The major pathway for BDE-209 entering the Arctic air

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Hayley Hung from Environment and Climate Change of Canada

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- Our point of view
- Conclusions

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- **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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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

Atmospheric Chemistry and Physics
Open Access

Prediction of gas/particle partitioning of polybrominated diphenyl ethers (PBDEs) in global air: A theoretical study

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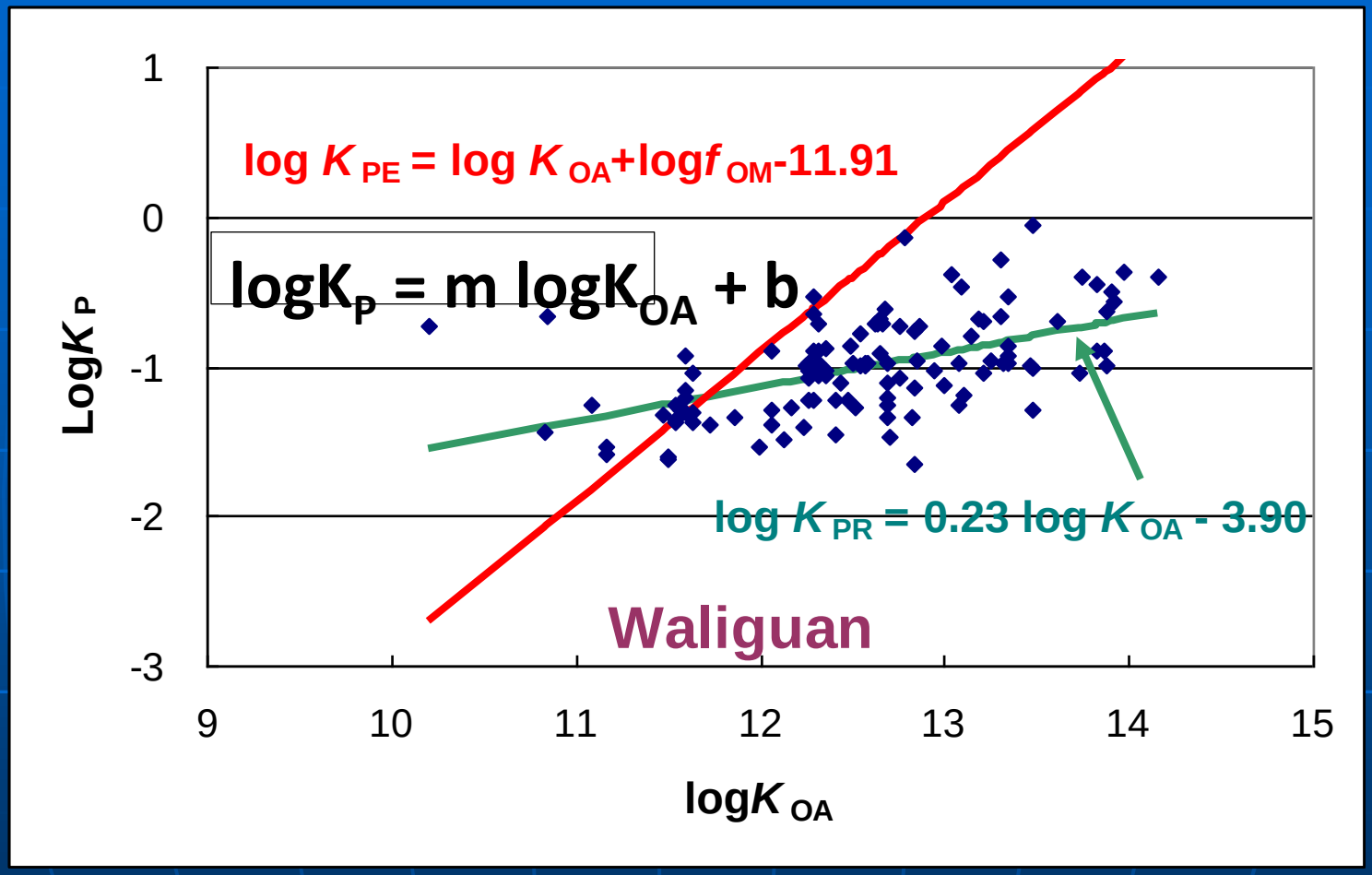
Equations at steady state： Important predictions

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

Li et al, 2015

Introduction：The slope *m*



The regression model (logK_{PR}) needs monitoring data to calculate the parameters m_O (0.23) and b_O (-3.90)

