

Interactive comment on “Treatment of non-ideality in the multiphase model SPACCIM – Part 1: Model development” by A. J. Rusumdar et al.

Anonymous Referee #2

Received and published: 21 July 2015

The authors have implemented the effects of solution non-ideality in aqueous-phase reaction kinetics in the SPACCIM modeling framework. This manuscript focuses on the model development and numerical aspects of the new treatments while a companion manuscript focuses on the results from detailed modeling studies. The manuscript is recommended for publication after the following minor comments are addressed.

The authors would like to thank the Anonymus Reviewer#2 for the careful consideration of the manuscript and for the constructive comments and suggestions made to improve the manuscript. Those are addressed below. Furthermore, we have added results of two new simulations (Figs. 8 and 9, new numbering) which emphasize the differences and identicalness between AIOMFAC, mod. LIFAC and SpactMod. Additionally, the applied SpactMod parameters are compiled in Appendix A.

Comments:

Page 4156, line 5: “...models do generally not consider...” sounds awkward. Suggest revising to “...models generally do not consider..”

Author's response:

The authors agree with reviewer's comment and have modified the manuscript according to the reviewer suggestion.

Page 4156, line 6: Please define SPACCIM (all acronyms should be defined at their first use).

Author's response:

The acronym of SPACCIM (“Spectral Aerosol Cloud Chemistry Interaction Model”) was added to the manuscript text and the whole manuscript was again checked for undefined acronyms and their definition at their first use. Furthermore, a list of all acronyms, indices and symbols are now provided in Appendix B (see also a comment below).

Page 4156, line 8: Revise “The present paper describes firstly, the performed model development including (i)...” to “The present paper firstly describes the model developments, including (i)...”

Author's response:

As recommended by the reviewer, the text has been modified in the suggested way.

Page 4156, line 9: the phrase “the kinetic implementation of the non-ideality in the SPACCIM framework” is confusing. Suggest revising it to “the implementation of solution non-ideality in aqueous-phase reaction kinetics in the SPACCIM framework.” Similar sentences elsewhere in the manuscript should also be revised appropriately.

Author's response:

We agree to the reviewers comment. The sentence has been rephrased. Furthermore, the whole manuscript was checked for similar sentences and those were revised correspondingly.

Page 4156, line 13: delete “performed”

Author's response:

Following the reviewers comment, we deleted “performed” in the manuscript text.

Page 4159, line 6: The “Zaveri et al., 2005” citation here should refer to “Zaveri, R. A., R. C. Easter, and A. S. Wexler (2005a), A new method for multicomponent activity coefficients of electrolytes in aqueous atmospheric aerosols, J. Geophys. Res., 110, D02201, doi:10.1029/2004JD004681,” which is presently missing in the list of references. Then on line 11, change “Zaveri et al., 2005” to “Zaveri et al., 2005b”, and make appropriate changes in the references.

Author's response:

The suggested reference was insert according to the reviewers comment.

Page 4160, line 4: The “Shrivastava et al., 2011” reference is inappropriately cited here as that work makes a highly simplified assumption for SOA partitioning and does not include interactions between organic and inorganic species. I suggest deleting it.

Author's response:

The authors agree to the reviewer’s opinion and deleted the reference (Shrivastava et al., 2011) in the manuscript text.

Page 4163, line 12: Please list the total number of particle and droplet classes used in the model. Also how is the size distribution represented in each class of particle/ droplet? Is it modal or sectional approach?

Author's response:

The SPACCIM framework allows representing the size distribution of particles by a sectional approach (see Wolke et al. 2005 for details). However, the simulations in the present paper consider only a mono-disperse particle population to focus on the influence of non-ideality. A number concentration of 10^8 cm^{-3} and an initial particle radius of 200 nm were used for the sensitivity studies as mentioned in Subsection 3.3.1.

This paper will greatly benefit by adding a list of all the notations used. There are many variables, subscripts, superscripts, and indices, which are difficult to keep track of without a systematic list of them.

Author's response:

The authors agree with the idea of the reviewer. Thus, the revised manuscript includes a list of symbols, indices and abbreviations used in the paper.

Table 1. What is m_s ? Should the activity of a solid be unity?

Author's response:

No, the activity of solid is not treated as unity. However, the corresponding activity coefficient is equal to unity. M_s represents to the molality of the corresponding solid. Due to the reviewer query, the revised Table 1 clarifies the issue now.

Figure 5. What model does the solid black line refer to? I believe it is AIOMFAC, but it’s is not indicated in the figure by an arrow.

Author's response:

The solid black line refers to E-AIM that was shown in the Figure. In the title, it was a mistake to mention the AIOMFAC. The authors apologize for this error. We have changed the text of the Figure caption in the manuscript concerning the remark of the reviewer.