

Interactive comment on “Molecular corridors and parameterizations of volatility in the evolution of organic aerosols” by Y. Li et al.

Anonymous Referee #1

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The authors have developed a new parameterization that predicts volatility of organic compounds containing oxygen, nitrogen and sulfur from the elemental composition that can be measured by soft-ionization high-resolution mass spectrometry. The parameterization is based on data from over 30,000 compounds taken from the National Cancer Institute (NCI) open database whose volatility was estimated by the US EPA's Estimation Programs Interface (EPI) Suite software. The newly developed parameterization is then used to predict volatility of 9053 organic compounds that were observed in various laboratory and field studies. The manuscript is well written and suitable for publication in ACP after addressing the following comments.

Comments

1) There is some confusion in the way the term “volatility” is used in this manuscript.

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Both EPI suite software and EVAPORATION model predict saturation vapor pressure, which depends only on the given chemical compound and temperature. On the other hand, the term “volatility” is now routinely defined in atmospheric organic aerosol literature as effective saturation vapor pressure, which is saturation vapor pressure multiplied by activity coefficient. The activity coefficient is often not known, but it depends on temperature and which other compounds (and their relative amounts) are mixed with the compound of interest.

While the authors have actually developed the parameterization for predicting saturation vapor pressures, the confusion arises by referring to it as volatility and discussing the term in the context of literature on various volatility basis set (VBS) frameworks that have been developed in the recent years (text on page 27879). The authors also state on line 26 on page 27879: “Volatility is a consequence of molecular characteristics of molar mass and chemical composition and structure,” which refers to “effective saturation vapor pressure” not “saturation vapor pressure.”

I suggest the authors replace “volatility” with “saturation vapor pressure” throughout the manuscript (including the title), except where the term “volatility” actually refers to “effective saturation vapor pressure.” The authors should also clearly define these two terms early in the manuscript to avoid any confusion.

2) Since the saturation vapor pressure for a given compound depends on temperature, please state the temperature at which the parameterization was developed. And so that it can be of practical use, please comment on how the parameterization might change with temperature.

Editorial comments:

Figure 1(c) legend: Please change to “tetary amine” to “tertiary amine”.

Figure 1(d) legend: Please change the first letter of the chemicals to small case.

In Figure 1, X-axis is volatility and Y-axis is molar mass. In Figures 5-9 the X and

Y axes are reversed. Please revise so that all figures have the same X and Y axes.
Figure 3 X-axis label: Please change “EPI suit” to “EPI suite”.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 27877, 2015.

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