Yang et al. 2013

IJRC-PTS

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

Li et al, 2015

Equations at steady state： Important predictions

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

Li et al, 2015

Prediction by Steady-State Model for PBDEs

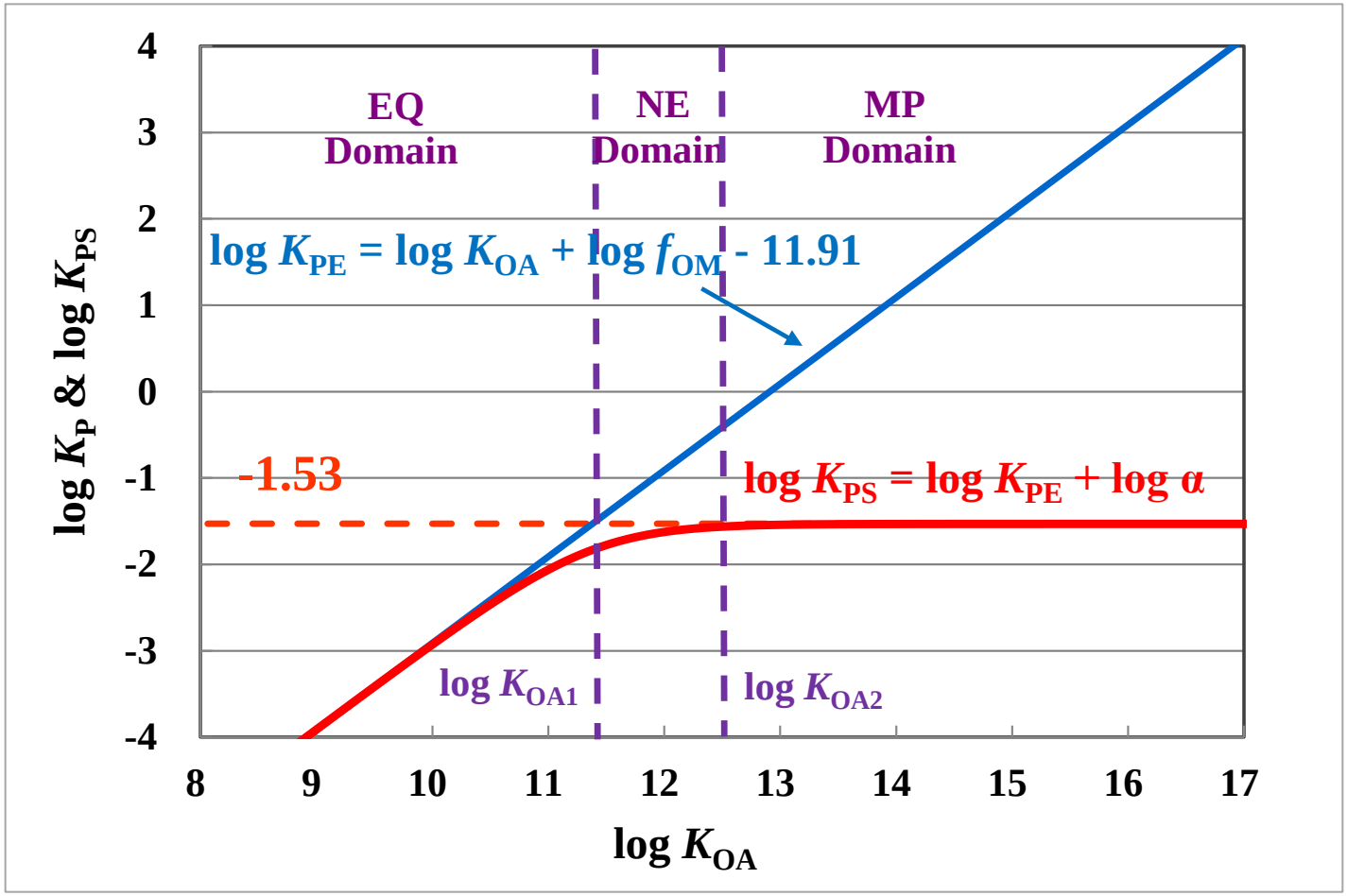


Figure 1. The G/P partition coefficients of PBDEs as functions of logK_{OA} calculated by two equations.

(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

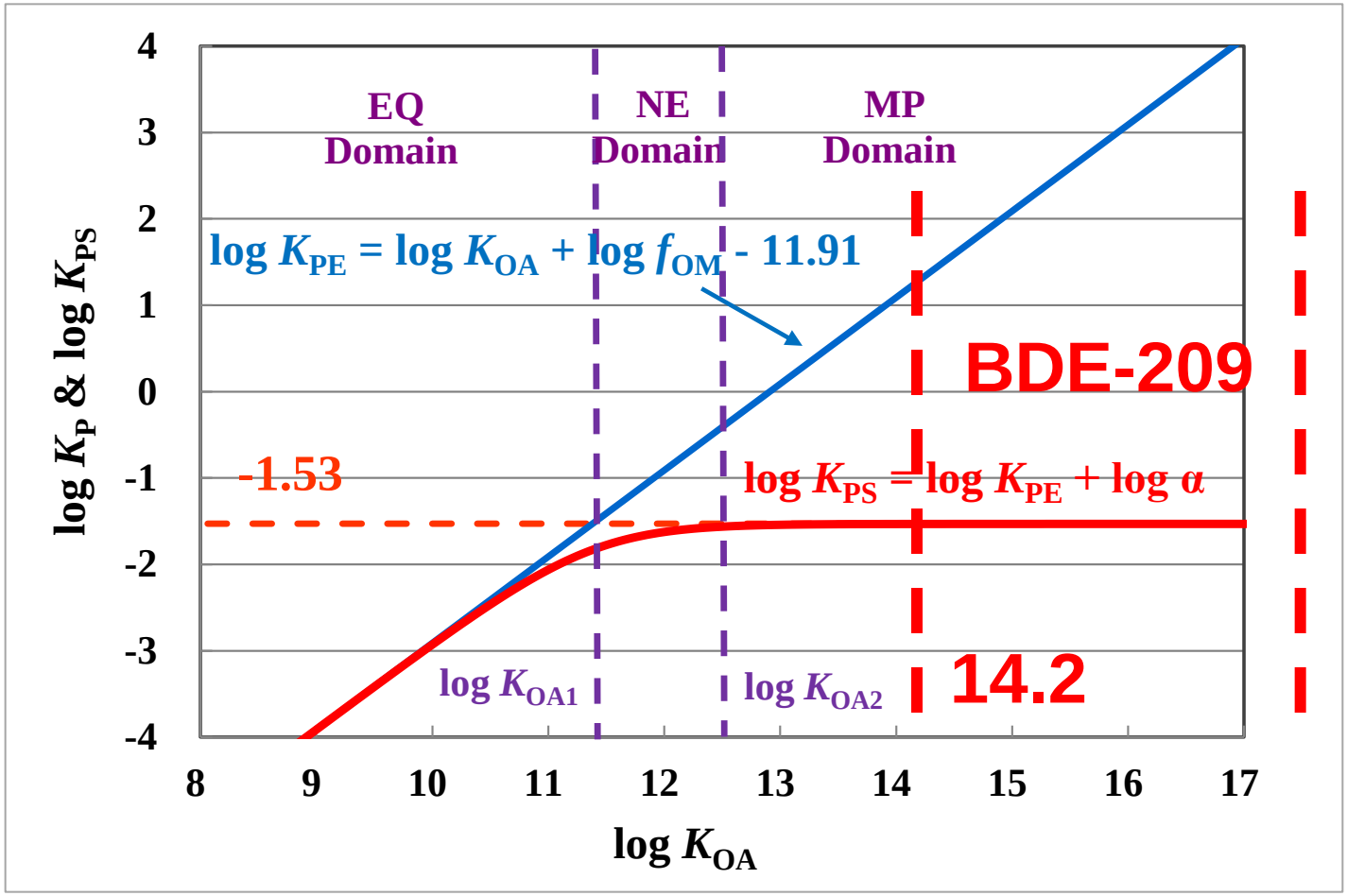
For BDE-209

$$\text{Log } K_{OA} = 14.2 \quad \text{at } +50^{o}C$$
$$= 20.0 \quad \text{at } -50^{o}C$$

