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# *Interactive comment on* "Distribution of gaseous and particulate organic composition during dark $\alpha$-pinene ozonolysis" *by* M. Camredon et al.

**S. Compernolle**

steven.compernolle@aeronomie.be

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The authors use as standard vapor pressure estimation method the Myrdal & Yalkowsky (MY) method combined with the Joback-Reid (JR) method to estimate boiling points. With this method, combined with the MCM chemical mechanism, they obtain much better results than Jenkin who used the same chemical mechanism, but a different vapor pressure method: the modified MacKay method (mM) combined with the Stein-Brown (SB) method to estimate the boiling point. This could lead to the suggestion that (1) the SB-Mm is less performant than the JR-MY method and (2) the MCM performs quite well in predicting SOA, provided that a 'good' vapor pressure method is used.

I want to note that the JR method is known to predict significantly too high boiling points

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for the less volatile compounds, basically because the boiling point is calculated as a sum of group contributions. This assumption gets worse the higher the boiling point is. Stein and Brown introduced a correction for this, such that the boiling point increases less than linearly with the number of group contributions. Other authors (eg. Cordes and Rarey 2002) used other correcting formulas, but with the same goal. Eg. in Fig. 2 of Cordes and Rarey (2002) a comparison is made between the JR method, other methods and experimental boiling points, where the overestimation of the JR method is clear.

Too high boiling points will lead to too low vapor pressures, provided the method for calculating vapor pressures from boiling points is more or less reliable. Very recently, Barley and McFiggans (2009) did a critical assessment of several vapor pressure methods, by comparing them with experimental vapor pressures of low-volatile compounds (although not as low volatile as typically found in SOA). All the methods using the JR boiling point importantly underestimate the vapor pressure. The JR-MY method actually performs best among the methods using JR, maybe because the MY method tends to overestimate vapor pressures (Barley and McFiggans 2009), but it still performs worse than all non-JR methods tested by Barley and McFiggans (2009). As a logical consequence, the SOA formation tests performed by Barley and McFiggans (2009) gives important overpredictions for all the JR methods, including JR-MY. As the compounds found in SOA are generally of lower volatility than the compounds tested by Barley and McFiggans (2009), the overestimation by the JR method of Tb will even be higher, and the underestimation of the vapor pressure will be more important.

As far as I could track down the references, the method that Jenkin used (SB-mM) is not investigated by Barley and McFiggans (2009) but they did investigate a method that is very close. The (in their notation) SB-BV method, uses the same boiling point method (Stein-Brown) and the same vapor pressure equation, needing boiling point and vaporization entropy as input, the only difference being that Jenkin's vaporization entropy was predicted from boiling point by the Vetere 1986 method (Baum 1998),

while in the SB-BV method, the Vetere 1995 method was used (Poling 2001). The SB-BV method was found to have a bias of only -0.03 and a standard deviation of 1.05, while the JR-MY method has a bias of -0.58 and a standard deviation of 1.38. While the SB-BV method is not the best from the comparison made by Barley and McFiggans (2009), it is certainly better than the JR-MY method. As the SB-BV method is probably very close to the SB-mM method, it is plausible that the SB-Mm method performs significantly better than the JR-MY method.

The relatively good agreement between model and experiment found by the authors is then possibly a combination of (1) too low vapor pressures predicted by the JR-MY method and (2) too few low-volatile compounds predicted by the MCM. I would say that the authors should include a discussion on the reliability of the JR-MY method, with reference to Barley and McFiggans (2009).

Wilfried Cordes and Jürgen Rarey, Fluid Phase Equilibria, 201, 409-433, 2002 M. H. Barley and G. McFiggans, Atmos. Chem. Phys. Discuss., 9, 18375-18416, 2009

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