

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 O_x production, hence this is looking at the effects on O₃ indirectly
- the tagging approach of Emmons et al. (2012), which looks at NO_x-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.

3 Results

4 Conclusions

References

- J. Coates and T. M. Butler. A comparison of chemical mechanisms using Tagged Ozone Production Potential (TOPP) analysis. *Atmospheric Chemistry and Physics Discussions*, 15(8):12389–12422, 2015.
- L. K. Emmons, P. G. Hess, J.-F. Lamarque, and G. G. Pfister. Tagged ozone mechanism for MOZART-4, CAM-chem and other chemical transport models. *Geoscientific Model Development*, 5:1531–1542, 2012.