Using exposure models to identify data gaps and develop knowledge infrastructure

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Emerging exposure science for developing chemical regulatory policy:

REACH, Biocides, TSCA reform

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SETAC

UNIVERSITY OF TORONTO SCARBOROUGH

International Society of Exposure Science

Science for Better Environmental Health

Presentation overview

- Chemical assessment programs
  - Objective: protect environment and human health
  - Method: quantify exposure and potential risk
  - Problem: large number of chemicals; few measure data, uncertainty is substantial, needs to be addressed, where to start?
- Mass balance and Quantitative Structure-Activity (Property) Relationship (QSA(P)R) models needed for screening and prioritization
  - "PBT categorization" & "holistic multimedia exposure"
- Multimedia exposure models and uncertainty analysis can be used to identify data gaps and "reduce uncertainty"
  - Case study: RAIDAR model and human exposure assessment

Evaluating "P": single compartment half-lives

e.g., Canada's "P" Regulations (2000):

Environmental Medium	Half-Life (*HL*)
Air	$\geq$ 2 days
Water	$\geq$ 182 days
Soil	$\geq$ 182 days
Sediment	> 365 days

Evaluate: compare medium specific *HL*s to criterion

"Pass / Fail"; uncertainty not addressed

Often process includes a fate model calculation, EQC

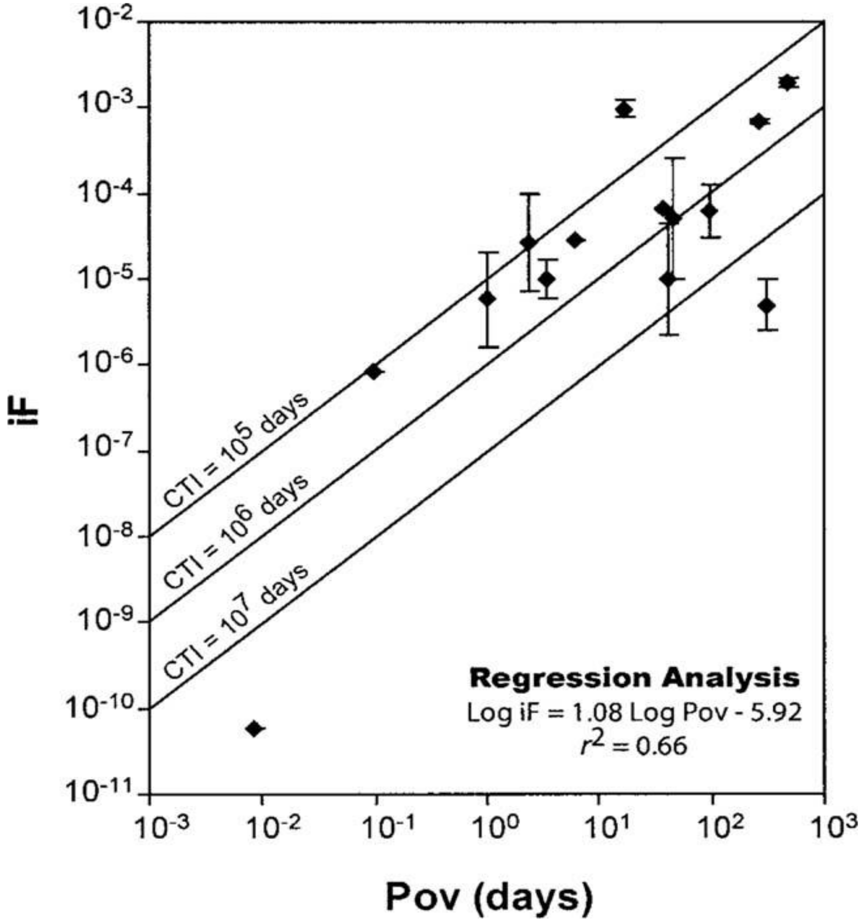
Data available for "P" assessments

- Case study:
- Canadian Domestic Substances List (DSL) ~11,000 organic chemicals (Categorization CD-ROM)
  - Water – Soil – Sediment half-lives:
  - "shake flask" biodegradation data, i.e., BOD (<10% of DSL)
  - **"Measured" environmental half-lives (12 DSL chemicals)**
  - Not a trivial task – high degree of variability and uncertainty
  - "QSARs" used in absence of measured data

P_{OV} – human *iF* relationships

Intake Fraction (*iF*) = Intake rate / Emission rate

Provides comparisons for <u>relative exposure potential</u>



CalTOX model

No strong relationships between *iF* and environmental medium specific half-lives

Suggests human far-field exposure potential is a function of the “whole environment”

MacLeod and McKone *ET&C* **2004**

Evaluating “B”: aquatic paradigm

e.g., Canada’s “B” Regulations (2000):

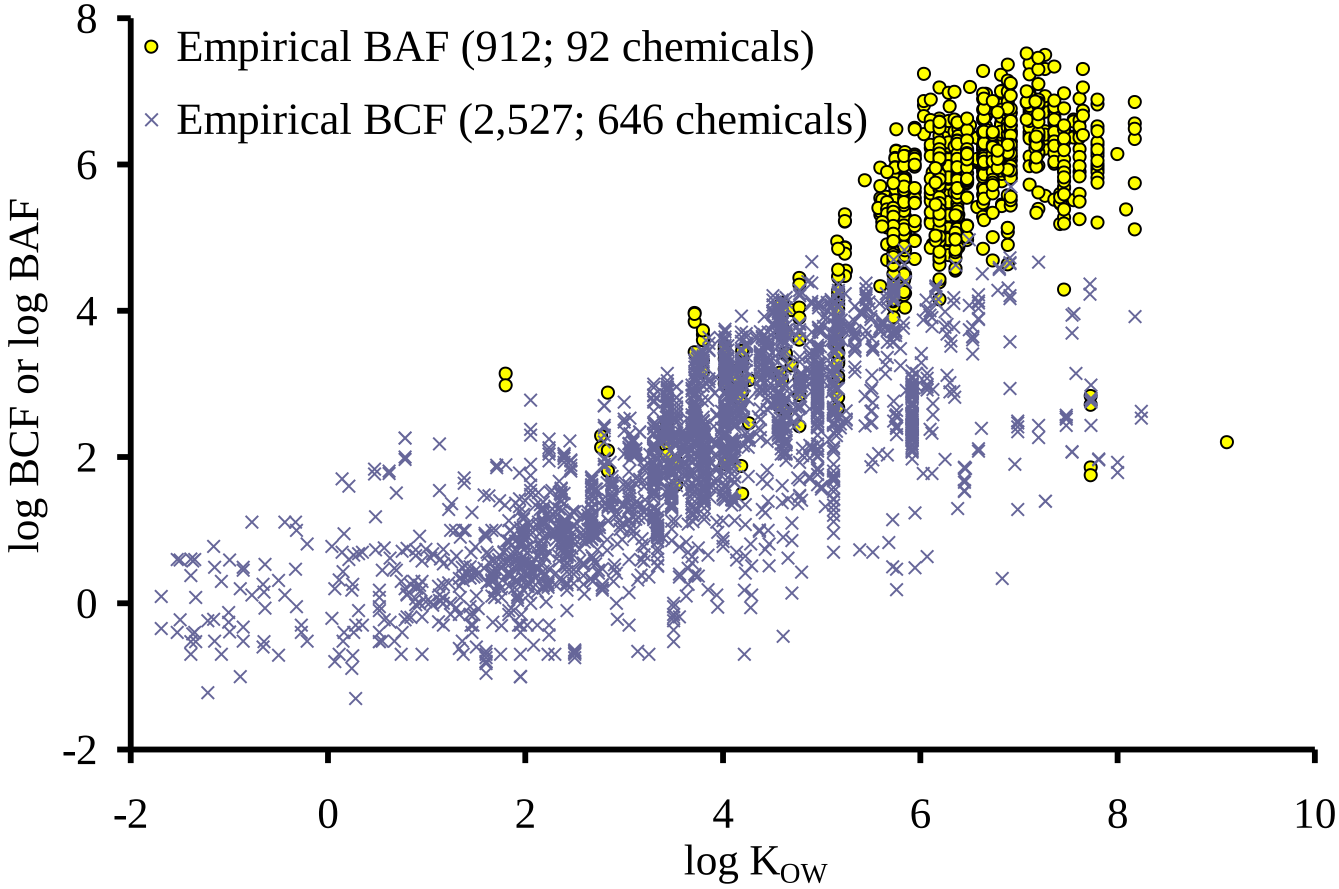
Parameter	Value
Bioaccumulation factor (BAF)	$\geq$ 5,000
Bioconcentration factor (BCF)	$\geq$ 5,000
Octanol-water partition coefficient (log K_{OW})	$\geq$ 5

