Recent advancements in modelling the impact of Carbonaceous Materials on bioavailability and food chain accumulation of POPs

Journal:	*SETAC Europe Annual Meeting 2007*
Manuscript ID:	SETAC-EU-0079-2007
Day and Time:	TUE AM2
Room:	Arrýbida Hall
Date Submitted by the Author:	17-May-2007
Complete List of Authors:	Egeler, Philipp

Recent advancements in modelling the impact of Carbonaceous Materials on bioavailability and food chain accumulation of POPs.

Bart Koelmans, Wageningen University, Wageningen IMARES

Mara Hauck, Radboud University, Nijmegen

Caroline Moermond, Wageningen University

Chiel Jonker, Utrecht University

Jan Hendriks, Radboud University, Nijmegen

Theo Traas, RIVM

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

Scope

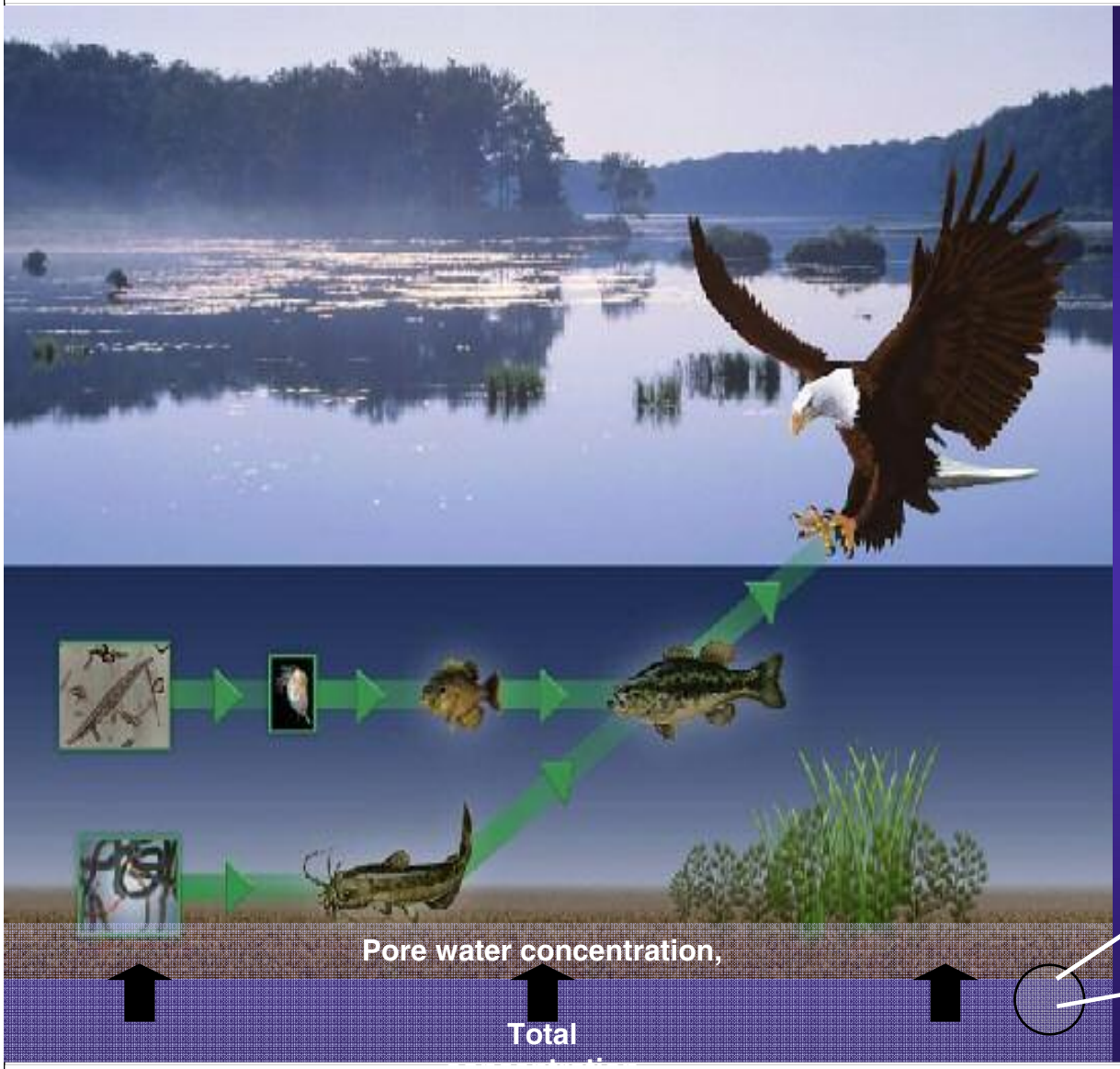
Bioaccumulation assessment of POPs:

Exposure (outside) + Toxicokinetics (inside) + Food web (among)

Modeling vs Measurement

Does accounting for black carbon sorption improve model simulations?

BC-inclusive Food Chain Accumulation Modeling



‘Soft, amorphous carbon’

‘Hard carbon’ (black carbon, coal, kerogen)

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

Basic model

Relate concentration in solid, *q*, to concentration in water, *C*, through dual sorption domain model:

$$q = f_{oc} K_{oc} C + f_{BC} K_{F,BC} C^{n_F}$$

Linear Term

= old EPT

Freundlich term

= new BC

Parameterisation:

