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Simulating chemistry using a hybrid approach in a Lagrangian particle dispersion model.

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The UK Met Office NAME model is a state of the art atmospheric dispersion modelling tool. The model uses a Lagrangian approach to advect abstract particles that can be used to represent emitted pollutants, such as radioactive nuclei or reactive organic compounds.

In this work we utilise the models ability to simulate the oxidation of volatile organic compounds under present day conditions for the South East UK. In this method Lagrangian particles are used to trace the trajectories of emitted and secondary produced species, whilst chemistry is performed on a fixed Eulerian subgrid. A wide range of test have been performed to assess the models suitability in simulating atmospheric composition for air quality purposes and the model has been shown to perform well compared with a range of other models and observations at surface locations.

In this presentation results from simulations using a reference chemical mechanism, based on the CRIv2-R5 scheme (traceable to the MCMv3.2), are compared to a reduced complexity chemical mechanism, highlighting the importance of the underlying assumptions made concerning the degradation of volatile organic compounds.

Results from further simulations highlight the specific importance of the representation of biogenic emissions and their oxidation mechanism to simulate summertime high ozone episodes across the UK.