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Theoretical characterization of the kinetics of the multiphase reaction of ozone with an aqueous maleic acid droplet

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Dicarboxylic acids are an essential component of tropospheric aerosols emitted directly or formed in chemical processes. Multiphase reactions of these organic molecules in atmospheric aqueous phases are governed by coupled kinetic processes between the gas-phase, the particle interface and its bulk. However, models of atmospheric aerosol reactivity often do not account for the coupled nature of multiphase processes. The goal of the present study is to investigate physiochemical properties and heterogeneous ozone oxidation of aerosol particles containing maleic acid (MA). Rate constants have been evaluated in different environments, in the gas phase, at the particle interface, and in the bulk, using a mixed quantum and classical approach. The presence of interfacial water molecules enhances the initial reaction step of MA + O_3, with a larger rate constant at the air-water interface than in the gas phase. By assuming a Langmuir-Hinshelwood behavior and comparing it with the bulk, the ozonolysis of maleic acid mainly occurs in the bulk, O_3 diffusion in the bulk being the limiting process. The calculated rates are compared with reported values. The original method presented here quantifies the influence of the heterogeneous environment on the reaction rates taking into account explicitly the heterogeneous environment.

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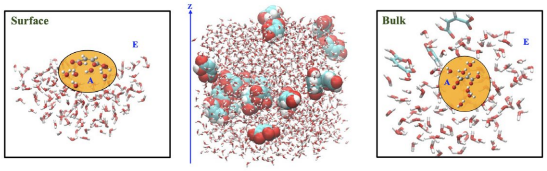

Figure: Snapshot of 20 maleic acid droplet and a schematic representations of the QM/QM' description of maleic acid at the surface and in the bulk.