

Interactive comment on “Explicit modeling of volatile organic compounds partitioning in the atmospheric aqueous phase” by C. Mouchel-Vallon et al.

Anonymous Referee #1

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This manuscript describes a very detailed atmospheric multiphase oxidation scheme. The employed chemical mechanisms are self-generating and therefore much larger than typically employed in atmospheric chemistry modeling exercises. An advantage is that individual chemicals are not "lumped" and the preservation of chemical identity preserves important chemical properties, in particular related to phase partitioning. The oxidation pathways for the studied systems is presented in the context of a 2-dimensional framework, and this is the first time this has been specifically done for aqueous phase atmospheric chemistry. The presentation is novel and the work should be published in ACP provided the comments below are addressed.

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Detailed comments: abstract line 11, does 2% refer to 2% of the total organic gas phase mass?

p.24096 "lack of knowledge concerning the aqueous phase contribution to atmospheric chemistry (Ravishankara, 1997). This is a bit overstated. The community knows that sulfate aerosol is formed through aqueous chemistry and SOA can form. There are certainly open questions but the community knows it happens. ...eg. as the authors point out inorganic reactions in the aqueous phase have been studied extensively. the sentence should be worded more carefully.

P24097 line 15 - please provide units for "L". It is also important to note that Ervens and Volkamer have confirmed this through modeling as stated by the authors, ... but as applied to a series of laboratory experiments conducted under different conditions in different labs.

P24097 section "i", it's not just that highly soluble species are *expected* to be found in atmospheric waters, they *are*found. The review paper by Chebbi and Carlier explains this in detail.

p.24098, line 6. There is a typo...constant"s" not constant

p24099 "in details" should be "in detail"

p. 24100, line 21: What species have $H > 10^{12}$?

p.24101, The diffusivity number for the reference compound is provided for a temperature of 298K. The authors set $T=278K$ in their model and use 278K for estimates of Heff values. What is a typical temperature for the (chemical) system in the atmosphere like the one studied here, and by how much would D_g (or kl ?)change? How does the difference in temperature for the different parameters limit or confound the findings here?

p. 24102, can the authors provide some brief details on how the acid/base equilibrium reactions are described kinetically and the influence of $[H^+]$ on phase partitioning?

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p.24102 what is the effect(s) of $z=0.05$? how sensitive are predictions to this value?

p. 24103 is an initial condition of $[O_3] = 40$ ppb representative of areas where individual alkane concentrations are 10ppb? Can the authors provide an example that this is the case? The same O_3 initial condition is used for all NOX scenarios? Can the authors justify this?

p.24104, line 12, number of lifetime"s"

p.24104, how is ' τ ', the lifetime defined? is it the chemical lifetime due to reaction with OH or does it combine OH/ O_3 and gas phase loss due to physical partitioning? is it the lifetime of the species in the gas phase or lifetime in the atmosphere prior to physical loss processes?

p.24104, please change multifunctional "ones" to "species", "moieties" or another more specific word. can the authors define a specific range for "moderately soluble"?

p. 24105, starting at Line 22. "dissolved organic matter is then likely subject to fast processing....this process is so far ignored in current atmospheric chemical models.' Is this statement accurate? The 3-dimensional photochemical models Geos-Chem (Fu et al., 2008) and CMAQ (Carlton et al., 2008) have some representation (simplified) of multiphase organic aqueous phase chemistry in their base versions.

Page 24106, Line 23 "Figure 2 shows that the dissolved organic content tends to increase with decreasing NOx concentration." This is a curious result. The authors state below (p. 24107) that "the degree of substitution of the organics ranges from 28% (low NOx scenario) to 38% (high NOx scenario)". Typically the more substituted an organic compound, the more soluble. Ervens et al. (2008) find that total solubility for an organic gas phase inventory is higher for low VOC:NOx (i.e., high NOx) and a paper currently in ACPD open discussion by Saylor shows results consistent with Ervens. Can the authors explain what appear to be discrepancies?

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