Technical University of Denmark

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UNEP/ SETAC partnership to advance the life cycle economy

Life Cycle Initiative

Development in methodologies for modelling of human and ecotoxic impacts in LCA

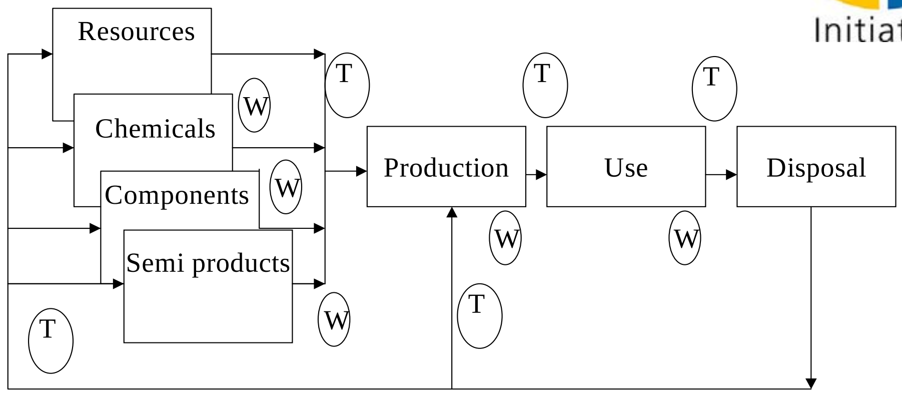
Michael Hauschild[1], Mark Huijbregts[2], Olivier Jolliet[3], Manuele Margni[4], Tom McKone[3], Dik van de Meent[2], Ralph K. Rosenbaum[4]

[1]Denmark, [2]Netherlands, [3]USA, [4]Canada

Inventory of emissions

		Emission	Emission
	CAS.no.	to air	to w ater
Substance		g	g
2-hydroxy-ethanacrylate	816-61-0	0,0348	
4,4-methylenebis cyclohexylamine	1761-71-2	5,9E-02	
Ammonia	7664-81-7	3,7E-05	4,2E-05
Arsenic (As)	7440-38-2	2,0E-06	
Benzene	71-43-2 (cur	5,0E-02	
Lead (Pb)	7439-92-1	8,5E-06	
Butoxyethanol	111-76-2	6,6E-01	
Carbondioxide	124-38-9	2,6E+02	
Carbonmonoxide (CO)	630-08-0	1,9E-01	
Cadmium (Cd)	7440-46-9	2,2E-07	
Chlorine (Cl2)	7782-50-5	4,6E-04	
Chromium (Cr VI)	7440-47-3	5,3E-06	
Dicyclohexane methane	86-73-6	5,1E-02	
Nitrous oxide(N2O)	10024-97-2	1,7E-02	
2,4-Dinitrotoluene	121-14-2	9,5E-02	
HMDI	5124-30-1	7,5E-02	
Hydro carbons (electricity, stationary combustic	-	1,7E+00	
Hydrogen ions (H+)	-		1,0E-03
i-butanol	78-83-1	3,5E-02	
i-propanol	67-63-0	9,2E-01	
copper (Cu)	7740-50-8	1,8E-05	
Mercury(Hg)	7439-97-6	2,7E-06	
Methane	74-82-8	5,0E-03	
Methyl i-butyl ketone	108-10-1	5,7E-02	
Monoethyl amine	75-04-7		7,9E-06
Nickel (Ni)	7440-02-0	1,1E-05	
Nitrogen oxide (NOx)	10102-44-0	1,1E+00	
NMVOC, diesel engine (exhaust)	-	3,9E-02	
NMVOC, pow er plants (stationary combustion)	-	3,9E-03	
Ozone (O3)	10028-15-6	1,8E-03	
PAH	ikke specifik	2,4E-08	
Phenol	108-95-2		1,3E-05
Phosgene	75-44-5	1,4E-01	
Polyeter polyol	ikke specifik	1,6E-01	
1,2-propylenoxide	75-56-9	8,2E-02	
Nitric acid	7782-77-6 ((	8,5E-02	
Hydrochloric acid	7647-01-0 ((	1,9E-02	
Selenium (Se)	7782-49-2	2,6E-05	
Sulphur dioxide(SO2)	7446-09-5	1,3E+00	
Toluene	108-88-3	4,8E-02	
Toluene-2,4-diamine	95-80-7	7,9E-02	
Toluene diisocyanat (TDI)	26471-62-5	1,6E-01	
Total-N	-		2,6E-05
Triethylamine	121-44-8	1,6E-01	
Unspecified aldehydes	-	7,5E-04	
Uspecified organic compounds	-	1,5E-03	
Vanadium	7440-62-2	1,8E-04	
VOC, diesel engine (exhaust)	-	6,4E-05	
VOC, stationary combustion (coal fired)	-	4,0E-05	
VOC, stationary combustion (natural gas fired)	-	2,2E-03	
VOC, stationary combustion (oil fired)	-	1,4E-04	
Xylene	1330-20-7	1,4E-01	
Zinc (Zn)	7440-66-6	8,9E-05	

