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# Approaches to investigate dynamics and delivery of multispecies evolving liquid aerosol mixtures

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**Abstract** Despite continuous progress in development of technologies allowing us to measure, characterize, and assess aerosol flows, many aerosol dosimetry phenomena in particular pertaining to the dynamics and evolution of liquid aerosols entering the human respiratory tract continue to challenge the scientific community. The complexity of this research domain can be attributed to factors ranging from the lack of standardized experimental approaches for in vitro aerosol exposure testing under human relevant exposure conditions, difficulties in developing radiolabeled aerosols, as well as the lack of validated computational models able to predict both the chemistry and physics of aerosols. Multidisciplinary efforts including expertise from aerosol science, physics, and experimental inhalation toxicology provide opportunities to jointly establish protocols to investigate the dynamics, delivery and deposition of aerosols entering the human airways and ultimately predicting the effective delivered doses. The approaches and methodologies applied are equally pertinent in toxicity assessment of aerosols as well as for targeted drug delivery strategies. We present our multidisciplinary approaches employed to understand the dosimetry of multispecies evolving liquid aerosol mixtures in the context of in vivo, in vitro and in silico aerosol research. In particular, we concentrate on the following three aspects: 1) Development of a computational fluid dynamic model (AeroSolved) capable to simulate formation, transport, evolution and deposition of aerosols. 2) Application of simulations for in vitro and in vivo exposure studies helping in characterization of used exposure systems and building predictive analytical models for the aerosol deposition/dosimetry. 3) Development of 3D printed casts for experimental research of aerosol dynamics in human lungs. By simultaneous and systematic use of the developed methods and tools, we hope to gain the much required insight into aerosol dosimetry of multispecies evolving liquid aerosol mixtures.

**CV** Francesco Lucci graduated in mechanical engineering from the University of Udine. In 2010 he obtained his PhD from the University of California, Irvine, working on Direct Numerical Simulations of fully resolved particles in Turbulent flows. After, he moved to Switzerland to study catalytic reactive flows, first in turbulent channels (ETH, Zurich) and later in open cell ceramic foams (EMPA, Dübendorf). In 2016 he joined the Aerosol Physics and Dosimetry group of the R&D department in Philip Morris International where he is currently leading the CFD team.

