

Assessment and improvement of plant uptake and cattle biotransfer models used in exposure assessment tools for soils contaminated with organic pollutants

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Contents of the talk

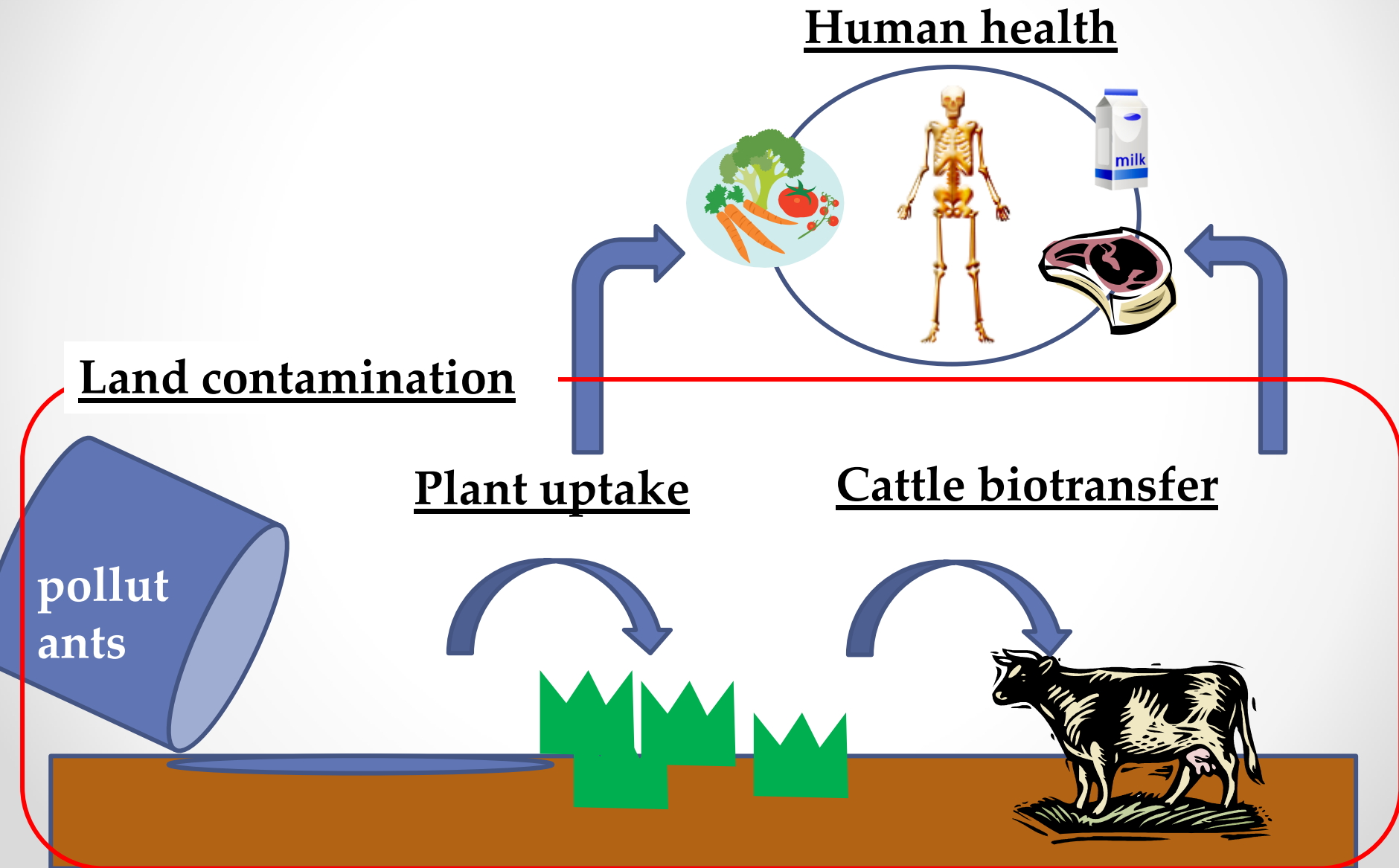
- Overview of my research
- Modelling on plant uptake
- Modelling on cattle transfer

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- **Overview of my research**
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Overall image of my research

~Exposure modelling, risk assessment and management of organic pollutants



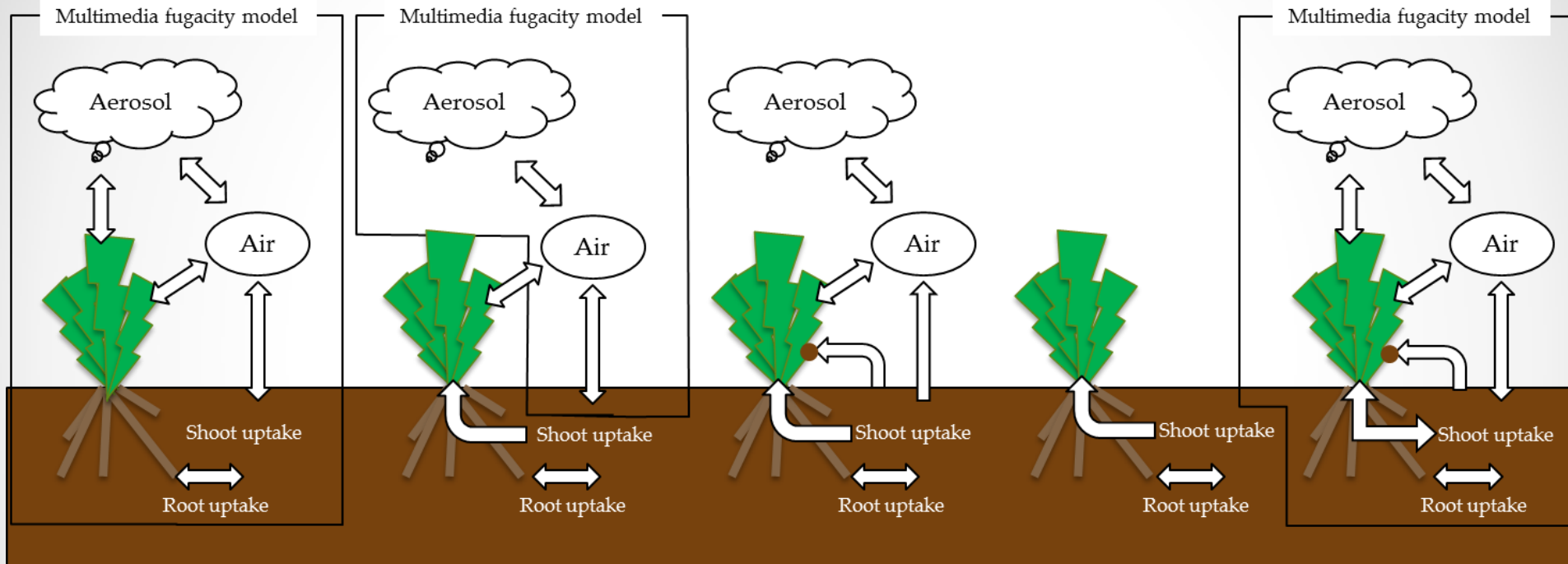
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- Modelling on cattle transfer

Plant uptake model

~Do existing models represent the real world ?

