

# MCM/GECKO-A: Development of a new modelling tool for atmospheric chemistry

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Organic compounds emitted in the atmosphere are oxidized through complex reactions involving a myriad of secondary organic compounds (SOC). Describing the oxidation of hydrocarbons with backbones larger than few carbon atoms involves millions of SOC, far exceeding the size of chemical mechanisms that can be written manually. Data processing tools can however be designed to overcome these difficulties and auto-generate consistent and comprehensive chemical mechanisms on a systematic basis. The Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A) has been developed for the automatic writing of explicit chemical schemes of organic species (Aumont *et al.*, 2005), and their partitioning between the gas and condensed phases (e.g. Camredon *et al.*, 2007, Mouchel-Vallon *et al.*, 2013, La *et al.*, 2016). These explicit mechanisms are useful tools to explore the fate of organic matter during its tropospheric oxidation and to examine how these organic chemical processes shape the composition and properties of the gaseous and the condensed phases. Furthermore, explicit mechanisms provide powerful benchmarks to design and assess simplified parameterizations to be included 3D model. GECKO-A can be viewed as an expert system that mimics the steps by which chemists might develop chemical schemes. GECKO-A generates chemical schemes according to a prescribed protocol assigning reaction pathways and kinetics data on the basis of experimental data and structure-activity relationships. In its current version, GECKO-A can generate the full atmospheric oxidation scheme for most linear, branched and cyclic precursors, including alkanes and alkenes up to C<sub>25</sub>. In collaboration with the University of York, the GECKO-A protocol is currently (i) updated on the basis of the current state of the art, (ii) extended to aromatic compounds and (iii) eventually improved to include a reduction protocol allowing the generation of the next version of the Master Chemical Mechanism (MCM, Saunders *et al.*, 2003, Jenkin *et al.*, 2015). Here the new protocol will be presented and first results from the updated MCM/GECKO-A version will be shown.

## References

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