

Interactive comment on “MATRIX-VBS: implementing an evolving organic aerosol volatility in an aerosol microphysics model” by Chloe Y. Gao et al.

Anonymous Referee #2

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General Comments:

The paper describes the implementation of a volatility basis set (VBS) approach within a box model version of the Multiconfiguration Aerosol TRacker of mIXing state (MATRIX) scheme.

The paper is generally well written but would benefit from careful proof reading to ensure that everything is written as concisely and accurately as possible. Whilst the paper fits within the scope of GMD, more detail would be needed for anyone to reproduce this study - I would recommend publication once the below issues have been resolved.

Specific Comments:

C1

- Page 3, line 3-6: This sentence is talking about the role of semi-volatile organics but mentions new particle formation - I would suggest moving the reference to new particle formation to the previous sentence about very low volatility organics, and including some additional references, i.e.: “It has been established that highly oxidised, low-volatility organics play a key role in new particle formation (Metzger et al., 2010; Riccobono et al., 2014; Kirkby et al., 2016) and particle growth (Trostl et al., 2016), while the range. . .” [this is alluded to in your Methods section but not clear here]

- Page 4, line 1-14: There are a few more details that would be useful to include in this model description. Specifically: Clarify whether this model tracks both aerosol number and aerosol mass? [I assume both from Figures 6 and 7] What are the “aerosol populations” – they seem to be specific modes of particular composition (perhaps refer the reader to Table 2 at this point)? What are the diameter ranges of these populations? (this also becomes relevant when interpreting Figures 6 and 7)

- Page 5, lines 25 - 30: Can you expand on what these mass-based emission factors represent? (enough for the reader to understand without having to refer to Shrivastava et al., 2008) To what is the additional factor of 1.5 applied?

- While the VBS scheme is outlined in the Model Description, it would be useful to include a brief description of how this influences, and what controls, the gas-particle partitioning among the different populations.

- Reaction with OH is mentioned as a mechanism for chemical aging of the organic species, is the OH concentration taken from GISS ModelE? How often are the concentrations updated? How does this process occur (does it occur at a specified reaction rate for each of the volatility bins of organic species?)

- Where do the products of the oxidation of biogenic organics go? Into the lowest volatility bin? Or are they treated entirely separately?

- Some of the information in Section 4 seems like it would be more appropriate in the

C2

model (i.e., description of the treatment of BC) / VBS description (i.e., description of the emission rates for the VBS species), rather than the discussion of the simulations?

- Page 6, lines 19 – 20: this currently sounds like each emission factor is 2.5 (which is not the case?), perhaps rephrase this to clarify what you mean

- In a couple of places, compounds that are low-, intermediate-, and high-volatility are referred to (e.g., Page 7, lines 13-15); in terms of the volatility bins used here, how are these categories defined?

- Page 22, Figure 2: Refer to Table 1 or Figure 1 to explain the legend entries and define OCAR Page 24/25, Figure 4/5: The layout of the columns doesn't quite match the description in the caption

Technical Suggestions:

I have a number of technical suggestions that may help improve the readability of the manuscript.

General comments:

On several occasions, quantities are referred to as "about" ##, it would be better to either refer to a more specific value or refer to this same value as "approximate".

Specific suggestions:

Page 1, line 21: should this be "high volatility" rather than "high volatile"?

Page 2, line 21: insert "the" between "with" and "hydroxyl"

Page 2, line 27: remove "it" from between "space" and "also"

Page 2, line 28/29: specify that the "it" being referred to here is the 2D-VBS?

Page 3, line 23: replace "terpenes emissions" with "emissions of monoterpenes" [if you are only referring to monoterpenes here]

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Page 4, line 21: remove the word "ones" from between "volatile" and "and"

Page 5, line 11: insert a hyphen into "nonvolatile"

Page 5, line 12-14: rephrase this sentence, it is currently not clear what you mean – and be consistent with writing numerical values as words or numbers, i.e. "eight" v. "8"

Page 5, line 18: you could replace "of different" with "and" ?

Page 5, line 19: you could move "(Mexico City)" to the end of this description (after "tropics") to avoid confusion

Page 5, line 23: you could separate this into two sentences, with the first ending after "Table 3" and the second beginning with "Here we do not include."

Page 6, line 30: replace "least one" with "least volatile"

Page 7, line 11: should this say "more oxidized" rather than "less oxidized"?

