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New CFD solution for aerosol simulations released on GitHub platform

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AeroSolved, the freely available software models the complex dynamics of aerosol mixtures in biomedical and environmental research

A new version of AeroSolved, a computational fluid dynamics (CFD) solution for aerosol simulations, has been released on the open-source GitHub platform. The freely available software models the complex dynamics of aerosol mixtures from their generation through evolution, transport, and deposition. AeroSolved can be used for the development, characterization, and assessment of inhalation devices, aerosol generators, and aerosol delivery systems. It can also be applied in an industrial context to support the reduction of emissions, as well as in other aspects of environmental and atmospheric science. AeroSolved has been funded by Philip Morris International (PMI) and developed jointly with the Department of Applied Mathematics, University of Twente, and the Nuclear Research and Consultancy Group (NRG), The Netherlands.

“Until now, publicly available CFD tools were limited in their ability to effectively model the wide range of physical processes involved in the multi-phase interactions of complex aerosol mixtures,” said Arkadiusz Kuczaj, Associate Professor, Industrial Computational Modeling, University of Twente, The Netherlands, and Manager, Aerosol Research and Dosimetry, PMI. “AeroSolved combines advanced techniques in physics modelling, mathematical representation, and computational processing to deliver cutting-edge aerosol simulations robust enough for a range of industrial applications. Crucially, AeroSolved is embedded in and compatible with OpenFOAM, an existing, widely used open-source CFD platform, allowing users to take advantage of extensive, highly developed libraries in their simulations.”

AeroSolved is able to simulate aerosol mixtures across gas, liquid, and solid phases. Modeling takes into account mass transfer, aerosol particle size distribution, particle velocity, and phase-coupled thermodynamic properties of aerosol mixtures (e.g. viscosity, heat capacity, heat conductivity, and surface tension). It offers modelling of aerosol nucleation (formation of particles), coagulation, condensation, and evaporation of liquid mixtures. It can also be used to assess the deposition of aerosol mixtures on surfaces by modelling impaction, sedimentation, and diffusion processes. By taking advantage of OpenFOAM’s extensive physics and chemistry modelling libraries, the unique computational power of AeroSolved offers entirely new possibilities in the exploration of the complex processes of aerosol physics.

AeroSolved has important applications in the biomedical sciences, particularly in the area of inhalation toxicology. In the investigation of aerosol deposition in the lungs, an *in silico* approach using AeroSolved software can complement *in vivo* and *in vitro* studies, potentially reducing the need for animal models in line with 21st Century Toxicology and the internationally recognized “3Rs”: replace, reduce, and refine the use of animals in research. It may also help to reduce the

costs of inhalation toxicology research and produce more timely results. PMI is using AeroSolved as part of its extensive development and assessment program for reduced-risk products, smoke-free products for existing smokers that have the potential to be much less harmful than cigarettes.

The release of AeroSolved is the latest milestone in a continuous effort from PMI to develop state-of-the-art computational tools and share them with the scientific community. Other recent releases include GladiaTOX, an open-source solution for analysis of high-content screening data in biomedical research, GenSA, an R package for processing complex optimization problems, and RGraph2js, a tool for dynamic visualization of networks and graphs. Other advanced computational tools are in development and expected to be released in due course.

AeroSolved can be downloaded for free via GitHub. Documentation and validation cases for selected physical processes are supplied, together with tutorial cases that demonstrate possible applications of the software.