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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.

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 #1

Received and published: 2 December 2014

Review of Li et al. on PBDEs in air

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Interactive Discussion

Discussion Paper

This paper builds on a recent publication by the authors cited on line 717. That publication provides a comprehensive set of data (700 pairs) on partitioning of PBDEs between gas (G) and particle (P) (aerosol) phases, mainly in China and over a wide range in temperature (-22 to 38 deg C). They test the dependence of the P/G partition coefficient Kp on the octanol-air partition coefficient Koa. The important conclusion is that equilibrium appears to apply at log Koa up to about 10 then Kp tends to level off and becomes constant at log Koa above about 12. This is novel and important information. They develop several empirical regression equations. They claim that the constant Kp regime is due to "saturation". I have a problem with their use of that word. To me, saturation implies an equilibrium state between two phases or, if one of the phases is a pure substance, a solubility limit. Clearly conditions are far from equilibrium or saturation. They recognize that in the intermediate regime conditions are "non equilibrium" but steady state. In my opinion there is an equilibrium region, a steady state region and between them lies a transition region.

The introduction is essentially a restatement of the work in the first paper. I find their derivation and discussion very long and convoluted and difficult to understand. This is not helped by reference to extensive Supplementary information with 18 figures.

They cite a paper by Rissler et al. On the kinetics of G - P trransfer. I would have expected other citations especially to the texts by Seinfeld & Pandis and Finlayson Pitts and Pitts.

I believe that a much shorter, higher impact and more understandable paper could be written that would do better justice to their excellent empirical studies. My suggestion is major revision.

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

This Review is the same as the one made by Anonymous Referee #1 under the initial manuscript evaluation before the paper was accepted for publication on the Atmospheric Chemistry and Physics Discussions (ACPD) website. We have re-

sponded these comments and some of their suggestions have been taken to revise our manuscript published on the ACPD website already, as shown below.

This paper builds on a recent publication by the authors cited on line 717. That publication provides a comprehensive set of data (700 pairs) on partitioning of PBDEs between gas (G) and particle (P) (aerosol) phases, mainly in China and over a wide range in temperature (-22 to 38 deg C). They test the dependence of the P/G partition coefficient Kp on the octanol-air partition coefficient Koa . The important conclusion is that equilibrium appears to apply at log Koa up to about 10 then Kp tends to level off and becomes constant at log Koa above about 12. This is novel and important information. They develop several empirical regression equations. They claim that the constant Kp regime is due to "saturation". I have a problem with their use of that word. To me, saturation implies an equilibrium state between two phases or, if one of the phases is a pure substance, a solubility limit. Clearly conditions are far from equilibrium or saturation.

RE: Agree! The term "saturation (SA)" was changed to "maximum partition (MP)" in the revised manuscript.

They recognize that in the intermediate regime conditions are "non equilibrium" but steady state. In my opinion there is an equilibrium region, a steady state region and between them lies a transition region.

RE: We do not agree. "Transition region" means the region is neither equilibrium nor steady state. Actually all the three regions (equilibrium, non-equilibrium, and the maximum partition region) are steady state, since all of them are solutions of the steady equation (9) (NG-P = NP-G + NP-S).

The introduction is essentially a restatement of the work in the first paper. I find their derivation and discussion very long and convoluted and difficult to understand. This is not helped by reference to extensive Supplementary information with 18 figures.

RE: The introduction presents the development of the study on gas-particle partitioning behavior for SVOC. Each equation (from (1) to (8)) represents a step forward in the development, which is important to lead the objectives of our present study.

They cite a paper by Rissler et al. On the kinetics of G - P trransfer. I would have expected other citations especially to the texts by Seinfeld & Pandis and Finlayson Pitts and Pitts.

RE: We cite the paper by Rissler et al. only for the mean diameter of 0.1 m for aerosols.

I believe that a much shorter, higher impact and more understandable paper could be written that would do better justice to their excellent empirical studies. My suggestion is major revision.

RE: Both the paper and the Supplementary were shortened.

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

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Interactive Discussion

Discussion Paper