Measure f_{oc} and f_{BC}

K_{oc} from K_{ow} regression

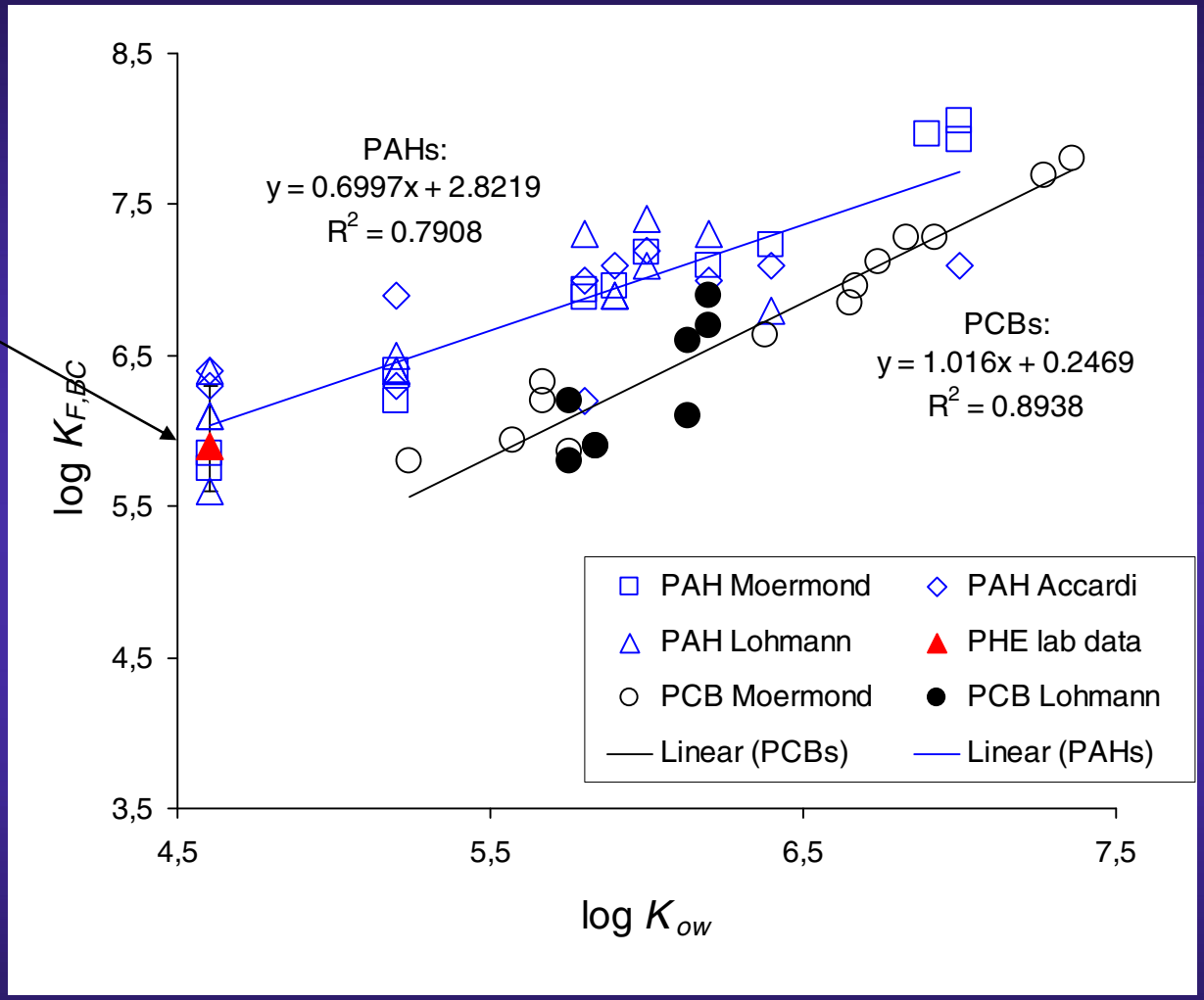
K_f from lab or field data ?

When *q* = measured, solve equation interatively for unknown *C*

Koelmans A.A., M.T.O. Jonker, G. Cornelissen, T.D. Buchelli, P.C.M. Van Noort and **Ö. Gustafsson**. 2006. Black Carbon: The Reverse of its Dark Side. *Chemosphere*, **63**: 365-377.

Estimation K_f from *in situ* sediment data

Lab values with attenuation factor



Consistency between 'attenuated' lab and field K_f data at n_F= 0.7

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

Koelmans A.A., M.T.O. Jonker, G. Cornelissen, T.D. Buchelli, P.C.M. Van Noort and **Ö. Gustafsson**. 2006. Black Carbon: The Reverse of its Dark Side. *Chemosphere*, **63**: 365-377.

Three cases

Increasing complexity and variability

1. PAHs in Manufactured Gas Plant (MGP) soils → Kp
   Laboratory data
2. PAHs in aquatic food chain → fish
   Data from 1 m^3 indoor model-ecosystems
3. PAHs in multiple species → chironomids, mussels, fish
   Field data