Both > logK_{OA2}=12.5

Li et al, 2015

Prediction by Steady-state model for PBDEs



The G/P partition coefficients of PBDEs as functions of logK_{OA} calculated by two equations.

(Li et al., 2015)

We predict

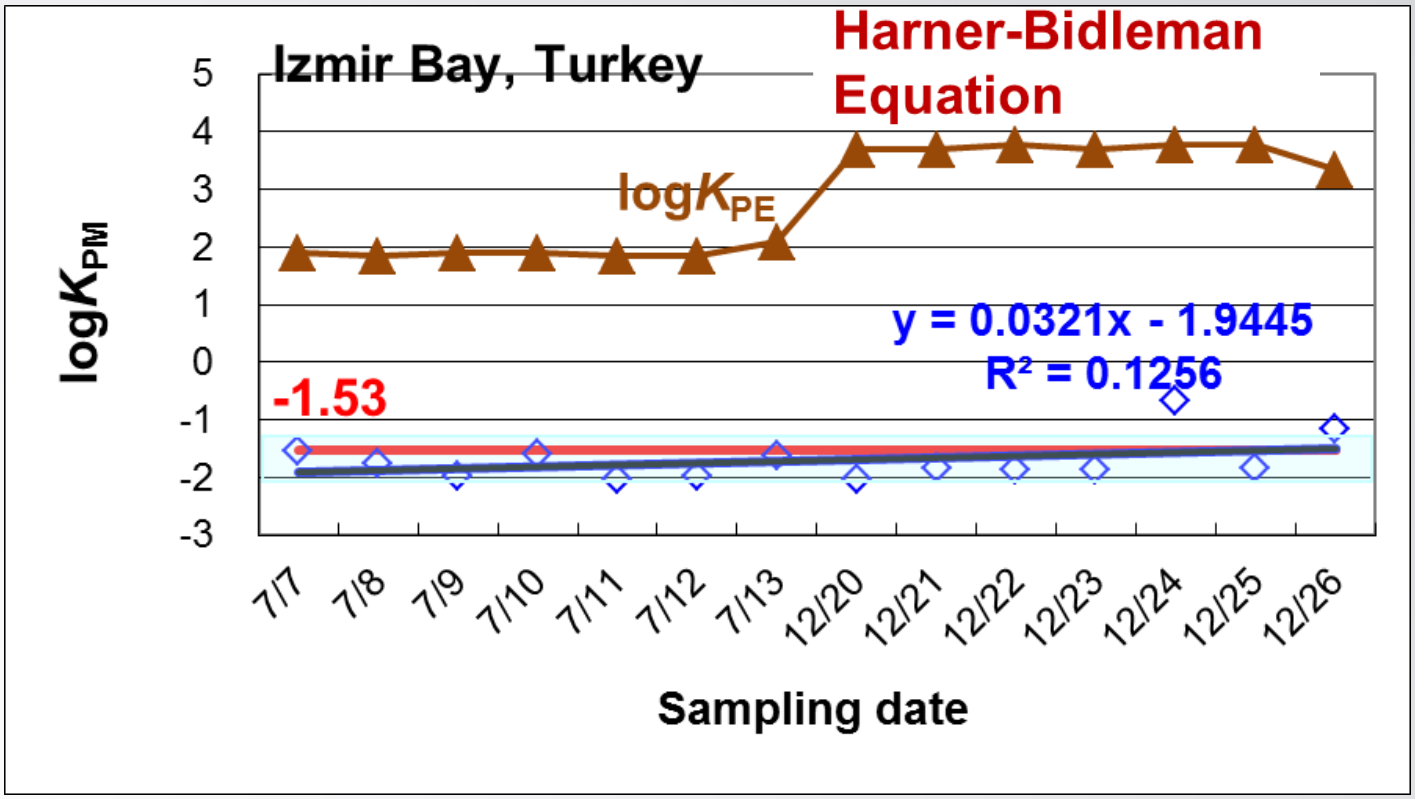
The logarithm of partition quotient ($\log K_P$) of BDE-209 is a constant (-1.53) at any ambient temperature and at any sampling sites.

(Li et al., 2017)

