

Interactive comment on “Formation of secondary aerosols: impact of the gas-phase chemical mechanism” by Y. Kim et al.

Y. Kim et al.

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We would like to thank W. Stockwell for his review.

Referee's comment: The authors should stress more strongly in the abstract and in the conclusion that they are not comparing the standard version of the CB05 mechanism with RACM2.

Our response: CB05 was modified by adding a higher molecular weight alkane (HC8), two biogenic alkenes (API and LIM) and their reactions. Our addition of reactions and species for SOA formation to RACM2 and CB05 involved some duplication of parts

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of the RACM2 mechanism into CB05. In order to have a more harmonized approach to the modification of both mechanisms for SOA formation, we have now modified our approach slightly by adding new reactions and species for SOA formation to both RACM2 and CB05. The results are not very different but by identifying clearly the chemical species linking the gas-phase mechanism (RACM2 or CB05) to the SOA species, the SOA formation module is now better described. An example of this modification is presented in the following revised Table 2a for toluene oxidation (similar modifications were made for the xylene oxidation).

The modifications added to both mechanisms (CB05 and RACM2) to account for SOA formation is now clearly stated in the conclusion: “Here, a harmonized approach was used when modifying the two mechanisms to handle SOA formation. Early treatment of SOA formation in air quality models used simple approaches where SOA formation was treated at the first oxidation step of the precursor species and only a few mechanisms have treated SOA formation at later oxidation steps (e.g. Griffin et al., 2002). We have attempted to reflect the current understanding of SOA formation by accounting for the NO_x -regime dependence of SOA formation from aromatic compounds and treating SOA formation at later oxidation steps. Accordingly, the future development of mechanisms for SOA formation will require chemical mechanisms that can account for the various gas-phase reaction steps that are important for SOA formation.”

Additional reference:

Griffin, R.J., Dabdub, D., Seinfeld, J.H.: Secondary organic aerosol. 1. Atmospheric chemical mechanism for production of molecular constituents, *J. Geophys. Res.*, 107, D17, 4332, doi:10.1029/2001JD000541, 2002.

Table 2a. Toluene oxidation chemistry for SVOC formation.

RACM2	CB05
$\text{TOL} + \text{HO} \rightarrow 0.25 \text{TOLPAEC}^* + \text{other products}$	$\text{TOL} + \text{OH} \rightarrow 0.25 \text{TOLPAEC}^* + \text{other products}$
$\text{TOLPAEC} + \text{HO}_2 \rightarrow 0.78 \text{AnClP} + \text{HO}_2^{**} \dagger$	$\text{TOLPAEC} + \text{HO}_2 \rightarrow 0.78 \text{AnClP} + \text{HO}_2^{**} \dagger$
$\text{TOLPAEC} + \text{MO}_2 \rightarrow 0.78 \text{AnClP} + \text{MO}_2^{**} \dagger$	$\text{TOLPAEC} + \text{MEO}_2 \rightarrow 0.78 \text{AnClP} + \text{MEO}_2^{**} \dagger$
$\text{TOLPAEC} + \text{ACO}_3 \rightarrow 0.78 \text{AnClP} + \text{ACO}_3^{**} \dagger$	$\text{TOLPAEC} + \text{C}_2\text{O}_3 \rightarrow 0.78 \text{AnClP} + \text{C}_2\text{O}_3^{**} \dagger$
$\text{TOLPAEC} + \text{NO} \rightarrow 0.053 \text{AnBIP} + 0.336 \text{AnBmP} + \text{NO}^{**} \dagger$	$\text{TOLPAEC} + \text{NO} \rightarrow 0.053 \text{AnBIP} + 0.336 \text{AnBmP} + \text{NO}^{**} \dagger$
$\text{TOLPAEC} + \text{NO}_3 \rightarrow 0.053 \text{AnBIP} + 0.336 \text{AnBmP} + \text{NO}_3^{**} \dagger$	$\text{TOLPAEC} + \text{NO}_3 \rightarrow 0.053 \text{AnBIP} + 0.336 \text{AnBmP} + \text{NO}_3^{**} \dagger$

*: new peroxy radical formed from toluene, **: oxidant species added as a product to retain the original gas-phase mechanism, †: new reactions added to both RACM2 and CB05 mechanisms for the SVOC formation.