

The major pathway for BDE-209 entering the Arctic air

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Contents

- Introduction
- The current point of view
- Our point of view
- Conclusions



Contents

- **Introduction**
- G-P partition Quotients for BDE-209
- BDE-209: Long-range transport
- Conclusions

Introduction:



The major pathways for POPs to enter the Arctic :

- ◆ **LRAT**: represented by α -HCH (MacDonald et al. 2002, Li et al., 1998, 2004; Li and Bidleman, 2003, Li and MacDonald, 2005)
- ◆ **LROT**: represented by β -HCH (Li et al. 2002, Li and MacDonald, 2005)



Introduction

How does BDE-209 enter the Arctic air?

LRAT

Is its gas phase or particle phase?

To answer this question, we need to understand the gas/particle partition.



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- Introduction: The question
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Models to predict G/P for SVOCs

- **Junge-Pankow model** (Junge, 1977; Pankow, 1987)

$$\varphi = c\theta/(P_L + c\theta)$$

**All these models predicted that BDE-209
in air is entirely sorbed to particles.**

- **Harner-Bidleman model** (Harner and Bidleman, 1998)

$$\log K_{PE} = \log K_{OA} + \log f_{OM} - 11.91$$

Current View

Previous view :

- ◆ BDE-209 is entirely sorbed in particles
- ◆ BDE-209 can only be found in source areas



Monitoring:

- BDE-209 was found in
- ◆ Remote areas
 - ◆ Arctic



Explanation:

it is particulate BDE-209 that enters Arctic through LRAT.



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Predicting Equation

Steady-state model

Atmos. Chem. Phys., 15, 1669–1681, 2015
www.atmos-chem-phys.net/15/1669/2015/
doi:10.5194/acp-15-1669-2015
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Prediction of gas/particle partitioning of polybrominated diphenyl ethers (PBDEs) in global air: A theoretical study

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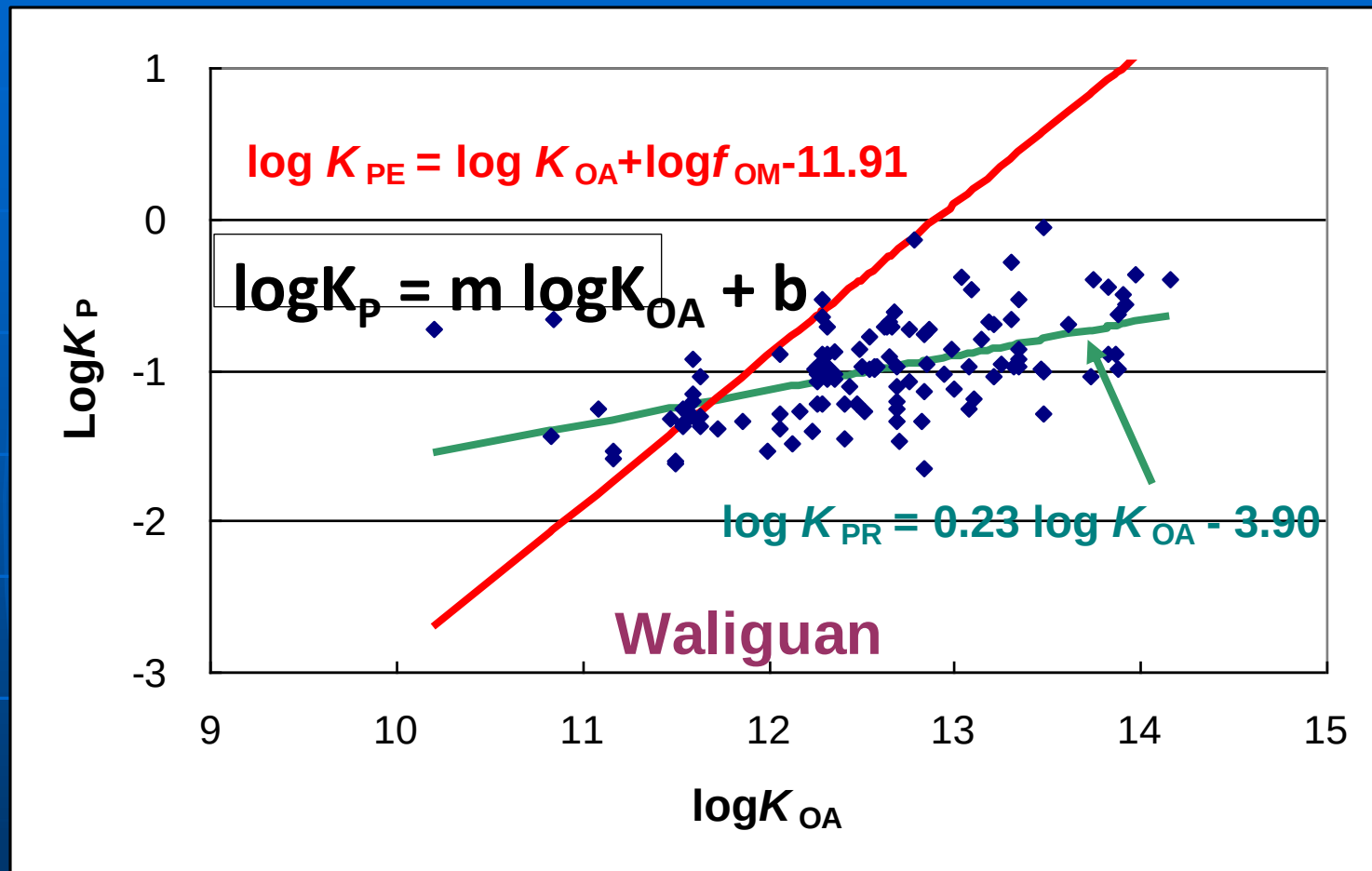
³IJRC-PTS-NA, Toronto, Ontario M2N 6X9, Canada



