

## ***Interactive comment on* “Simulation of semi-explicit mechanisms of SOA formation from glyoxal in a 3-D model” by C. Knote et al.**

### **Anonymous Referee #2**

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The authors have performed a detailed study of glyoxal contributions to SOA formation in California during CARES/CalNex using a version of WRF-Chem which they have updated for this purpose. The work should be suitable for publication in ACP after the following issues are addressed.

- It is my understanding that cloudwater processing of glyoxal to form SOA was not considered in this study (this was confirmed on line 396 but should be made clear earlier in the manuscript). The authors should discuss the potential errors (or lack thereof) introduced by this choice. Could this contribute to the overestimation of glyoxal concentrations above 2000 m (line 381)?

- Line 16 – this statement is a bit misleading: “surface uptake is found to be the main

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contributor. . .” This sounds as if a glyoxal SOA formation mechanism that scales with aerosol surface area was shown to provide the best agreement with the field data, which I don’t believe was the case. Yes, the surface uptake mechanism was shown to result in higher yields of glyoxal SOA than the other pathways, and this may be what the authors meant to say. However, perhaps the emphasis on this mechanism should be reduced a bit, considering that in the conclusions of the manuscript (line 631-634) the authors state that, until additional experimental evidence exists to support this modeling approach, it may not be justified and models which rely on this mechanism may overestimate glyoxal SOA formation.

- Line 19-20, abstract: This point is stated in such a way that it may be interpreted incorrectly. Glyoxal uptake at high salt concentrations is still high enough to be considered “substantial,” even if it no longer increases linearly with salt concentration due to kinetic limitations. No one would argue that an  $H^*$  of  $\sim 10^7$  M/atm is insubstantial.

- Line 37-38 – Quite a few seminal laboratory studies are missing from this list: Kroll et al. (2005), Liggio et al. (2005), Galloway et al. (2009), Volkamer et al. (2009). McNeill et al. (2012) doesn’t belong in this list - it was a modeling study (see below).

- Line 45 – The box model simulations of McNeill et al. (2012) should be included in this list.

- Line 65-66 – It’s not correct to say there is no previous study of glyoxal-SOA formation in a 3D regional model. Formation of SOA by glyoxal via cloudwater processing has been modeled in CMAQ by Carlton and coworkers (studies which should be cited here). Perhaps what the authors mean to say is that SOA formation by glyoxal via aerosol phase processes has not been studied in a 3D regional model.

- Line 142 - the authors should clarify what is meant by “inversion-based emissions”

- Line 163- The way that this is worded, it sounds like uptake of glyoxal into particles in the model does not impact the gas-phase glyoxal concentration. I don’t believe that

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this is the case after reading section 4.3.3., so some clarification may be in order. If this is the case, please justify

- Line 189 – “There is no clear scientific consensus on how glyoxal might form SOA.” This is an overstatement. SOA formation by glyoxal has been one of the most intensely studied topics in atmospheric chemistry over the past 8 years or so. The scientific community knows quite a lot about its mechanisms, and there are only a few points of controversy.

- Line 193 - What does “interactions between irreversible and reversible formation pathways are still unknown” mean? These pathways simply interact via their competition for glyoxal monomer in the aqueous phase.

- Fig 3 – please change the quotation marks on “salting-in” to the English style.

- Line 234 – The ammonium-catalyzed pathway presented by Noziere et al. and related studies such as Galloway et al. (2009) has been observed to be reversible. The authors should provide a rationale for treating it as irreversible here and mention it in the text.

- Line 256 – The authors need to offer more insight into the physical underpinning of the photochemical surface uptake mechanism for glyoxal. Without any insight into the nature of this uptake, it’s impossible to evaluate the modeling approach or know whether or not it is appropriate to extrapolate parameters derived from chamber studies to the environment. A speculative list of plausible physical mechanisms that could motivate this modeling approach, but which need further study, would be sufficient.

- Line 505 – “constant” should probably be “content”

- Line 526 – “. . .40% of glyoxal. . .” I think there is a word missing here. SOA?

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