

Workpacke WP M: Modelling

Lead: TU Graz

The principal objective of WP M is the development of a model for aerosol transport allowing the fate of airborne nanoparticles to be predicted. The particles may be released from liquid formulations by drying. The model should become a candidate for a standard in MNM risk assessment in real-life applications. A second objective is to model the deposition of the nanoparticles on human tissue, such as skin and lung mucosa.

WP M cooperates with the experimental WPs PC and E and, on the basis of their input, produces computational data that can, in turn, be verified experimentally. Modelling the aerosol should allow inference on the state of the MNM during spraying and after deposition. Important factors are the rate of evaporation of liquids and the agglomeration of nanoparticles. High concentrations of nanoparticles in the spray liquid, and locally in individual droplets, can favour the formation of agglomerates. Agglomeration influences the physical state of the MNM, the physicochemical properties, and hence their fate and effects in the environment. The data generated should reveal similarities and differences between different spray scenarios which can be validated experimentally using exemplary data points.

For the second objective of the WP, the deposition of MNM and their uptake into lung tissue will be modelled as an example for an environmental fate of high concern. The MPPD model allows for the computation of such particle fate in mice and human airways. Human airways have certain exclusion sizes regarding particles and droplets, depending on their size. According to the model, particles in the range of 5 nm – 250 nm have a high probability to move into the alveoli, the most distal compartment of the lung. In this region, only the surfactant and few cells separate the gaseous phase from the blood, allowing for particles to cross the blood-air barrier.