Equations at steady state: **Important predictions**

1. The threshold values predict the equilibrium or nonequilibrium states ($\log K_{OA1,2}$ vs. the values of m (Slope))
 - For the first time, we have the threshold values of $\log K_{OA1,2}$ to classify the equilibrium or nonequilibrium states for PBDEs, or other SVOCs in future

Introduction: The slope m



The regression model ($\log K_{PR}$) needs monitoring data to calculate the parameters m_o (0.23) and b_o (-3.90)

Yang et al. 2013



Equations at steady state: **Important predictions**

- 1.
2. The relationship between $\log K_p$ and $\log K_{OA}$ (and $\log P_L$) are not linear



Equations at steady state: **Important predictions**

- 1.
- 2.
3. **The existence of the maximum domain for PBDEs in which $\log K_p = -1.53$**

Prediction by Steady-State Model for PBDEs

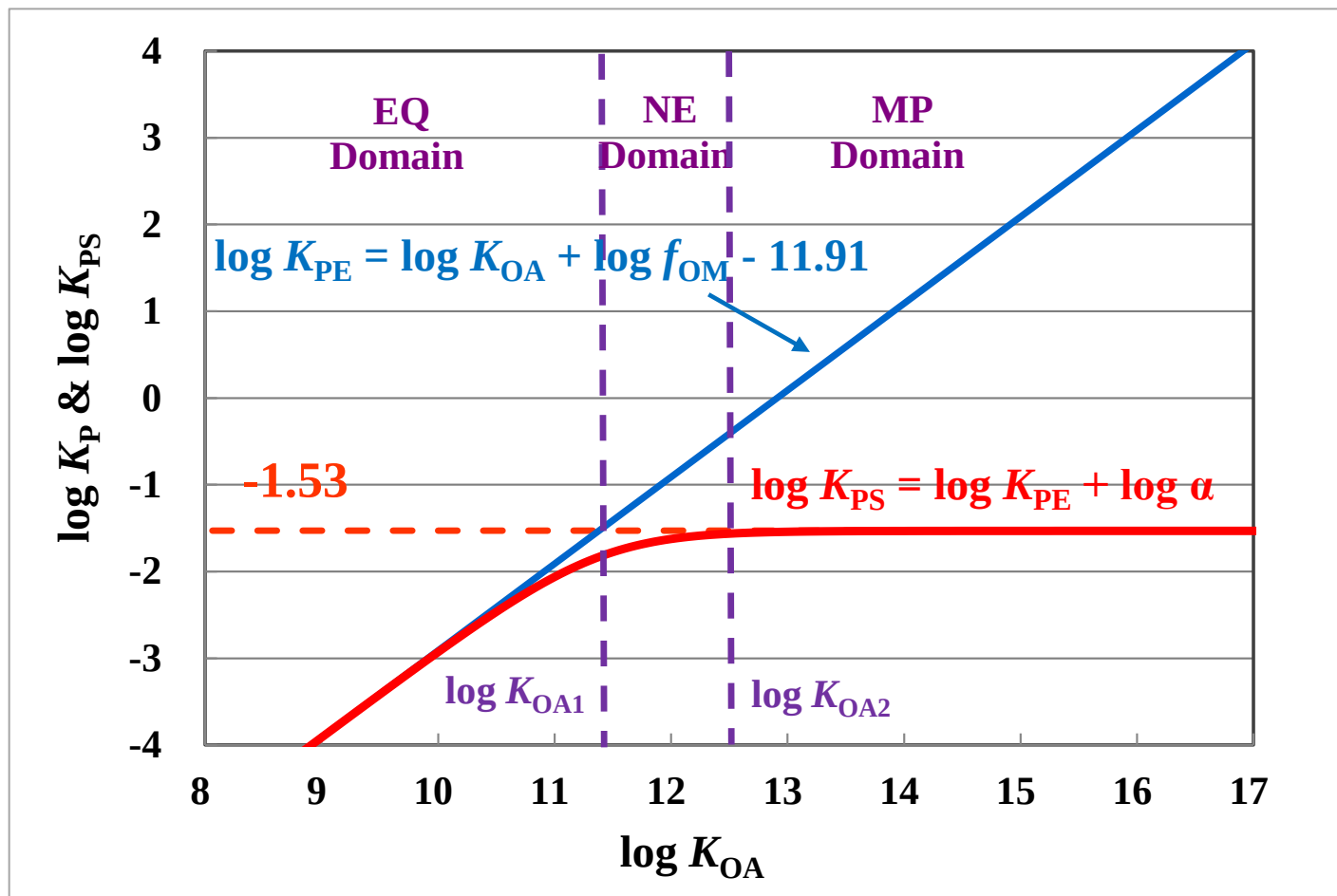


Figure 1. The G/P partition coefficients of PBDEs as functions of $\log K_{OA}$ calculated by two equations.
(Li et al., 2015)



Equations at steady state: Threshold Values

$\log K_{OA}$ range

- $\log K_{OA1}=11.4$: The first threshold value, separating equilibrium (**EQ**) and nonequilibrium (**NE**) domains
- $\log K_{OA2}=12.5$: The second threshold value, the start of the maximum partition (**MP**) domain

Li et al, 2015

Prediction by Steady-state Model for PBDEs

Important predictions:

- The existence of MP domain is the most important prediction by the Steady-state Model



(Li et al., 2015)