All endpoints with respect to aquatic organisms, i.e., fish

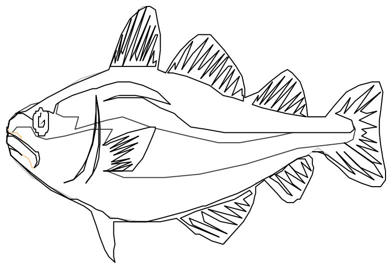
“Pass / Fail”; uncertainty not addressed

Data available for "B" assessments

Measured BCF or BAF < 4% of DSL



Measured K_{OW} < 10% of DSL



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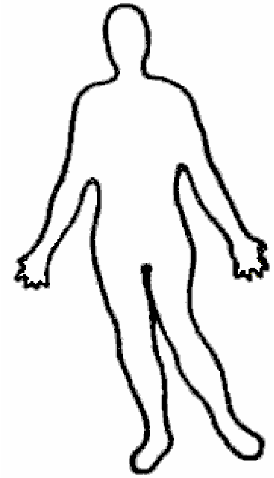

Environ. Sci. Technol. 2007, 41, 4019−4025

A Terrestrial Food-Chain Bioaccumulation Model for POPs

JAMES M. ARMITAGE AND
FRANK A. P. C. GOBAS*

criterion for identifying
Because empirical BCFs do
of commercial substances i
has applied an aquatic
model to derive the BAF of
Domestic Substances List.
riate for identifying bio

Environ. Sci. Technol. 2001, 35, 325−334

Bioaccumulation of Persistent Organic Pollutants in Lichen—Caribou—Wolf Food Chains of Canada's Central and Western Arctic

BARRY C. KELLY AND
FRANK A. P. C. GOBAS*

concentrations in higher trophic level organisms that exceed those concentrations in the organism's prey (*4−8*). Many of these compounds are also resistant to chemical degradation, giving them long half-lives in the environment. Long-lived organic contaminants that can biomagnify in food chains and may ultimately cause toxic effects have since been classified as persistent organic pollutants (POPs).

Regulatory agencies in Canada, the United States, and Europe have attempted to control the use of first-generation POPs (e.g., PCBs, dioxins, DDT) by either banning or reducing their emission into the environment. Canada's recently promulgated Toxic Substance Management Policy (TSMP)

Environ. Sci. Technol. 2011, 45, 197–202

Bioaccumulation of Organic Contaminants in Humans: A Multimedia Perspective and the Importance of Biotransformation†

MICHAEL S. MCLACHLAN,*,‡
GERTJE CZUB,‡ MATTHEW MACLEOD,§
AND JON A. ARNOT‖

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(mol L−1). The *BAF* includes dietary and aqueous exposure, whereas the *BCF* includes only aqueous exposure. Strong correlations between the *BCF* and *BAF* and the octanol:water

Environ. Sci. Technol. 2004, 38, 2406−2412

Bioaccumulation Potential of Persistent Organic Chemicals in Humans

GERTJE CZUB† AND
MICHAEL S. MCLACHLAN*,†,‡

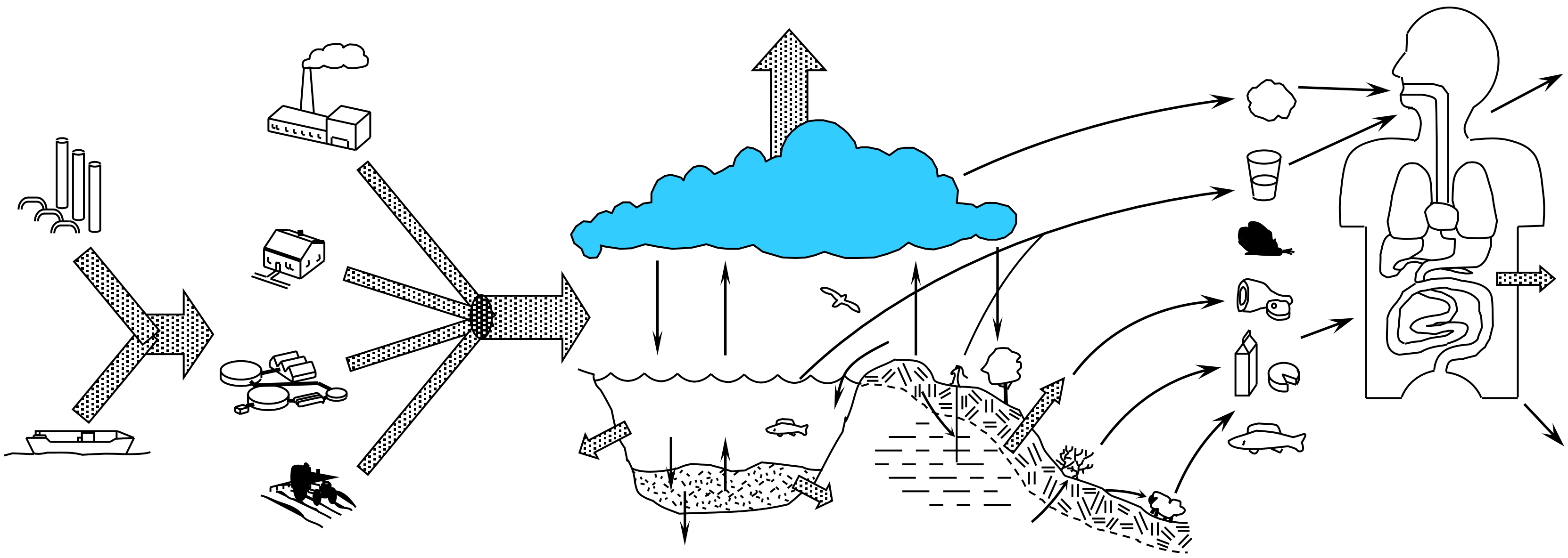
and management of chemicals. In this paper we explore measures of bioaccumulation.