- 5 models for estimating plant uptake



RAIDAR

EUSES

CSOIL

CLEA

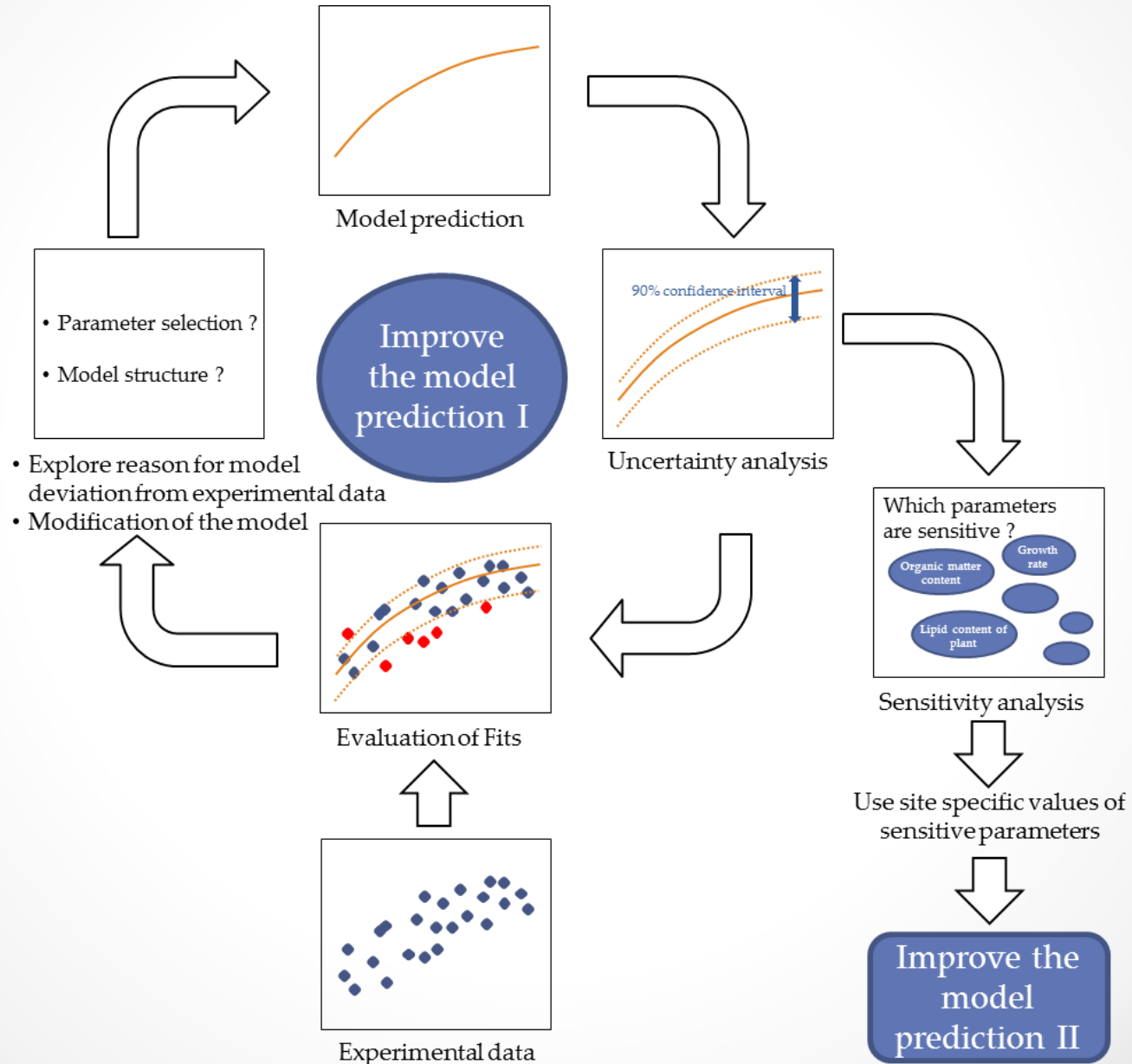
CalTOX

- 74 chemical data for root uptake
- 39 chemical data for shoot uptake (PCBs, PAHs, CBs, pesticides)

Bioconcentration factor (BCF) = concentration in plant / concentration in soil

Plant uptake model

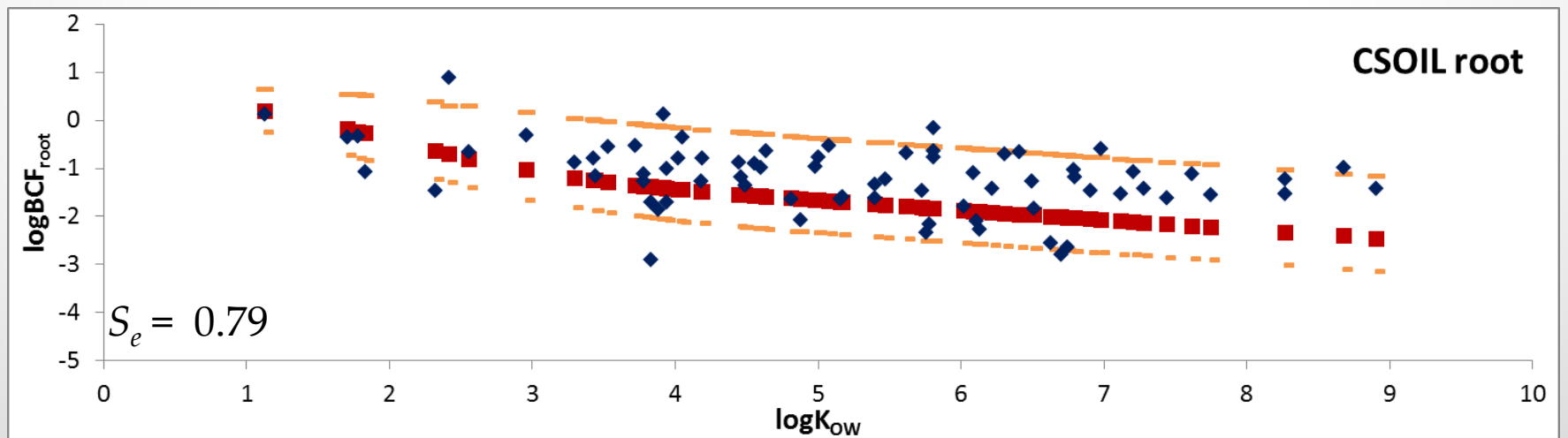
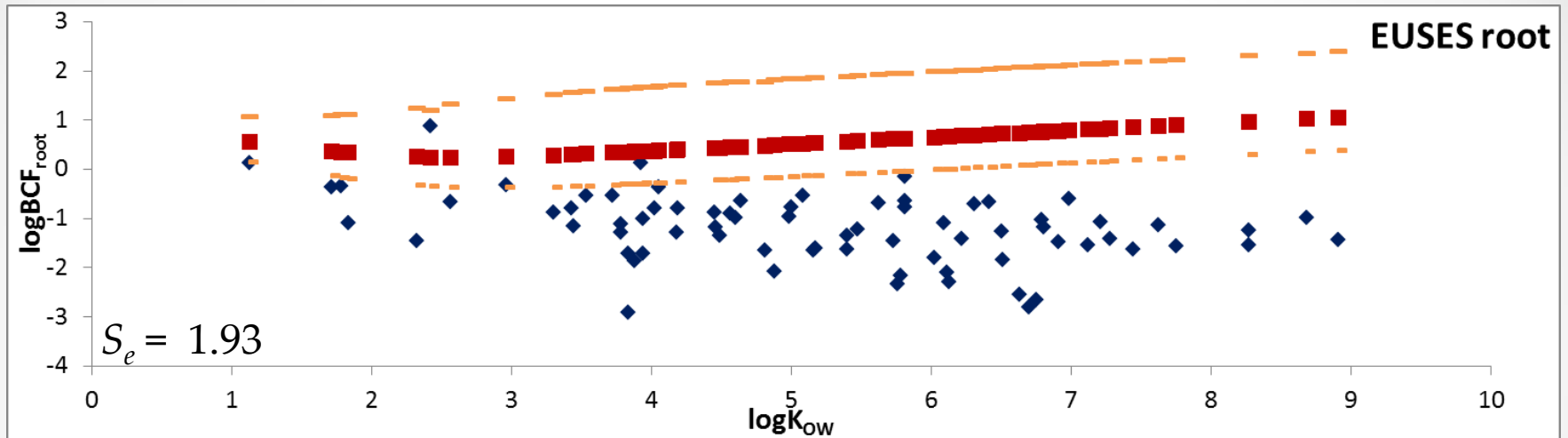
~Do existing models represent the real world ?



Root uptake model

~Do existing models represent the real world ?