Equations at steady state: **Threshold Values**

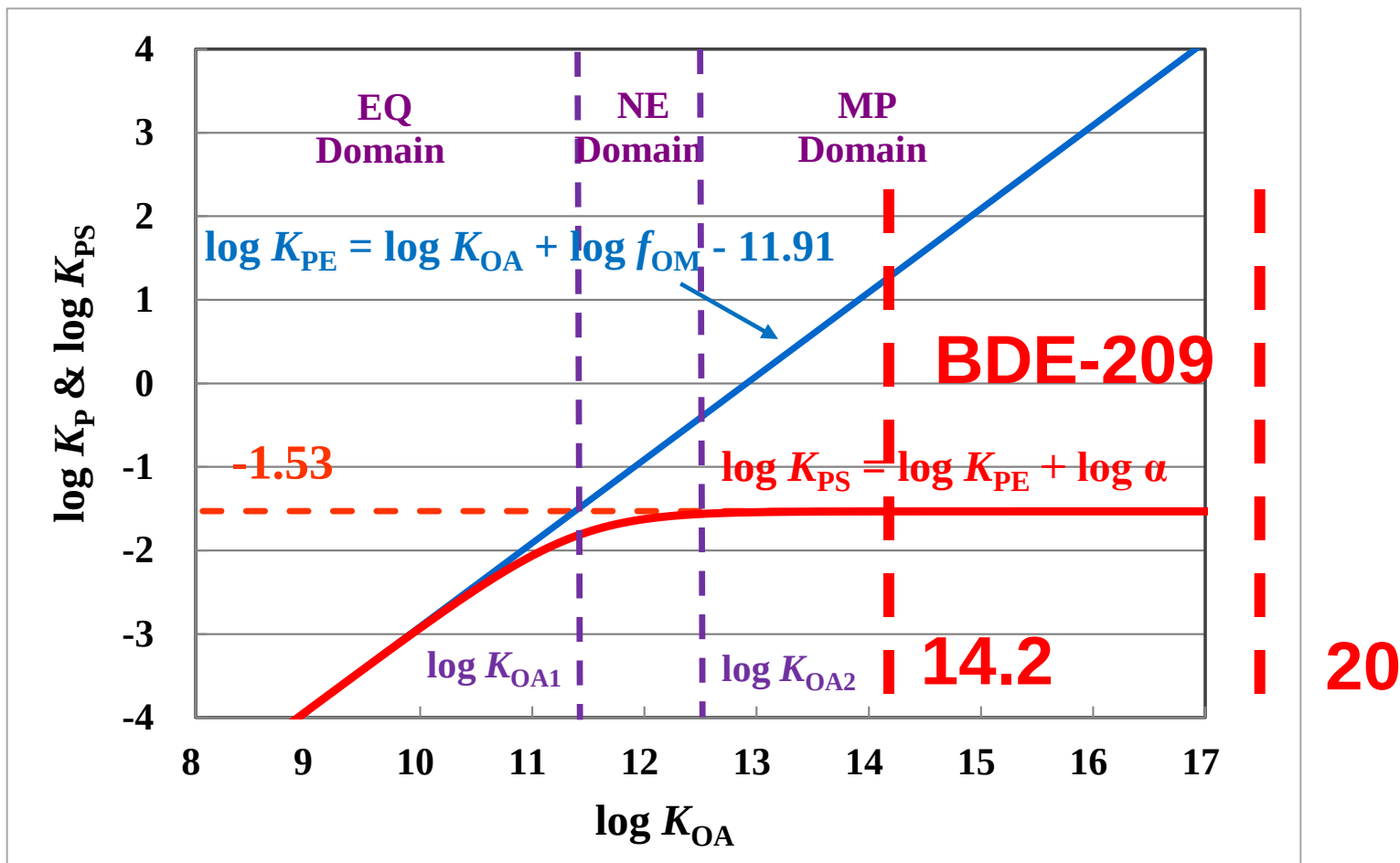
For BDE-209

$$\begin{aligned}\text{Log } K_{OA} &= 14.2 && \text{at } +50^{\circ}\text{C} \\ &= 20.0 && \text{at } -50^{\circ}\text{C}\end{aligned}$$

$$\text{Both} > \log K_{OA2} = 12.5$$

Li et al, 2015

Prediction by Steady-state model for PBDEs



The G/P partition coefficients of PBDEs as functions of $\log K_{OA}$ calculated by two equations.

(Li et al., 2015)

We predict



The logarithm of partition quotient ($\log K_p$) of BDE-209 is a constant (-1.53) at any ambient temperature and at any sampling sites.