The product life cycle



Characterised impact profile of product

Global warming	174.000	kg CO_2-eq
Ozone depletion	0	kg CFC11-eq
Acidification	868	kg SO_2-eq
Photochemical ozone formation	200	kg C_2H_4-eq
Nutrient enrichment	3.576	kg NO_3^--eq
Human toxicity	$3{,}40 \cdot 10^{11}$	m^3 air
Ecotoxicity	$2{,}16 \cdot 10^{7}$	m^3 water
Land use	170	ha·yr
Volume waste	9.450	kg
Hazardous waste	248	kg

Background

- Characterisation factors (CFs) express potential impact on human health or ecosystems
- For comparison of chemicals (relative scale)
- Different characterisation methods give very different results
- CFs missing for many of the substances encountered in inventories for products
- → unsatisfactory treatment of chemicals in LCA
- Chemicals often not included in Life Cycle Impact Assessments (LCIAs)
- Results often inconclusive
- … Environmental LCA in practice often Energy LCA

About the *Life Cycle Initiative*

Joint initiative between United Nations Environment Programme (UNEP) and Society of Environmental Toxicology and Chemistry (SETAC):

Enhancement of the availability of sound LCA data and methods and guidance about their use.

For toxic impacts:

Recommended characterisation models and factors for human toxicity and ecotoxicity

- applicable on a world-wide basis
- for a large number of substances

Goal

- Identification of good modelling practice
- Harmonisation of existing models
- Recommendation of characterisation model
- Recommendation of characterisation factors
- Provision of characterisation factors for many substances
- Guidance on use of characterisation factors

LCIA and ERA of chemicals

Similarities

- Multimedia, multi compartment fate and exposure models
- Same type of physico-chemical and biological substance data (Kow, H, DT50, EC50, …)

Differences:

	ERA	LCIA
Scope of impacts	Chemical exposure of humans and ecosystems	All known environmental impacts
Scope of substances	Focused on one or a few substances	Focused on life cycle inventory (hundreds of substances)
Issue addressed	Is there a risk of critical exposure?	Largest potential impact - A or B? How much larger?
Modelling assumptions and parameter choices	Conservative assumptions (“realistic worst case)	Best estimate (avoid bias in comparison with other impacts)
Spatial differentiation	Often site-*dependent*	Normally site-*generic*

Process

- Consensus created through joint efforts on
  - Identification of state of the art
  - Identification of good modelling practice
  - … Monthly teleconferences keep the process going
- Review workshops with external experts
- Need for model comparison identified
- Need for consensus model identified
- Sponsorship obtained
  - ICMM
  - ACC
  - UNEP
- … seed money which supported a huge voluntary effort from the participants

Model comparison

Existing models compared on their results and main sources of differences in their output identified

- CalTOX **(McKone et al., USA)**
- IMPACT 2002 **(Pennington et al., Switzerland)**
- USES-LCA **(Huijbregts et al., Netherlands)**
- BETR **(MacLeod et al., Canada)**
- EDIP **(Hauschild et al., Denmark)**
- WATSON **(Bachmann et al., Germany)**
- EcoSense **(Droste-Franke et al., Germany)**

