Influence of the geometry of the aerosol conducting system on the deposition of particles from inhalable aerosols on cellular surfaces in vitro

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Within the last decade the air liquid interphase (ALI) cell culture technology became the state-of-the-art method for in-vitro testing of airborne substances. Cells are cultured on microporous membranes and thereby get efficiently into contact with the test atmosphere while being supplied with nutrients and being humidified from the basal side of the membrane. Biological models like cell lines from the human lung or complex *ex vivo* models like precision cut lung slices (PCLS) can be applied. Sensitivity and relevance of the basic technique for use with chemical gases were demonstrated in round-robin prevalidation studies in Germany including laboratories from Fraunhofer, academia and governmental institutions (BfR and BAuA). However, especially for the application of this basic technology on the testing of a broader range of airborne materials like droplet and particle aerosols, there is still no general scientific consensus on the question of the most suitable exposure design. Concepts including complex physical phenomenons like electrostatic deposition of particles or thermophoresis have been introduced to address specific scientific questions. To develop a concept for a more general application of the ALI culture technology for all kinds of airborne materials in the long run, this study aimed in a first step at the characterization of the influence of the aerosol conduction system on the particle deposition by the use of computational fluid dynamics (CFD).

In the CFD simulation models applied within the scope of this project the fluid air is treated as an incompressible continuum in an Euler frame of reference and as a laminar flow. The particles are regarded as solid spheres of different size in a Lagrangian frame of reference. As the particles are dispersed and the portion of volume is rather small in the continuous phase the influence of the dispersed phase on the continuous phase is neglected. The particles exhibit inertia and are exposed to drag, pressure and gravity forces. The particle diameters are defined by a cumulative distribution function. Due to the result of a simulation of an experimental setup, it could be shown that particles do not cover the border areas of the tubes, when they are reaching the cell culture device. Because of this the injection distribution of particles for partial models omitted areas close to the tube walls. The behaviour of particles which hit or touch a wall was defined as "stuck", so that these particles were removed from the flow field and were accumulated on the wall for visual and numerical evaluation. For the simulations the CFD software STAR-CCM+[3] was applied.

Concerning the deposition behaviour of the particles on the cell culture membrane, several geometries were investigated. All geometries had a 180° deflection of the flow in common, but other geometrical details like the inlet nozzle design were modified and simulated in order to increase and smooth the deposition rate. However the deposition rate showed a very robust behaviour, as the resulting differences encountered were rather small. Two geometries showed a smoother but also a lower deposition rate at the same time. The other geometries with partially exceeding designs were fairly equivalent. Due to the partially submicronic size of the particles, it is now planned to proceed with simulations accounting for brownian motion and thermophoresis applying temperature gradients. As STAR-CCM+ does not support the above described effects, FLUENT[4] will be applied for these simulations. Thus it is the aim by accounting for these effects in the numerical simulations to investigate if one of the geometrical structures is predominant.

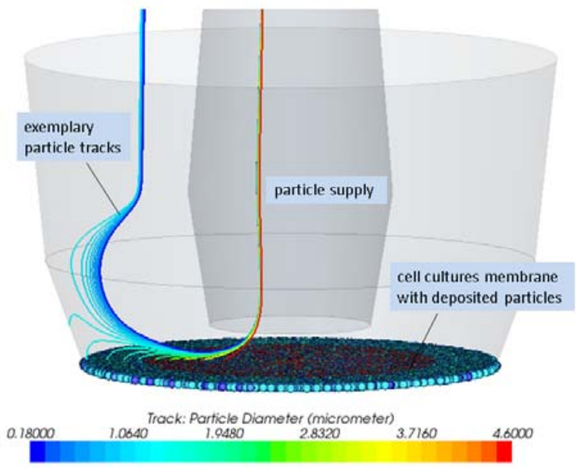

Figure 1: CFD of particle deposition on cell culture membrane with STAR-CCM+

[3]STAR-CCM+ is registered trademark of CD-adapco
[4]FLUENT is registered trademark of ANSYS, Inc.