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Atmospheric
Chemistry
and Physics
Discussions

Interactive comment on "Organic particulate matter formation at varying relative humidity using surrogate secondary and primary organic compounds with activity corrections in the condensed phase obtained using a method based on the Wilson equation" *by* E. I. Chang and J. F. Pankow

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General Comments

The authors present work here to account for variations in activity coefficient, molecular weight and water uptake on semivolatile organic partitioning in atmospheric aerosol (based on a contribution-method Wilson equation). This work constitutes an important contribution to the area of organic aerosol modeling and would be of interest to the atmospheric community. Publication is recommended after the following comments are addressed.

Page 3, "…hypothetical lumped product": Please add a reference here.

Page 4, end of paragraph 1: Please add a brief discussion on the findings of the Bowman and Melton (2004) study (especially on the computational requirements).

Page 4, "is thus problematic.": It would be useful to report (if possible) a potential range of uncertainty in partitioning associated with this kind of assumption.

Page 9: The iteration process (Eq. 5 to 10) is important for the whole paper. It would be nice if the steps are explained a bit more.

Page8-10: Acronyms such as "SIPSOL.1" and "CP-Wilson.1" should be clearly defined in the text.

Page 12, 8 lines before end of page: Replace "significantly more computationally economical" with "significantly faster"

Page 13, "Some degree of caution should therefore be exercised with considering predictions made using CP-Wilson.1 for nitrate-containing compounds." The authors are clear in justifying the reason to be cautious when nitrate groups are present, but do not give any guidelines on caution should be exercised. Should activity coefficients computed with CNO2 groups be independently evaluated?

Page 13: "At some point …CP-Wilson.2". This is future work, and should be moved to the end section of the manuscript.

Page 13, second line before end: Would the system always separate in two phases? The Gibbs phase rule allows for more than 2 or 3 phases to be present.

Page 14, end of section 2.3: Was "further optimization" carried out by further reducing the step size?

Page 15: Is it possible that more than 2 aerosol phases exist?

Page 17: “was obtained 10,000 . . . system resource availability”: this could be reduced a bit, perhaps as ” was repeated 10,000 times to obtain a representative average calculation time”

Page 19, end of section 3.1: Can you give a brief explanation why phase separation is likely at high x_i?

Page 21, end of section 3.4: Would P6 “not being comfortable” in each phase suggest that further phase separation is possible?

Page 23: The implication of the new method on predicted SOA is particularly significant, especially since the sensitivity at low M_o is enhanced. For this to have an even stronger impact to the reader, it would be useful to point out the SOA increase for “atmospherically-relevant” levels of M_o.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 995, 2008.

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