Interactive comment on “Development of a protocol for the auto-generation of explicit aqueous-phase oxidation schemes of organic compounds” by P. Bräuer et al.

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Received and published: 23 March 2019

1 General comments

The paper presents an interesting extension of existing auto-generation mechanisms to include aqueous-phase reactions. The work is novel, and fits well within the scope of ACP. Thorough literature review work is presented, evaluating data and rate constant prediction methods, carefully discussing the limitations and rationalising the choices made for the new CAPRAM/GECKO-A protocol. The new mechanism is also evaluated against experimental chamber data. Overall, the paper is well-structured, though rather long. I would recommend trying to shorten the manuscript before publication by scanning for any obviously repeated concepts and superfluous content, as well as carefully reviewing the grammar and ensuring all sentences are easy to parse (I cannot guarantee to have caught all typos, grammatical mistakes, and unclear sentences, but the ones I have are highlighted below – there are also some excess commas in places; please proofread the article again carefully). However, it is definitely suitable for publication in ACP subject to revision.

2 Specific comments

While I have found the written text (despite the reservations above) for the most part easy to follow, I believe some of the figures used are quite difficult to read and interpret, and would benefit from reploting.

This applies in particular to Figure 1, where I am struggling to see what the different boxplots represent. Figures 3, 4, 5, 7, S1, S3, S4, S5, S6 and S7 would benefit from using different symbols as markers rather than just different colours, as some of the colours are quite difficult to distinguish. Figure 8 could be made clearer by using more significantly different markers (rather than crosses with different orientations). The figures showing simulation data can only be understood in conjunction with careful reading of the main text, and would benefit from more detailed descriptions in their labels.

I would try to move more of the detail into the ESM, as the main text is currently very long. For example, at present, sections discussed at length in the ESM are still discussed in a lot of detail in the main text (e.g page 2 and page 7), when referencing the ESM should be enough. The text also feels unnecessarily long when sections are introduced carefully, and then go on to repeat the context mentioned previously.

The new “advanced” Evans-Polanyi correlation strikes me as unusual, in that it can no
doubt usefully scale with molecular size – but it would intuitively seem to me that we are losing most of the useful information that the individual bond enthalpies provide by lumping them into one sum. There ought to be a “better” way of accounting for more than the weakest bond than using the sum of BDEs, and perhaps this will be something that can be further improved in the future.

3 Technical corrections

p1, line 19: change “was” to “were” for consistency with plural usage of “data” elsewhere
p1, line 30: add “The” at start of sentence
p1, line 39: add “a” before “supplementary tool”

C4
p23, line 9: “let” should say “led”
p32, in Table 3, entry for “Monomolecular decay of alkoxy radicals”: “breaking” not “braking” and “an”, not “and”
p32, in Table 3, entry for “Decomposition of acyloxy radicals”: “breaking” not “braking”
p33, Table 4 caption: review use of articles; as stands, add “the” before “start”; correct “UC” to “UV”
p40, Figure 7 caption (line 3): “there” should say “their”
p41, Figure 8 caption (line 4): “cross” should say “crosses”
p41, Figure 8 caption (line 5): add “an” outlier
ESM, p15, p18, p20, p21, p22, p23: throughout (including the labels of Tables S3, S5, S6, S7), $R^2$ is mistakenly referred to as the correlation coefficient
ESM, p18, line 5: review “tropospheric relevant organics compounds”
ESM, p18, line 12: change “prove” to “proof”
ESM, p18, line 17: review commas
ESM, p18/19, line 21/1: review sentence
ESM, p19, Figure S2 caption (line 6): when referring to subfigure c likely should be referring to subfigure d, and when referring to subfigure d should be referring to subfigure e
ESM, p20, line 4/5 and beyond: unsure what is going on here – where is the start of the sentence? This whole paragraph repeats the same exact content already described earlier in different words
ESM, p20, line 5: insert “it”
ESM p20, line 10: Figure S4 is not the figure described – should this refer to Figure C7

S8?
ESM, p20, line 23: “Figure S2d” should say “Figure S2e”
ESM, p25, Table S9, p27, Table S10, p28 Tables S11 and S12: please check the units; I can understand those in Table S8, even though it would perhaps make more sense to say $C^\prime$ itself is dimensionless (etc.) unless the division by its units is also added into the equation; for these other tables, the volume part of the units does not seem to add up correctly
ESM, p26, Figure S6 caption (line 6): correct the spelling of “respective”
ESM, p30, Figure S9 caption (line 7): “give” should say “given”
ESM, p31, Figure S10 caption: expand “orig”
ESM, p33, Figure S14 caption: correct the spelling of “investigating”
ESM, p34, line 3: “these type”, inconsistent use of singular/plural
ESM, p34, line 4: correct the spelling of “initialised”
ESM, p34, line 9: insert “the” only reaction pathway