3 expert review workshops and 3 model comparison workshops

Using a test set with broad organic chemical representation

Main sources of difference identified, unintentional sources eliminated

A UNEP/SETAC toxicity scientific consensus model created – **USEtox™**

The principles behind USEtox™

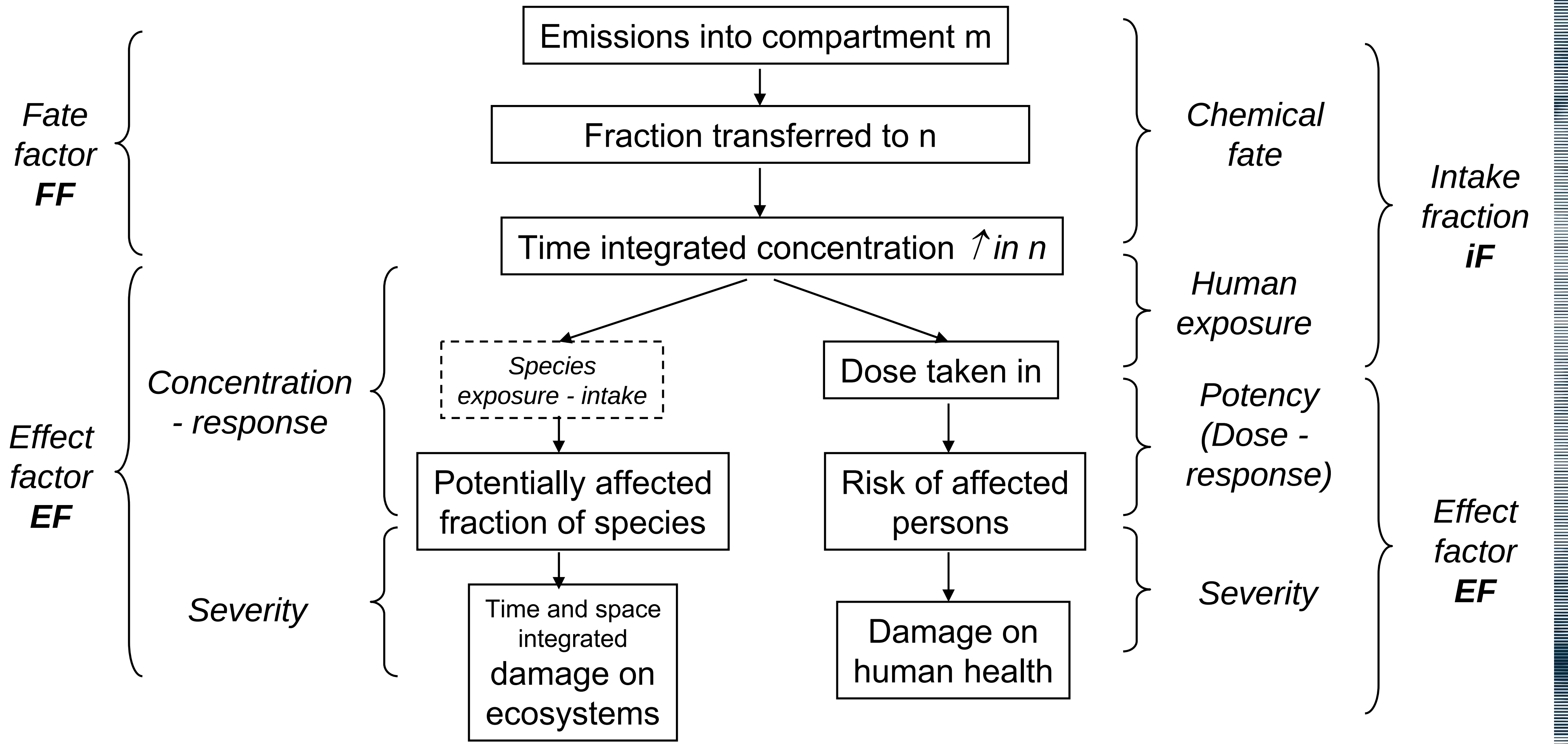
Parsimonious **– as simple as possible but as complex as needed – containing only the most influential model components;**

Mimetic **– not differing more from the original models than these differ among themselves;**

Evaluated **– providing a repository of knowledge through evaluation against existing models;**

Transparent **– being well documented, including the reasoning for model choices.**