C/P partition quotient

Monitoring data

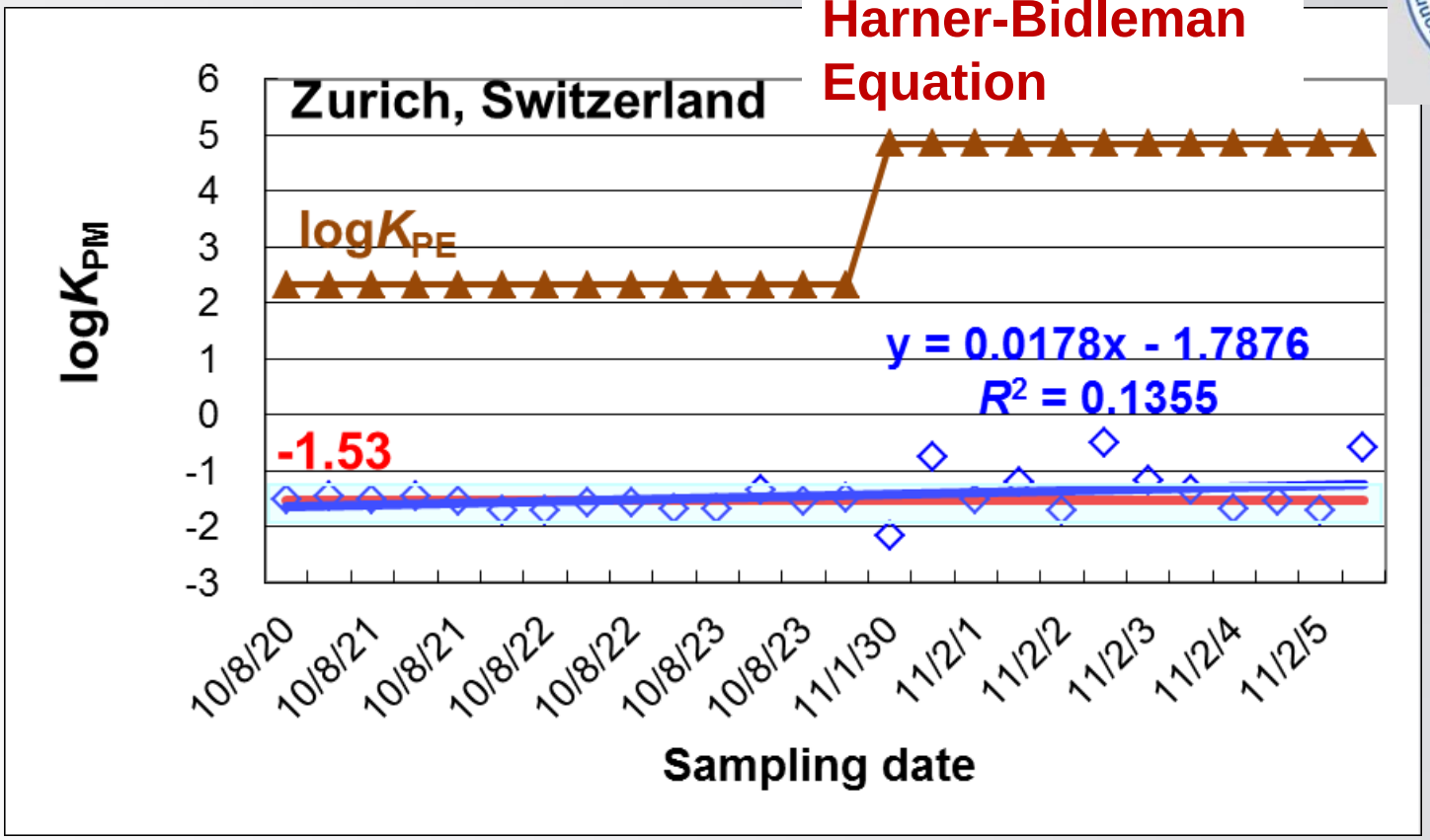
Izmir Bay, Turkey



The values of logK_P of BDE-209 versus sampling date in Izmir Bay, Turkey in 2005. Assuming that the values of *TSP* at the site were 30 μg/m³ in summer and 50 μg/m³ in winter.

