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Geoscientific
Model Development
Discussions

Interactive comment on "Partial Derivative Fitted Taylor Expansion: an efficient method for calculating gas/liquid equilibria in atmospheric aerosol particles – Part 2: Organic compounds" *by* D. Topping et al.

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We thank the referee for the comments made which are addressed in the following:

'Technical comments: p. 1766, lines 24-28: The analysis of the binary vs. ternary vs. UNIFAC statistics described here is not clear. The authors state that the ". . .average predictions from ternary are smaller than those from binary..." Does that mean that overall the ternary model is more accurate (which is what is shown in Table 4, referenced in the same sentence, but has already been stated)? Or does it mean that the

ternary model predicts smaller deviations from unity (which would be interesting but not shown anywhere...)?' Response: Apologies for the lack of clarity here. This is a typo, the text should read 'average percentage deviations from ternary...' which means the ternary model is more accurate. This has been corrected.

'The authors then say, "For example, for "4", "5" and "8" the difference between both variants is large. . .", which suggests the comparison of binary vs. ternary looking for compounds with either the largest difference between the bi- nary and ternary percentage deviations (though the word "both" is confusing) or the compounds for which both the binary and ternary predictions are poorest; the listed compounds (when compared with other compounds in Table 4) do not really serve to clarify.' Response: Again many apologies for the lack of clarity here, the reference to compounds 4, 5 and 8 is wrong and was a poor oversight. This sentence was referring to the fact that for one sample compound (7), the ternary model shows maximum deviations of 2.2%, whereas for one instance, the binary model experiences deviations of -73%. This was trying to re-iterate how whilst the ternary model is better performing, the binary model can display a large range of deviations. This sentence has now been changed to the following: 'For example, for compound 7 used in this study, and listed in table 4, the percentage deviation on changing from the ternary to the binary model can increase from 2.2% to -73.3%.'

'Finally, the authors then reference the reported percentages for compound "7" which is not listed (but supports the suggestion of identifying the largest differences in the percentage deviations; though not clear then how that supports the first sentence).' Response: Yes, see above.

'p. 1769, line 11: Is compound "12" dominant with and without the consideration of activity coefficients? It is recommended that a clarification be made here (e.g., "12" is the dominant compound in the ideal case") and if another compound became dominant in the non-ideal case it may be interesting to note or discuss. This may be particularly interesting given that the compounds chosen were the most abundant particle-phase compounds in a modeling study that (presumably) neglected activity. Note: "domi-

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nate" should be "dominant".' Response: The reviewer has raised an interesting point here. In the non-ideal case this compound shared that majority of the condensed phase abundance with Compound 11 (which had around 70% of its abundance in the condensed-phase), while in the ideal case it alone was the most dominant semi-volatile compound. The sensitivity study used to provide the example compounds only assumed ideality, using a wide range of anthropogenic and biogenic scenarios and ambient conditions to predict the most abundant compounds in the condensed phase. If we had picked compounds derived through explicit treatment of non-ideality, we might expect the benchmarking against UNIFAC to somewhat improve the percentage deviations on comparison with PDFiTE. This might form an interesting study to perform, whether the choice of compounds from a non-ideal complex system improves benchmarking tests. There have been some theoretical studies to assess the change in component ranking with and without the assumption of ideality in absorptive partitioning, however generalizing the end result is dependent on the initial abundance in the gas phase. This is partly why the benchmarking comparisons against UNIFAC were constructed using many random initializations even though the dynamic testcase was informed by the original sensitivity study. In the paper we will adjust the following text: Line 11, Page 1769: '. . .in this example. . .' will be changed to '. . .for both the ideal and non-ideal runs in this example. . .'

'Were there any significant differences in the mass or number size distributions between the ideal and non-ideal cases? While it would be difficult to generalize from such differences, it may add weight to the significance of including activity coefficient corrections.' Response: The mass in the non-ideal case does decrease (by around $\sim$15%) compared with the ideal case. However this change is very scenario specific, and depends greatly on the gas-phase abundance of the condensing species, so we don't think that a discussion of the change in mass size distribution would add anything to this paper.

'Comments on Section 2: Overall it is recommended that the authors review each of the

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symbols and indices used in Equations 2-15 to ensure that they are unique, defined, and complete. Some examples of symbols/indices needing revision follow.' Response: Yes we do apologise for these errors. The errors listed are part of a list supplied by referee #1 and have been corrected accordingly. Those which are unique to this review are the following:

'p. 1764, line 23: "compound" should be "compounds"; line 24: suggest that "as defined within the MCM" be placed in parenthesis'. Response:These have been changed.

p. 1765, line 10: Replace "A example" with "An example"; line 28: "computational" should be "computationally". Response:This has been changed

p. 1765, line 12: Replace "Figs" with "Figures". p. 1767, line 5: "PD-FITE" should be "PD-FiTE". Response:This has been changed

Tables and Figures:

Table 2: Polynomials for only 12 compounds are listed. Response:Apologies, the missing compound has been added.

Please check all Table numbers and references in citations. Table 4 is referenced in the text as Table 5; Table 5 is referenced as Table 6, etc. More description is needed in the Table 4 header (e.g., describing that values are averages over multiple runs/RH values, etc.). Response:These have been corrected, and table 4 now has the text: 'Statistics averaged across 100 random initializations at ten relative humidities (10, 20, 30, 40, 50, 60, 70, 80, 90, 99%), providing 1000 datapoints'.

Fig. 1: The color scale is not defined/described (Figs 1-3). "xB" in figure should be "xâA ÌĘšB". Response:This has been corrected.

Fig.2:"xâA ÌĘšB"infigureshouldbe"xâA ÌĘš3"and"lnfA"shouldbe"lnf1"(inFig.3too). Response:This has been corrected

Fig.3:"xâA ÌĘšB"infigureshouldbe"xâA ÌĘš4". Response:This has been corrected

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Fig. 4: It is recommended that the compounds in Fig. 4 be specified; may have implications for future applications and understanding robustness of binary vs. ternary approach for specific compounds. Response:We have added compound number references to the compounds with the largest deviations on comparing the binary and ternary models.

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