Models used : RAIDAR, EUSES, CSOIL, CLEA, CalTOX

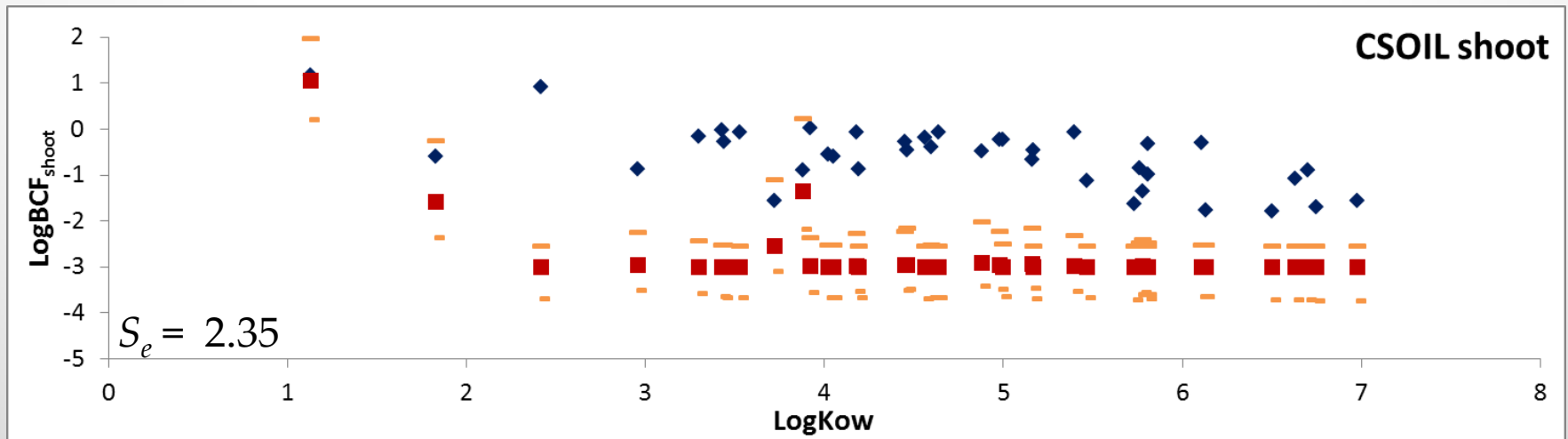
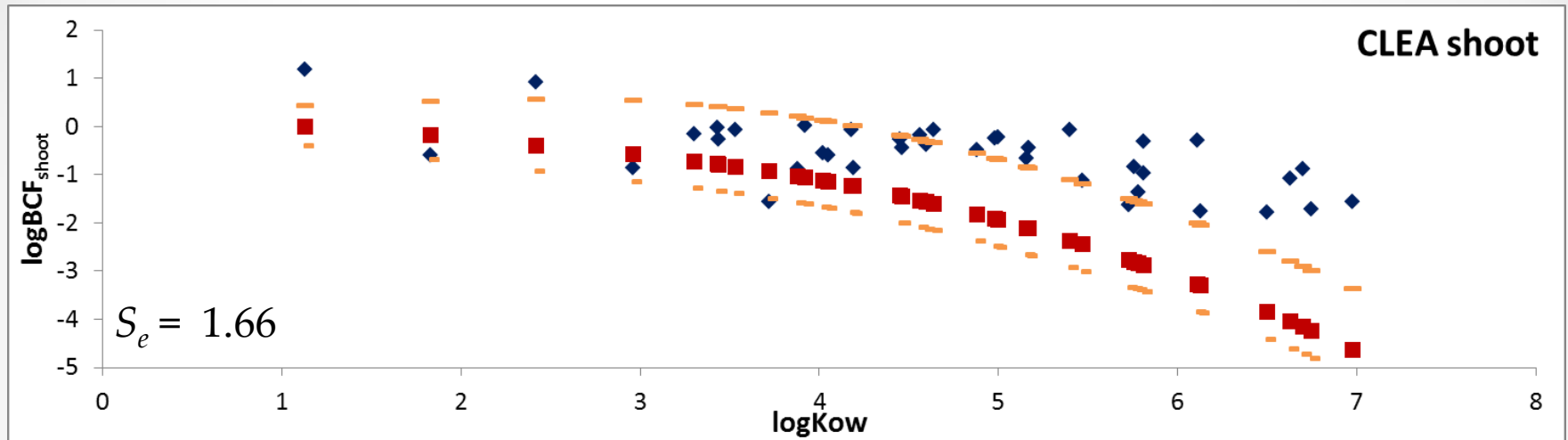


● Blue : experimental data, Red : model prediction, Orange : 90% prediction interval ●

Shoot uptake model

~Do existing models represent the real world ?

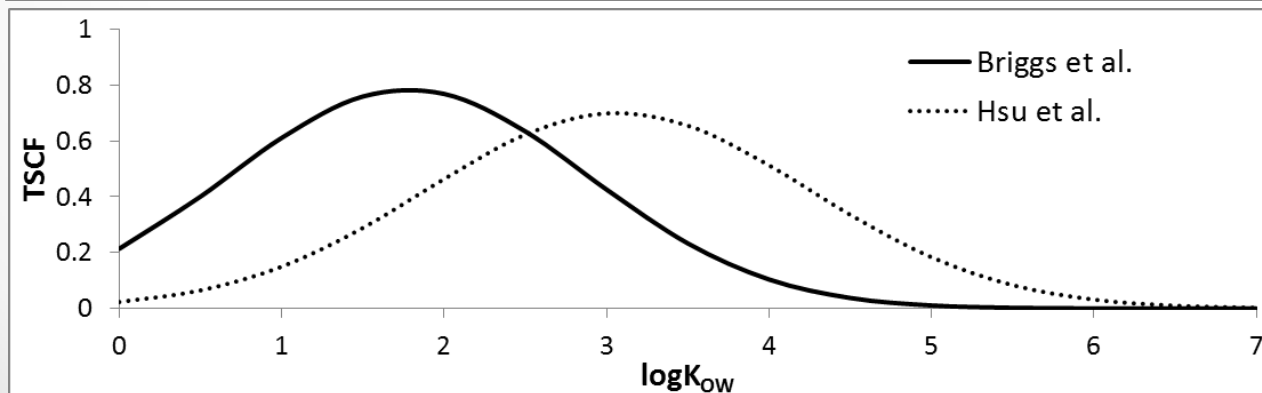
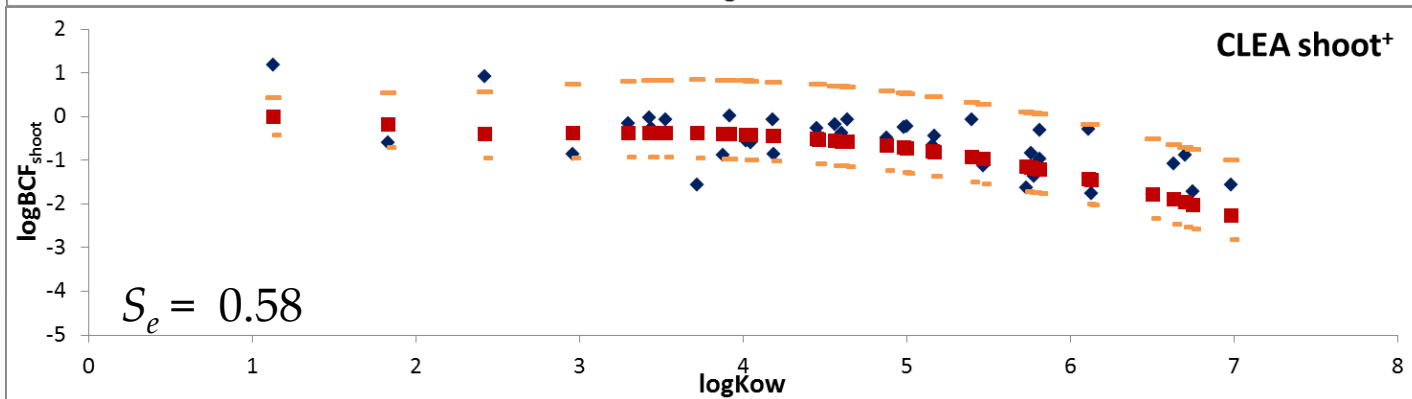
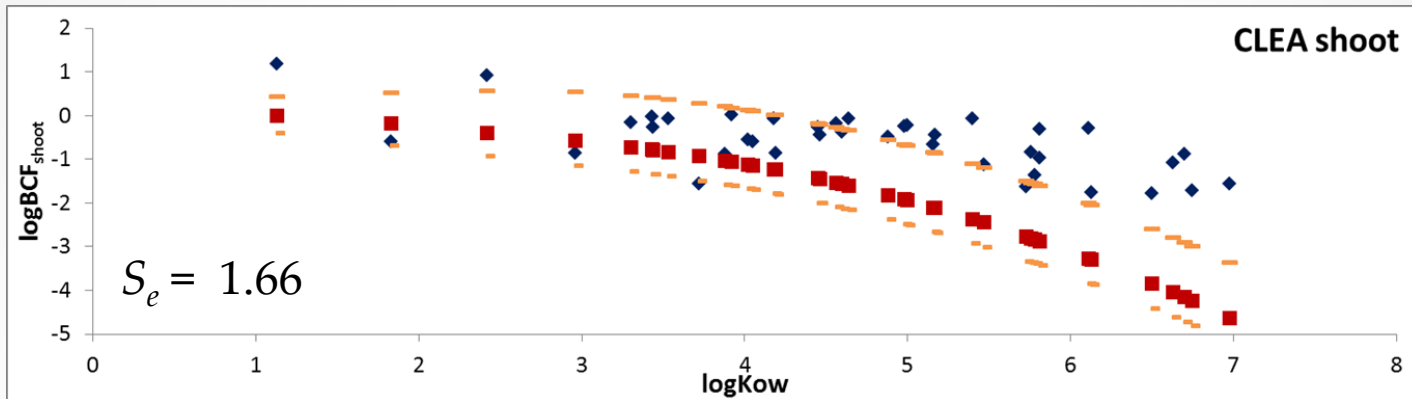
Models used : RAIDAR, EUSES, CSOIL, CLEA, CalTOX



