Response to the comments of Dr. Krieger:

Comment:

I enjoyed very much reading the interesting paper. However, I am missing a paragraph discussing and referring the readers to the problem that our knowledge of saturation pressures of low-volatility compounds are limited because of measurement challenges, e.g. Bilde et al. (2015). All estimation methods rely on training sets of well-established vapor pressures. Those are typically biased toward compounds with saturation vapor pressures in the range of 10^3 to 10^5 Pa. For partitioning we are however, mostly interested in compounds with saturation vapor pressures in the range of about 10^{-7} Pa to 1 Pa (O'Meara et al. 2014). Those with larger saturation pressure are entirely in the gas phase whereas those with lower saturation pressures will partition entirely into the aerosol. The authors state that the EPI Suite software is "...accepted as a good estimation method of volatility of organic compounds...". In panel (a) of the Fig. 1 I plot the estimated vapor pressures of the EPI Suite versus the experimental values taken from the PHYSPROP database that is part of the EPI Suite for the pressure range mentioned above. (Please also note, that these data are often just extrapolations from high temperature measurements.) In panel (b) the estimation error histogram is plotted. Clearly, there is a significant bias of the EPI estimation towards higher pressures even when comparing it with the training data set. Again, that is because for atmospheric applications we are interested in pressures below the majority of the pressures used in the training data set for the EPI suite. Hence, I recommend to the authors to use in Fig. 4 of their paper not (only) a comparison of their parametrization to another estimation method but (additional) also to the data available.

Responses:

We thank Dr. Krieger for the positive evaluation of our manuscript and the helpful comment. Based on your suggestions, we will compare the vapor pressure

estimated by our method with the PHYSPROP database (Fig. 4b). We will expand discussions in the revised manuscript as detailed below.

"Figure 4(b) shows the comparison between C_0 estimated by our parameterization and the experimental data. The experimental C_0 values of 1729 organic compounds with heteroatoms including N or S are taken from the PHYSPROP database that is part of the EPI Suite (http://esc.syrres.com/interkow/EpiSuiteData.htm). Our method gives a good performance with R of 0.84, MB of -0.41, and MAGE of 1.24. As shown in Fig. 4(b), the estimation error increases as the saturation mass concentration decreases. An accurate prediction of low vapor pressure is difficult due, in large part, to the limitation caused by measurement challenges. For example, the measured vapor pressure of dicarboxylic acid, a low-volatility compound commonly found in atmospheric aerosols, disagreed by up to two orders of magnitude between different measurement techniques (Krieger et al., 2012; Huisman et al., 2013; Bilde et al., 2015). The effects of functionalization, phase states (crystalline, amorphous, (subcooled) liquid), and molecular structure need to be considered in future experimental studies (Huisman et al., 2013; Bilde et al., 2015). The vapor pressure estimation methods could give very divergent predictions for the same compound (Clegg et al., 2008; O'Meara et al., 2014). Another difficulty in predicting low vapor pressure is that most estimation methods, including the EPI Suite, are constrained by databases heavily biased toward mono-functional compounds with saturation vapor pressures in the range of $\sim 10^3 - 10^5$ Pa (Barley and McFiggans, 2010; Krieger et al., 2012). The EPI Suite uses the PHYSPROP database as its training data set. When comparing with the PHYSPROP database, the estimation error of EPI Suite increases as the vapor pressure decreases, especially when the vapor pressure decreases below 10^{-4} Pa (http://www.epa.gov/sab/pdf/sab-07-011.pdf).

Despite of some limitations as described above, the new estimation parameterization derived from a large dataset in this study is sufficiently good to predict C_0 for various structural organic classes as shown by overall good correlation.

In the next section, the saturation mass concentration of ambient OA (e.g., the compounds with elemental composition measured by high-resolution mass spectrometry techniques) is estimated using Eq .(2)."
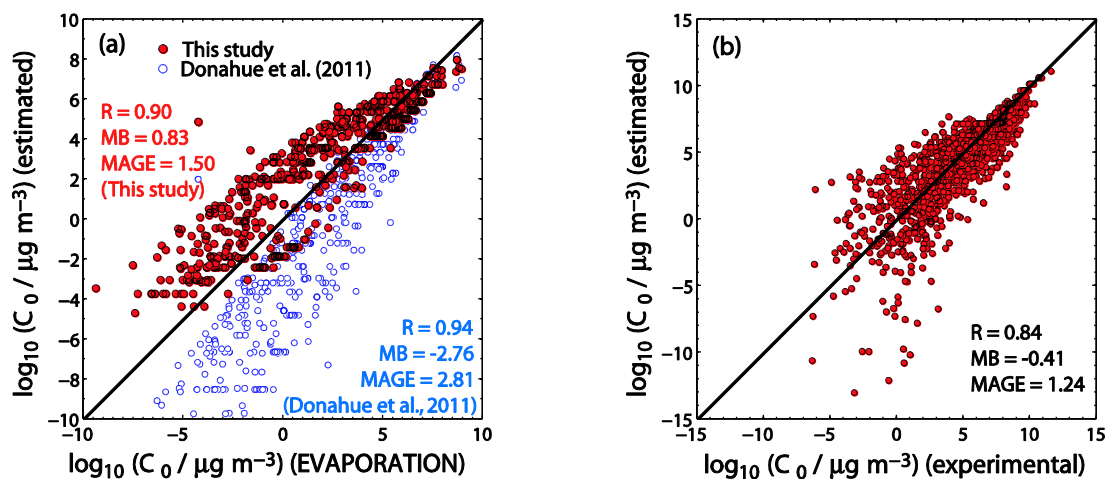

Figure 4. (a) Saturation mass concentration (C_0) of CHO compounds predicted by Eq. (2) with the coefficients from this study and with the coefficients from Donahue et al. (2011) plotted against C_0 computed by the EVAPORATION model (Compernolle et al., 2011). The data comprise 704 SOA oxidation products from biogenic (isoprene, α-pinene, limonene, glyoxal) and anthropogenic precursors (C12 alkanes) as presented in Shiraiwa et al. (2014). (b) Comparison of C_0 predicted by Eq. (2) in this study and experimental values taken from PHYSPROP database (http://esc.syrres.com/interkow/EpiSuiteData.htm).