1. Modeling MGP Soil Kd's: Default parameter set

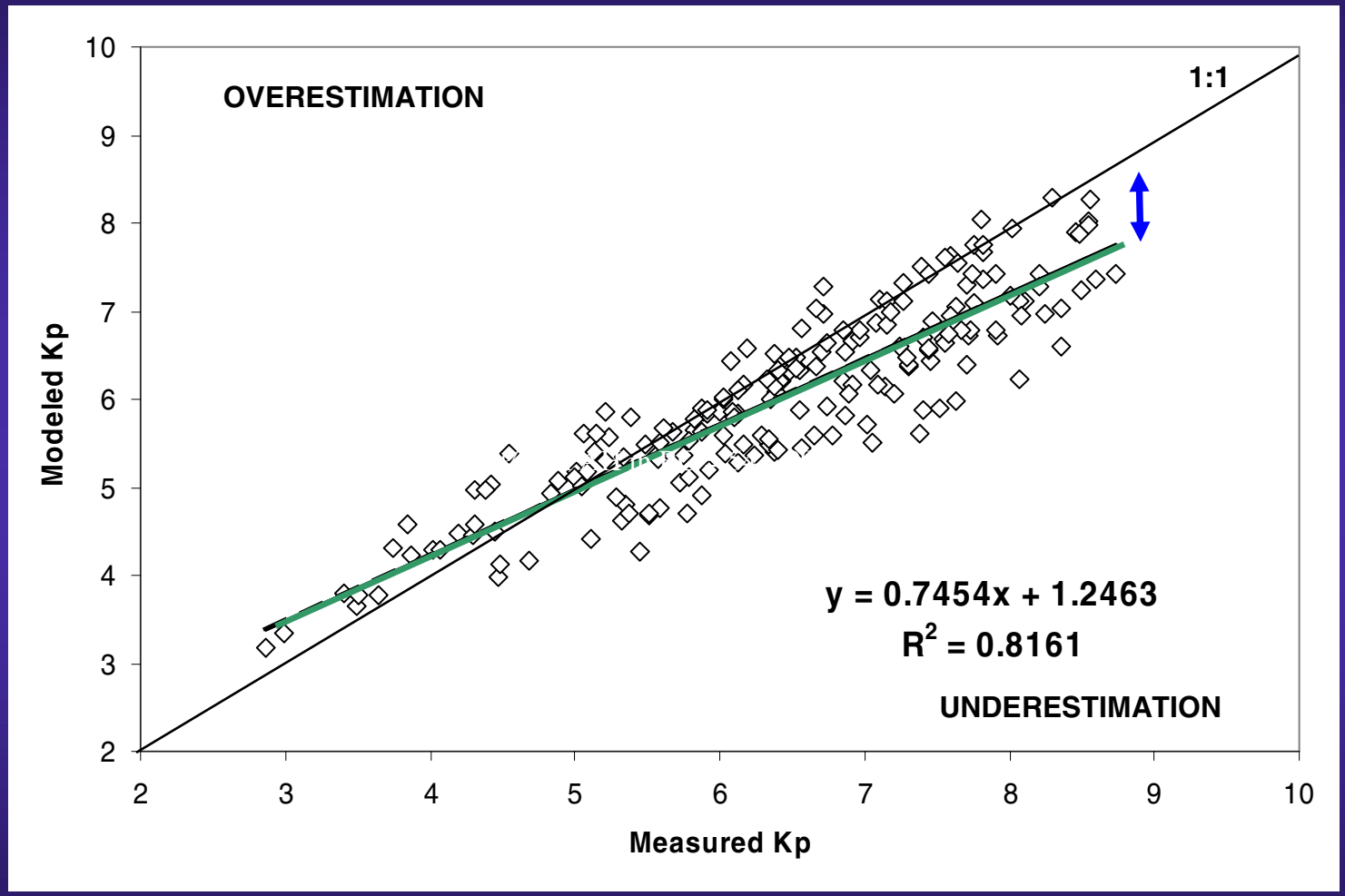
→ Dataset from Jonker *et al, submitted*

→ 15 MGP soils x 13 PAHs = 195 cases

→ Pore water concentration measured using SPME

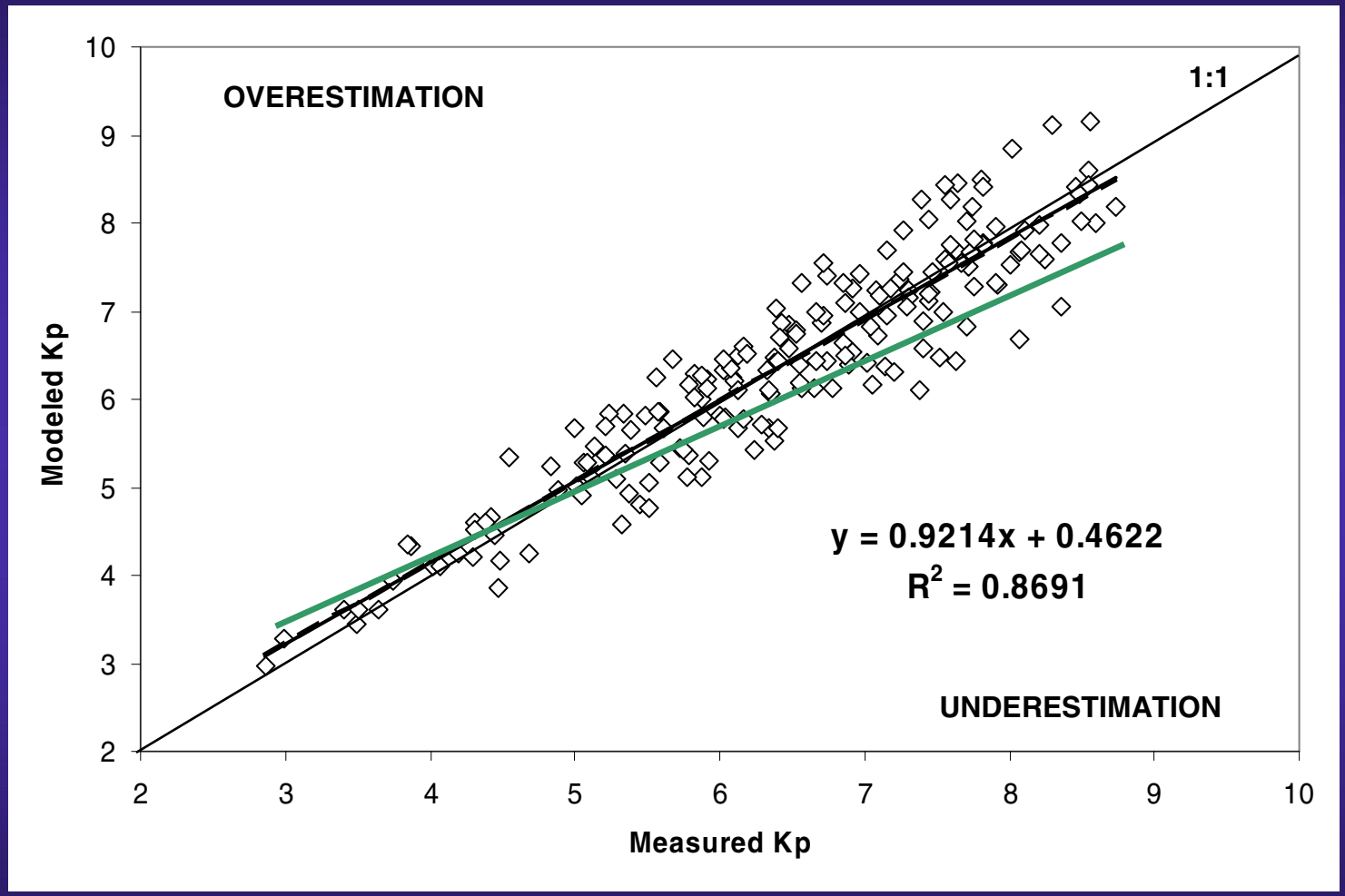
f_{oc} = 0.02 – 0.87, f_{BC} = 0.003 – 0.38, BC/TOC = 0.13 – 0.60

