New Tagging

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Abstract

1 Introduction

2 Methodology

2.1 VOC Tagging Approach

- boxmodel set-up, initial conditions, VOC emissions same as in Coates and Butler (2015)
- only difference is the tagging approach used; Coates and Butler (2015) determine effects of VOC on O3 by inferring the effects of VOC on Ox production, hence this is looking at the effects on O3 indirectly
- the tagging approach of Emmons et al. (2012), which looks at NOx-tagging has been adapted to VOC tagging by Shuai and Tim and now the effects of VOC on O3 mixing ratios can be directly compared
- Tagging the VOC degradation of MOZART-4 was achieved using the same technique as S&T but using the KPP version of MOZART-4, including the modifications to MOZART-4 outlined in Coates and Butler (2015) such as using MCM v3.2 inorganic chemistry, using only reactions relevant to tropospheric processes.
- From the gas-phase reactions in the KPP version, we have the full set of non-tagged reactions – the "real" chemistry – and appended this with reactions where the degradation reactions

of a VOC are tagged for the VOC in order to trace the effects of the VOC degradation on O3 and Ox production.

- The tagging approach requires extracting the set of reactions where reactions of the VOC products with members of the Ox family are also included.
- We define the Ox family to include O3, O, O1D, NO2, NO3, N2O5, HNO3, ISOPNO3, ONIT, ONITR, HO2, HO2NO2.
- The set of tagged chemistry which runs parallel to the "real" chemistry was then added to the KPP version of MOZART-4 chemical mechanism described above.
- This chemistry was then implemented in the boxmodel and then tested to determine that the tagged chemistry does not influence the "real" chemistry by comparing the mixing ratios of tagged species to their non-tagged counterparts. If the chemistry is correctly set-up then there should be no difference.
- The next testing stage was that this new chemistry set-up gives the same results as the previous chemistry (i.e. the results in Coates and Butler (2015)) by comparing the mixing ratios of the "real" chemistry in the new set-up to that in Coates and Butler (2015) and again there should be no differences as the boxmodels are set-up in exactly the same way.

2.2 Vertical Mixing with Diurnal Boundary Layer Height

- A parameterisation of the diurnal profile of the planetary boundary layer (PBL) height over Los Angeles was provided by Boris Bonn based on data from the CARES field campaign (, CARB) .
- The PBL height was calculated at every time point for the model run and then read into the boxmodel at each time point .
- The concentrations of the chemical species within the PBL are diluted due to the larger mixing volume when the PBL height increases at the beginning of the day, also the increasing PBL height induces mixing of chemical species from the free troposphere with those chemical species within the PBL i.e. vertical mixing. When the PBL height collapses during night giving the stable nocturnal boundary layer, this traps the chemical species into a smaller volume thus increasing the concentrations of the chemical species.

check if reference correctly

include plot

- This vertical mixing scheme was implemented into the boxmodel using the same approach of Lourens (2012).

- The mixing ratios of the chemical species in the free troposphere were taken from the MATCH-MPIC chemical weather forecast model on the 27th March (the start date of the simulations). The model results (`http://cwf.iass-potsdam.de/`) at the 700 hPa height were chosen and the daily average was used as input into the boxmodel.

check about reference and if this is appropriate

3 Results

4 Conclusions

References

California Air Resources Board (CARB). 2010 CalNex White Paper: Research at the Nexus of Air Quality and Climate Change. Technical report, California Air Resources Board, 2008.

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