

Inhalable carbon fibres – CF aerosol generation, characterisation, and numerical simulation of deposition on cell surfaces exposed at air-liquid interface

S. Mülhopt¹, M. Hauser¹, M. Wexler¹, J. Mahl¹, W. Baumann¹, S. Klein¹,
B. Gutmann², C. Schlager², T. Krebs², and D. Stapf¹

¹Institute for Technical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, 76021, Germany

²Vitrocell Systems GmbH, Waldkirch, 79183, Germany

Keywords: ALI, air-liquid interface, WHO fibres, aerodynamic diameter

Presenting author email: muelhopt@kit.edu

Carbon fibres (CF) and CF-reinforced plastics (CFRP) are innovative materials, which are increasingly produced, used and therefore recovered and disposed. In these processes particles and fibres which could fulfil the criteria of the World Health Organisation (WHO) to be potentially carcinogenic (so-called WHO fibres, critical aspect ratio $> 3:1$, length $\geq 5 \mu\text{m}$ and diameter $\leq 3 \mu\text{m}$) can possibly be released. This raises serious concerns about potentially harmful effects upon inhalation. Therefore, in this study investigations of CF under thermal and mechanical stress are carried out.

Polyacrylonitrile based carbon fibres were treated in a defined process to reproducibly generate aerosols. For this purpose, the CF were cut by hand, thermally treated in nitrogen or air and comminuted in a planetary ball mill. This bulk material was dispersed into dry air by a segmented belt aerosol generator. The resulting CF aerosol passed a PM_{10} inlet when introducing to an exposure station. Inside the exposure station, the inhalable fraction of the CF material was delivered to the air-liquid interface (ALI) of human lung cells, where toxicological investigations were carried out, i.e., directly on the apical surface of cell cultures, in order to simulate lung-like conditions. Lung epithelial, macrophage and fibroblast cell cultures in mono- and co-culture were used for toxicological evaluation of respirable CF fragments focussing on determination of cytotoxicity, gene expression analyses and determination of pro-inflammatory, profibrotic and genotoxic potential (Friesen et al., 2023).

The aerosol inside the exposure system was sampled on filters to determine the exposure dose. For assessing the cell surface dose on the one hand the online dose measurement employing a quartz crystal microbalance was used, on the other hand empty cell culture inserts were exposed. Both samples, the membranes from the inserts as well as the filters from the aerosol phase were analysed by digital microscopy.

The images of the fibre fragments were analysed regarding length and thickness using two methods, the Feret diameters on one hand and the rectangle model on the other hand. These values derived from the images were used to calculate the aerodynamic equivalent

diameter and to sort the objects in size classes resulting in histograms for the three fractions fibres fulfilling the WHO criteria, fibres of other geometries and particles. The deposition efficiency was determined by calculating the ratio of the deposited dose to the exposure dose class by class. The deposition behaviour of the three fractions of the carbon fibre aerosol was measured on the one hand and simulated by numerical methods on the other.

For the numerical simulation of fibre deposition, the shape factor X was implemented into the calculation of the drag force. Simulations were performed for fibre diameters ranging from some nanometres to a few microns with aspect ratios between 1 and 20. Model validation is conducted through comparison with experimental data.

Carbon fibres in the aerodynamic equivalent diameter theoretically achieve deposition efficiencies in the range of around 1 % (e.g., $\omega_0(d_{ae} = 1.08 \mu\text{m}) = 0.91 \%$) to 80 % (e.g., $\omega_0(d_{ae} = 10.8 \mu\text{m}) = 82.4 \%$). When using an electrostatic field, the deposition efficiencies can be increased up to $\omega_0 = 100 \%$, depending on the size and particle charge. In comparison, the measured deposition efficiencies show lower values and will be discussed regarding influences of sampling and image analyses.

Parts of this work were financed by the Federal Ministry of Education and Research under project number FK03XP0195 and by the project FINEST funded by the Investment and Networking Fund of the Helmholtz Association under grant agreement no. KA2-HSC-10 which is gratefully acknowledged.

Friesen, A., et al. (2023): *Int. J. Mol. Sci.* 24 (3), S. 1927. DOI: 10.3390/ijms24031927.