1. Modeling MGP Soil Kd's: Default parameter set



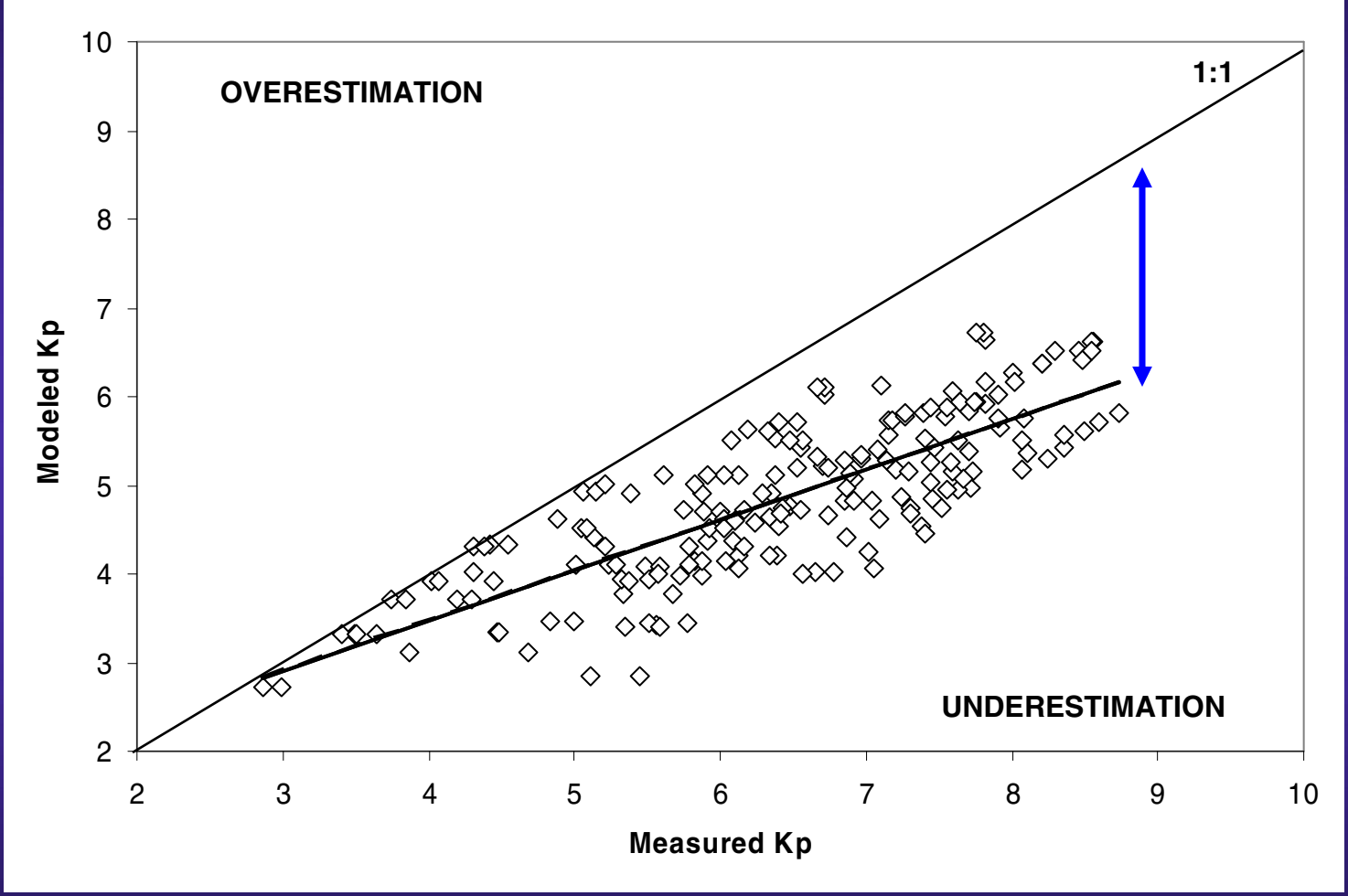
Modeled % of PAH in BC = 54 – 99 %, Average 90.5 %