Currently the criterion for identifying bioaccumulative chemicals is a bioaccumulation factor or a bioconcentration factor in aquatic organisms in excess of 5000 or, if these data

Food Web–Specific Biomagnification of Persistent Organic Pollutants

Barry C. Kelly,[1] Michael G. Ikonomou,[2] Joel D. Blair,[1] Anne E. Morin,[1] Frank A. P. C. Gobas[1*]

Conceptual model: far-field human exposure



Chemical emissions

Environmental fate/transport, distribution, degradation, food web bioaccumulation and exposure to humans

Mackay 2001

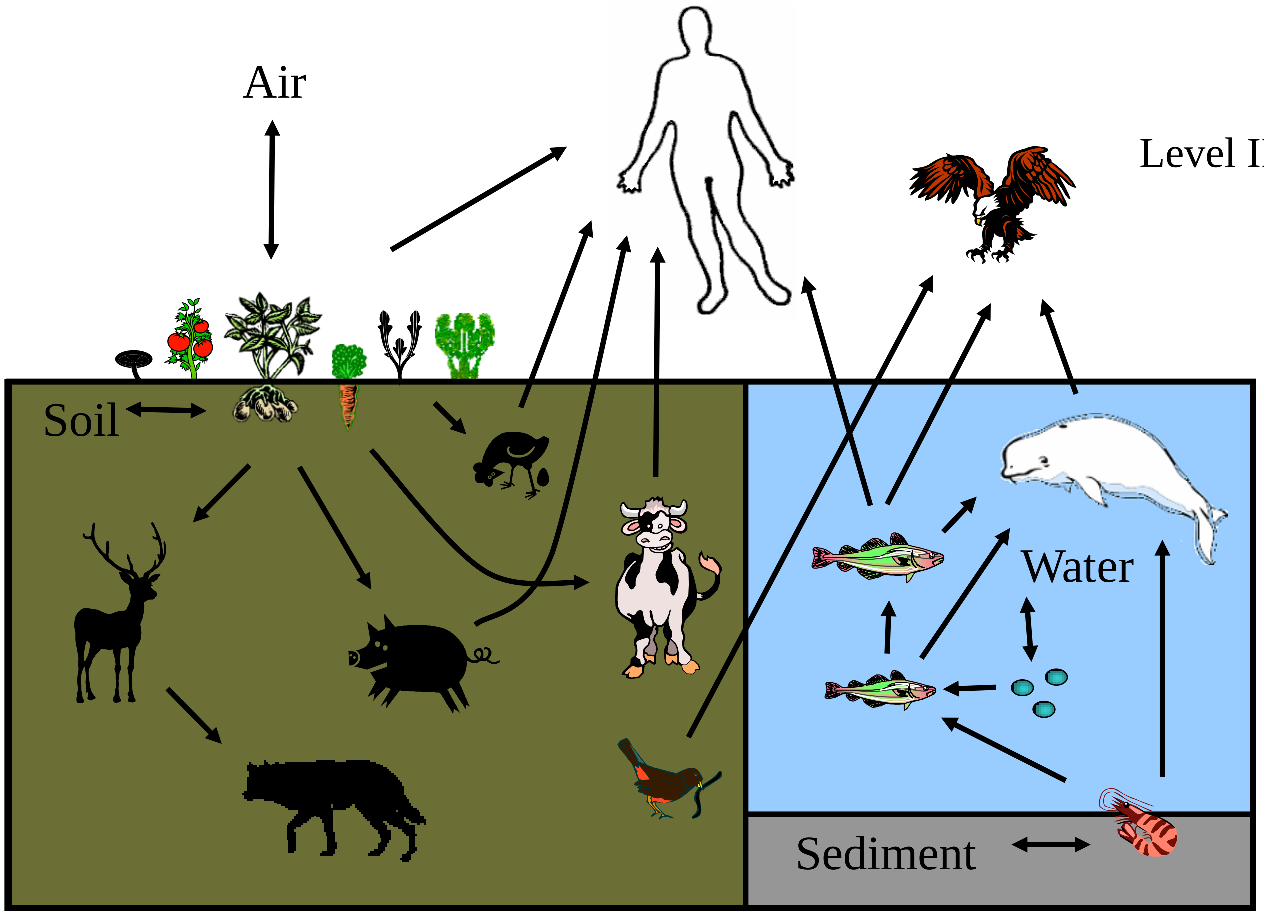
Mass balance exposure models, e.g., RAIDAR

Combined mass balance fate and food web bioaccumulation models for ecological and human exposure (and risk) assessment

