

Research Interests – Simon Rosanka

In the past decades, global atmospheric models have been established as a key tool to improve our understanding of the Earth's atmospheric processes and to address the influence of anthropogenic activities on the Earth's climate. Especially, the adequate modelling of atmospheric chemistry is an important aspect to tackle humanity's current and upcoming challenges related to climate change and air pollution. One well known tropospheric greenhouse gas is ozone. In the troposphere, ozone is of special interest since close to the ground, it is a pollutant that directly impacts human health (e.g. respiratory problems) and the ecosystem's productivity. Additionally, ozone absorbs radiation and, therefore, has a direct climate impact and is known to have made the third largest greenhouse gas contribution to the radiative forcing since preindustrial times. Notably, global models tend to overpredict tropospheric ozone concentrations.

My primary research thus focuses on improving the representation of physical and chemical processes influencing ozone and other gases within global atmospheric chemistry models. Since ozone is not directly emitted by natural or anthropogenic activities, its tropospheric abundance depends on its chemical production, chemical loss, deposition, and the influx by stratospheric-tropospheric exchange. The chemical production of ozone strongly depends on the emission of its precursors, like carbon monoxide, nitrogen oxides, and volatile organic compounds. In general, the latter are a large group of organic chemicals (e.g. ketones, aldehydes, alcohols) that are directly emitted by natural and anthropogenic activities or chemically produced within the atmosphere. Among other aspects, a realistic simulation of tropospheric ozone, and other greenhouse gases, in global atmospheric models thus relies on the realistic representation of volatile organic compounds.

I therefore evaluate and improve the representation of volatile organic compounds within the global ECHAM/MESSy Atmospheric Chemistry model. Such improvements include the development of parts or completely new chemical mechanisms. A recent prominent example for this is my development of the Jülich Aqueous-phase Mechanism of Organic Chemistry. Many oxygenated volatile organic compounds are highly soluble and partition into warm clouds, where they are quickly oxidised. This leads to elevated concentrations of the superoxide anion, which is known to destroy the rather insoluble ozone. So far, no global model, including the global ECHAM/MESSy Atmospheric Chemistry model, adequately represented this process. In order to overcome this deficit, I developed the Jülich Aqueous-phase Mechanism of

Organic Chemistry, which is the first explicit in-cloud oxygenated volatile organic compound oxidation scheme available for global simulations that are affordable with modern supercomputing facilities (Rosanka et al., 2021a). Developing such a mechanism always follows a similar procedure. First, the mechanism is derived and developed based on chemical kinetic data, which are obtained from the literature or quantum chemical and theoretical kinetic calculations. Afterwards, the resulting mechanism is implemented into a box model. Here, the box model represents a single air parcel using predefined conditions. Its simulation results are compared to measurements or reviewed using earlier studies. Once the mechanism properly represents the added chemistry, it is optimised with respect to its computational costs and implemented into the global ECHAM/MESSy Atmospheric Chemistry model. The improvement due to the new mechanism in this model is then evaluated using ground based, airborne, and spaceborne observations. In the case of the Jülich Aqueous-phase Mechanism of Organic Chemistry, I found that the representation of oxygenated volatile organic compounds like methanol greatly improves. Further, the enhanced uptake of ozone into cloud droplets reduces the tropospheric ozone model bias by up to 20%. Global models, which neglect in-cloud oxygenated volatile organic compound oxidation, will thus underestimate clouds as an ozone sink (Rosanka et al. 2021b, 2020).

In my future work, I plan to build on my gained experiences and my developed chemical mechanisms to further improve the representation of volatile organic compounds and trace gases in global models. Currently, the use of the Jülich Aqueous-phase Mechanism of Organic Chemistry is limited to warm cloud droplets. Therefore, I would like to apply a modified version of it to the liquid phase of aerosols. Such implementation will allow to address the importance of aqueous phase oxygenated volatile organic compound oxidation to the formation of secondary organic aerosols. The induced changes in their abundance will influence the Earth's climate, since they absorb and scatter solar radiation, and alter cloud microphysical properties, which influence the Earth's radiation balance. By comparing simulation results to measurements and by using experimental results testing existing chemistry schemes, I plan to refine and further increase the schemes' complexity for global model applications. In this way, I stay committed to use novel approaches for advancing and promoting knowledge in atmospheric pollution and chemistry-climate interactions.