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Sticking of HO_2 on fatty acids aggregates

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Models of atmospheric chemistry are widely used to perform projections of future changes in the chemical composition of the global troposphere, including changes in climate related greenhouse gases and aerosol particles. However, large uncertainties are still associated with the chemistry implemented in these models, which in turn can lead to inaccurate long-term predictions. The proposed work seeks to improve our understanding of the oxidative capacity of the atmosphere, which drives the lifetime of trace gases, and therefore atmospheric composition.

Recent measurements [1] of free radicals made in forested environments characterized by low levels of nitrogen oxides (NO_x = NO and NO_2) indicate that current models of atmospheric chemistry tend to overestimate the concentration of peroxy radicals (HO_2 and RO_2). An overestimation of peroxy radicals is an important issue since these radicals are the main precursors of the hydroxyl radical (OH), the most important atmospheric oxidant during daytime. This issue could lead to a significant overestimation of the oxidative capacity of the global atmosphere since more than 86% of the Earth surface is covered by forests, oceans, and polar regions.

An analysis of this dataset indicates that the missing sink could be due to an underestimation of the rates of RO_2+HO_2 reactions, and/or the uptake of peroxy radicals onto aerosol particles. A thorough evaluation of scientific studies published in the literature shows that there is a lack of kinetic and mechanistic data to correctly assess the contribution of these two loss pathways of peroxy radicals in low NO_x environments.

Classical molecular dynamics simulations, using the Gromacs package [2], are performed to study the interaction of HO_2 with organic (carboxylic acid) aerosols. The effect of the presence of water molecules on the surface are also be investigated. These calculations provide theoretical values for observable quantities such as uptake and mass accommodation coefficients.

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