Cetin and Odabasi, 2007

Zurich, Switzerland

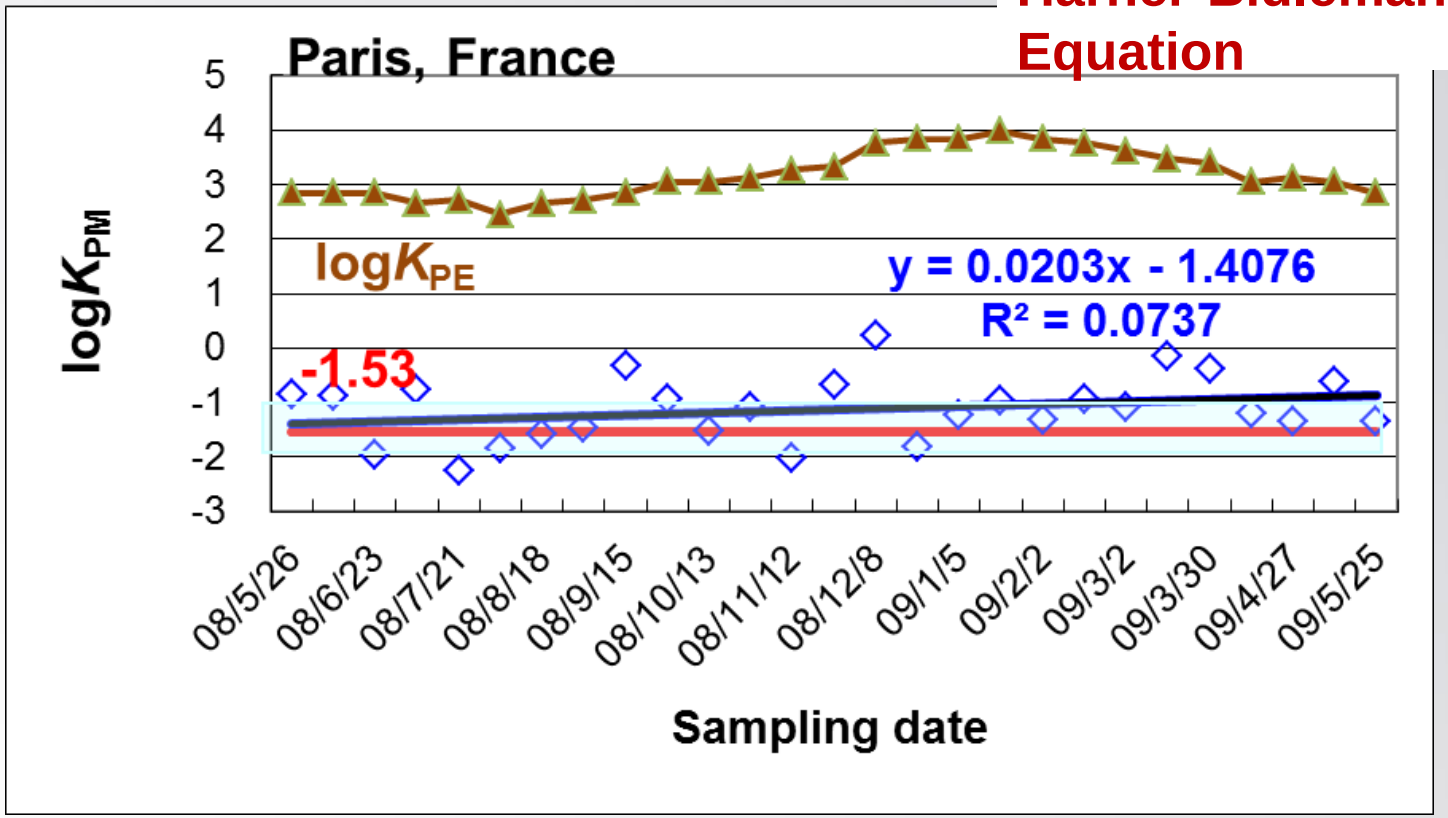


The values of logK_{PM} of BDE-209 versus sampling date in Zurich, Switzerland in 2010. Assuming that the values of *TSP* in this city were 30 μg/m^3 in summer and 50 μg/m^3 in winter.

Bogdal 2014

Paris, France

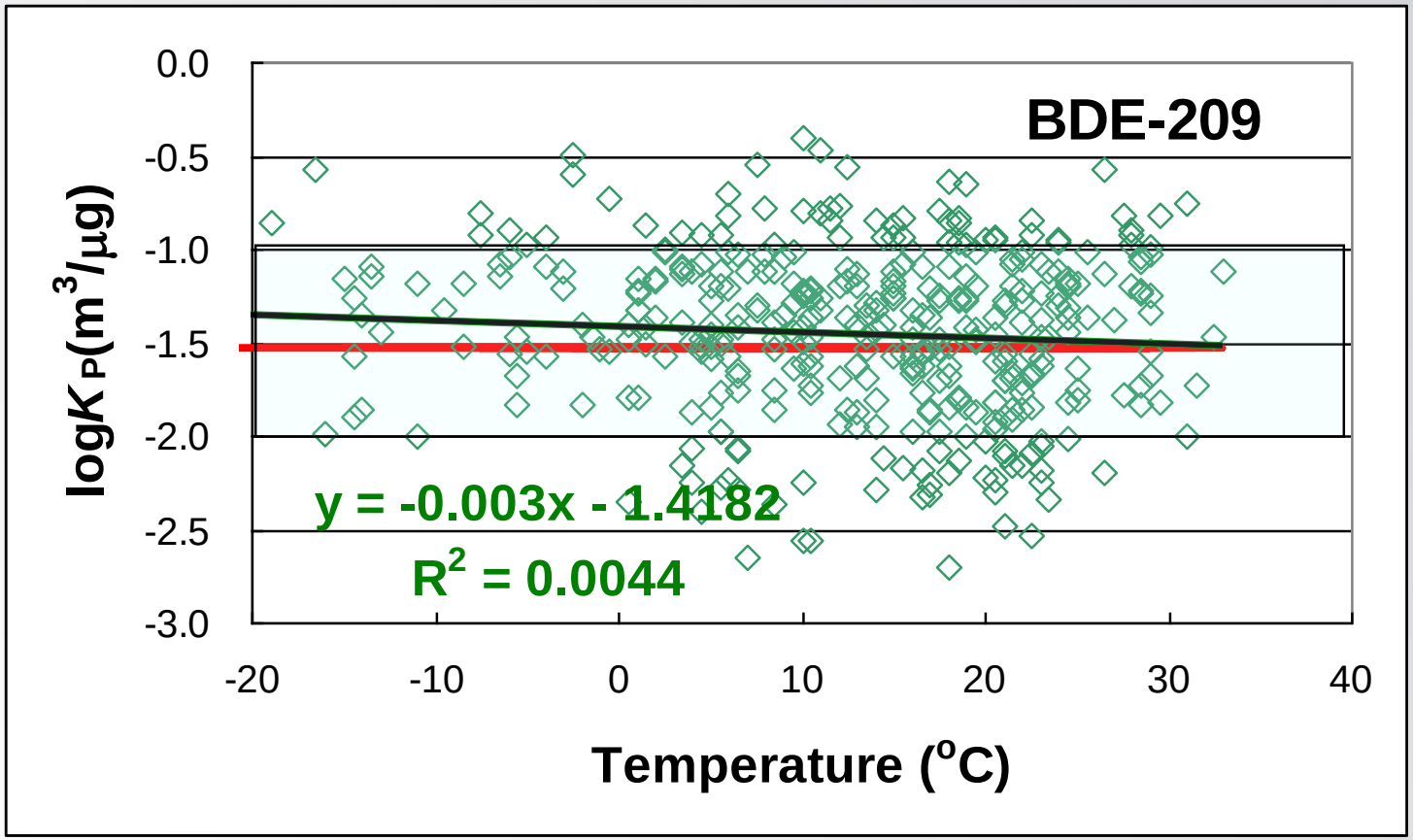
Harner-Bidleman Equation



Variation of logK_{PM} for BDE-209 versus sampling date in downtown Paris, France. Assuming that the values of *TSP* in this city were 50 μg/m^3 in summer and 100 μg/m^3 in winter.

