Simulations of SOA formation from alpha-pinene ozonolysis and photo-oxidation in chamber experiments

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Model description

We present here simulations of secondary organic aerosol formation from ozonolysis and photo-oxidation of alpha-pinene in a smog chamber. Simulations were performed using the MANIC model (Lowe et al., 2009), which uses gaseous VOC photochemistry from the MCM (Jenkin et al., 1997; Saunders et al., 2003) coupled to aerosol microphysics through mass transfer driven by Raoult's Law using predicted vapour pressures. The aerosol size distribution and size-resolved composition are represented by 16 size bins, which can use either moving-centre or moving-grid numerical schemes to follow particle growth.

Results

Two nucleation (i.e. unseeded) test cases will be presented:

1. ozonolysis of 100 ppb alpha-pinene by 135 ppb ozone, in the absence of NOx. This experiment was performed in the EUPHORE chamber, and is taken from Jenkin et al. (2004). Measurements of ozone, alpha-pinene and aerosol mass are compared with model output.

2. photo-oxidation of 55 ppb alpha-pinene, with initial concentrations 15 ppb NO2, 3 ppb NO and no ozone. This experiment was performed in the University of Manchester aerosol chamber, and measurements of NO, NO2, O3 and aerosol concentration are compared with the simulated quantities.

In both test cases, simulated aerosol mass concentrations reproduced measured aerosol mass concentrations to within a factor of 5, without the need to tune vapour pressures. Aerosol nucleation rate was tuned to the measured number concentration, and wall loss rates were also derived from the measured aerosol number distributions (Verheggen et al., 2006).

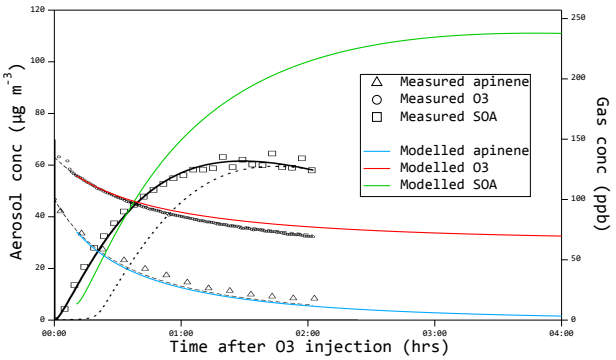

Figure 1: Preliminary results from the ozonolysis simulation. SOA mass is over-predicted by a factor of two.

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