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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Photochemical degradation of iron(III)-citrate/citric acid aerosol quantified with the combination of three complementary experimental techniques and a kinetic process model" *by* Jing Dou et al.

Anonymous Referee #3

Received and published: 16 September 2020

The authors of manuscript acp-2020-799 studied the photochemical degradation of iron(III) carboxylates (with iron(III) citrate as a proxy) via 3 complementary methods. The mass loss of single particles was measured using an electrodynamic balance, the oxidation state of single particles was determined using STXM/NEXAFS, and HOÂů2 production was monitored using a coated wall flow tube experiment. These results were all used to validate a novel Photochemical Reaction and Diffusion (PRAD) model. The model reproduces experimental results within stated levels of uncertainty. The experimental data shows that O2 uptake and mobility, influenced by particle viscosity

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and size, is a significant factor in the degradation of iron containing aerosols.

The combination of experimental and modelling work done together is a compelling way to debut the PRAD model. Manuscript acp-2020-799 is constructed well and supported with clear figures (both in the manuscript and SI) and should be published after the following comments are addressed.

Major Comments:

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1) The PRAD model was developed (presumably) for modeling iron degradation but the framework can be used in other particle/gas reaction systems. Some discussion on how general this model is/can be and which systems it could be successfully applied to would be good. It would also be helpful to add statements about what this model does well, like which parameters are known with the most certainty or which conclusions are the strongest, to help the reader understand the PRAD model's place among other similar models (both those already existing and those yet to be developed).

2) Some additional discussion about the sensitivity that the manual tuning of certain parameters in the PRAD model has would be useful. Quantifying the sensitivity would be excellent but at least something to help the reader gauge the effect that a slight mistuning might have. In a similar vein, adding a column to table 1 showing the uncertainties in each of these parameters (if they're available) would be good.

3) Line 322-323 and Figure 7 shows a statistical agreement with 95% confidence between the model and the data, but it is just on the edge of significance. Even though a 95% confidence level is commonly used, it is ultimately arbitrary. A sentence or two giving some extra context or how the estimate could improve would be helpful in making the conclusion (that jcalc is a good estimator for jobs) more robust.

Minor Comments:

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Line 45: “humic like” should be hyphenated Line 57: “time resolved” should be hyphenated

Line 72: The chemical formula of iron(III) citrate is FeC6H5O7 but the structural formula written shows an incorrect number of Carbon and Hydrogen atoms. Please revise the structural formula.

Line 99: reword: “The PRAD model allows to simulate”

Line 201: The denominator in the expanded version of equation (4) uses “r” as a subscript, it shows “0.5(rr+1 – ri-1)” should it read “0.5(ri+1 – ri-1)” instead? Also why use 0.5(ri+1 – ri-1) instead of (ri+1 – ri)?

Line 209: Shouldn’t the radius should be squared in equation (6) as part of the sphere surface area equation? This continues through equations (8), (9), (13), (14), and (16). A brief clarification would help.

Line 248: If cn is molar concentration (as defined in line 205), then Nn should be the number of moles, not the number of molecules.

Line 270: Because concentration was defined as a subscripted “c” (i.e. cn in line 205) replace the nCit values with cCit for consistency.

Figure 6: The caption colors do not correspond to the figure colors.

Line 304: “The degradation progresses. . .” should be “The degradation processes. . .”

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