1. Modeling MGP Soil Kd's: Optimized parameter set



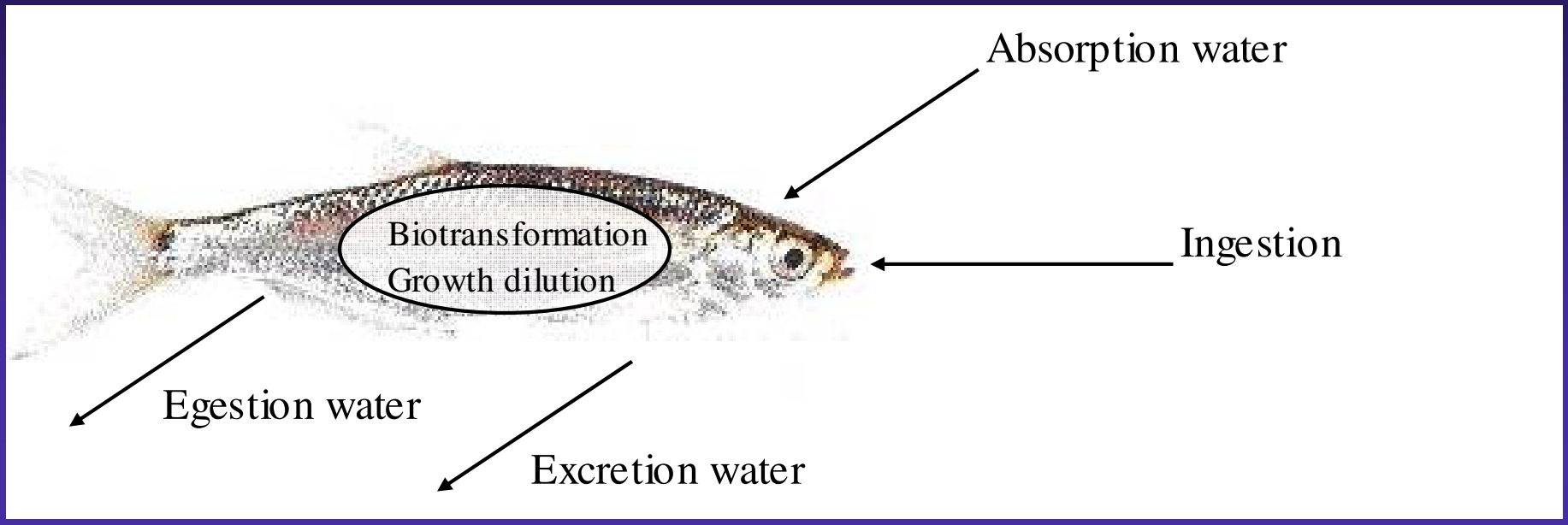
Better fit, parameters still realistic, but improvement not significant

1. Modeling MGP Soil Kd's: Ignore BC contribution



No BC: Underestimation up to 2-3 orders of magnitude

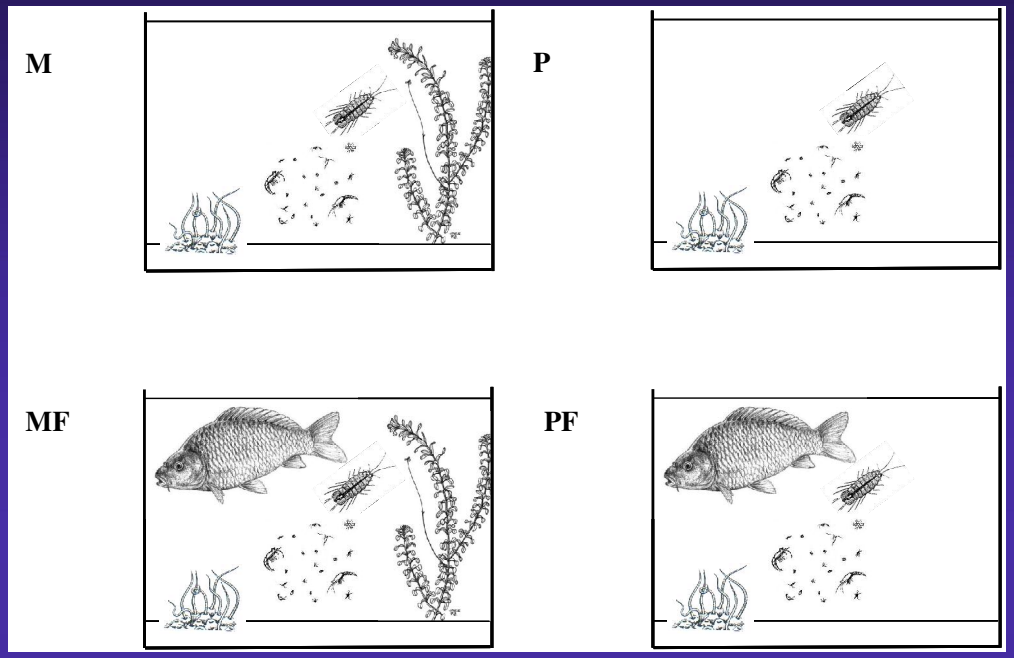
BC-inclusive Food Chain Accumulation Modeling: 'add food chain'



$$\frac{dC_i}{dt} = k_{0,x,in} * C_w + k_{1,x,in} * C_{i-1} + k_{2,x,in} * C_{sed} - \sum_{j=0}^{j=3} k_{j,x,out} * C_i$$

$$q = f_{oc} K_{oc} C_w + f_{BC} K_{F,BC} C_w^{n_F}$$

2. BC-inclusive PAH Food Chain Accumulation Modeling in laboratory cosms



- → Dataset from Moermond & Roessink *et al, In press*
- → 4 ecosystem structures on same contaminated sediment x triplicate x 13 PAHs = 156 cases
- → PAHs in sediment and biota, BC in sediment

