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Constraining the production rate of reactive oxygen species from air pollution in the human lung with EPR spectroscopy and mechanisms in cloud chemistry models

Ashmi Mishra, Eleni Dovrou, Steven Lelieveld, Ulrich Pöschl, and Thomas Berkemeier
Multiphase Chemistry Department, Max Planck Institute for Chemistry, 55128 Mainz, Germany

Inhalation of fine particulate matter (PM2.5) can cause adverse health effects.[1] PM2.5 contains redox-active components which trigger the formation of reactive oxygen species (ROS) in the lungs. In the presence of transition metals, H_2O_2, the most stable ROS, is converted into the highly reactive OH radical through Fenton chemistry. Many of these reactions are known from cloud chemistry models,[2] however, the kinetics of the reactions in the human body are also affected by the presence of antioxidants and proteins. Antioxidants may scavenge ROS, but also enable efficient redox cycling of transition metals, perpetuating Fenton chemistry. Situationally, this may lead to an increase or reduction of ROS production in the human lung.

We performed electron paramagnetic resonance (EPR) studies of the Fenton reaction with a spin-trapping agent at physiologically relevant conditions using antioxidants and proteins as a cell-free surrogate for lung lining fluid. By applying a kinetic model, these complex reaction mechanisms can be constrained through inverse modelling, the process in which model parameters are determined from fitting to experimental data.[3] We describe how this method can be used to constrain chemical rate coefficients and how it can help to direct laboratory experiments.[4] As further constraint to the inferred reaction rates, we harness the extensive chemical mechanism available in cloud chemistry models.[2] We implement the rates of the reactions between antioxidations, transition metals, and ROS into the KM-SUB-ELF model[5,6] to infer the oxidative stress of PM2.5, the key component of air pollution that interconverts stable ROS (H_2O_2) to the noxious OH radical.

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