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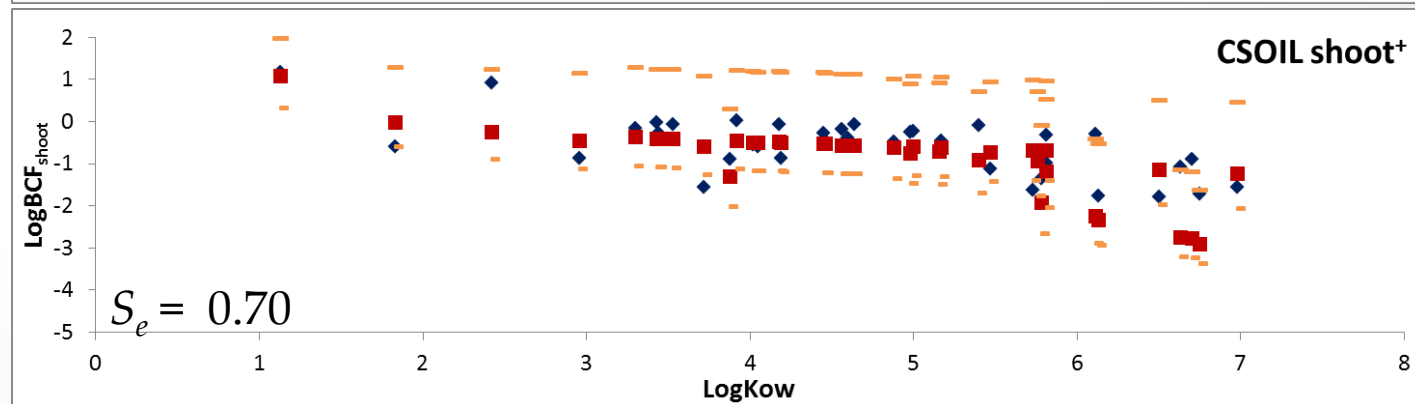
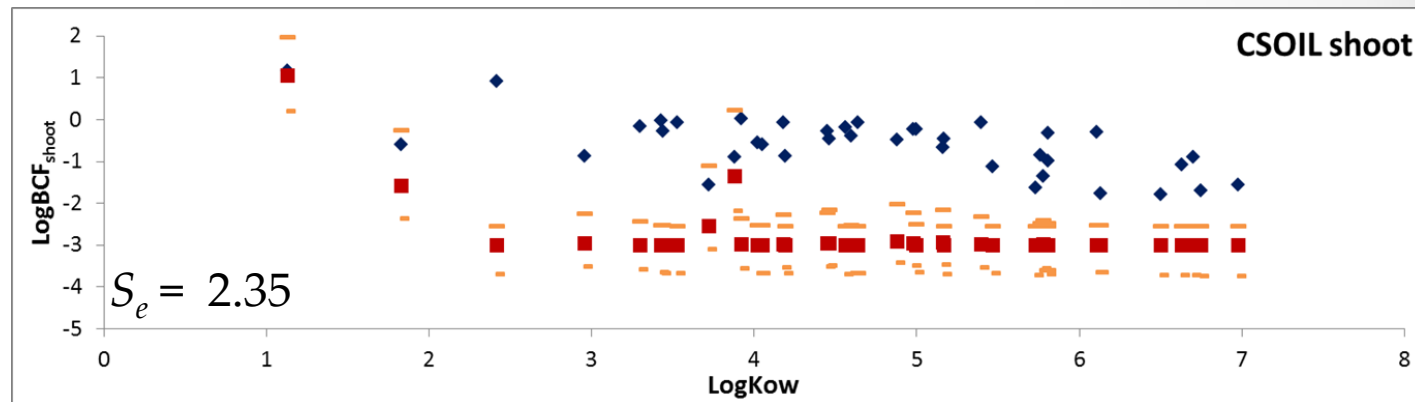
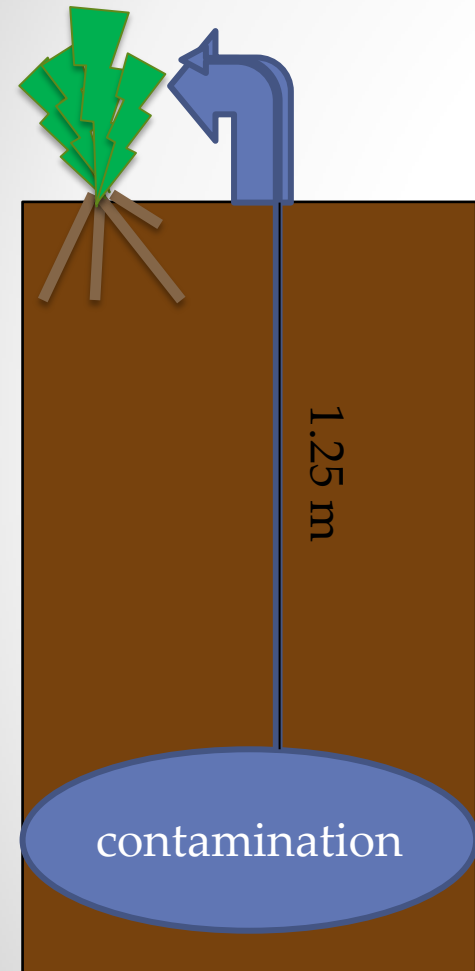
Modification of CLEA shoot model

~ focus on transpiration stream concentration factor (TSCF)



Modification of CSOIL shoot model

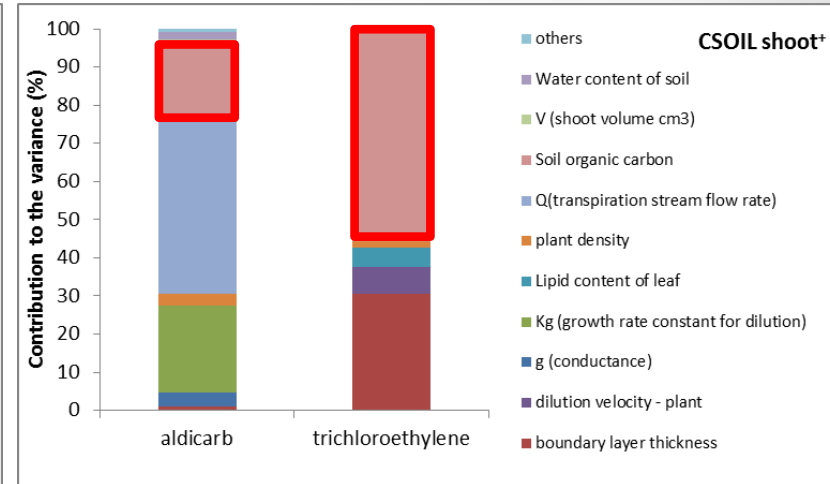
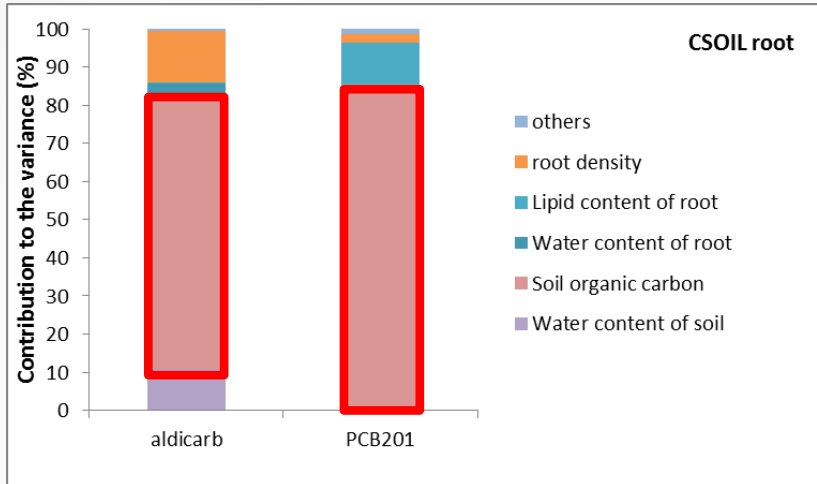
~ focus on soil-air-plant pathway