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

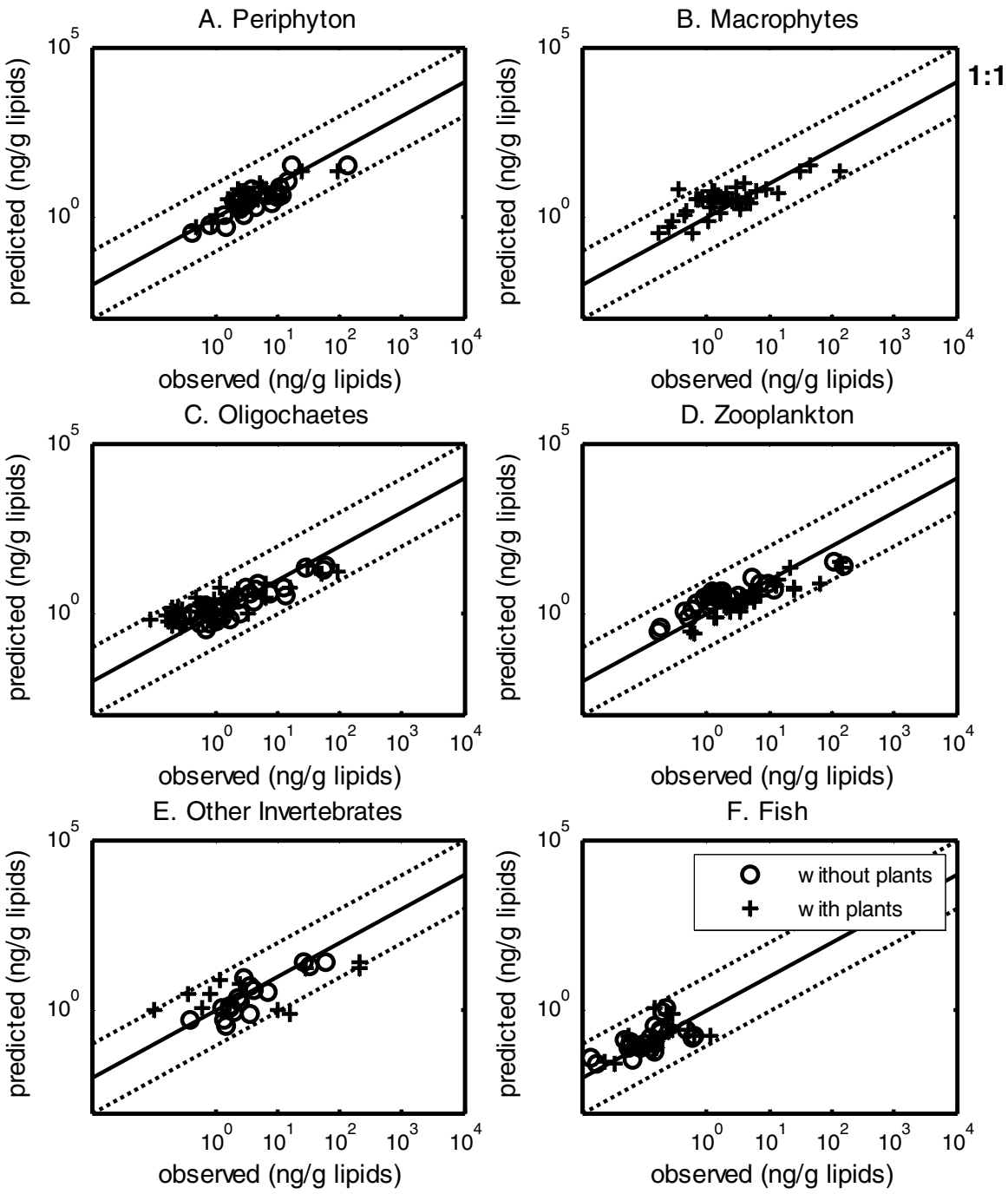
Moermond C.T.A., T.P. Traas, Ivo Roessink, K. Veltman, A.J. Hendriks and **A.A. Koelmans**. 2007. Modeling decreased food chain accumulation of HOCs due to strong sorption to carbonaceous materials and metabolic transformation. *Environ. Sci. Technol. In press.*

2. Modeling ac

Default parameters

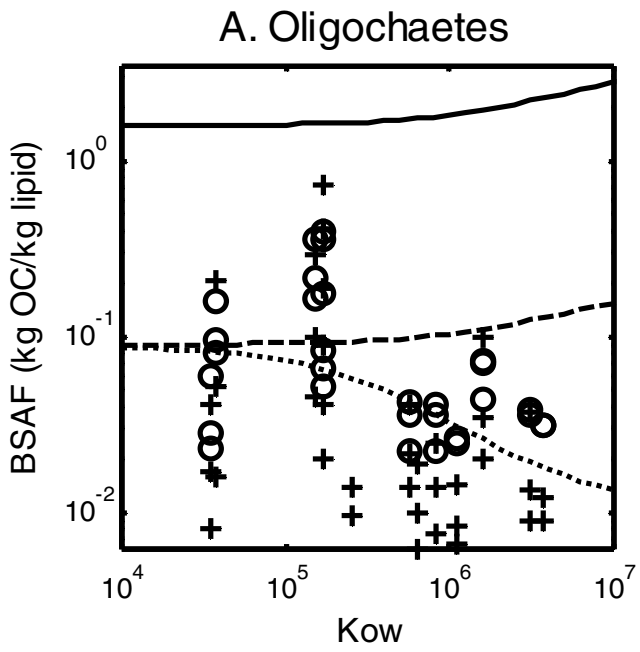
→ good fits for macrophytes, periphyton, algae (no biotransformation)

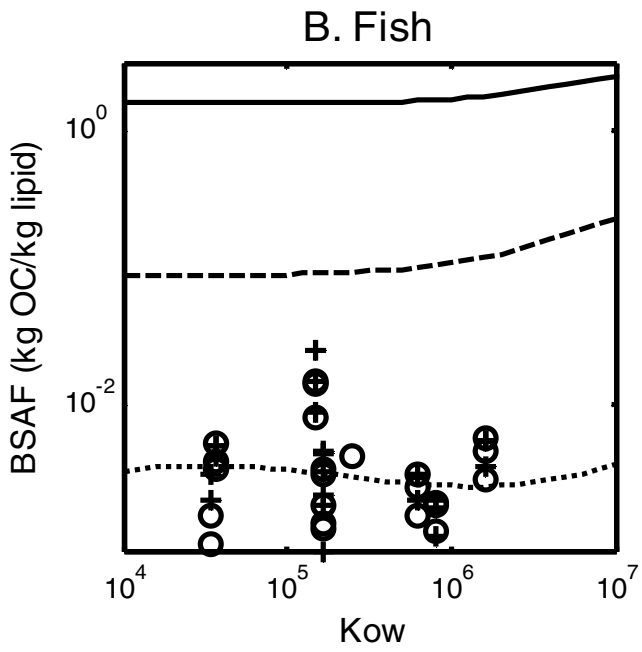
→ For macrofauna & fish known to metabolize PAHs, biotransformation k_m was fitted



WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

2. BC-inclusive PAH Food Chain Accumulation Modeling in laboratory cosms





___ Traditional model overestimates data

---- BC included

….. BC and biotransformation included

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

Moermond C.T.A., T.P. Traas, Ivo Roessink, K. Veltman, A.J. Hendriks and **A.A. Koelmans**. 2007. Modeling decreased food chain accumulation of HOCs due to strong sorption to carbonaceous materials and metabolic transformation. *Environ. Sci. Technol. In press.*

