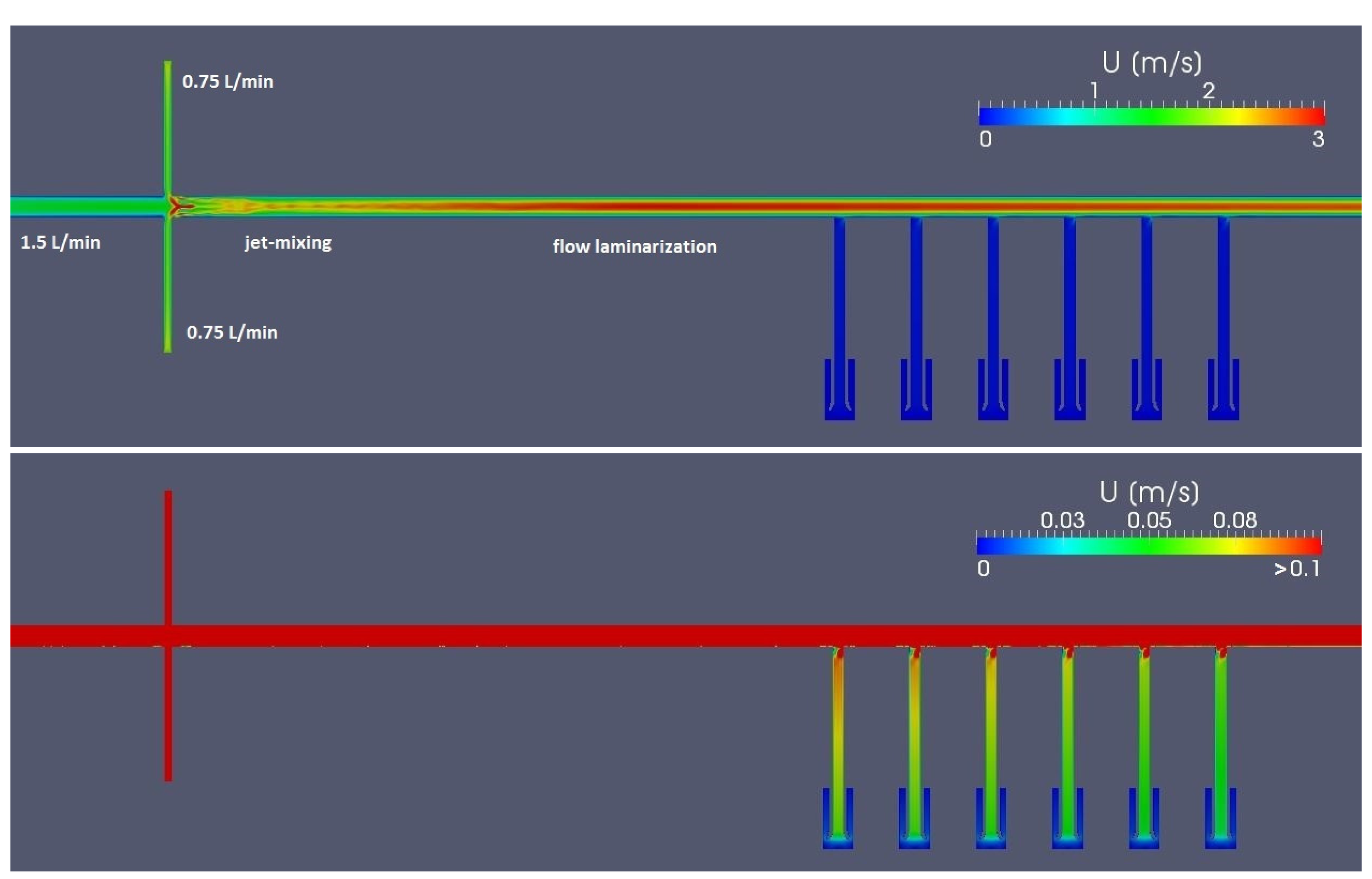
Schematic drawing



Representative geometry for single row

Flow assessment in the dilution/distribution unit

Direct Numerical Simulations (DNS) for various flow rates (Reynolds numbers) for the aerosol inlet and dilution legs performed in the dilution/distribution unit representative for the exposure system.