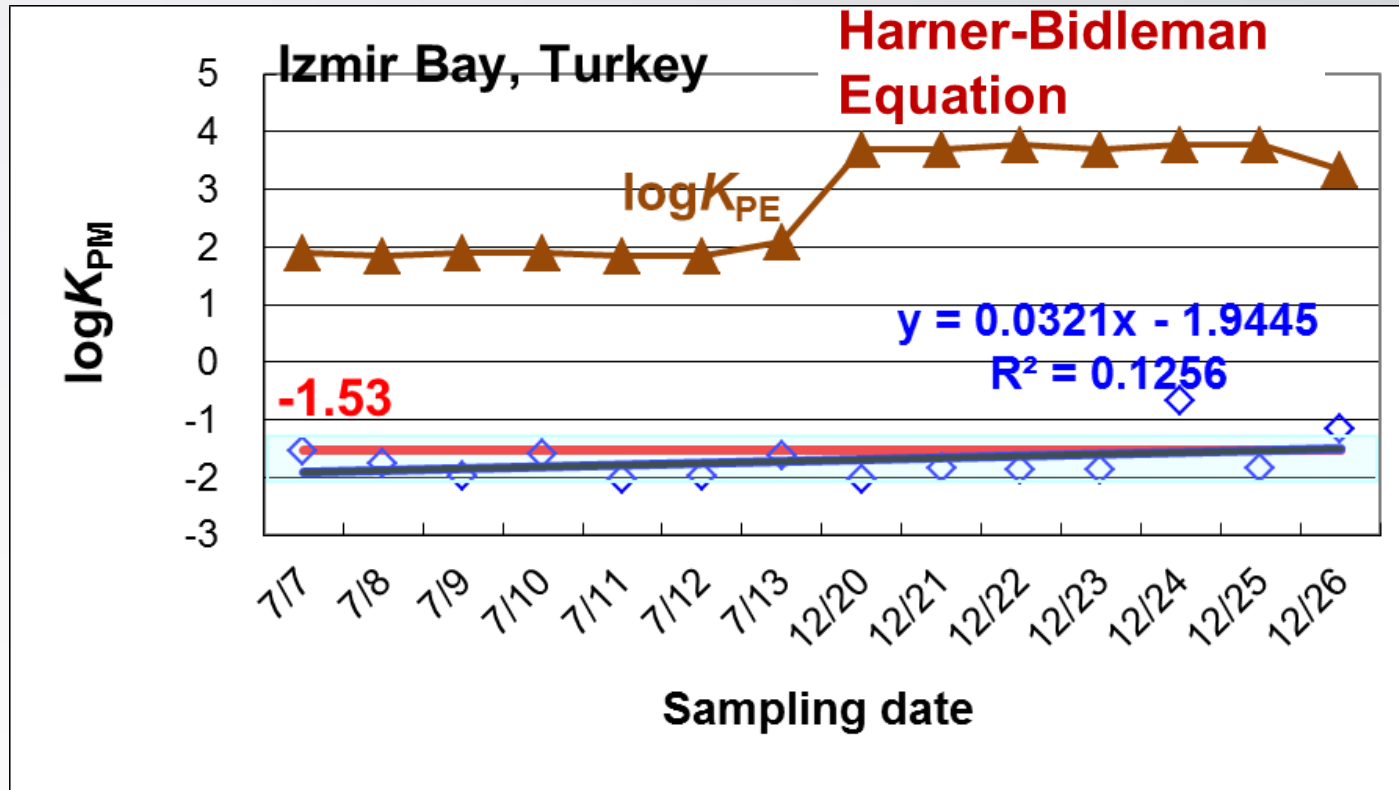
(Li et al., 2017)