100,00 km^2 regional area

Level II or Level III fate calculations

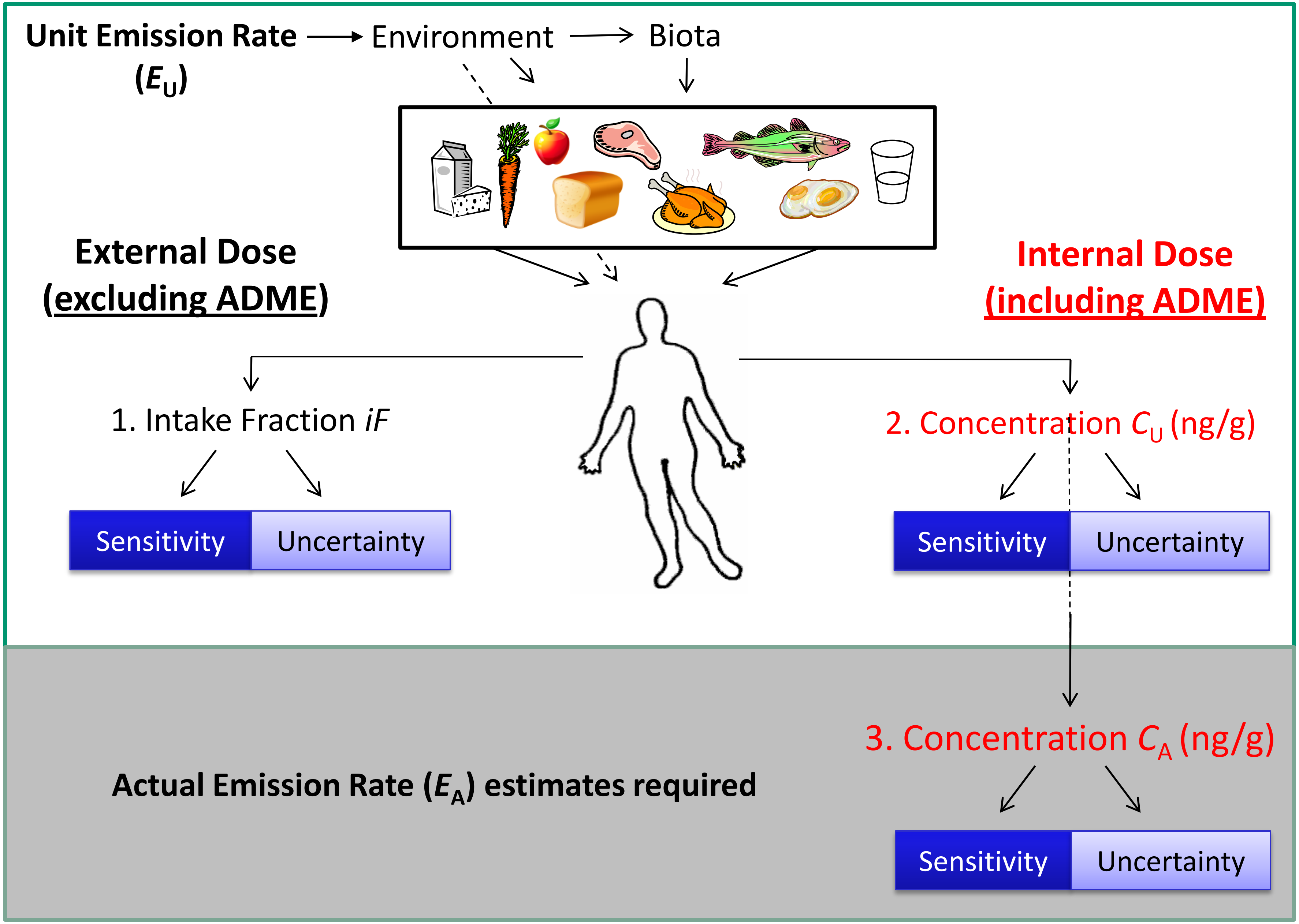
~ CEMC EQC model



Environ Sci & Technol **2006** (V.1.0)

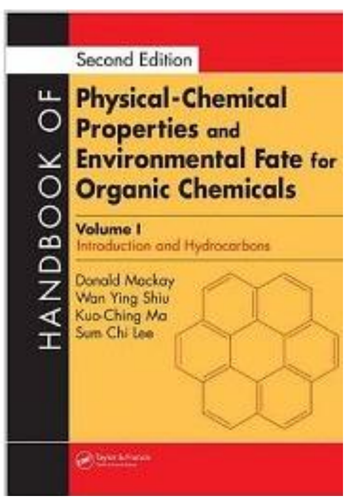
Environ Sci & Technol **2008** (V.2.0)

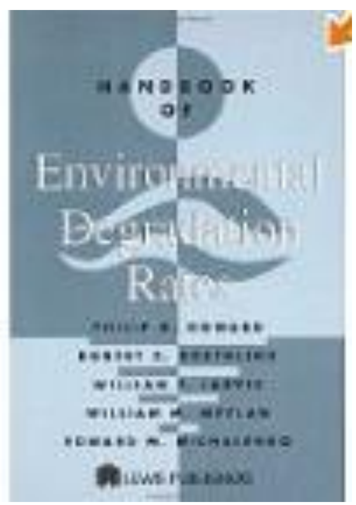
e.g., RAIDAR Human Far-field Chemical Exposure Metrics

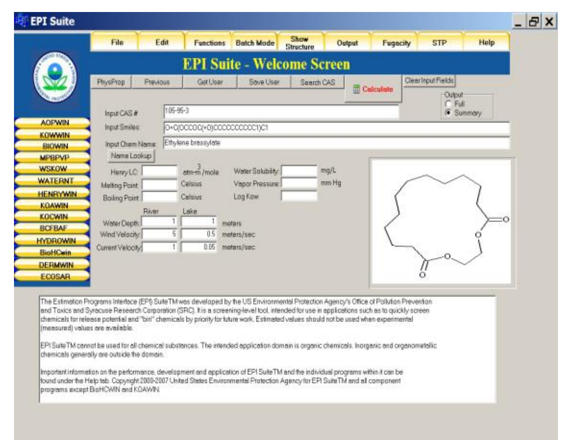


Input requirements for multimedia exposure models

- Phys-chem properties: MW, K_{OW}, K_{AW} (or P and Sw), K_a
- Reaction half-lives (*HL*): air, water, soil, sediment and *biotransformation half-lives in vertebrates*
- Same input parameters required for typical "P&B" categorization model assesments
- C_A estimates require "actual" emission rate estimate (E_A)