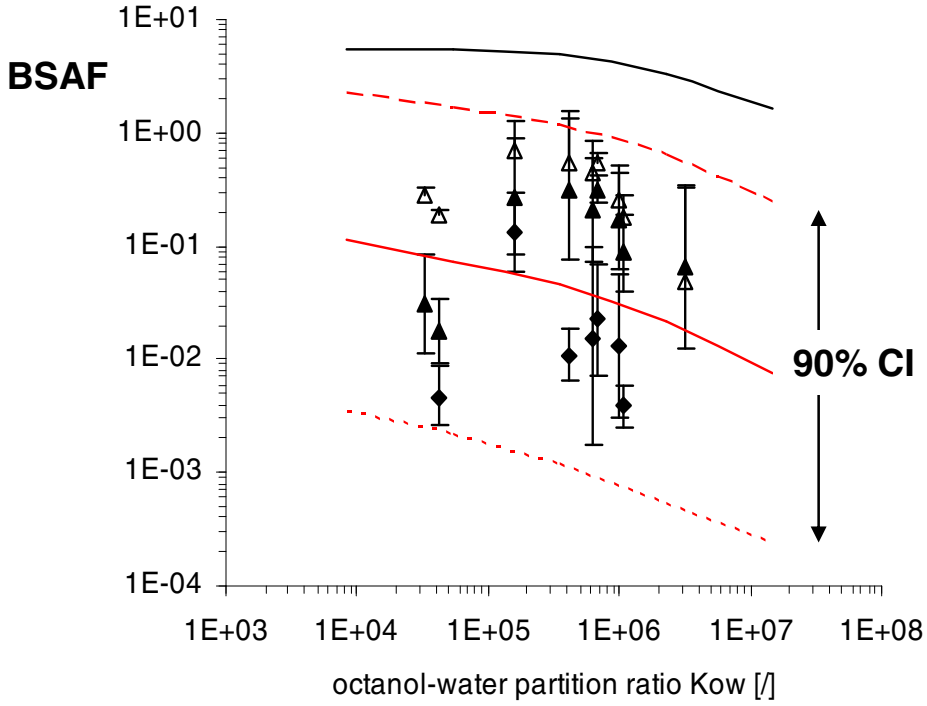
3. BC-inclusive Probabilistic Modeling of PAH Food chain accumulation in the field

- → Dataset from Hauck *et al*
- → 518 measured BSAFs from six studies
- → Marine field experiments, marine ecosystem, freshwater ecosystems, forest soils
- → Uncertainty analysis BC parameters, K_f, n_F, f_{BC}, using Monte Carlo simulations

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

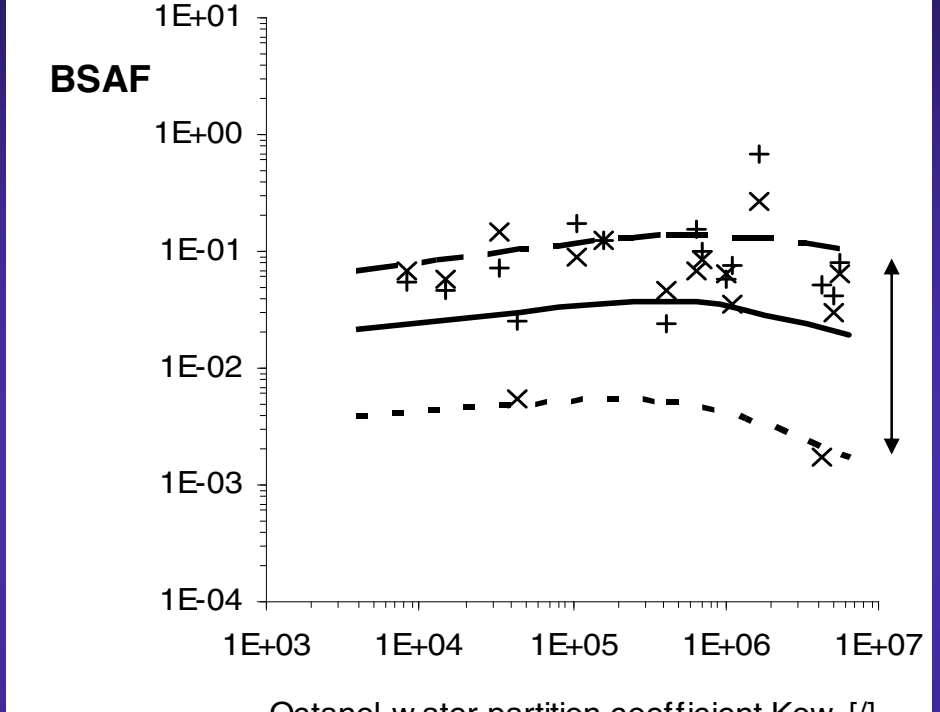
Hauck M., A.J. Hendriks, M.A.J. Huijbregts, A.A. Koelmans, M.J. Van de Heuvel-Greve, C.T.A. Moermond, K. Veltman, A.D. Vethaak. 2007. Including sorption to black carbon in modelling bioaccumulation of polycyclic aromatic hydrocarbons: Uncertainty analysis and comparison with field data. *Environ. Sci. Technol.* **41**:2738-2744.