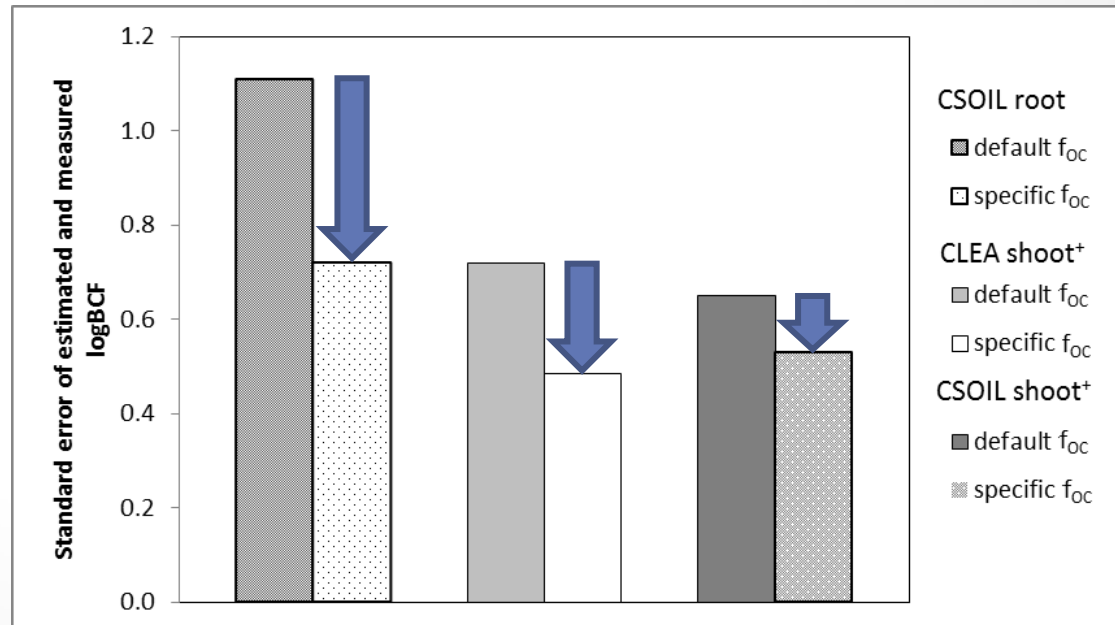
Improvement of the model performance

~ focus on the sensitive parameter (soil organic carbon content (f_{OC}))

Sensitivity analysis



Soil organic carbon content:
Default value → Specific value



Summary of the modelling on Plant uptake

- Model assessments identified the CSOIL model to reproduce the observed root uptake of organic chemicals most accurately.
- None of the models simulated the observed shoot uptake of chemicals well.
- Modifications to transpiration and volatilisation for shoot uptake enable a much improved performance of the CSOIL and CLEA models.
- Soil organic carbon content was a particularly sensitive parameter in all the models tested, and using a site specific value reduced the standard errors substantially between model estimation and observations.



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- **Modelling on cattle transfer**

Cattle biotransfer model

~Do existing models represent the real world ?

- 10 models for estimating milk and beef transfer

Regression-based models

- Travis & Arms
- EUSES
- CalTOX
- Maclachlan & Bhula
- RTI
- Dowdy et al.



Mechanistic models

- RAIDAR
- ACC-HUMAN
- OMEGA
- CKow

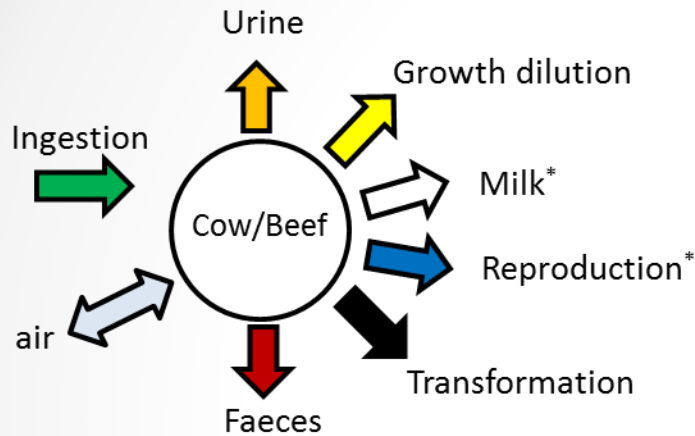
- 129 chemical data for milk transfer
- 91 chemical data for meat transfer (PCBs, PCDD/Fs, PBDEs, pesticides...)

Biotransfer factor (BTF) = concentration in milk or meat / chemical daily intake

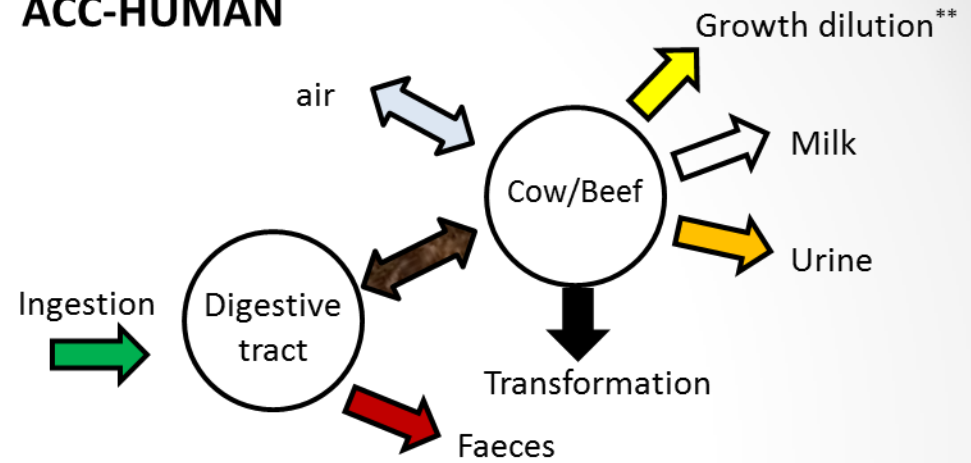
Cattle biotransfer model

~Do existing models represent the real world ?

