

Conceptual simplification of mechanism complexity: a new paradigm for understanding the tropospheric ozone budget.

P. M. Edwards^{1*} & M. J. Evans^{1,2}

¹ Wolfson Atmospheric Chemistry Laboratories, Department of Chemistry, University of York, York, UK

² National Centre for Atmospheric Science, Department of Chemistry, University of York, York, UK

* Corresponding author: pete.edwards@york.ac.uk

The chemistry of the troposphere has huge chemical complexity due to the myriad of oxidation products formed from primary emitted compounds. Simplifications are necessary when representing this chemistry in chemical transport models; however, these schemes still frequently contain many hundreds of reactions. This complexity often clouds attempts to diagnose the chemical processes occurring with implications for our understanding of air quality and climate.

Understanding the production of tropospheric ozone is central to atmospheric chemistry research, and a major focus of this work involves trying to understand the differences between its representation in different models. Unfortunately current diagnostics focusing on the rate of NO to NO₂ conversions within the model have provided little in terms of process level detail. Conceptual simplification of the complexity is needed to enable a more detailed analysis of the ozone budget, and thus enable a process level diagnostic. Here we construct a novel ozone production diagnostic based around the fundamental principle of conservation of molecular spin and its implications for the atmospheric processing of emitted bonds. This approach tracks the efficiencies of the key mechanistic steps of tropospheric oxidation leading to ozone production: namely the emission of oxidisable bonds; the conversion of bonds into peroxy radicals; and the reaction of these peroxy radicals that convert NO into NO₂.

Using this new approach in the GEOS-Chem model we diagnose the processes responsible for changing ozone production under different emissions of nitrogen oxides and hydrocarbons. This provides significantly more detail than the traditional diagnostic, most notably highlighting significant model artifacts and the importance of an accurate representation of peroxy radicals and their reservoir species. We hope that this new diagnostic tool will better highlight reasons why global models of tropospheric chemistry differ thus allowing improvements in model formulation.