C/P partition quotient



Monitoring data

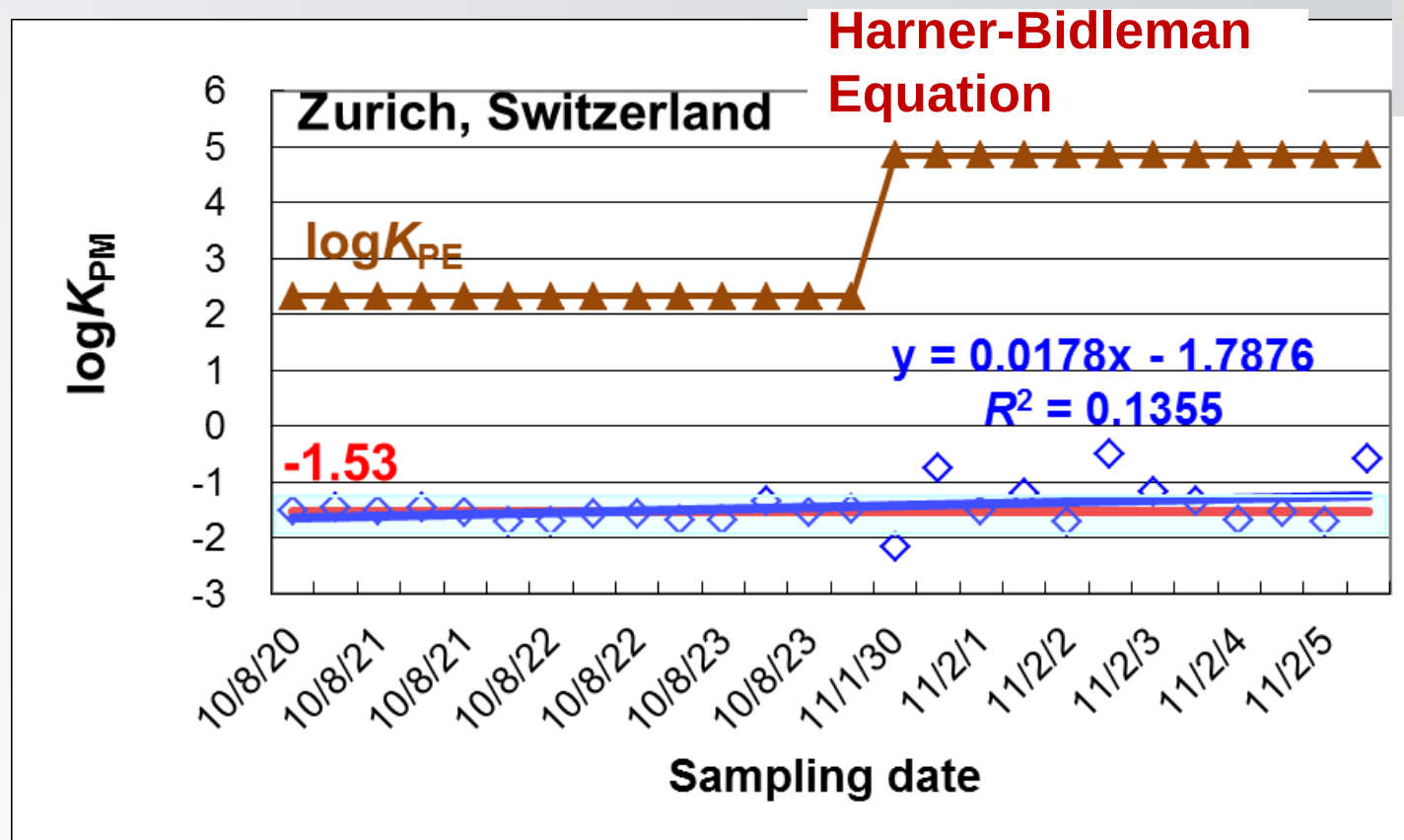
Izmir Bay, Turkey



The values of $\log K_p$ of BDE-209 versus sampling date in Izmir Bay, Turkey in 2005. Assuming that the values of TSP at the site were $30 \mu\text{g}/\text{m}^3$ in summer and $50 \mu\text{g}/\text{m}^3$ in winter.

Cetin and Odabasi, 2007

Zurich, Switzerland

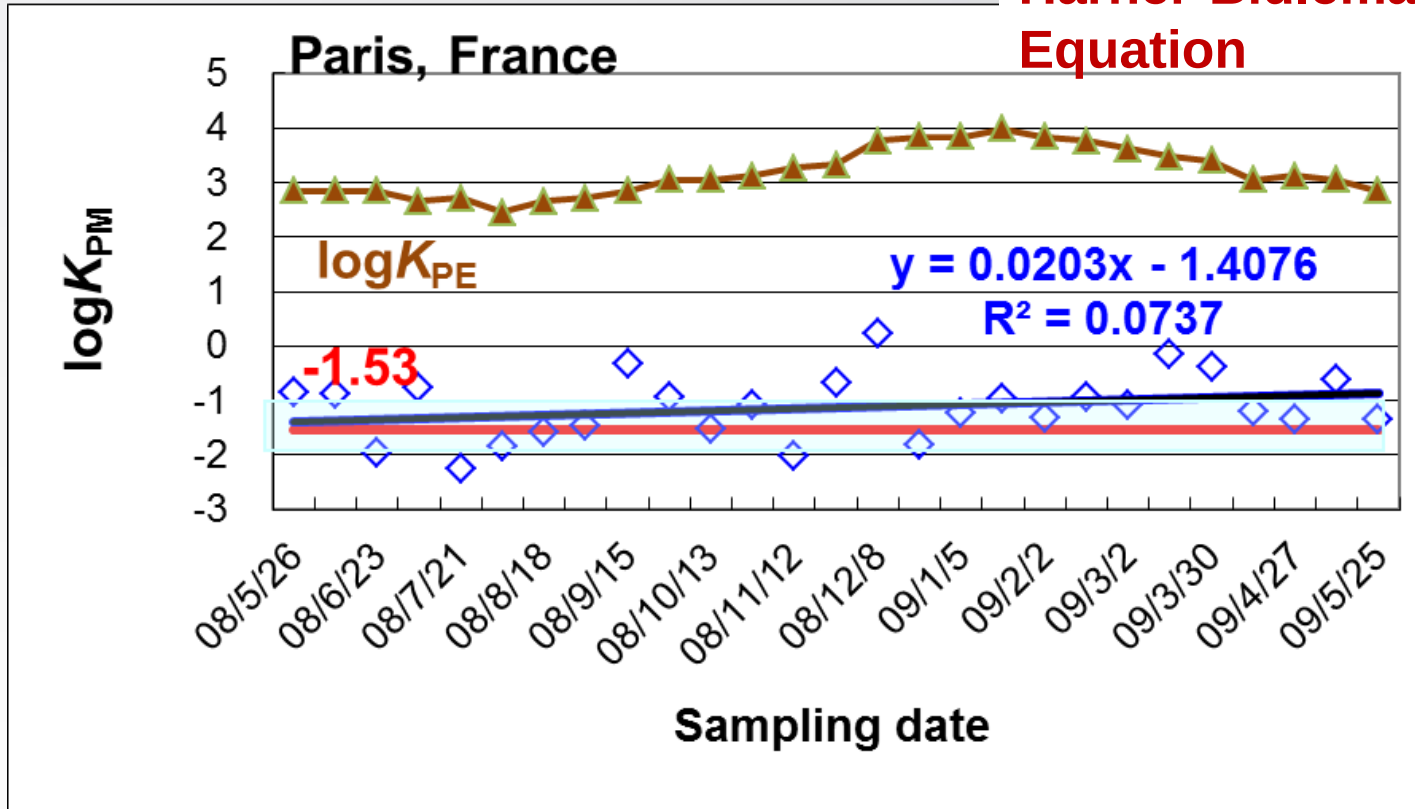


The values of $\log K_{PM}$ of BDE-209 versus sampling date in Zurich, Switzerland in 2010. Assuming that the values of TSP in this city were $30 \mu\text{g}/\text{m}^3$ in summer and $50 \mu\text{g}/\text{m}^3$ in winter.