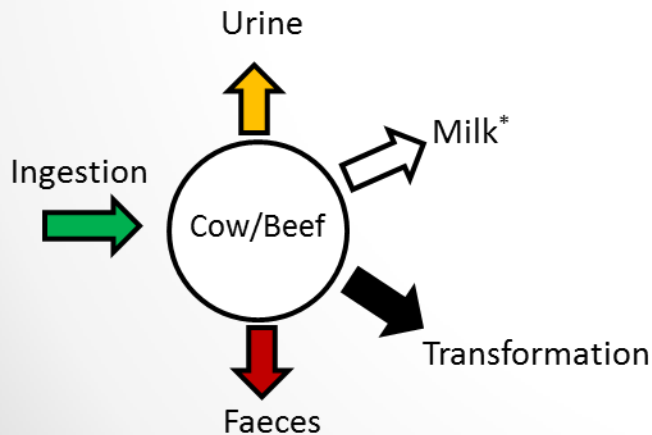
RAIDAR



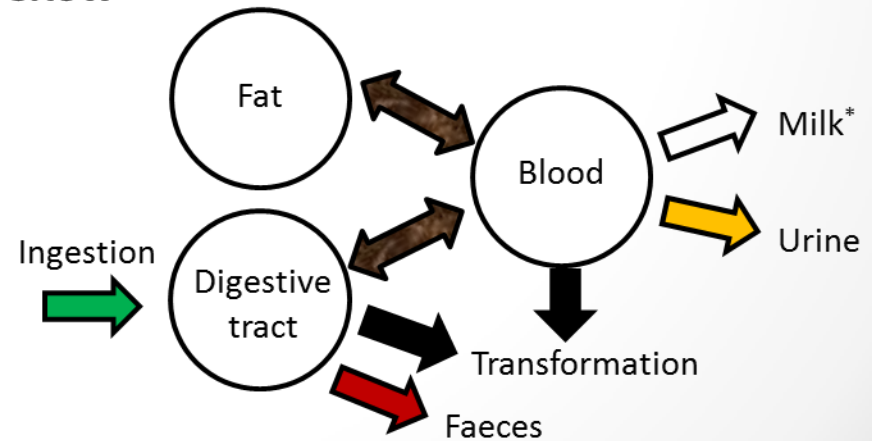
ACC-HUMAN



OMEGA



CKow

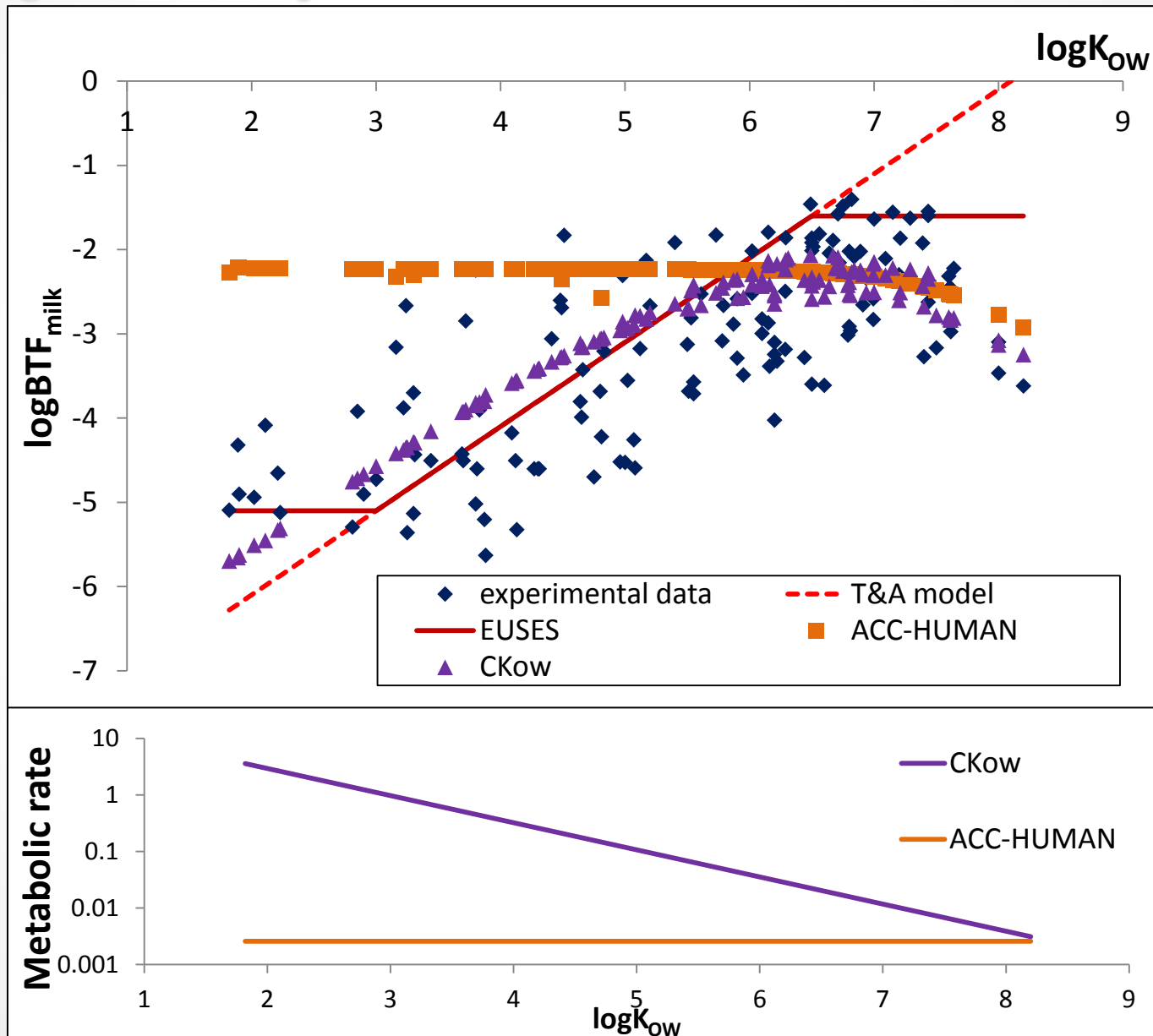


*Only for lactating cow. **Only for non-lactating beef

Cattle biotransfer model

~Do existing models represent the real world ?

