Geophysical Research Abstracts,
Vol. 10, EGU2008-A-02904, 2008
SRef-ID: 1607-7962/gra/EGU2008-A-02904
EGU General Assembly 2008

Explicit modelling of the SOA/VOC/NOx system

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Our current understanding of SOA formation is limited by the lack of knowledge of gaseous secondary organics involved in gas/particle partitioning. SOA formation involves a multitude of semi-volatile organic compounds (SVOC). Their complex molecular structures and low atmospheric concentrations cause analytical difficulties. Here, we developed an explicit model to explore (i) the potential for products of multiple oxidation steps contributing to SOA, and (ii) the behaviour of the SOA/VOC/NOx system. The model is based on the coupling of detailed gas-phase oxidation schemes (the Self Generating Master Mechanism) with a thermodynamic condensation module. Such a model allows prediction of SOA mass and speciation on the basis of first principles. The SOA/VOC/NOx system is studied for the oxidation of various hydrocarbons under atmospherically relevant concentrations. The results suggest that volatile precursors lead to significant SOA formation via multiple oxidation steps of the parent hydrocarbons.