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Atmospheric Chemistry and Physics Discussions

Interactive comment on "SIMPOL.1: A simple group contribution method for predicting vapor pressures and enthalpies of vaporization of multifunctional organic compounds" *by* J. F. Pankow and W. E. Asher

Anonymous Referee #2

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General Comments:

This paper describes the development of a simple group contribution method for calculating the vapor pressures and heats of vaporization of oxidized organic compounds that have the potential to form secondary organic aerosol (SOA). The method is based on the premise that the effects of functional groups on vapor pressure are multiplicative and independent of their location in a molecule and the presence of other groups (higher order terms to correct for these effects are not included, in order to maintain a level of simplicity appropriate for the available knowledge of atmospheric aerosol

composition and because a sufficient database is not available). This approach allows vapor pressure to be estimated for a particular structure by multiplying factors characteristic of the functional groups and the number of times they appear in the structure. When presented in log form, this becomes a summation of terms. The values of the factors for groups present in atmospheric aerosol have been determined in this study by fitting a large literature database of measured vapor pressures of mono- and multifunctional compounds to the vapor pressure and heat of formation (i.e., temperature dependent vapor pressure) equations. The agreement between the values obtained by calculations and the original data are then evaluated and the factors optimized.

There is not much I can say about the technical aspects of the paper, since it primarily consists of a description of the theory and fitting procedures. The theory is straightforward and intuitively sensible, and I assume the computations were carried out correctly. The comparison of the results with the original data looks good, and suggests that the parameter values should work reasonably well for the wide array of complex compounds that are found in aerosol particles. There have been a number of previous attempts to use a similar approach for studies of gas-particle partitioning, but they were much more limited in scale. I think this paper will become a highly cited reference in the aerosol field, and, given the time and effort required for this endeavor, it is unlikely that anyone will attempt to improve on the approach presented here.

The paper is written very well, it is clear and concise, and the figures, tables, and references are appropriate. I highly recommend the paper for publication in Atmospheric Chemistry and Physics. I have just a few other minor comments.

Specific Comments:

1. It would probably be worthwhile to mention in the conclusions that besides the inherent uncertainties in the vapor pressures estimated using this method, gas-particle partitioning is also affected by the activity coefficient of the compound in a particular matrix. If, based on their own experience or the literature, the authors have additional

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comments on the order of magnitude expected for activity coefficients and their uncertainty, this would also be helpful in allowing readers to determine how much confidence they might place in gas-particle partitioning calculations.

Technical Comments:

1. Page 11846, first paragraph: Since logP decreases by ˜ -0.5 for each carbon number, P decreases by ˜1/3 of an order of magnitude (i.e., a factor of ˜3). This is much different than 1/2 of an order of magnitude when applied to a long carbon chain. This relation is one that is easy to remember (as a rule of thumb), so the value should be stated accurately.

2. Table 6, superscript d: This should be primary, secondary, and tertiary nitrate group, not nitro group.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 11839, 2007.