3. BC-inclusive Probabilistic Modeling of PAH Food chain accumulation in the field



▲,Δ mussels; ♦ chironomids; ___ No soot sorption

- Uncertainty: 3 orders of magnitude
- Devation from model up to factor ten



+ *A. marina*; x *C. edule*

- Uncertainty: 2 orders of magnitude
- Devation from model up to factor three

WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

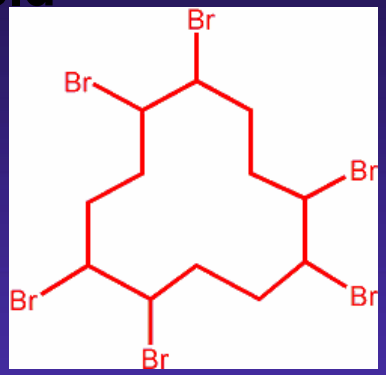
Hauck M., A.J. Hendriks, M.A.J. Huijbregts, A.A. Koelmans, M.J. Van de Heuvel-Greve, C.T.A. Moermond, K. Veltman, A.D. Vethaak. 2007. Including sorption to black carbon in modelling bioaccumulation of polycyclic aromatic hydrocarbons: Uncertainty analysis and comparison with field data. *Environ. Sci. Technol.* **41**:2738-2744.

Conclusions from sensitivity / uncertainty analyses:

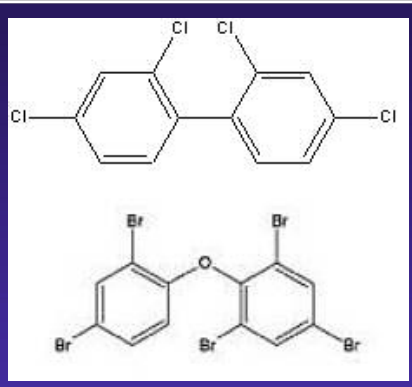
- Soil-lab data Kp (manual SI):
  $K_{F,BC} > n_{F,BC} >> K_{OC}$
- Indoor Mesocosm data fish (Monte Carlo SI):
  $n_{F,BC} > K_{F,BC} >$ biotransformation rate k_m
- Field data (f_{BC} estimated) (Monte carlo UA):
  $f_{BC} >> n_{F,BC} = q > K_{F,BC}$

Thank you

4. BC-inclusive Dynamic Modeling of Brominated Fame Retardants in the field

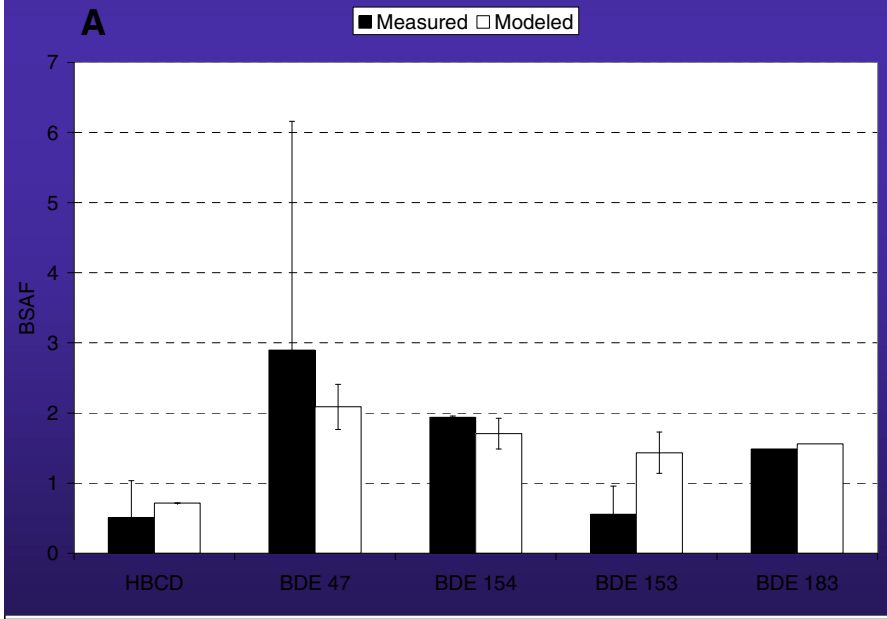


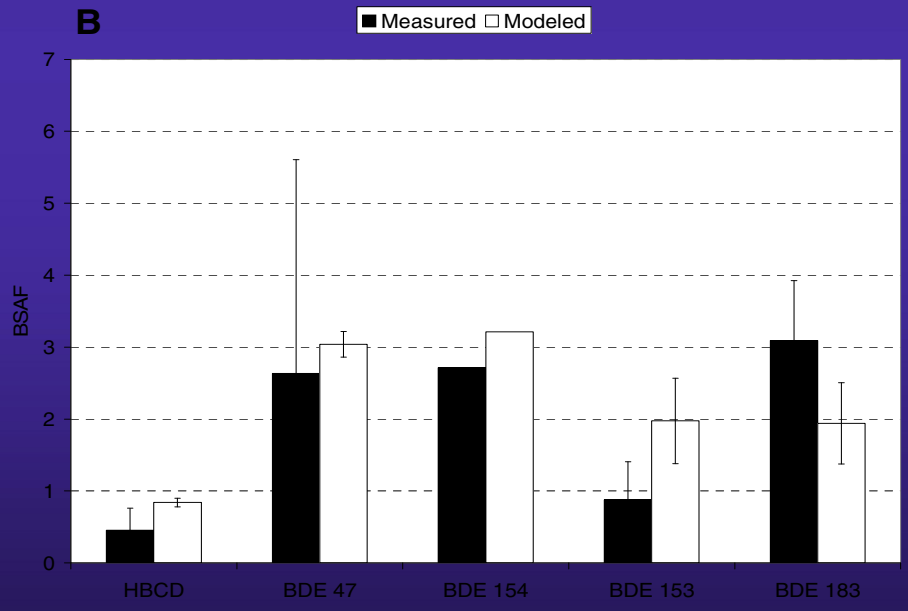
→ Barbel and Bleak, Cinca river, Spain



HBCD Hexabromocyclododecane

PBDE Polybromodiphenylether 47, 100, 153, 154, 183





WAGENINGEN UNIVERSITY
ENVIRONMENTAL SCIENCES

Van Beusekom O.C., E. Eljarrat, D. Barceló and **A.A. Koelmans**. 2006. Dynamic modelling of food chain accumulation of brominated flame-retardants in fish from the Ebro river basin, Spain. *Environ. Toxicol. Chem.* **25**:2553-2560.