Atmospheric
Chemistry
and Physics
Discussions

Interactive comment on "RH-dependent organic aerosol thermodynamics via an efficient reduced-complexity model" *by* K. Gorkowski et al.

Anonymous Referee #1

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Gorkowski et al. developed a very useful model BAT that can treat the non-ideal mixing of organics and water and can predict the liquid-liquid phase separation, which is very important in SOA partitioning. The BAT model uses the measurable organic aerosol properties (oxidation state, molar mass and vapor pressure) as inputs and the simulated results agree with a comprehensive thermodynamic model AIOMFAC. The BAT model is successfully coupled with the VBS model predicting the gas-particle partitioning. The topic of this study is timely and highly relevant in improvement of thermodynamic aerosol treatment in chemical transport models. I recommend this manuscript for publication after the following comments can be addressed.

Major comments: My major concern goes to the method of Functional Group Translation: P12, Line 10-11: Can the "functional group translation" also treat the nitrogen-

or sulfur-bearing functional groups? P14, Line 8-10: I suggest adding a more detailed description to explain how to do "a distinct multifunctional translation". How the functional group translation is calculated for C97OOH in Fig.4(b)? The translated O:C ratio and molar mass can be added in Tables S5 and S6 in the supplement. P14, Line 22-25: Is Fig.4a based on the carboxy-based, ketone-based, etc parameterizations? The shaded grey area and the purple line in Fig. 4a are not explained in the main text. Please help me understand Fig.4a.

Minor comments: (1) P5, Line 21: It is not proper to describe Eq. (6) as the effective volatility of "all species". It is still the effective volatility of the compound j but includes water and inorganics in the absorbing phase. (2) P9, Line 9: Could the authors explain more how you get the scaling factor in the form of [s1(1+O:C)s2]? From Section 3.2 it seems s1 and s2 are fitted by the training dataset generated by the AIOMFAC model, instead of experimental data as you wrote here on Line 9. (3) P10, Line 31: The authors wrote "the light green domain starts at $\sim$ 20% of the O:C ratio reached at the miscibility limit and covers up to the blue domain", but from Table S1, it seems the light green domains starts from O:C of 0.05 and covers up to the O:C of 10% of the miscibility line? In the excel file, the mid O:C region is "0.05 < O:C < 0.1+ miscibility line", which is different from Table S1 (0:05 < O: C< 0.1 miscibility line). (4) P11, Line 8-10: Could the authors explain in a more detailed way how the equation (S14) is derived to calculate the limit of miscibility line? How you determined the O:C range of 0.05~0.45? (5) P11, Line 29: The sentence is correct but the (aw > xw) confuses me as from Fig.3, for the higher O:C region, the predicted aw is smaller than xw. (6) P12, Line 6-7: I couldn't see this result from Fig.3 and I don't quite understand the grey areas in Fig.3. Could the authors help explain it? (7) P14, Line 11: It is better to describe the Fig.4 from Fig.4(a) to (c). (8) Figure 6: Should ξ_j be ξ_{jguess} in the output of the VBS neural network? I also suggest add aw,sep in the program outline.

Technical corrections: (1) P2, Line 31: "remains" should be "remain". (2) P10, Line15: should be organic $\leftrightarrow$ organic interactions. The latter "organic" is missing. (3) P31, Line

1: There are two "the" at the beginning of the sentence.