

# Novel generation and visualisation tools for understanding atmospheric chemistry

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The chemistry of the troposphere underlies a range of environmental issues, which have substantial societal and economic impacts. Whether it is a changing climate, a reduction in air quality or the degradation of ecosystems due to air pollution the details of the chemistry determines the severity of the impact. Numerical models of atmospheric chemistry lie at the heart of our ability to understand, predict and hence mitigate these problems. The description of the chemistry occurring within these models is known as the ‘mechanism’. Different models use different levels of chemical complexity and approximation in deriving these mechanisms, depending on their individual science and/or policy foci.

These models make differing predictions for the composition of the atmosphere, and more importantly its sensitivity to policy options. One reason for the variation in model predictions lies in the differences between the mechanisms used. Knowledge in the impacts of these different mechanisms is essential if we are to have faith in the science and policy decisions made with these models and their limitations.

In order to further understand the underlying chemistry, and how different models perform over a range of conditions, requires detailed inter-comparisons to be performed. ‘Big Data’ mapping techniques, such as force-directed graphs, have been successfully applied in the fields of neuroscience, social-media and genome analysis (1-3) – all of which resemble the complexity of model gas-phase chemical interactions – in order to extract underlying properties of an otherwise intricate system. However, visualisation of an evolving chemical system is difficult owing to the number of species involved and applicable timescales.

We have used these developments in graph and network theory to look at new ways of exploring model chemical mechanisms. Applications of these allow the visual simplification of such systems, whilst enabling the user to compare physicochemical properties (e.g. reaction fluxes) for a range of times, locations and mechanistic parameters. These tools allow mechanisms to be explored in detail and provide rapid assessment of their pros and cons.

## References

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