Atmos. Chem. Phys. Discuss.,
doi:10.5194/acp-2016-68-RC1, 2016

Atmospheric Chemistry and Physics
Discussions

Interactive comment on "Evaluation of gas-particle partitioning in a regional air quality model for organic pollutants" *by* C. I. Efstathiou et al.

Anonymous Referee #1

Received and published: 21 March 2016

This manuscript presents an evaluation of alternative gas-particle partitioning schemes in a modified version of the WRF-CMAQ model run for Benzo-a-pyrene (BaP). The authors compare modeled BaP concentrations within a European model domain under 5 different gas-particle partitioning schemes and also compare model results to measurement data from EMEP monitoring sites.

The novel aspect of this work seems to be announcing that the different gas-particle partitioning schemes have been incorporated into CMAQ. The more complicated schemes apparently provide the best model performance relative to measurement data, but the authors state that the disagreements between measurements and the model are likely mostly attributable to uncertainties in emission estimates. Therefore it is difficult to draw conclusions about which partitioning scheme is best based just on results reported in this paper.

I have two scientific concerns about the paper. I think both are significant, but possibly #1 arises from unclear presentation in the paper.

1) I understand Table 2 and the text to say that Scenarios 3, 4 and 5 include both the Junge-Pankow adsorption model *and* the Harner-Bidleman Koa absorption model. Is that correct? If so, I think the model is perhaps adding two redundant descriptions of gas-particle partitioning.

It has been a while since I looked at the JP model, but my recollection is that it includes a fitting parameter that was derived from empirical data under the assumption that all partitioning was by adsorption to aerosol surfaces. But, the assumption that adsorption dominates could not be confirmed. Xiao and Wania (http://www.sciencedirect.com/science/article/pii/S1352231003002139) later showed that vapor pressure and Koa both describe sorption to organic matter equally well. Therefore, I think partitioning schemes that include both vapor pressure and Koa as chemical parameters are likely including redundant information, and could easily be over-fitted.

2) The authors state that soot-air partition coefficients were calculated as the ratio of soot-water adsorption constants (Ksw) and the Henry's Law constant. Kai Goss has pointed out that applying a thermodynamic triangle for a solid interface in contact with water and the same solid interface in contact with an adjacent gaseous phase is a conceptual mistake that can lead to very large errors (http://pubs.acs.org/doi/abs/10.1021/es0301370).

I actually do not see a good option for the authors to overcome this problem, since the Lohmann & Lammel (2004) and the Dachs & Eisenreich (2000) papers that are the basis for the gas-particle partitioning scheme applied in this paper are both based on thermodynamic triangles that Goss argues (convincingly!) are invalid.

Interactive comment on Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2016-68, 2016.