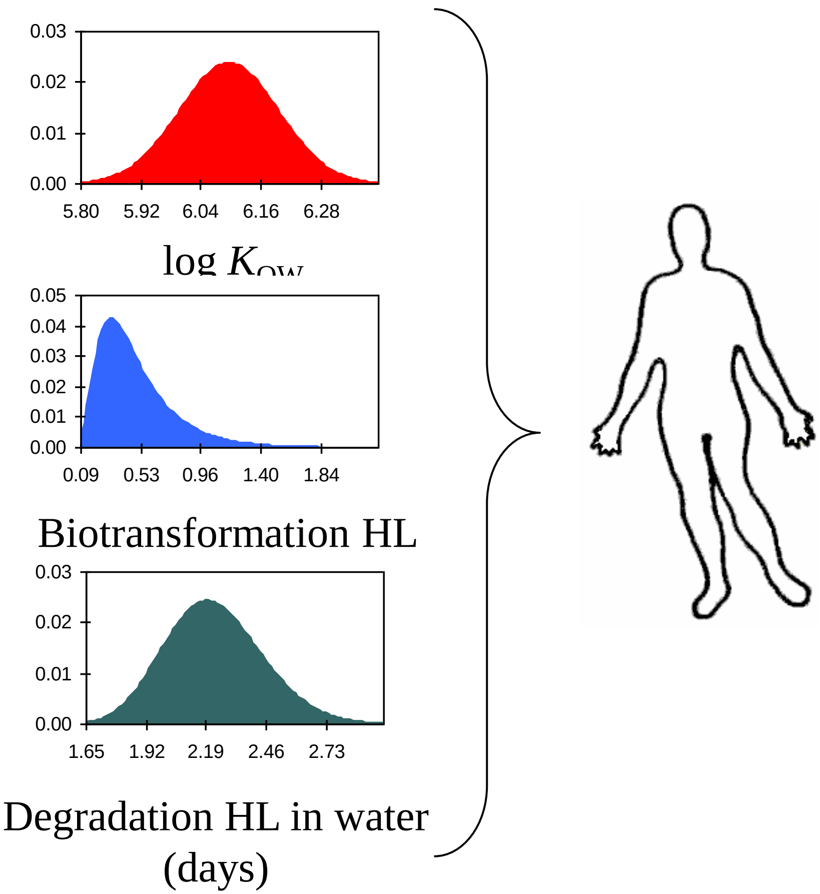


Uncertainty analysis

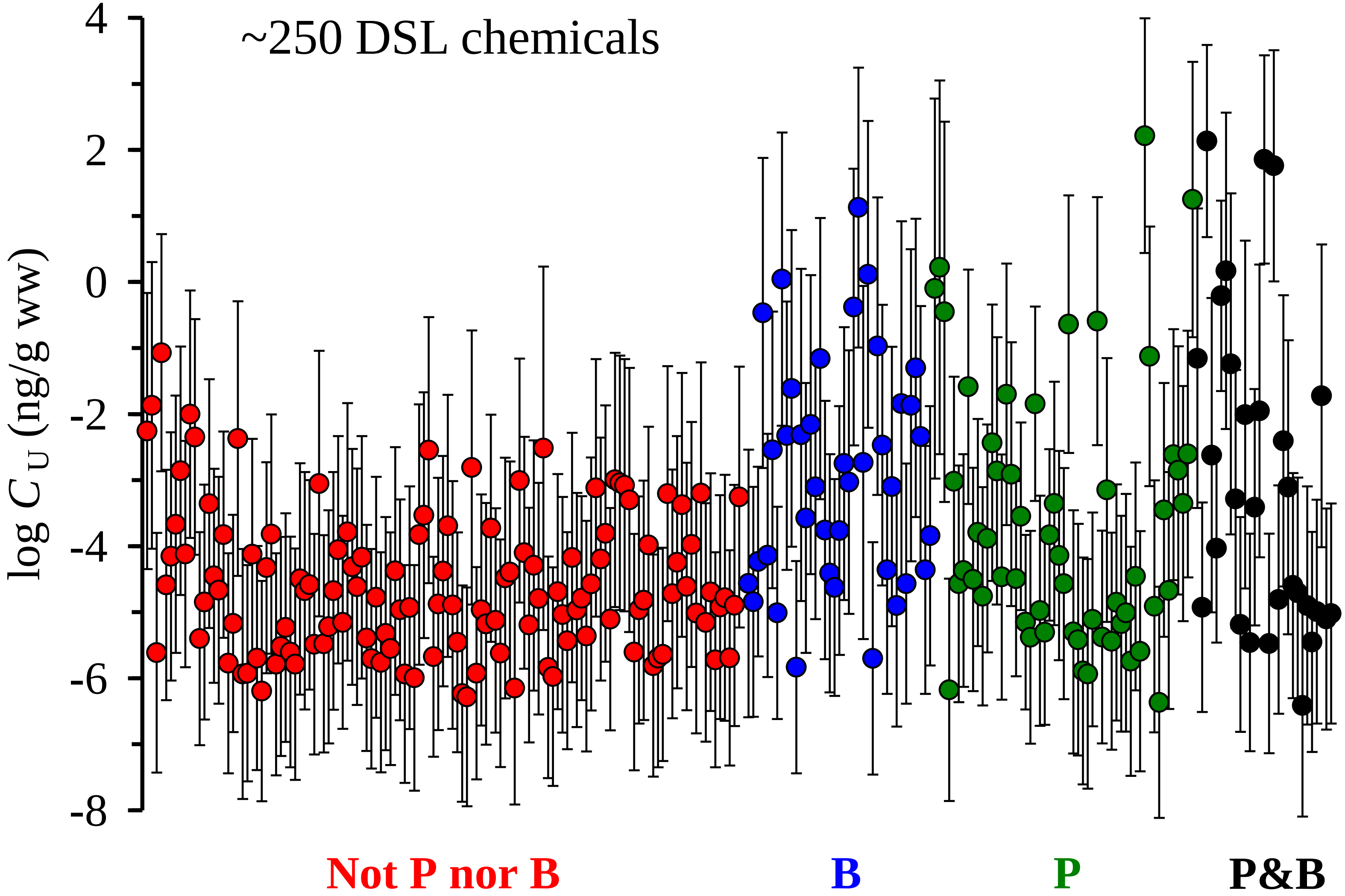
Linking "emissions-to-exposure" provides unique opportunities to address uncertainty

Contribution of Variance (*CV*): propagation of uncertainty of all model input parameters on model output, e.g., C_U

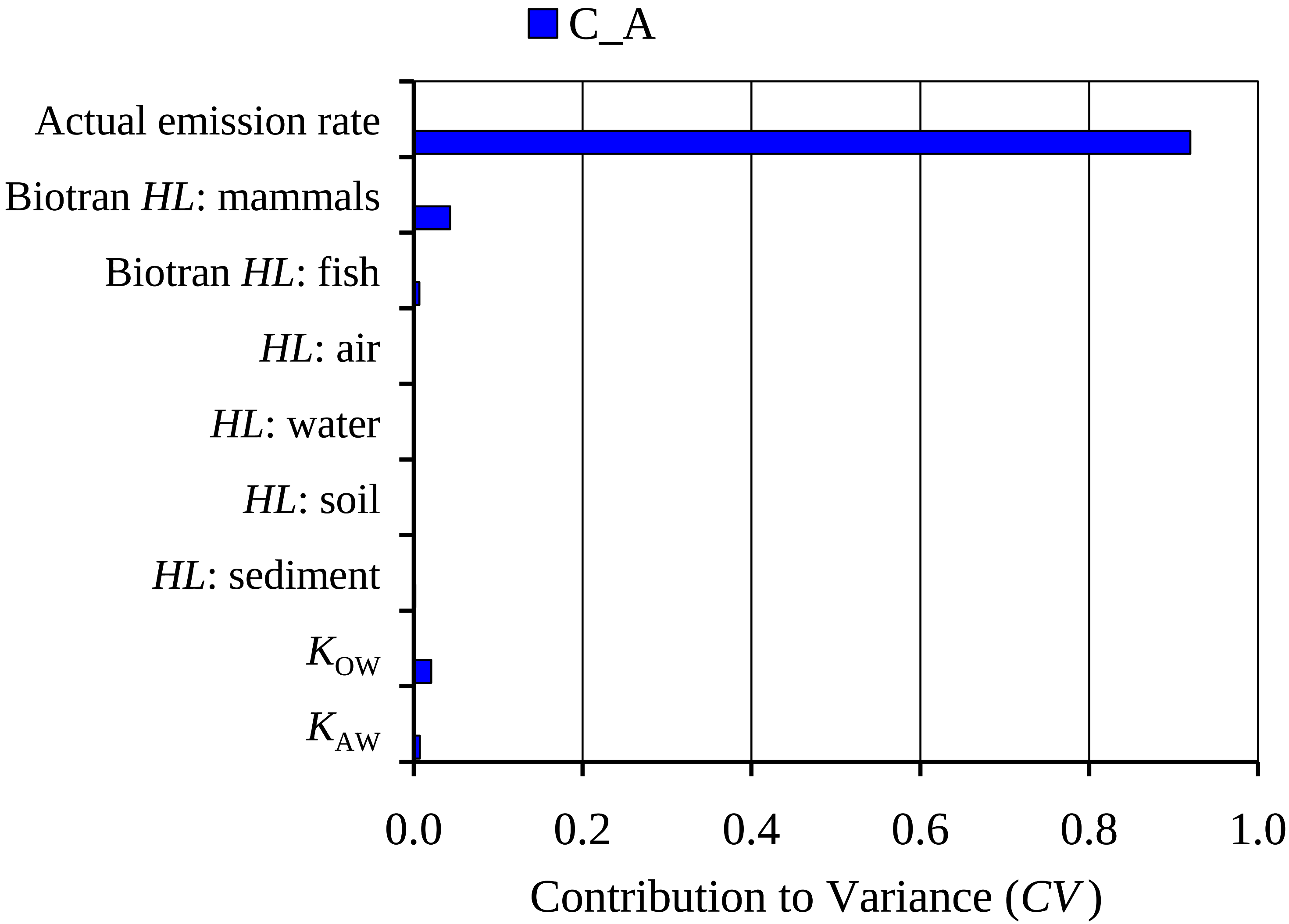
Distributions (uncertainty) for model input parameters may require professional judgment, particularly for incomplete datasets



