Geophysical Research Abstracts,
Vol. 11, EGU2009-12114, 2009
EGU General Assembly 2009

Evaluation of the EMEP gas/particle SOA mechanism for alpha-pinene

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The EMEP MSC-W model for secondary organic aerosol (SOA) has so far made use of a semi-explicit gas/particle partitioning scheme for α-pinene, in which the α-pinene chemistry is represented by 30 reactions between 17 species. The so-called Kam-2 mechanism, described in Andersson-Sköld and Simpson (2001), was based upon a dark-chemistry scheme for α-pinene presented by Kamens et al. (1999), but with additional reactions added to represent OH-chemistry and dimer formation. The original mechanism was tested against 11 smog-chamber experiments, and found to reproduce observed SOA quite well across a wide-range of temperature and α-pinene levels.

In recent years a number of new studies have become available which necessitate revisions and new testing of the EMEP SOA scheme. As shown in Simpson et al. (2007), assumptions concerning the vapour pressure of specific compounds can have pronounced effects on predicted SOA amounts. The Kamens group has also presented new ideas for the α-pinene mechanism (e.g., Li et al., 2007). Finally, a large number of new smog-chamber data has become available in recent years, allowing a better understanding of the dependencies of SOA formation upon initial conditions, NOx levels, light, relative humidity, and wall-losses (e.g., Pathak et al., 2007).

The EMEP SOA scheme is being re-written in the light of these new developments, and we present results for revised SOA schemes compared to recent smog-chamber data. We also discuss some key uncertainties associated with the development and use of such chemical mechanisms.

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