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Atmospheric Chemistry and Physics Discussions

Interactive comment on "An efficient approach for treating composition-dependent diffusion within organic particles" *by* Simon O'Meara et al.

Anonymous Referee #1

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The authors have developed a correction factor for the analytical solution for particle phase diffusion to account for the composition dependence of the particle phase diffusion coefficient. The topic of the manuscript is timely and is well suited for ACP. The developed correction has weaknesses regarding the generality of the solution and this limits the applicability of the correction to wider range of the conditions. However, these limitations are described in the manuscript, and within the suitable range of conditions the correction works well. The methods used in the study seem in general valid and the manuscript can be published in ACP after addressing below comments.

Specific comments:

P. 1. L. 12-13: Authors state "Until such time as a general solution is found, caution should be given to sensitivity studies that assume constant diffusivity." I interpret this

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as a critique towards using constant diffusivity approach. However, as the authors themselves admit that they were not able to derive a general composition dependent description, it would seem to me that constant diffusivity assumption is better choice at the moment than using a composition dependence that might not be suitable for the given conditions.

P. 5, L. 12-14: Authors chose e-folding state as the reference “time point”. Did the authors test if the choice of this reference point affects the comparison results? Also, correct ‘or’ -> ‘of’ (L. 14)

P. 6, L. 7: It is stated that analytical solution was fit by eye to Fi-PaD results. Is fitting by eye enough accurate method for this? Why not using a more mathematical method for fitting the curve?

P. 6, L. 11-12: It says “An interpolation method was developed to estimate parameters for the correction equation between the values of dxs,sv and log10(D0nv/D0sv) used for the equation derivation”. This developed interpolation method needs to be described. I assume this refers to Tables A3 and A4. However, these tables and their captions require clarification. For instance, please clarify what it means when it says “whether the log10 of parameter values was taken” and “whether the log10 of the variable was taken” in the table captions.

P. 7, L. 16-17: Why is the metric for proximity to equilibrium different for +ve and –ve cases?

P. 12, L. 3-9 and Figure 9: Is the % error presented in Fig. 9a comparing analytical constant D version to Fi-PaD results or to analytical composition dependent D version? Based on text and use of eq. 9 it seems that comparison point would be Fi-PaD, but based on figure caption it sounds like comparison point is the analytical solution with composition dependent D.

P. 14, eq. 12: Please explain why was this particular functional form chosen for the p4.

P. 15, L. 18-19: “In both solutions (numerical and analytical), diffusion rates have a square dependence on particle size”. If one substitutes eq. 6 to eq. 3 the diffusion rate in eq. 3 is dependent on Rp not Rpˆ2. Did the authors test the CD for different sizes?

P. 15-16, from P. 15 L. 27 to P. 16 L. 3: If I understood correctly, the effect of different molar masses was tested by using the fitting parameter values that where determined from assuming both molar masses where 100 g/mol, and this CD did not work when M of semi-volatile was varying from that of non-volatile. Is it so that the correction factor CD simply doesn’t work if M of compounds are different or would the CD work for the different M values if p parameters were fitted by using the M values that are of interest?

Technical notes:

P. 4, L. 24: Here it says subscript s refers to surface of particle, but eq. 3-5 do not contain subscript s. Is there a typo either in the equations or in the text?

P. 6, L. 3-4: Explain here what +ve and –ve mean.

P. 13, L. 13 and Fig. 10: I recommend naming the x-curves with some other symbol than p. Use of p here is confusing as also the fitting parameters for CD are marked with p.

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