EGU22-6553
https://doi.org/10.5194/egusphere-egu22-6553
EGU General Assembly 2022

Can simple machine learning methods predict concentrations of OH better than state of the art chemical mechanisms?

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Concentrations of the hydroxyl radical, OH, control the lifetime of methane, carbon monoxide and other atmospheric constituents. The short lifetime of OH, coupled with the spatial and temporal variability in its sources and sinks, makes accurate simulation of its concentration particularly challenging. To date, machine learning (ML) methods have been infrequently applied to global studies of atmospheric chemistry.

We present an assessment of the use of ML methods for the challenging case of simulation of the hydroxyl radical at the global scale, and show that several approaches are indeed viable. We use observational data from the recent NASA Atmospheric Tomography Mission to show that machine learning methods are comparable in skill to state of the art forward chemical models and are capable, if appropriately applied, of simulating OH to within observational uncertainty.

We show that a simple ridge regression model is a better predictor of OH concentrations in the remote atmosphere than a state of the art chemical mechanism implemented in a forward box model. Our work shows that machine learning may be an accurate emulator of chemical concentrations in atmospheric chemistry, which would allow a significant speed up in climate model runtime due to the speed and efficiency of simple machine learning methods. Furthermore, we show that relatively few predictors are required to simulate OH concentrations, suggesting that the variability in OH can be quantitatively accounted for by few observables with the potential to simplify the numerical simulation of atmospheric levels of key species such as methane.