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 #2

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General comments

The manuscript describes the application of community air quality model CMAQ to study atmospheric transport of B(a)P and effects of gas-particle partitioning and degradation. Several gas-particle partitioning models were implemented in the CMAQ model extending its capabilities with respect to modeling of PAHs. Though the subject of the study is of importance with regard to existing air quality problems in Europe, description of this study suffers from obscurity and thus requires substantial revisions.

First of all, I would mention not clear enough description of parameters applied in the equations 10 and 11, related to gas-particle partitioning (e.g. KOA, KSA). Secondly, evaluation of the effects of several GPP mechanisms through their incremental testing (incremental testing is defined in section 3.2 and Table 2) is not quite clearly described

with regard to sensitivity of CMAQ model output to particular partitioning mechanisms in model simulation scenarios. In some cases abbreviations, defined for GPP models and scenarios and used throughout the analysis, are mixed like e.g. DE model and DE scenario. This leads to problems with understanding what is presented, for example, in the second column of tables 4 and S8 called 'Model'. There are both abbreviations for scenarios and models (for example, JP-W and DE, HB, etc.). Finally, the underestimation of observed B(a)P concentrations in air is explained by low emissions. At the same time, there is no discussion of potential problems of emission data used, no comparison of total annual emissions with other studies, for example, with similar studies e.g. Aulinger et al. (2007) and others.

Specific comments

Page 3, line 12-13: "CMAQ contains modules representing advection, eddy diffusion, in-cloud, and precipitation processes". It would be better to use 'in cloud and below-cloud scavenging with precipitation'.

Page 3, line 26: 'gas phase reactions' instead of 'gas reactions'.

Page 4, line 23: Though the equation 2 follows the publication of Aulinger et al. (2007), it is not clear how the particulate fractions in each mode i, fi, are obtained, because in the cited work (Cooter and Hutzell, 2002) similar equation is written for the sum of partition coefficients, but not for fractions of a compound in particulate phase.

Page 5, equation 7: fOM is used without index i. Does it mean that the fraction of organic matter in aerosol particles is the same in each of three modes?

Page 6, line 3: assumptions used here for ratio of activity coefficients and ratio of mean molar weights of organic matter of the particles and octanol (that they are equal unity) need to be discussed with regard to their uncertainties as it was shown in e.g. (doi: 10.5194/acpd-14-21341-2014).

Page 6, line 14-15: Soot-air partition coefficients were calculated as the ratio of soot-

water adsorption constants KSW and the inverse Henry's Law constant (HâĂŠ), with KSA values adopted from Bärring et al. (2002). Concerning the way of deriving the KSA it would be important to provide estimates of uncertainties that would be introduced by this assumption. Moreover, it is unclear how this adopting was performed for B(a)P since the publication of Bärring et al. (2002) was focused on experimental determination of the soot–water distribution coefficients for PCDDs, PCDFs, and PBDEs.

Page 6, line 16: There would be a need to describe more clearly these two parameterizations for KOA (e.g. to give equations, to show difference).

Page 10, line 6: It would be better to provide the difference (relative or absolute) between the maps in Figures 2a and 2b instead of direct comparison.

Page 21, Table 1: it is not shown from where the values for Ksoot-water, Ksoot-air, and OH reaction rate were taken.

Page 22, table 2: Table 2 does not correspond to its description in section 3.2 for 4th and 5th scenarios.

Page 27, figure 3: Please, correct the abbreviations JB-W and DL, as they were not defined earlier. The same for figure S5. Concerning the maps, it would better to show the difference between them in relative units.

Table 4 and Table S8 do not present mean modeled and observed B(a)P concentrations. In the column 'Model' both abbreviations for scenarios and for GPP models are used (for example, JP-W and DE, HB, etc.). Please, provide equations or references for IOA etc.