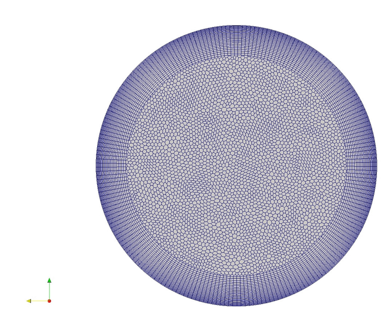


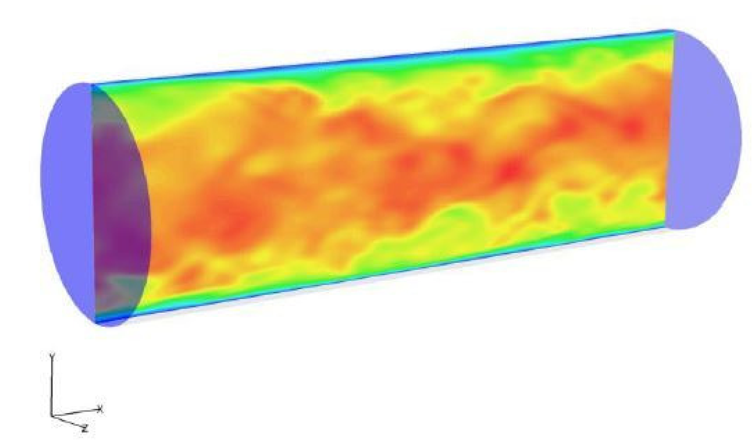
- **Jet-mixing regime for efficient turbulent mixing guaranteed by double mixing tee configuration**
- **Flow laminarization depending on Reynolds number for considered flow rates (3-12L/min)**

Validation of computational approach

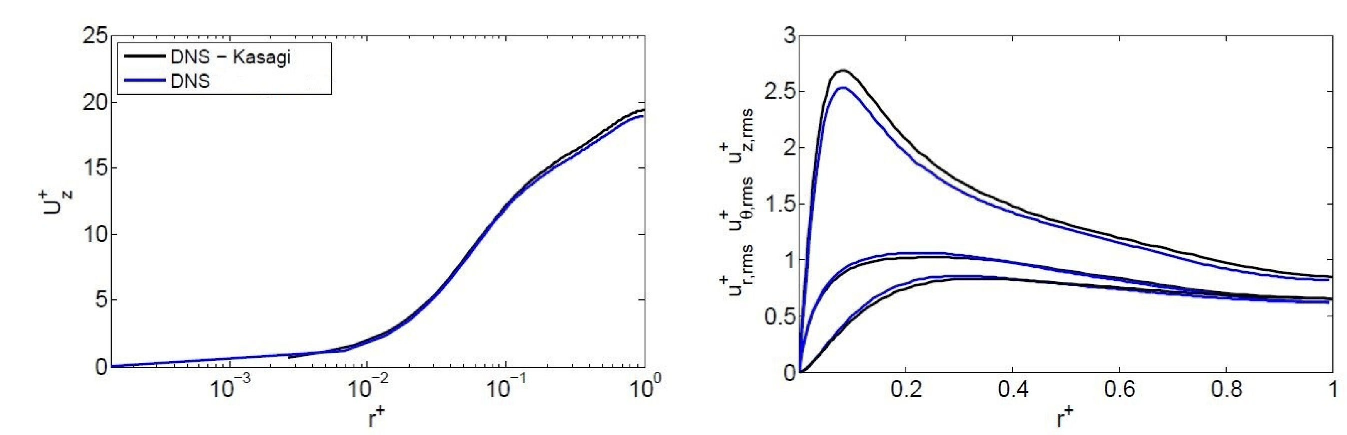
Developed compressible low-Mach Navier-Stokes aerosol drift-flux OpenFOAM® solver ([1, 3]) validated for pipe geometry flow by comparison with DNS results (boundary Reynolds number $Re_\tau = 180$).

Extruded polyhedral mesh and snapshot of velocity magnitude:



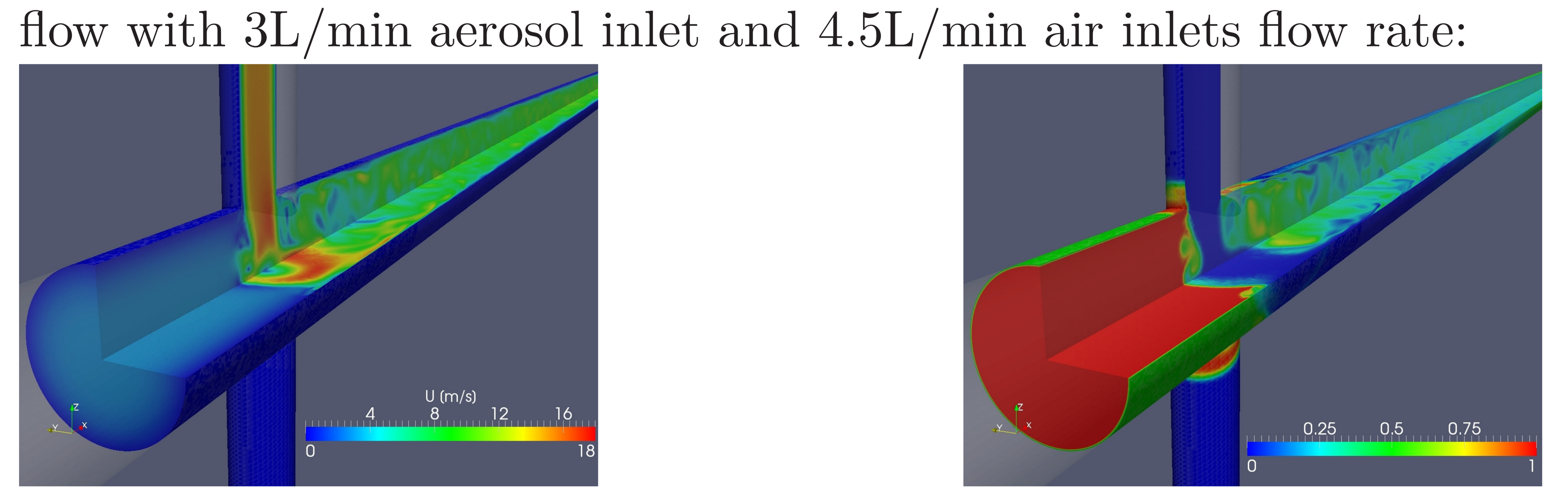


Comparison of in-house results with Direct Numerical Simulations by Kasagi [2] for the mean flow and r.m.s. velocity fluctuations:

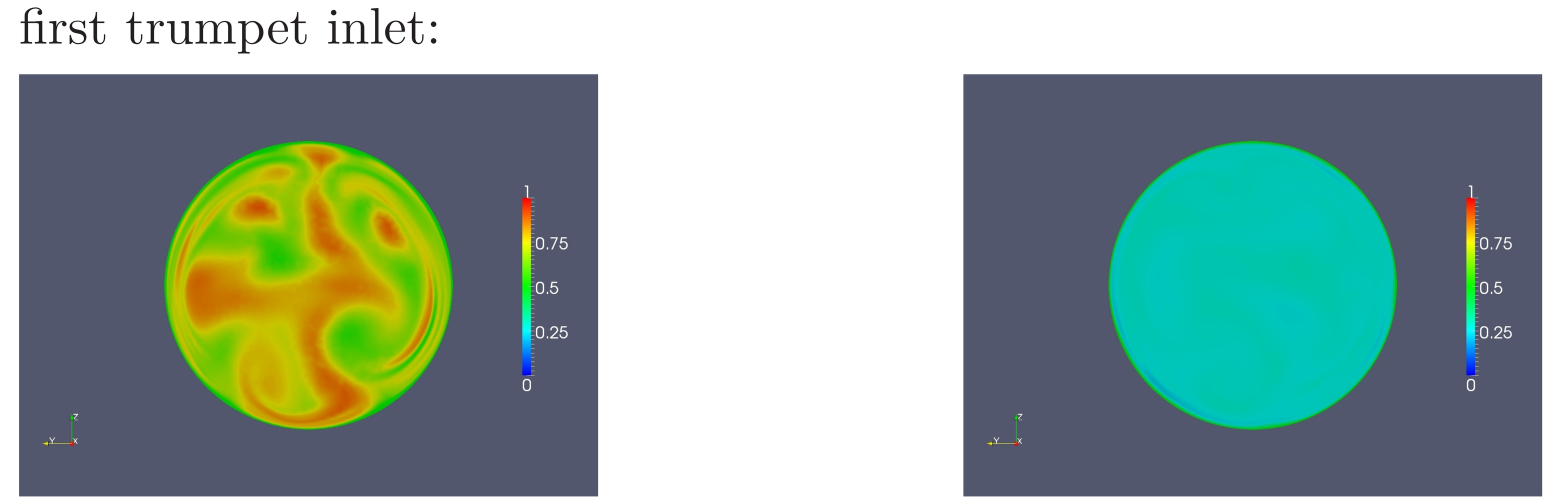


Mixing in the dilution unit

Turbulent flow (left) and mixing of passive scalar (right) for 12L/min flow with 3L/min aerosol inlet and 4.5L/min air inlets flow rate:

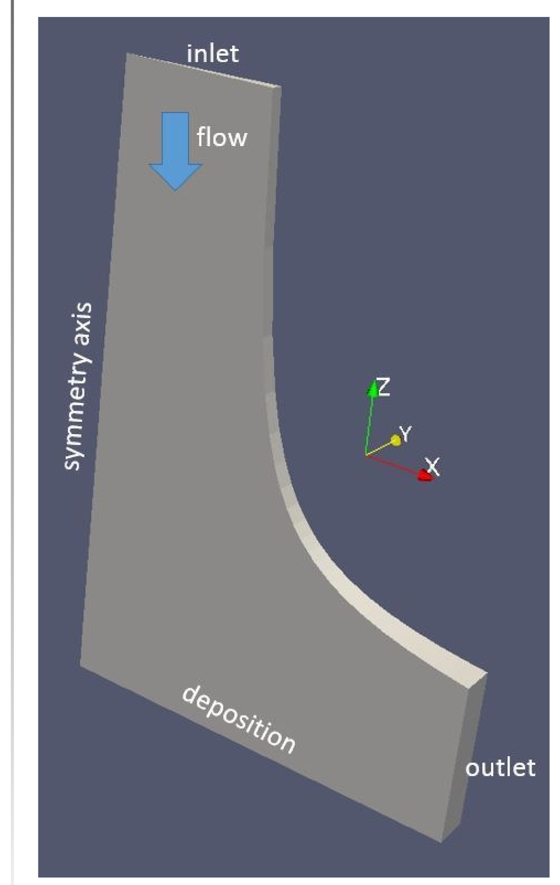


Mixing uniformity for 12L/min flow with 1.5L/min (left) versus 4.5L/min (right) air inlet flow rates at a cross-section prior to the first trumpet inlet:

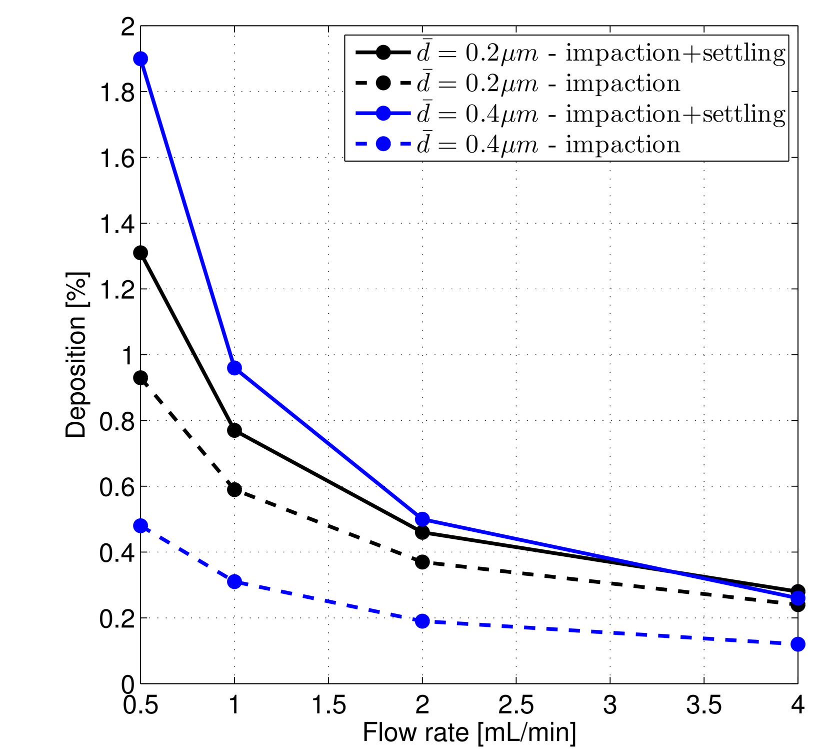


- **Mixing uniformity is controlled by equipartitioning of flow rates between inlets**

Aerosol flow in delivery system



Axi-symmetric representation of trumpet geometry



Deposition of two different aerosol mean particle sizes $\bar{d}$ taking into account impaction and gravitational settling for four various flow rates

Conclusions

- Aerosol mixing and uniformity in the exposure system can be controlled via proper adjustments of flow rates
- Developed computational framework allows for accurate computations of aerosol flow and deposition in exposure systems
- Future: application of developed platform for complete evaluation of in-vitro exposure studies

References

[1] E.M.A. Frederix, M. Stanic, A.K. Kuczaj, M. Nordlund, and B.J. Geurts. Extension of the compressible PISO algorithm to single-species aerosol formation and transport. *International Journal of Multiphase Flow*, Submitted, 2014.

[2] K. Fukugata and N. Kasagi. Highly energy-conservative finite difference method for the cylindrical coordinate system. *Journal of Computational Physics*, 181:478–498, 2002.

[3] Ch. Winkelmann, M. Nordlund, A.K. Kuczaj, S. Stolz, and B.J. Geurts. Efficient second-order time integration for single-species aerosol formation and evolution. *International Journal for Numerical Methods in Fluids*, 74(5), 2014.

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