

## ***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

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  $K_p$  on the octanol-air partition coefficient  $K_{oa}$ . The important conclusion is that equilibrium appears to apply at  $\log K_{oa}$  up to about 10 then  $K_p$  tends to level off and becomes constant at  $\log K_{oa}$  above about 12. This is novel and important information. They develop several empirical regression equations. They claim that the

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constant  $K_p$  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 transfer. 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.

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

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