Bogdal 2014

Paris, France

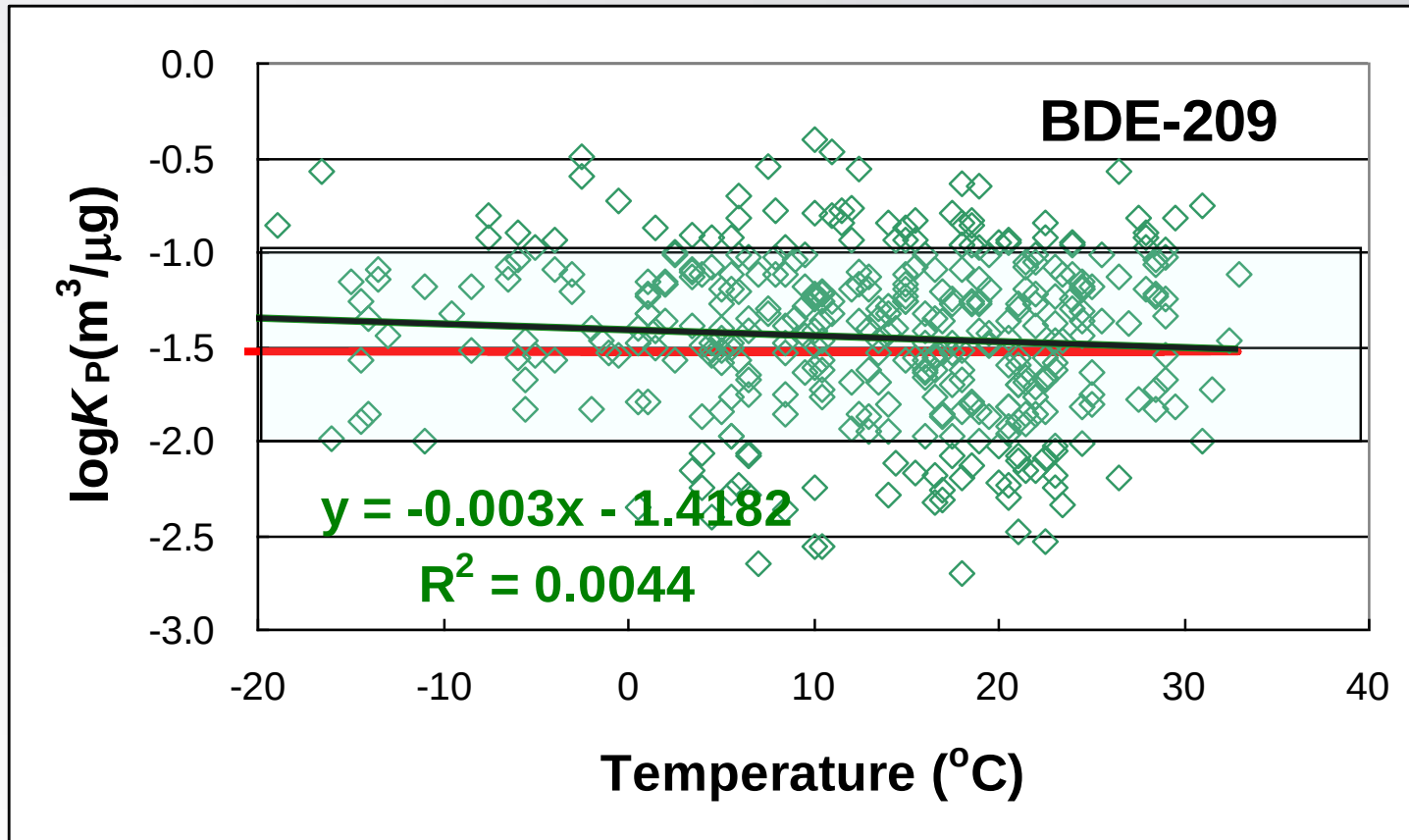
Harner-Bidleman Equation



Variation of $\log K_{PM}$ for BDE-209 versus sampling date in downtown Paris, France. Assuming that the values of TSP in this city were $50 \mu\text{g}/\text{m}^3$ in summer and $100 \mu\text{g}/\text{m}^3$ in winter.