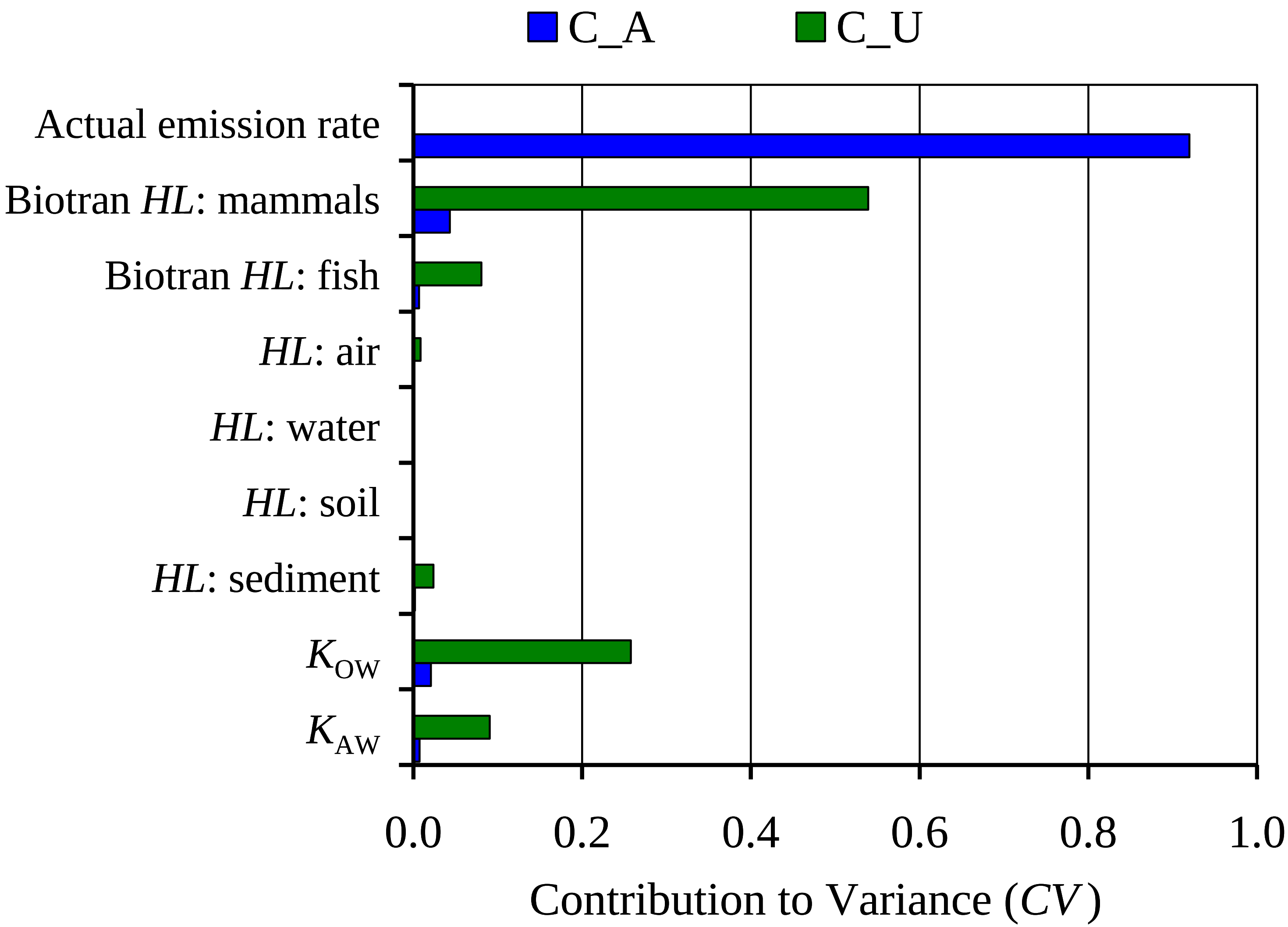
Include uncertainty in human far-field exposure assessment (e.g., C_U)



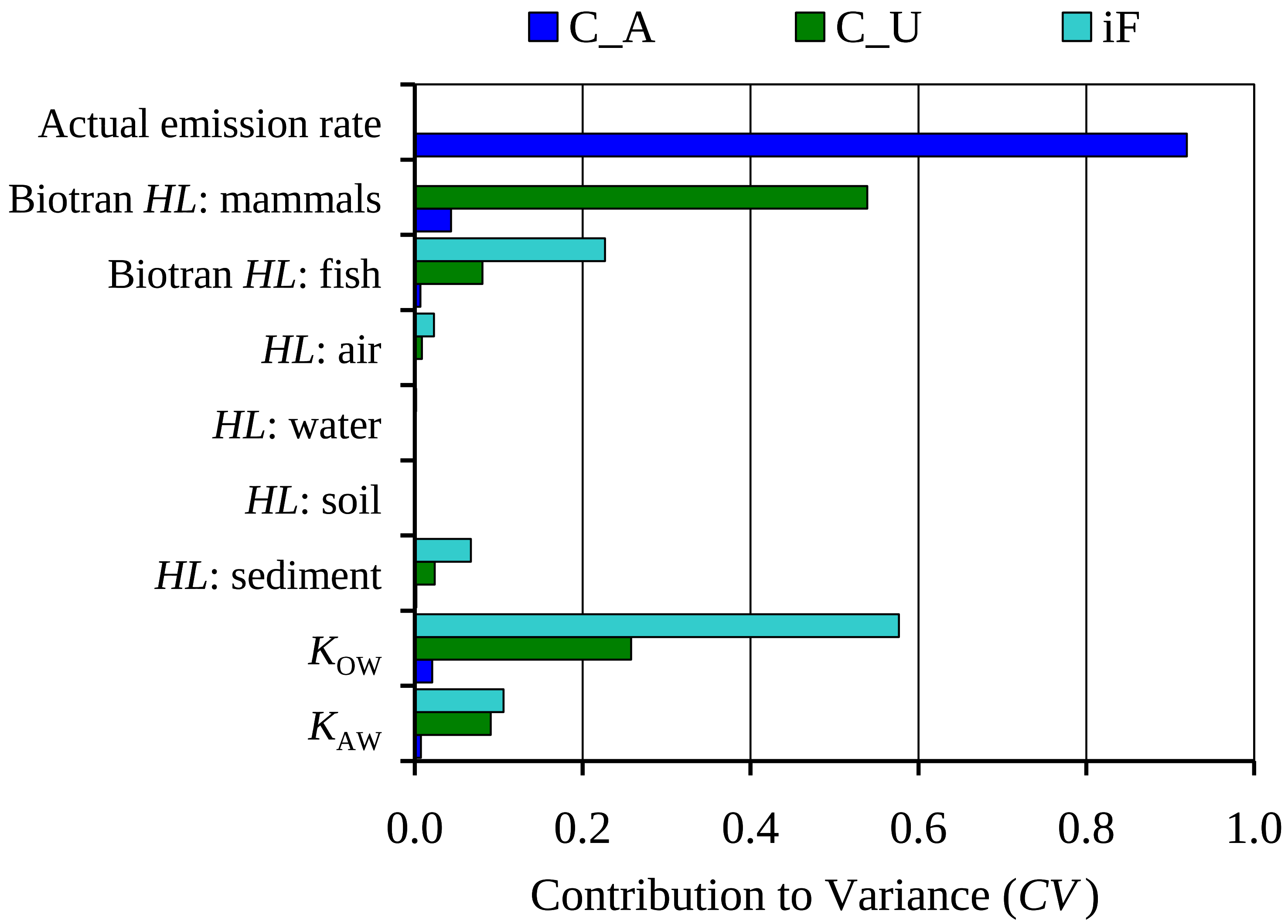
Uncertainty analysis: one chemical - HCB