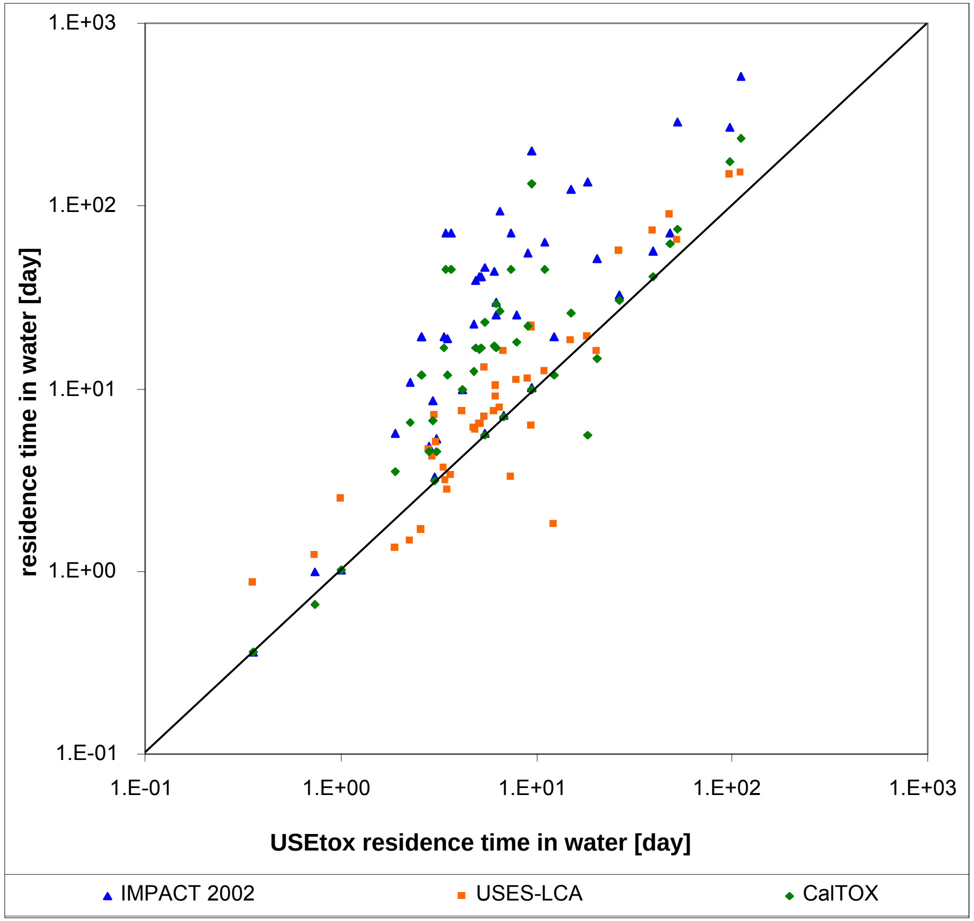
Framework

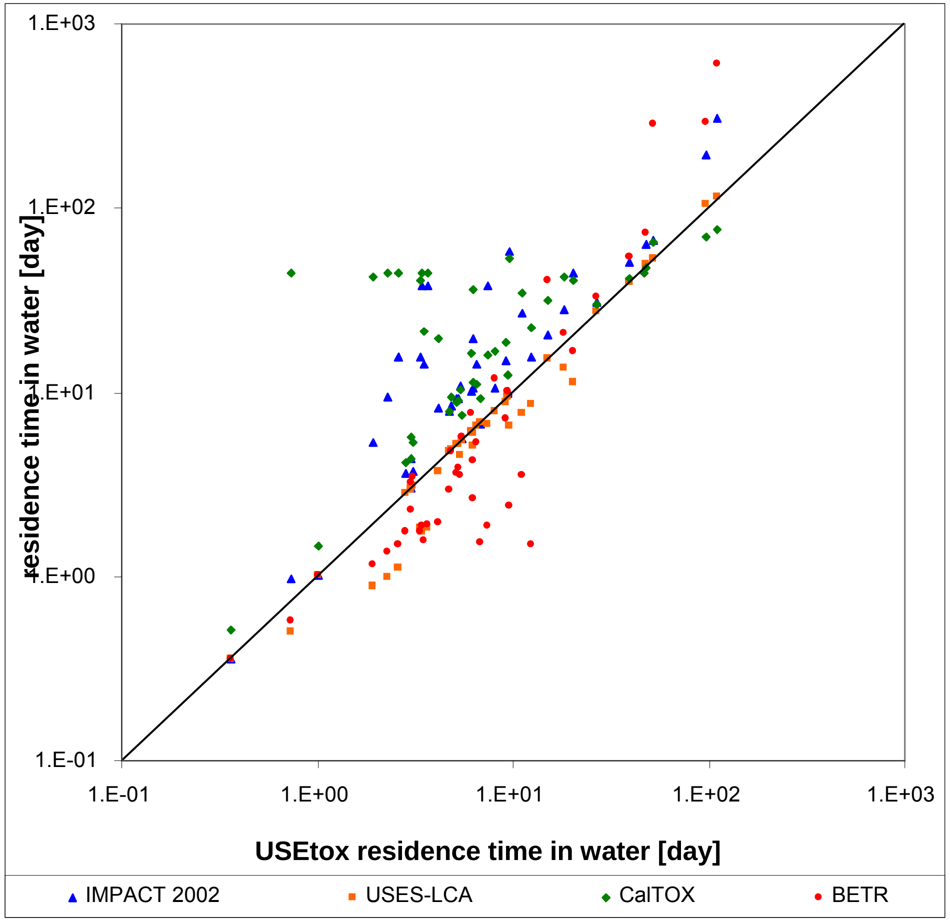


Ecotoxicity: CF=FF·EF

