EGU21-8865
https://doi.org/10.5194/egusphere-egu21-8865
EGU General Assembly 2021

Investigation of atmospheric hydrogen cyanide: a modelling perspective

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Hydrogen cyanide (HCN) is one of the most abundant cyanides present in the global atmosphere, and is a tracer of biomass burning, especially for peatland fires. The HCN lifetime is 2–5 months in the troposphere but several years in the stratosphere. Understanding the physical and chemical mechanisms of HCN variability is important due to its non-negligible role in the nitrogen cycle. The main source of tropospheric HCN is biomass burning with minor contributions from industry and transport. The main loss mechanism of atmospheric HCN is the reaction with the hydroxyl radical (OH). Ocean uptake is also important, while in the stratosphere oxidation by reaction with $O(^1D)$ needs to be considered.

HCN variability can be investigated using chemical model simulations, such as three-dimensional (3-D) chemical transport models (CTMs). Here we use an adapted version of the TOMCAT 3-D CTM at a 1.2°x1.2° spatial resolution from the surface to ~60 km for 12 idealised HCN tracers which quantify the main loss mechanisms of HCN, including ocean uptake, atmospheric oxidation reactions and their combinations. The TOMCAT output of the HCN distribution in the period 2004-2020 has been compared with HCN profiles measured by the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) over an altitude grid from 6 to 42 km. HCN model data have also been compared with ground-based measurements of HCN columns from NDACC FTIR stations and with in-situ volume mixing ratios (VMRs) from NOAA ground-based measurement sites.

The model outputs for the HCN tracer with full treatment of the loss processes generally agree well with ACE-FTS measurements, as long as we use recent laboratory values for the atmospheric loss reactions. Diagnosis of the individual loss terms shows that decay of the HCN profile in the upper stratosphere is due mainly to the $O(^1D)$ sink. In order to test the magnitude of the tropospheric OH sink and the magnitude of the ocean sink, we also show the comparisons of the model tracers with surface-based observations. The implications of our results for understanding HCN and its variability are then discussed.