Page 7, line 18: replace "same with that" as "same as that"

Page 8, line 19: replace "much more" with "higher concentrations"

Page 8, line 20: replace "is also very different" with "are also very different"

Page 9, line 18: replace "effects" with "affects"

Page 9, line 29: replace "reason of this" with "reason for this"

References:

Kirkby J; Duplissy J; Sengupta K; Frege C; Gordon H; Williamson C; Heinritzi M; Simon M; Yan C; Almeida J; Trostl J; Nieminen T; Ortega IK; Wagner R; Adamov A; Amorim A; Bernhammer AK; Bianchi F; Breitenlechner M; Brilke S; Chen X; Craven J; Dias A; Ehrhart S; Flagan RC; Franchin A; Fuchs C; Guida R; Hakala J; Hoyle CR; Jokinen T; Junninen H; Kangasluoma J; Kim J; Krapf M; Kurten A; Laaksonen A; Lehtipalo K; Makhmutov V; Mathot S; Molteni U; Onnela A; Perakyla O; Piel F; Petaja T; Praplan

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AP; Pringle K; Rap A; Richards NAD; Riipinen I; Rissanen MP; Rondo L; Sarnela N; Schobesberger S; Scott CE; Seinfeld JH; Sipilä M; Steiner G; Stozhkov Y; Stratmann F; Tomé A; Virtanen A; Vogel AL; Wagner AC; Wagner PE; Weingartner E; Wimmer D; Winkler PM; Ye P; Zhang X; Hansel A; Dommen J; Donahue NM; Worsnop DR; Baltensperger U; Kulmala M (2016) Ion-induced nucleation of pure biogenic particles, *Nature*, 533, pp.521-526. doi: 10.1038/nature17953

Pierce, J. R., Riipinen, I., Kulmala, M., Ehn, M., Petäjä, T., Junninen, H., Worsnop, D. R., and Donahue, N. M.: Quantification of the volatility of secondary organic compounds in ultrafine particles during nucleation events, *Atmos. Chem. Phys.*, 11, 9019-9036, doi: 10.5194/acp-11-9019-2011, 2011.

Riccobono F; Schobesberger S; Scott CE; Dommen J; Ortega IK; Rondo L; Almeida J; Amorim A; Bianchi F; Breitenlechner M; David A; Downard A; Dunne EM; Duplissy J; Ehrhart S; Flagan RC; Franchin A; Hansel A; Junninen H; Kajos M; Keskinen H; Kupc A; Kürten A; Kvashin AN; Laaksonen A; Lehtipalo K; Makhmutov V; Mathot S; Nieminen T; Onnela A; Petäjä T; Praplan AP; Santos FD; Schallhart S; Seinfeld JH; Sipilä M; Spracklen DV; Stozhkov Y; Stratmann F; Tomé A; Tsagkogeorgas G; Vaattovaara P; Viisanen Y; Vrtala A; Wagner PE; Weingartner E; Wex H; Wimmer D; Carslaw KS; Curtius J; Donahue NM; Kirkby J; Kulmala M; Worsnop DR; Baltensperger U (2014) Oxidation products of biogenic emissions contribute to nucleation of atmospheric particles, *Science*, 344, pp.717-721. doi: 10.1126/science.1243527

Tröstl J; Chuang WK; Gordon H; Heinritzi M; Yan C; Molteni U; Ahlm L; Frege C; Bianchi F; Wagner R; Simon M; Lehtipalo K; Williamson C; Craven JS; Duplissy J; Adamov A; Almeida J; Bernhammer A-K; Breitenlechner M; Brilke S; Dias A; Ehrhart S; Flagan RC; Franchin A; Fuchs C; Guida R; Gysel M; Hansel A; Hoyle CR; Jokinen T; Junninen H; Kangasluoma J; Keskinen H; Kim J; Krapf M; Kuerten A; Laaksonen A; Lawler M; Leiminger M; Mathot S; Moehler O; Nieminen T; Onnela A; Petäjä T; Piel FM; Miettinen P; Rissanen MP; Rondo L; Sarnela N; Schobesberger S; Sengupta K; Sipilä M; Smith JN; Steiner G; Tome A; Virtanen A; Wagner AC; Weingartner E; Wimmer D;

C5

Winkler PM; Ye P; Carslaw KS; Curtius J; Dommen J; Kirkby J; Kulmala M; Riipinen I; Worsnop DR; Donahue NM; Baltensperger U (2016) The role of low-volatility organic compounds in initial particle growth in the atmosphere, *Nature*, 533, pp.527-531. doi: 10.1038/nature18271

Interactive comment on *Geosci. Model Dev. Discuss.*, doi:10.5194/gmd-2016-171, 2016.