Tlili et al., 2011

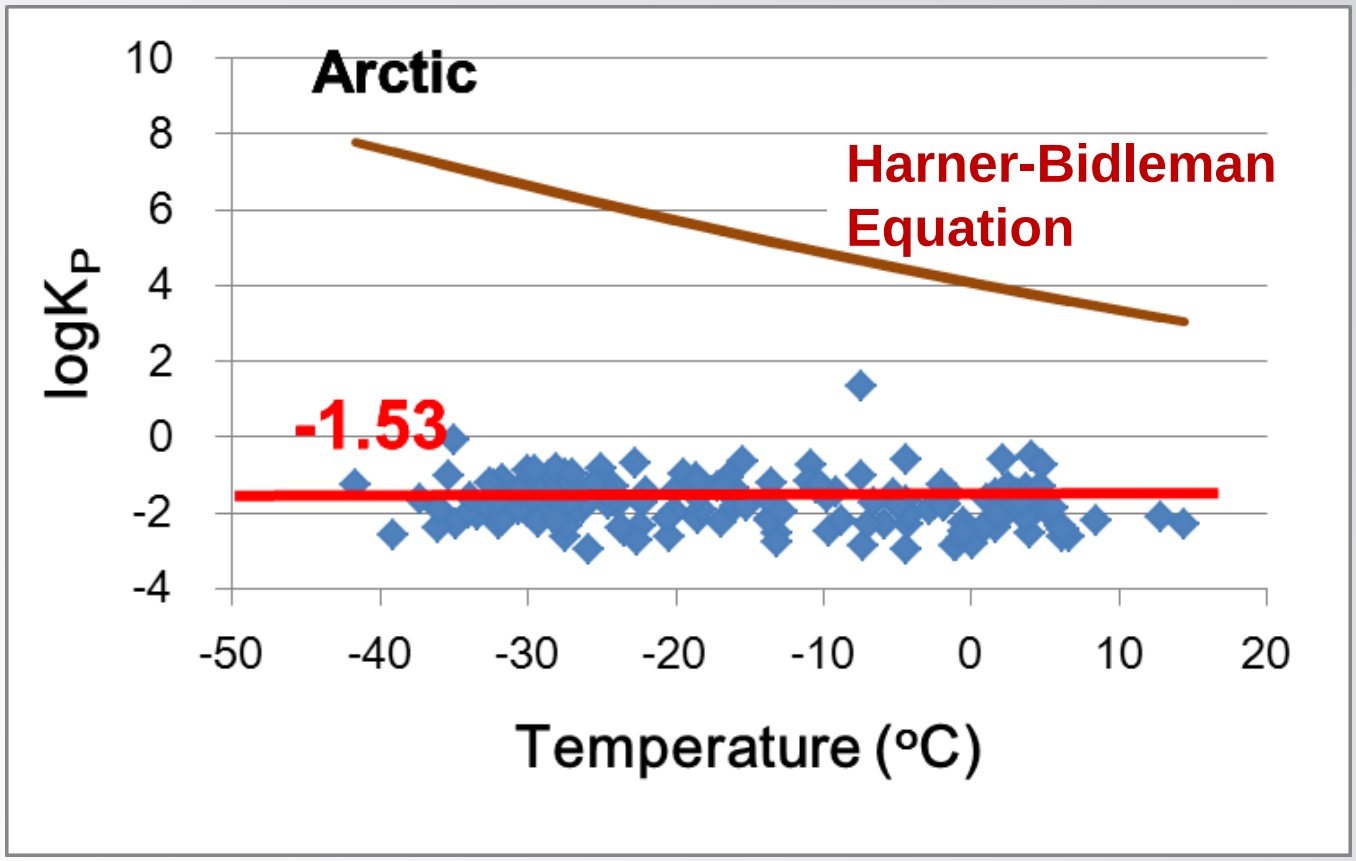
SAMP-II, China



Variation of logK_{PM} for BDE-209 versus sampling date in China.

(Li et al., 2017)