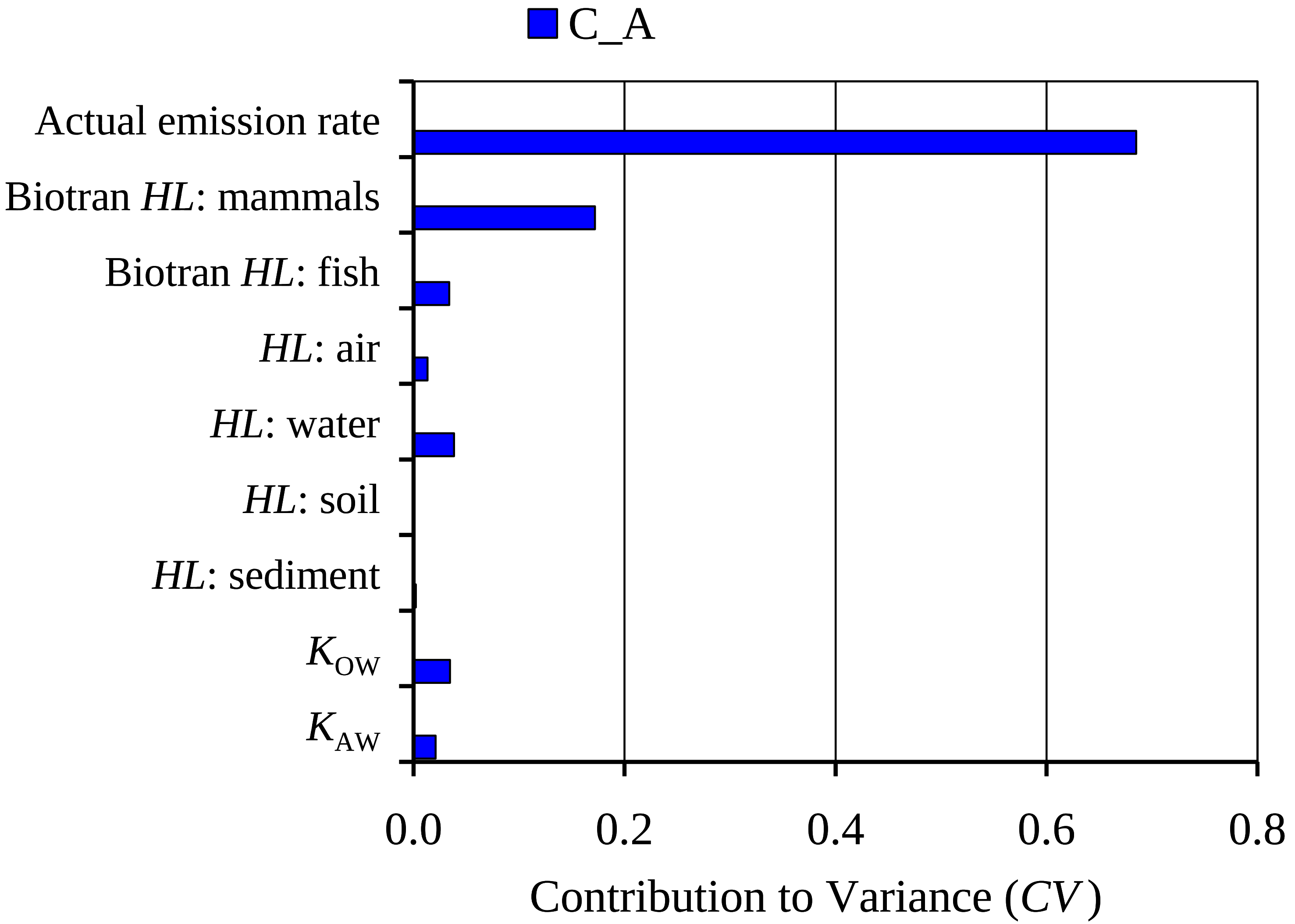
Uncertainty analysis: one chemical - HCB