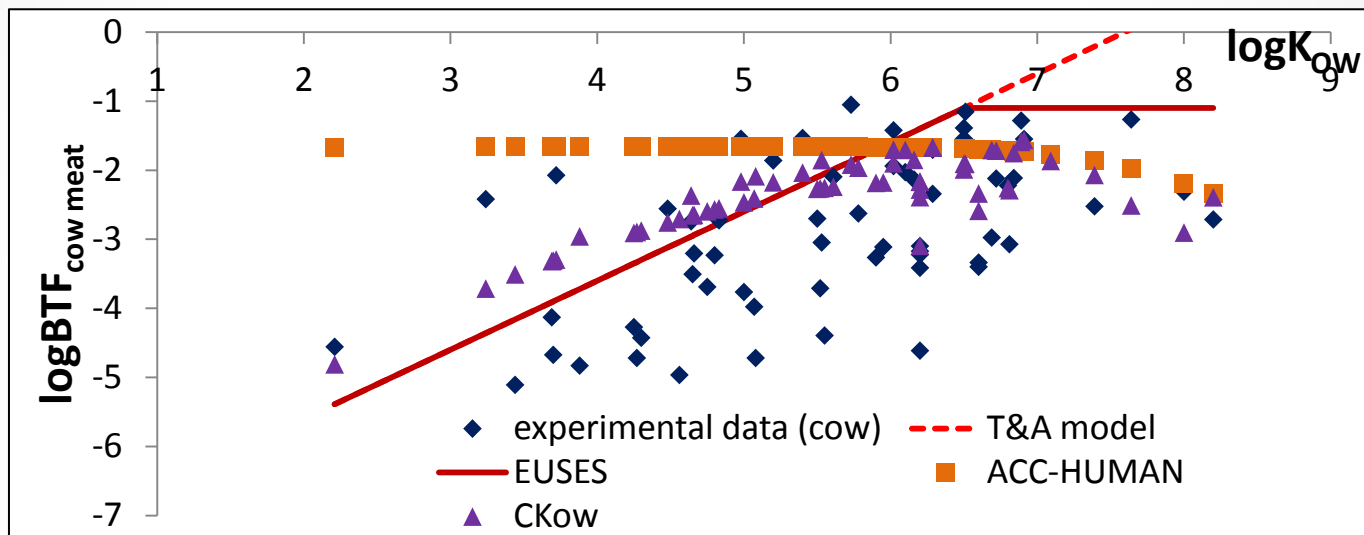
Milk



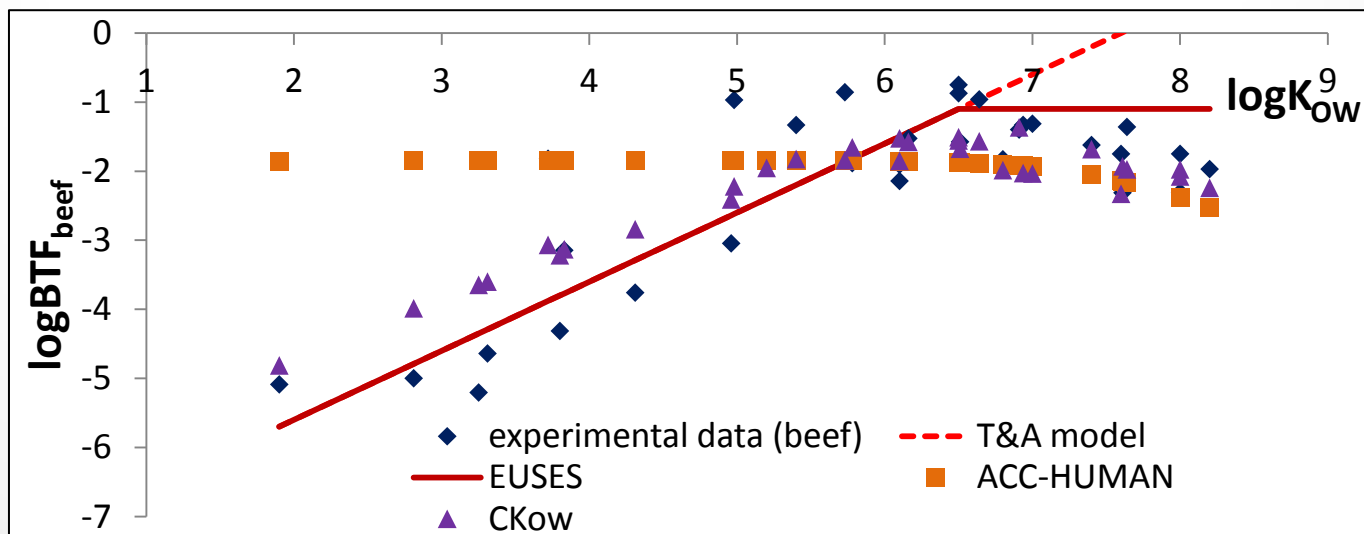
Cattle biotransfer model

~Do existing models represent the real world ?

Cow meat

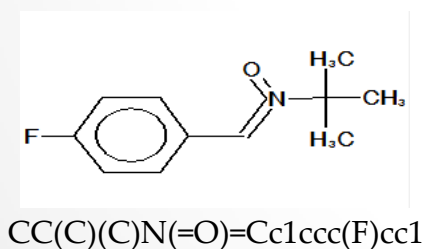
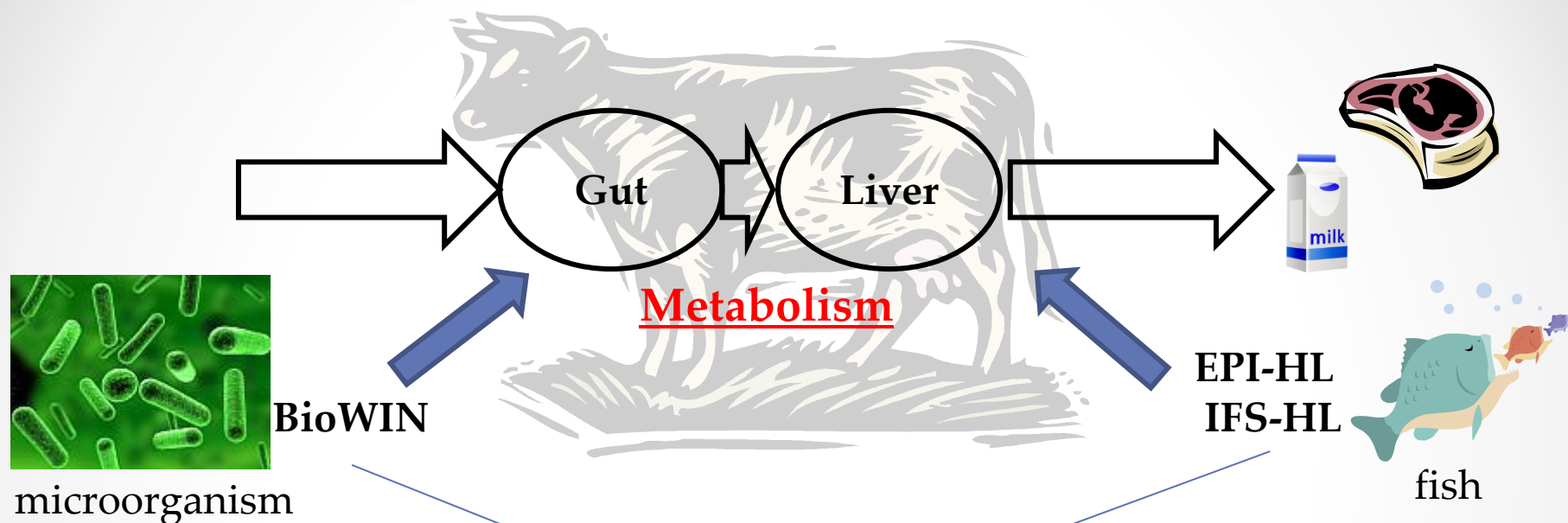


Beef

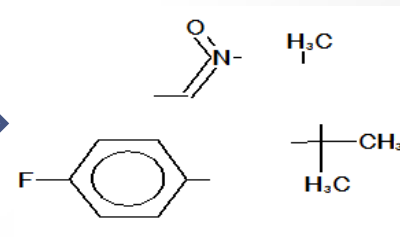


Cattle biotransfer model

~ Can the metabolic rate in cattle be simply predicted?



