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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.

Anonymous Referee #1

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General comments:

This paper presents a methodology (organic PD-FiTE) for calculating activity coefficients of organic compounds in aqueous mixtures. This method is more efficient than the ubiquitous UNIFAC model. Organic PD-FiTE is based on a methodology originally applied to inorganic compounds (PD-FiTE) in a publication by the same authors. While organic PD-FiTE could be very useful to atmospheric modeling, especially given the difficulty of thermodynamic predictions of organic mixtures, the manuscript itself contains some flaws. As detailed in "specific comments," I hesitate to recommend pub-

lication until thorough justifications for using (1) the Taylor Series expansion and (2) the chosen concentration scales are made for organic systems. There are also a large number of errors throughout the manuscript that require careful attention (addressed in "technical corrections").

Specific comments:

The work by Zaveri et al., 2005 (the MTEM model) is specific to aqueous inorganic electrolytes systems only. It is also specific to an ionic mole fraction concentration scale. The observation of linearity noted in the current manuscript (p1757, lines 10-13) was appropriately used by Topping et al., 2009 (the PD-FiTE model) for inorganic systems, but is inappropriately used here for organic systems. Before the PD-FiTE methodology is applied to organic systems (p1757, lines 23-25), proof of a linear dependence of the logarithm of the activity coefficient on some specific concentration scale is required.

p1759, lines 9-11: It is stated that "[f]or the organic model, binary activity coefficients and interaction are expressed as a function of water mole fraction." The "two-fold" reasons for the change from water activity (RH) to water mole fraction are both reasons of convenience. A mathematical or physical reason to justify the change from water activity (RH) to water mole fraction is required.

p.1760, line 17: It is stated that "[a]s the dry mole fraction of solute "B" approaches zero, the term . . . converges to zero." How would the reader know that the change of the log of the activity coefficient with respect to the concentration of the other species tends to zero as the concentration of the other species tends to zero? Justification is required here.

Technical corrections:

p 1756, line 15. "up to" not "upto".

Equation 2: The upper bound of the summation, 'N', has not be defined in the text. A sentence should be added to the text defining 'N' as the number of distinct compounds.

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p1758, line 5: The functional dependency on “(RH)” should be included (c.f. line 6 on the same page). Also, here and on p1760, line 14, “ln” should not be italicized.

p1758, line 7: “x”j” should be “x”i”, or “component i” should be “component j”.

Equation 3: Subscript “i’ should not be used both to define the species (LHS) and to index the summation (RHS).

Equation 4 & 5: Again, the upper bound of the summation, m, is not defined. Please correct.

Equations 6-9: It is not clear why the concentration notation changed from “equivalent mole fraction” (x”) in equation 1 to “associated mole fraction”, (x) in equations 6-9.

Equation 6: The dependency on RH should be made explicit (similar to the way the xw dependency is given in equation 7).

p1759, line 22: “water as the solvent 6 becomes” should be “water as the solvent, Eq. (6) becomes”.

Equation 9: The sum is over index ‘j’, however, there are no subscripts ‘j’. The summation is not needed.

p1760, line 4: “With” not “WIth”.

p1760, line 14: The partial derivative should be taken with respect to “xB” or “x’B”, not “B”.

p1760, line 21: The constant of differentiation should read “xw = c” not “xw”.

The LHS of eq. (14) and should not be in parentheses.

Equation (15): The polynomial order superscript should be on the dry mole fraction, not on the subscript.

p1762, line 2: lnfA(x’B,. . .xw) should read “lnfA(x’B, xw)”.

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p1762, line 11: the arguments of beta should not be subscripted.

p1763, line 24-25. The original ZSR paper is Zdanovskii's 1936 paper, not Zdanovskii's 1948 paper. Please correct the citation.

Equation (17): The argument of the mole fraction of water should not be subscripted.

p1764, line 12. In this line, eq. (B1) is referenced, but this is the same as eq. (13). At this point in the manuscript, it makes more sense to refer the reader back to an earlier equation, rather than forward to the appendix.

p1771, line 3: "Focused", not "Focus".

p1773, line 16: "Cloud", not "CLoud" (the "L" in VOCALS comes from the word "Land").

Figure 1: The caption and text say "x'B" (dry mole fraction of B), but the x-axis uses "XB" (the mole fraction of B). Please be consistent.

Figures 2-3: Although it is explained in the text, it is confusing to use 1, 3, and 4 in the captions and A and B in the figures. A note similar to that seen with Tables 6-7 would be helpful.

Figure 4: The caption refers to subscripts "b" and "t", but "b" and "t" are not actually subscripted in the figure. Please correct.

Figure 6: "RH)" instead of "RH))".

Interactive comment on Geosci. Model Dev. Discuss., 4, 1755, 2011.