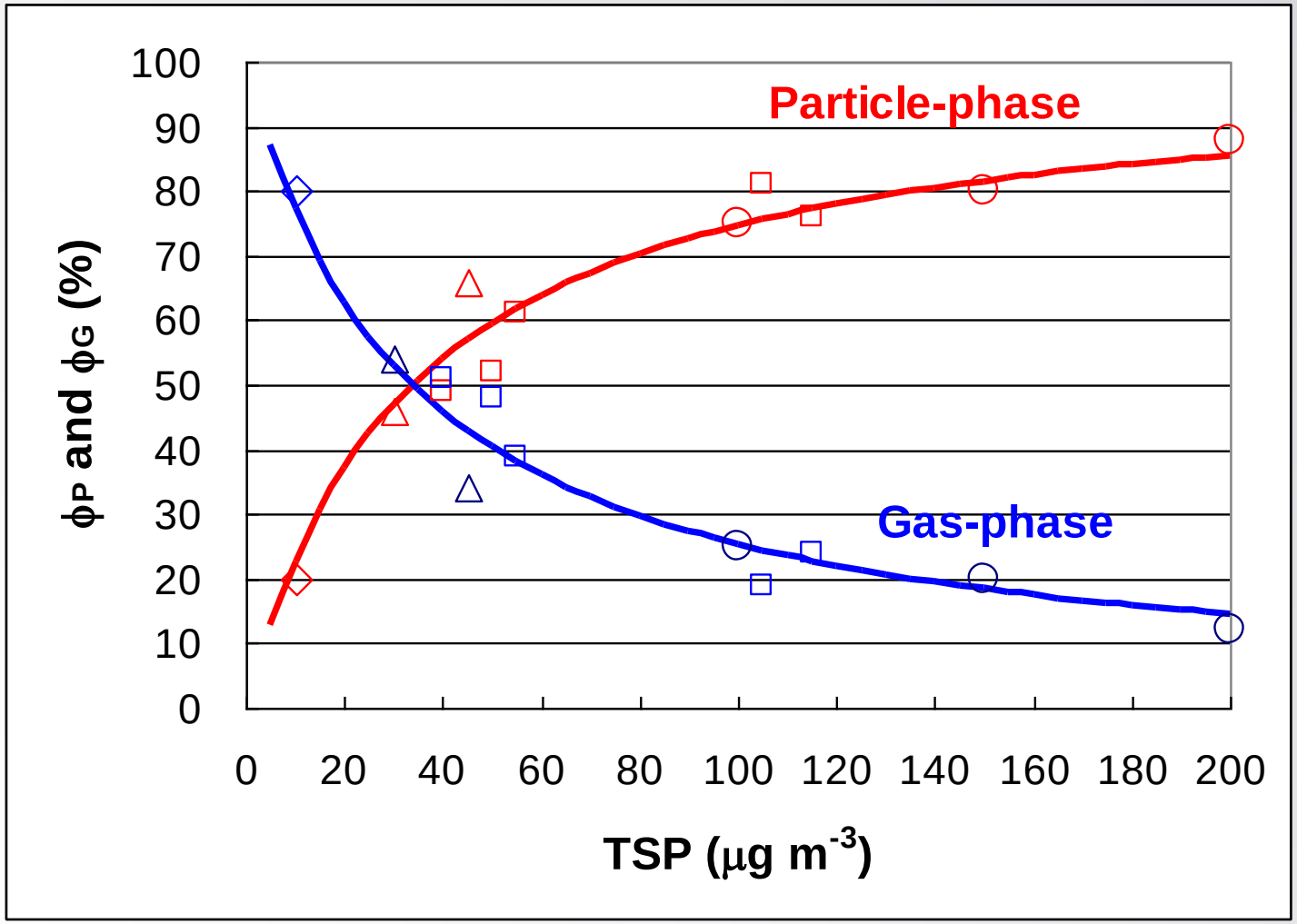
Arctic air



Variation of logK_{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 Izmur 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 TSP=5 μg/m^3 to 14.5% when TSP=200 μg/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

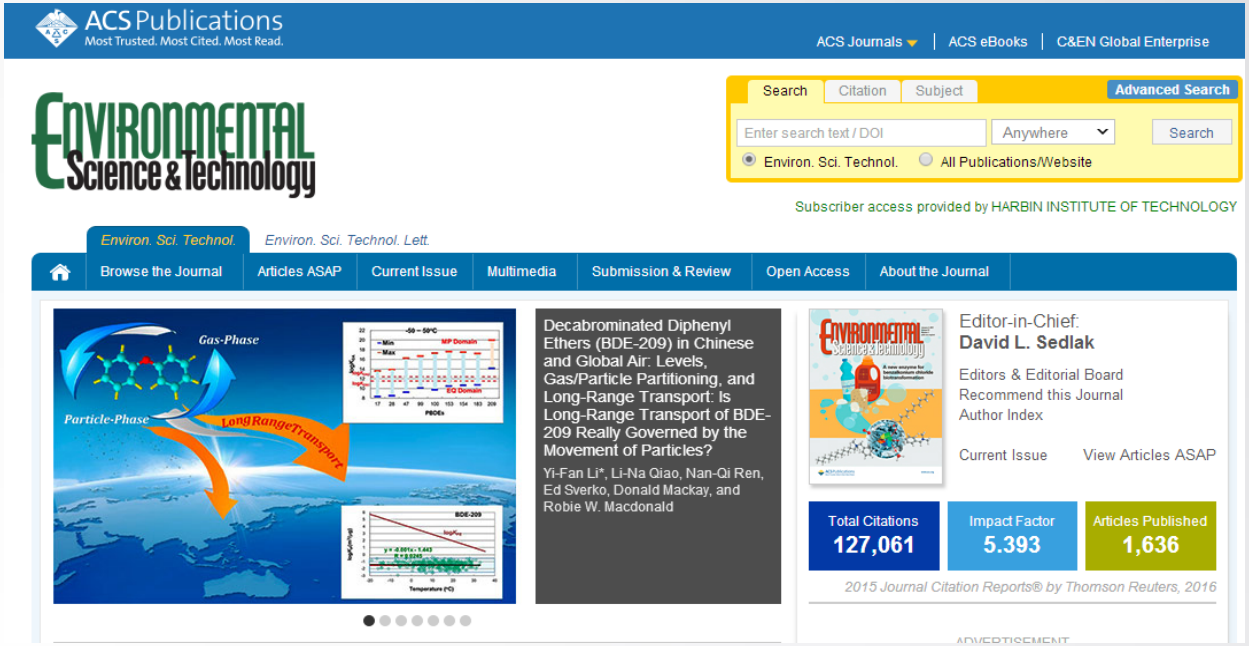
Thus, it is mainly the gaseous not particulate BDE-209 that enters the Arctic atmosphere via LRAT.

(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?

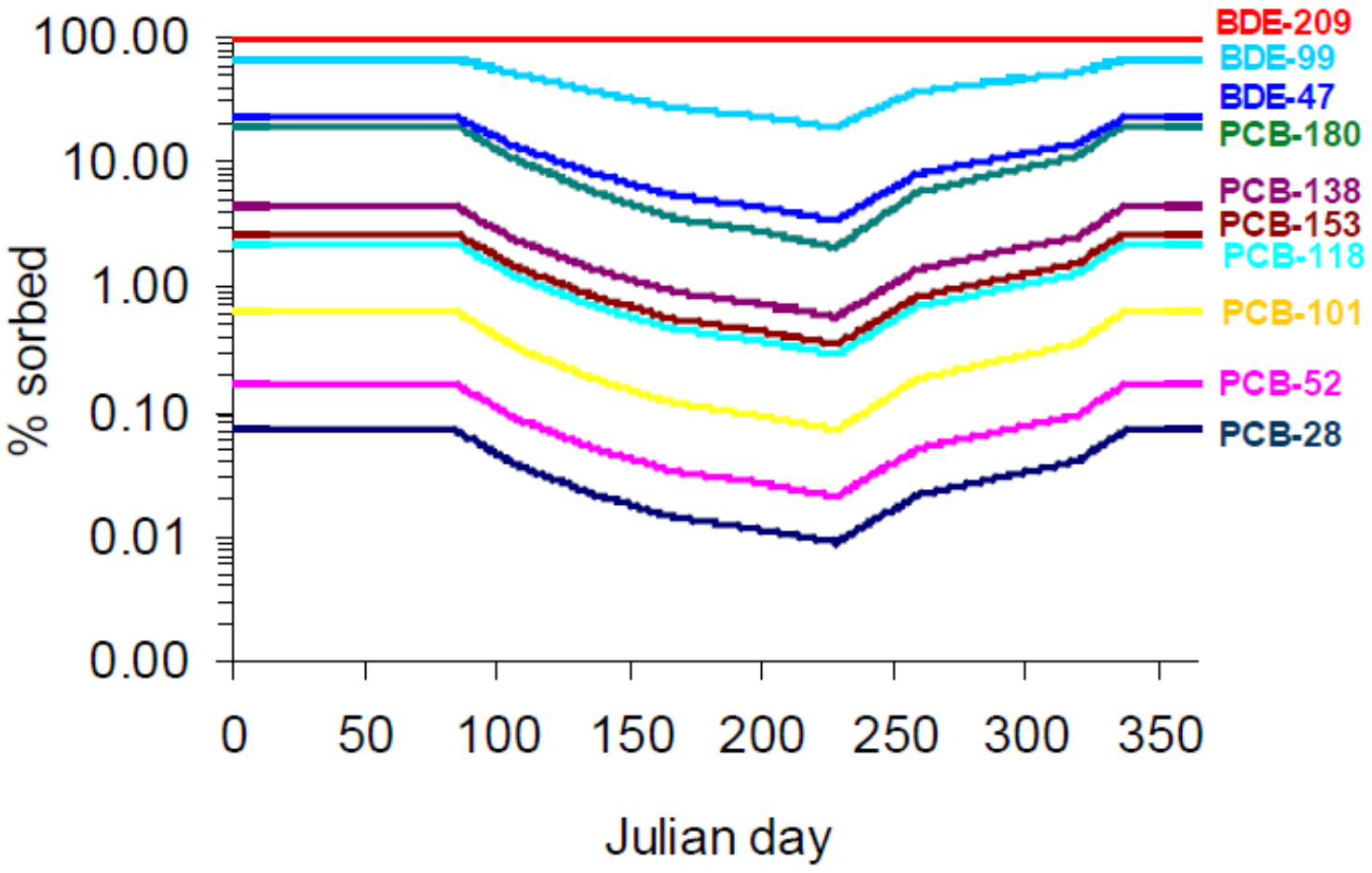
Environmental Science & Technology, 51, 1035-1042, 2017



