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Interactive Comment

Interactive comment on "A group contribution method for estimating the vapour pressures of α -pinene oxidation products" by M. Capouet and J. F. Müller

Anonymous Referee #2

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General comments

The paper describes an estimation method for the determination of vapour pressures of multifunctional organic compounds, which are formed by the oxidation of alpha-pinene in the atmosphere. The oxidation products of this monoterpene are also representative for the reaction products of other monoterpenes and sesquiterpenes. The vapour pressure is a crucial parameter for gas-particle partitioning prediction. In case of semi- and non-volatile biogenic compounds, the vapour pressure has been experimentally determined only for a few compounds and usually a UNIFAC method is used for the pre-



diction. Especially for multifunctional compounds with low volatility this method tends to overestimate the vapour pressure. Capouet and Müller have developed another method based on group contribution principles, taking also the effect of different carbon structures into account, not solely the additive effects of functional groups. The estimated vapour pressures of their method show better agreement with experimental values than the UNIFAC method. I recommend the publication in APCD with some minor revisions given below.

Specific comments

Page 11250, line 4/5: and throughout the text: hydroperoxide (the compound) should be replaced by hydroperoxy (the functional group).

Page 11250, line 5: and throughout the text: the term "acid" should be replaced by "carboxylic acid" or by the proper expression "carboxy" for the functional group.

Page 11256, line 17: and throughout the text "alkanoic compound" should be replaced by "hydrocarbon" or "alkane".

Page 11261, line 27: "carboxylic diacids" should be replaced by "dicarboxylic acids".

Page 11273, Fig. 2: The pinic acid parent compound has one carbon atom too much.

Technical corrections

Page 11251, line 22/23: ...several oxygenated groups among the carbonyl... should be written: ...several oxygenated groups among them carbonyl...

Page 11254, line 24: Bilde et al. (2003) has shown... should be replaced by Bilde et al. (2003) have shown...

Page 11257, line 26: remove "the" from ...whose the structure is shown...

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 11249, 2005.

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