Biodegradation
QSAR Model

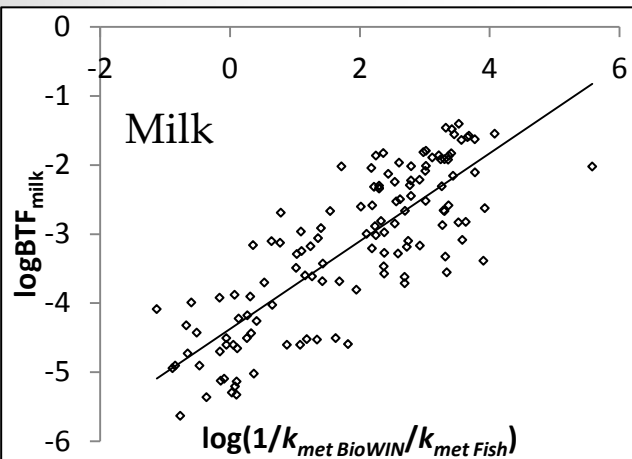


Half life, Metabolic rate

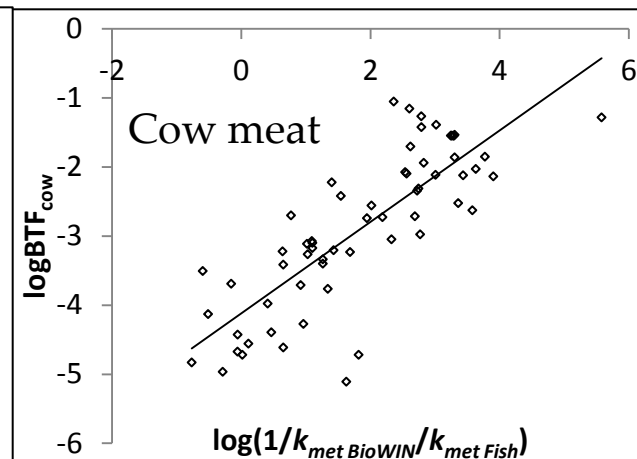
Cattle biotransfer model

~ Brand new regressions using simulated metabolic rate

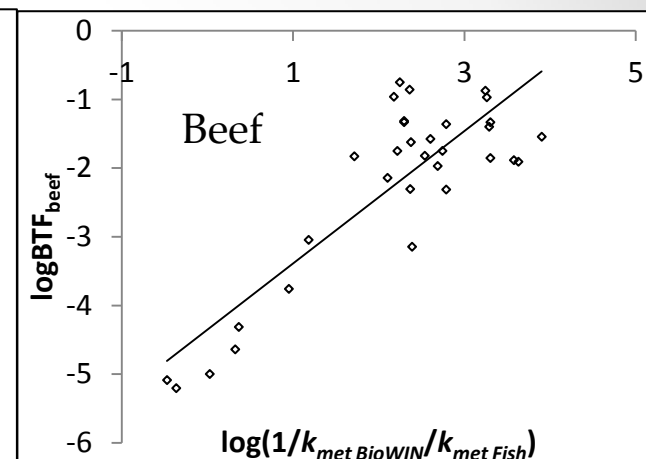
Simulated metabolic rate v logBTF



$$R^2 = 0.68, S_e = 0.63$$

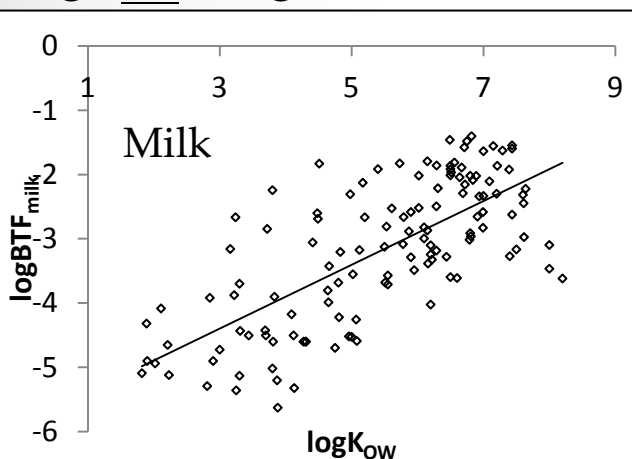


$$R^2 = 0.65, S_e = 0.67$$

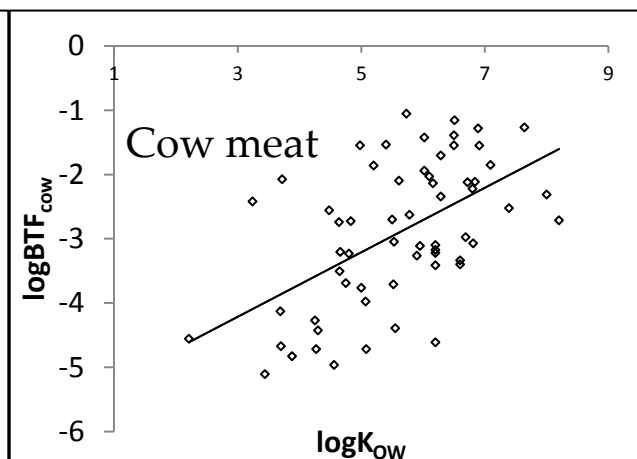


$$R^2 = 0.73, S_e = 0.70$$

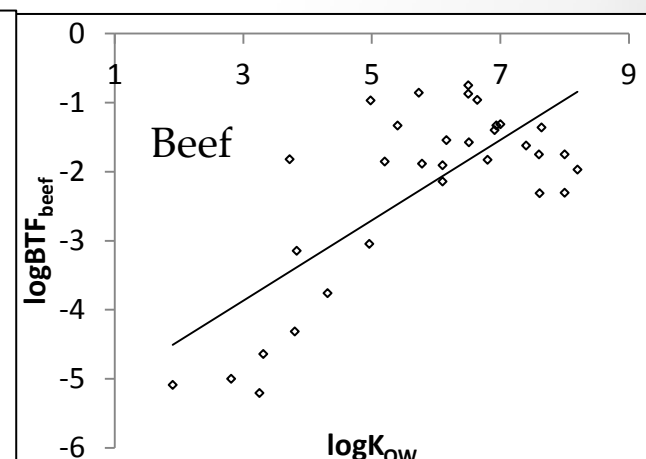
logK_{OW} v logBTF



$$R^2 = 0.51, S_e = 0.78$$



$$R^2 = 0.30, S_e = 0.94$$

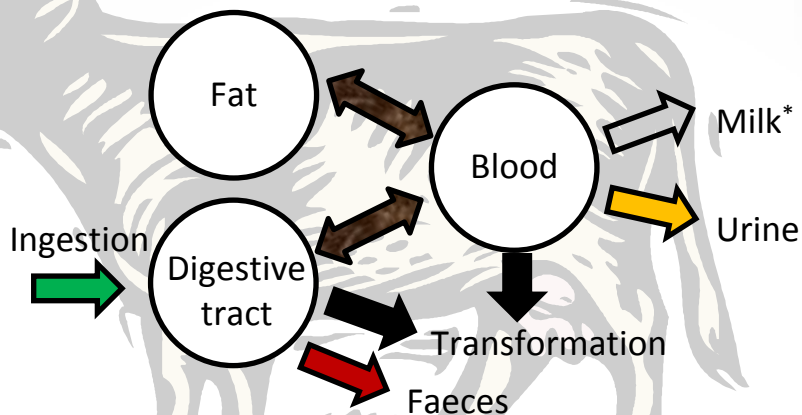
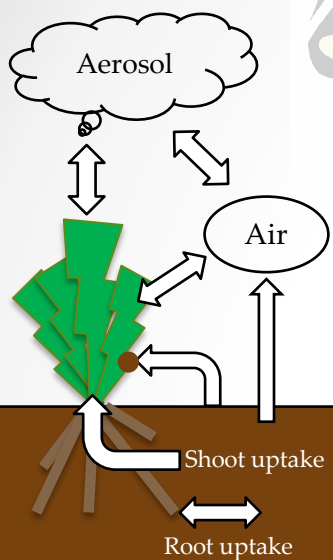


$$R^2 = 0.55, S_e = 0.90$$

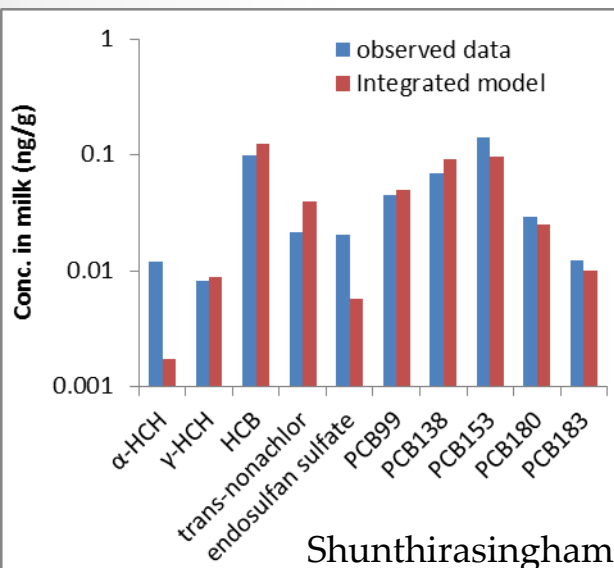
Summary of the modelling on Cattle transfer

- About 130 chemical data showed that cattle biotransfer of organic pollutants has too much variability to be estimated well by existing models.
- Metabolic rate in cattle was a crucial parameter to estimate the biotransfer but it could not easily be obtained.
- The metabolic rate in cattle was simulated using biodegradation QSAR models and the brand new regressions for the simulated metabolic rate showed the best performance of all models including the most popular K_{OW} regression.

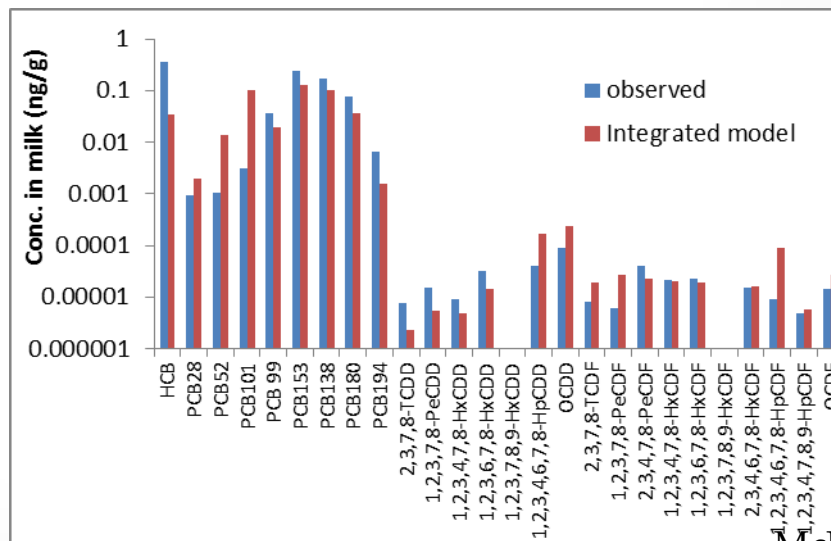
Integrated model



Given : concentration in soil (and air)
 Predicted: concentration in milk and meat



Shunthirasingham et al. 2013



McLachlan 1996

Thank you very much !