Uncertainty analysis: one chemical - HCB

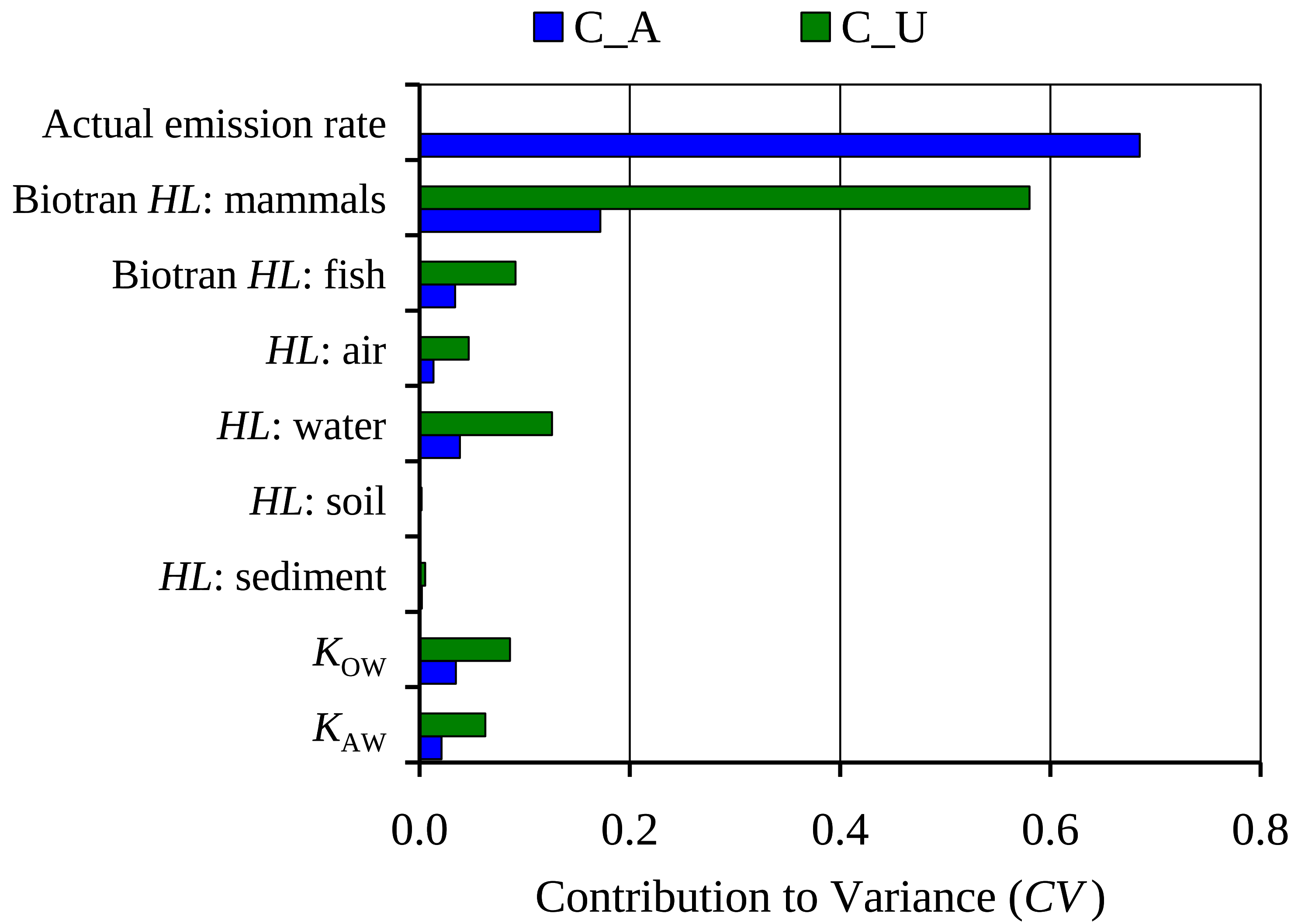


Uncertainty analysis: average ~ 13,000 chemicals



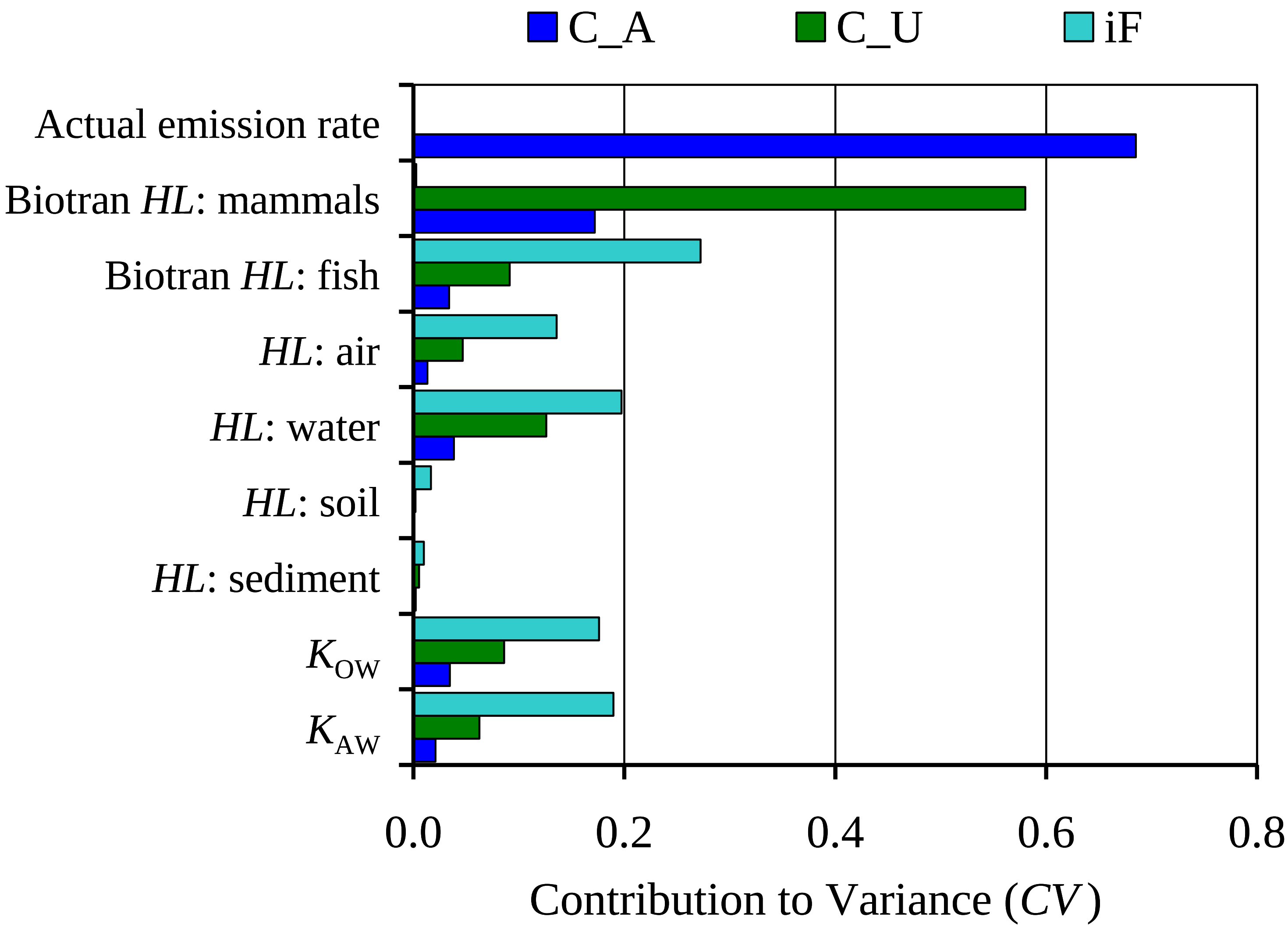
"ScreenPOP"

Uncertainty analysis: average ~ 13,000 chemicals



"ScreenPOP"

Uncertainty analysis: average ~ 13,000 chemicals



"ScreenPOP"

Publicly available screening-level exposure model input data sources, e.g., QSARs

????

Actual emission rate	A few, e.g., EU TGD
Biotran *HL*: mammals	0
Biotran *HL*: fish	1
HL: air	1
HL: water	1
HL: soil	1
HL: sediment	1
K_{OW}	~10
K_{AW}	~3

Summary

- Multimedia mass balance exposure models can screen and prioritize chemicals and provide hypotheses for testing (model evaluation)
- Combining exposure models and uncertainty analysis provides defensible guidance to address data gaps and develop knowledge infrastructure
- Chemical property (input) parameters, but can include other parameters, e.g., environmental properties, human contact rates
- Results based on "what we think we know", conceptual models, exposure model assumptions, input parameter uncertainty assumptions
- Need "near-field exposures" for humans for truly "holistic" exposure
- Reliable reaction half-life data and QSARs needed!!!
- Accurate emission rate data also needed for exposure assessment
- Integrated emissions, monitoring and modelling programs for further model evaluations and refinements, e.g., Cefic-LRI ECO.13

Thank you for your attention!

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