Tlili et al., 2011

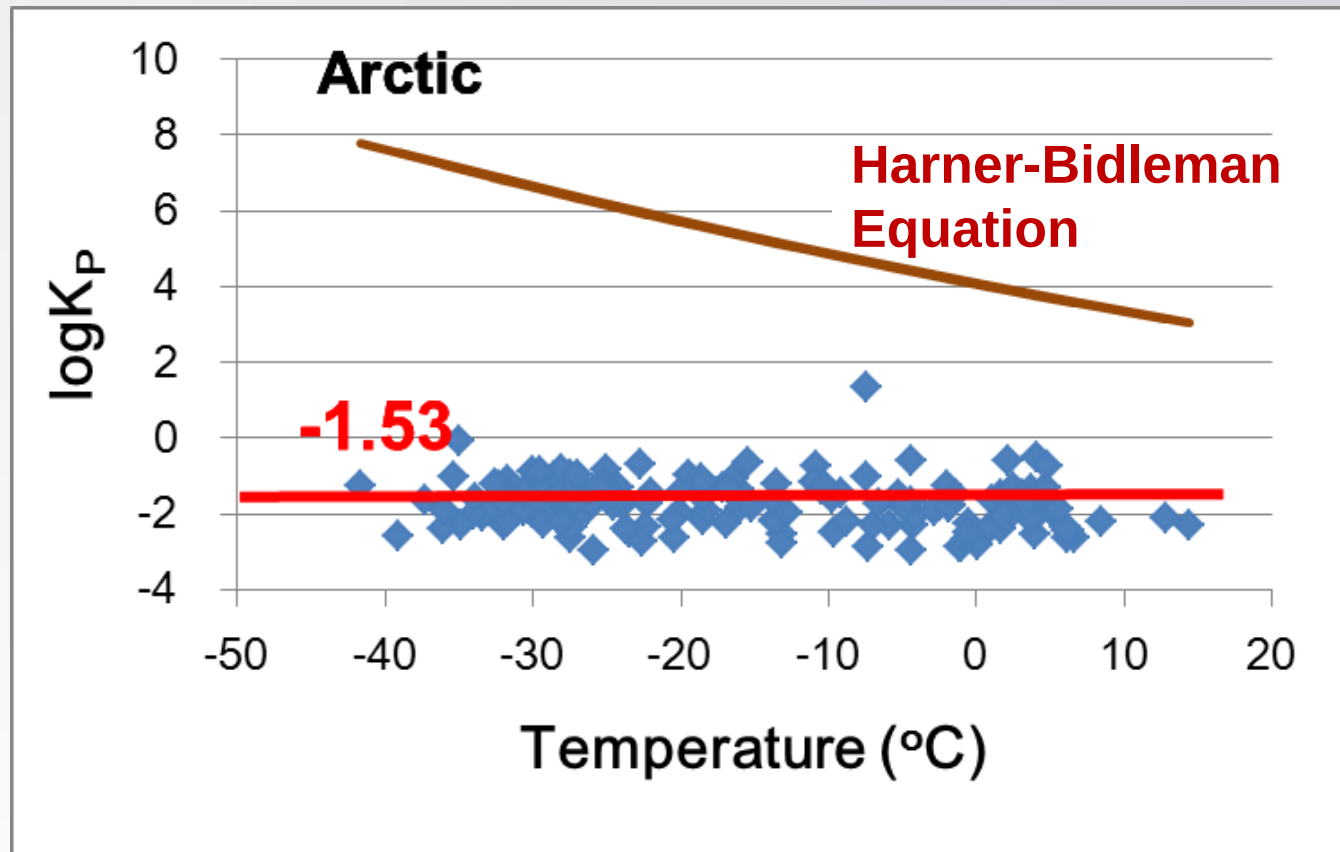
SAMP-II, China



Variation of $\log K_{PM}$ for BDE-209 versus sampling date in China.

(Li et al., 2017)

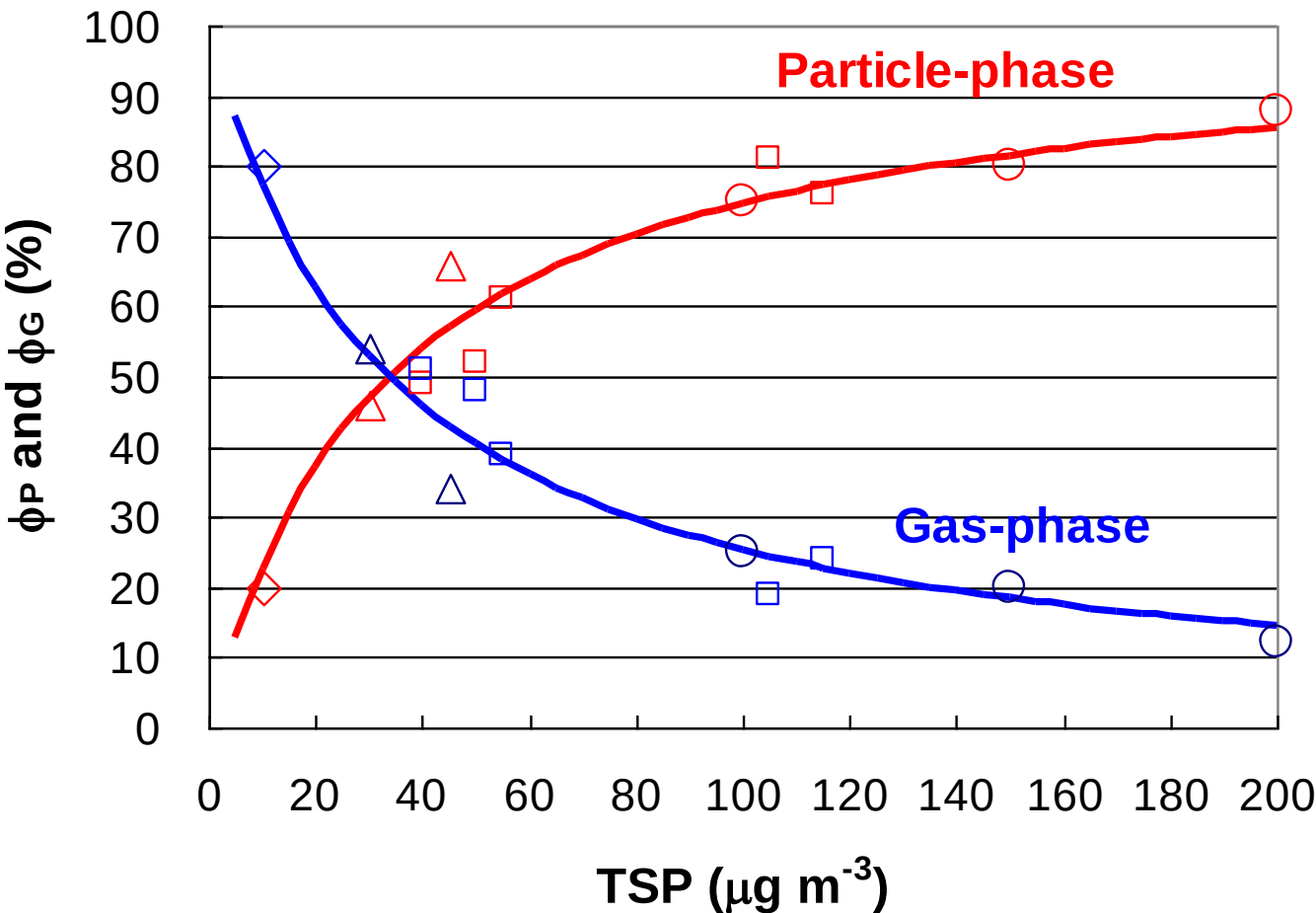
Arctic air



Variation of $\log K_{PM}$ for BDE-209 versus temperature at Alert, Canada from 2006 to 2012

