

Interactive comment on »Development of a protocol for the auto-generation of explicit aqueous-phase oxidation scheme of organic compounds»

General comments

In the paper, a new CAPRAM/GECKO-A (Chemical Aqueous Phase Radical Mechanism /Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere) protocol for mechanism auto-generation of chemical processes of organics in the aqueous phase is presented. An extensive literature review of kinetic data of the aqueous-phase reactions of hydroxyl radical and nitrate radical with organic compounds was done. Further, different methods (i.e., gas-aqueous correlations, homologous series of various compound classes, radical reactivity comparisons, Evans-Polanyi-type correlations, and structure-activity relationships (SAR)) for the prediction of kinetic and mechanistic data for aqueous-phase reactions with organics were evaluated. On the basis of evaluation, in a new CAPRAM/GECKO-A protocol hydroxyl radical reactions with organics were estimated with SAR by Doussin and Monod (2013) supplemented by SAR from Minakata et al. (2009); while to describe nitrate radical reactions with organics the advanced Evans-Polanyi-type correlations were used. In addition, the extensive tests on essential and uncertain parameters were performed, and also the oxidation of 1,3,5-trimethylbenzene (TMB) at high RH conditions was carried out in the aerosol chamber LEAK.

Although the current understanding of atmospheric organic chemistry, especially for the gas phase, is much better, there is still a big gap to understand aqueous-phase mechanisms. Thus, I think the manuscript is highly suitable for publication in Atmospheric Chemistry and Physics, which I recommend after addressing the following comments:

Specific comments

The manuscript is very extensive with a lot of material including also ESM; I would suggest to shorten a bit if possible (especially the text/sentences, which are repeated can be deleted).

Further, I strongly suggest a separate list of abbreviation, which would be very helpful. The full name should be used at the beginning, and after abbreviation can be used throughout the manuscript.

I suggest also checking the English language.

Abstract:

Page 1, line 19: processes instead of mechanisms.

Page 1, line 33: Instead of mesitylene I would use 1,3,5-trimethylbenzene or TMB later in the manuscript.

1.Introduction:

Page 2, line 38: Use “auto-generation” throughout the manuscript. “Auto-construction” is not a good choice.

2. Evaluation of kinetic data:

Page 3, lines 12-15 (Overall, a database...) can be deleted; the same is written below (lines 30-32).

Page 3, lines 9-11: If aromatics are excluded here, then this sentence can be deleted.

Page 5, line 1: Correct the sentence.

3. Sensitivity runs:

Page 10, line 12/13: The compound is missing... “the main degradation product of the OH initiated oxidation of” ? (2-oxo-3-hydroxy-succinaldehyde)

Page 10, line 15: Figure 11c/d shows...(not show)

Page 11, lines 29-41: Please, rewrite this section to make it clearer.

Page 13: Why do you use HLC abbreviation for the Henry’s Law coefficient and not as it is usually used?

4. The new multiphase mechanism generator GECKO-A

In Table3 “automated mechanism self-generation” is used; in line 17 (page 15) “automated aqueous-phase mechanism generation”, but mostly “auto-generation” is used. I would suggest using the same through the whole article.

5. Validation...

Page 19, line 10: How OH radicals are formed from the photolysis of O₃ in the gas phase? During photolysis, O atom is formed, which with H₂O forms OH (RH 75%)?

Page 19, line 30: Check the unit for Henry’s law coefficient.

Page 20, line 1:...carboxyl functional groups and not “functions”.

The meaning of UPT, RNX, etc. sensitivity runs should be involved in the list of abbreviations.

Page 20, line 41: From Fig. 19, the particle growth (red color) in the model run TMB cannot be seen.

Page 20, line 67/68: Correct the whole sentence: “Furthermore, uptake processes...”

Page 22, line 5: Do you have an idea how malic acid is formed?

Page 22, line 27: ...has been developed and tested.

Page 23, line 12: Check the unit for Henry's law coefficient.

Table 4: ^(c)...by switching of the UV-C

Figure 9: ..5-dicarbonlys

Figure 13: Add conditions or at least mark cloud and non-cloud periods. This should be done also for other figures.

Figure 19 & 20: TMB cannot not be seen.

ESM

Page 19: First two lines?

Page 24, line 6: Dashed lines in subfigure d (not c).

Page 20: line 10: ...plotted as box model in ? (Where?)

Page 24, line 76: The grey dashed-dotted line is not visible.

Page 30: Figure S9: Give the reference for the standard SAR.

Page 31: Correct the title for Figure S10.

Page 32: Figure S12: It is good to shortly explain alpha, beta and gamma scenarios also here.