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Discussions

Interactive comment on "Prediction of gas/particle partitioning of polybrominated diphenyl ethers (PBDEs) in global air: a theoretical study" *by* Y.-F. Li et al.

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(1)comments from Referees

Interactive comment on "Prediction of gas/particle partitioning of polybrominated diphenyl ethers (PBDEs) in global air: a theoretical study" by Y.-F. Li et al.

Anonymous Referee #2 Received and published: 15 October 2014

A steady-state model is developed in this study to model gas/particle participation of PBDEs in air. In addition to the chemical transfer from gas to particles, the competing dry and wet depositions of particles are taken into account in quantifying gas/particle

participation. The study concludes that the equilibrium state is a special case of the steady state when particle depositions are negligible relative to gaseous transfer. The steady-state model shows better performance in fitting field measurements than the equilibrium model published previously. The authors present a list of equations to substantiate the development of the steady-state model. The findings are novel and could be applied to model environmental behaviour and fate of PBDEs. The manuscript is recommended for publication in ACP.

1.Line 5 on page 23418, defining Kpm is not really necessary since this parameter is not used in any equations. The readers can be easily confused by so many newly defined parameters such as Kpr, Kpe or Kpp.

2.Line 25-28 on page 23418, fOM is not a constant and it varies significantly from one site to another, similar to TSP. As such, fOM needs to be monitored as well in real environment.

3.Line 12 on page 23420, the parameters A and B in Eq. (8) vary among different PBDE congeners. Consider deriving another equation of logKpp(t), similar to Eq. (8), since ambient temperature is more readily available than logKoa, and can thus be readily used by modellers.

4.Line 16-18 on page 23441, consider re-wording this sentence.

5.Line 25 on page 23424, it appears arbitrary to introduce the constant C in Eq. (21). What is the physical meaning of C? How could this parameter be subjectively changed from 5 to 50 at Waliguan site? A bit more explanation and justification is needed here for the constant C.

6. Typos: (1). Line 4 on page 23416, replace 'routs' with 'routes'. (2). Line 2 and 4 on page 23419, consider replacing 'Eq. (3)' with 'Eq. (2)'. (3). Line 21 on page 23419, replace'are" with 'is'. (4). Line 4-7 on page 23440, consider replacing 'steady' with 'steady state'. (5). Line 12 on page 23441, replace 'planed' with 'planned'.

(2)author's response and (3) author's changes in manuscript

General

We thank the Referee #2 for his remark on the novelty of our paper, the support to publish this paper in ACP, and also the comments on the weak points and errors made in the paper. We response these comments in the following.

1. In this paper, many new parameters of KP, including KPM, KPR, KPE, and KPS, have been defined for establishing the steady-state model for G/P partitioning study. KPM is directly calculated using the monitoring data. Although KPM has not been used in any equation in the paper, but it is used to derive Eq. (2) and also in Figures 5, S11, S13, and S15.

2. In our study, the value of fOM was assumed as 0.1 as suggested by Mackay 2001. Although the real values of fOM at sampling sites were most likely different from 0.1, but this did not affect the application of the steady-state equations, as discussed in Section "4.5 The limitation of application". Actually we did the sensitivity analysis for parameter fOM, and it was found that the final results are not sensitive to the variation of the parameter fOM. In the future, however, we will try to monitor the values of fOM.

3. We derived the equation to calculate logKpp(t) in our previous paper (Li and Jia, 2014), which has the form $logKPP(t) = (0.011A–0.135)t–2.74B/(t+273) +0.263A+0.011B–5.006$

Reference: Li Y. F. and Jia, H. L.: Prediction of Gas/Particle Partition Quotients of Polybrominated Diphenyl Ethers (PBDEs) in north temperate zone air: An empirical approach, Ecotoxic. Environ. Safety, 108, 65-71, 2014.

4. "As equilibrium is an idealized scenario not presenting in real environment, the steady state discussed here is also an ideal one, since only dry and wet depositions were discussed." has been changed to "It should be borne in mind that the steady state discussed here is an idealized scenario since only dry and wet depositions were

discussed in the study, other factors, such as humidity and artifacts, will also play roles to a certain extent to affect the G/P partitioning."

5. "The value of C will be determined later" has been changed to "Thus the term CBa is the chemical's molecular diffusivity for the particle film in air, and the value of C will be determined later". More discussions on C can be found in the section "4.5 The limitation of applications".

6. All typos except Typo (2) have been corrected. For Typo (2), we didn't make the replacement, because Eq. (3) is right.

Interactive comment on Atmos. Chem. Phys. Discuss., 14, 23415, 2014.