Hung et al, NCP 2013

BDE-209: Fractions in gas and particle phases



Arctic
 (average for 6-year data, NCP, 2013)
 Izmir Bay and Izmir City
 (Cetin and Odabasi, 2007)
 Zurich
 (Bogdal, 2014)
 China (Li et al., 2015)

(Li et al., 2017)



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BDE-209: Long-range transport



- Gaseous BDE-209 are abundant in air (from 87.1% when $\text{TSP}=5 \mu\text{g}/\text{m}^3$ to 14.5% when $\text{TSP}=200 \mu\text{g}/\text{m}^3$ from our equation), and dominant over all PBDE congeners in gas phase in many populated areas, like China, Turkey, Switzerland, and other countries.
- Similarly to other SVOCs, **this compound in gas phase is subject to LRAT** from warmer to colder areas.

(Li et al., 2017)

BDE-209: Long-range transport



Thus, it is mainly the gaseous not particulate BDE-209 that enters the Arctic atmosphere via LRAT.

(Li et al., 2017)

Headline Paper:

Decabrominated Diphenyl Ethers (BDE-209) in Chinese and Global Air: Levels, Gas/Particle Partitioning, and Long-Range Transport: Is Long-Range Transport of BDE-209 Really Governed by the Movement of Particles?

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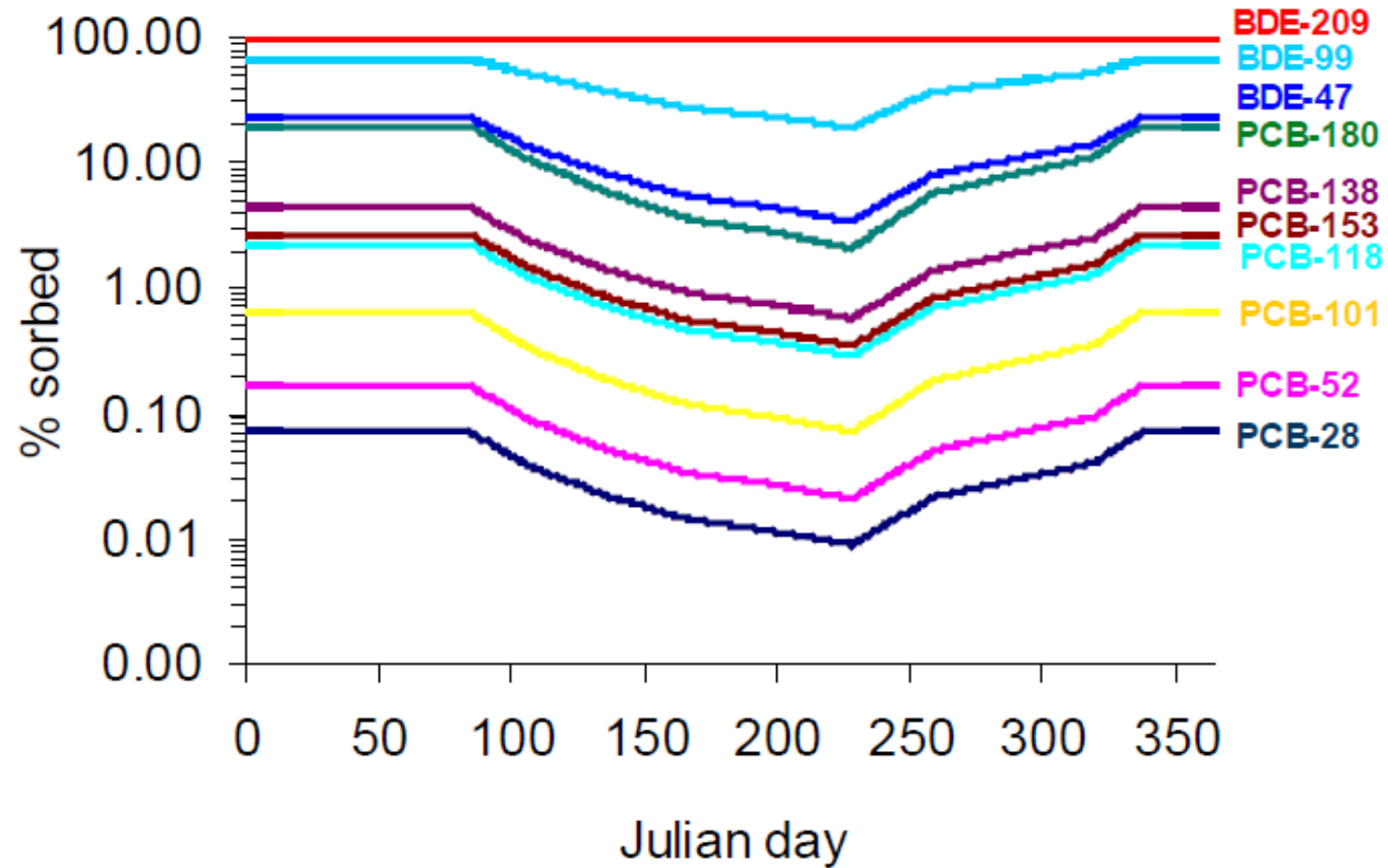
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Models to predict G/P for SVOCs



(Breivik et al, 2006)

Threshold Values

