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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Influence of non-ideality on aerosol growth" *by* S. Compernolle et al.

S. Compernolle et al.

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We would like to thank the anonymous referee for his or her input. His comments/questions are repeated here in italic.

Specific Comments

Section 2.3: The fitting to the SPARC data produced a complete set of UNIFAC parameters which could have been used in the comparison. Why was this not done?

As explained by table 4, the fitting to SPARC data generated only interaction parameters between

- alkane group - known functional groups.

- alkane group - new functional groups.
- known functional groups - new functional groups.
- new functional groups - new functional groups.

Hence what is missing for a complete set of SPARC-derived parameters are interactions between known functional groups - known functional groups such as data from e.g. alcohol-acid, alcohol-keton, ... mixtures. This would amount to a lot of new SPARC online calculations to obtain data and subsequent fitting of the UNIFAC formula. This would be quite some additional work, while it would only provide a test on SPARC's performance for known functional groups. Since this was not the primary scope of the paper, this was not done.

Page 17072, eq. 17: Why is total molar concentration of the particulate organics not in this equation? If equation 3 is used, partitioning coefficients should be multiplied by the total concentration.

There was indeed a mistake in the righthandside of eq. 17, which has been corrected. We thank the referee for his alertness. For the same reason, we have replaced $\kappa_{p,j}$ by $\kappa_{p,j}c_{om}$ on line 11 after eq. 17 and $\kappa_{p,w}$ by $\kappa_{p,w}c_{om}$ at page 17073, line 25. Finally, we have also replaced capital C, reserved for mass concentrations, by c, used for molar concentrations, in eq. 17 and at lines 11 and 14.

Page 17072, eq. 18: Why is the non-volatility fraction not defined as the ratio of total particulate concentration and total gas and particulate concentration?

This would not describe the same quantity. Our defined non-volatility measure $\overline{f}_{om}$ indicates if the aerosol is mainly composed of low-volatile components (value close to 1), or high volatile (value close to zero). There is no direct link with the gas phase concentrations. The ratio of total particulate concentration and total gas and particulate concentration, $\sum_i c_{p,i} / \sum_i (c_{g,i} + c_{p,i})$, describes a quite different quantity. One could

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e.g. imagine a system where the aerosol consists mainly of low-volatile components, but where there is also a much larger quantity of many high-volatile, almost uncondensable, gases present. In that case our quantity $\overline{f}_{om}$ would be close to 1, while $\sum_i c_{p,i} / \sum_i (c_{g,i} + c_{p,i})$ would be close to zero. We compared the quantities for a few SSCEs and found that they are indeed very different.

Technical Corrections

All pages: The usage of term vapor pressure should be checked or at least explained. Saturation vapor pressure is better term for most of the cases in this paper.

"vapor pressure" has been substituted with "saturation vapor pressure".

Page 17062, lines 7 and 11: Sentences starting in these lines should be clarified

The text is extended for clarification.

Page 17063, line 11: Sentence starting in this line should be clarified

The text is extended for clarification.

Page 17068, line 26: Case should be cases

"case" changed in "cases"

Page 17071, Section 3.2: This section is quite long and partly not well organized. For example, sentences in the first paragraph have rather loose connections. Fourth paragraph (page 17072, line 20) is not clear by itself; it could be combined with the previous one. There are no clear connections between the short paragraphs in page 17073; some of these could be combined.

We admit that the connections between paragraphs could have been better. We have modified the section according to the suggestions of the referee.

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Interactive Comment

Page 17077, line 32: Title of the article and journal abbreviation should be checked

The journal abbrevation J. Phys. Chem.-US (instead of J. Phys. Chem.) was implemented by the ACP Production Office, as it is the ISI-convention which is followed by ACP. "water" replaced by "Water in title.

Page 17078, line 7: No space before comma

Space deleted.

Page 17078, line 25: Mixtures should be written by lower case letters

Mixtures changed into mixtures.

Page 17079, line 20: UNIFAC in should be in capital letters, journal abbreviation

Unifac changed into UNIFAC. The same error was present -and is corrected- page 17078, line 28. The journal abbrevation Ind. Eng. Chem. Proc. DD. (instead of Ind. Eng. Chem. Proc. Des. Dev.) was implemented by the ACP Production Office, as it is the ISI-convention which is followed by ACP.

Page 17079, line 23: AICHE should be AIChE

AICHE changed into AIChE.

Page 17080, line 21: Should HuffHartz be Huff Hartz?

Indeed. The name is corrected.

Page 17087, Table 6: Reference should be to Table 5

Reference changed into Table 5. Idem for reference in caption of Table 7.

Page 17093, Fig. 3: Different colors should be used for the ideal and UNIFAC-Hansen mass yield lines

The color for UNIFAC-Hansen is changed.

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Interactive comment on Atmos. Chem. Phys. Discuss., 8, 17061, 2008.

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