IRC-AEE

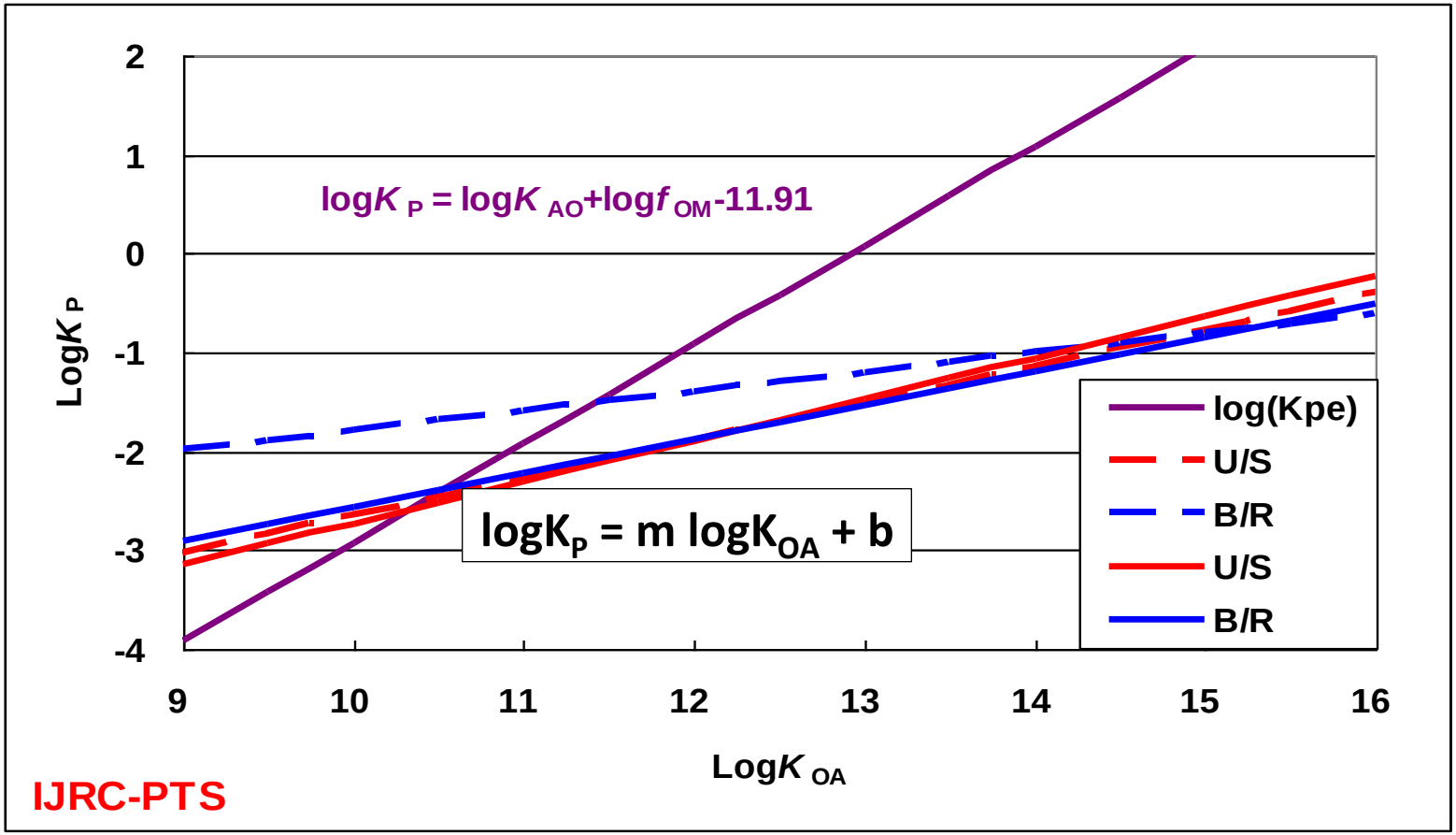
Thank you for your attention!

Models to predict G/P for SVOCs



(Breivik et al, 2006)

Threshold Values



(Li and Jia., 2014)