Human toxicity: CF=iF·EF

FFs Aquatic environment

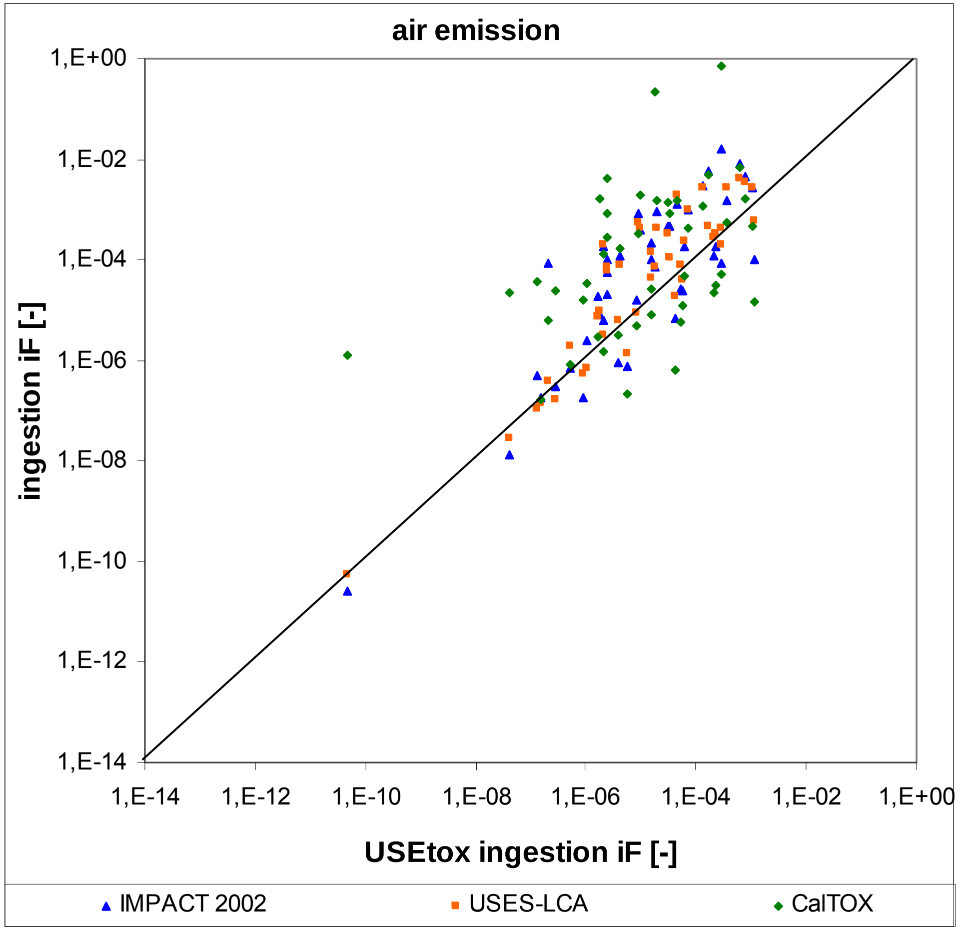




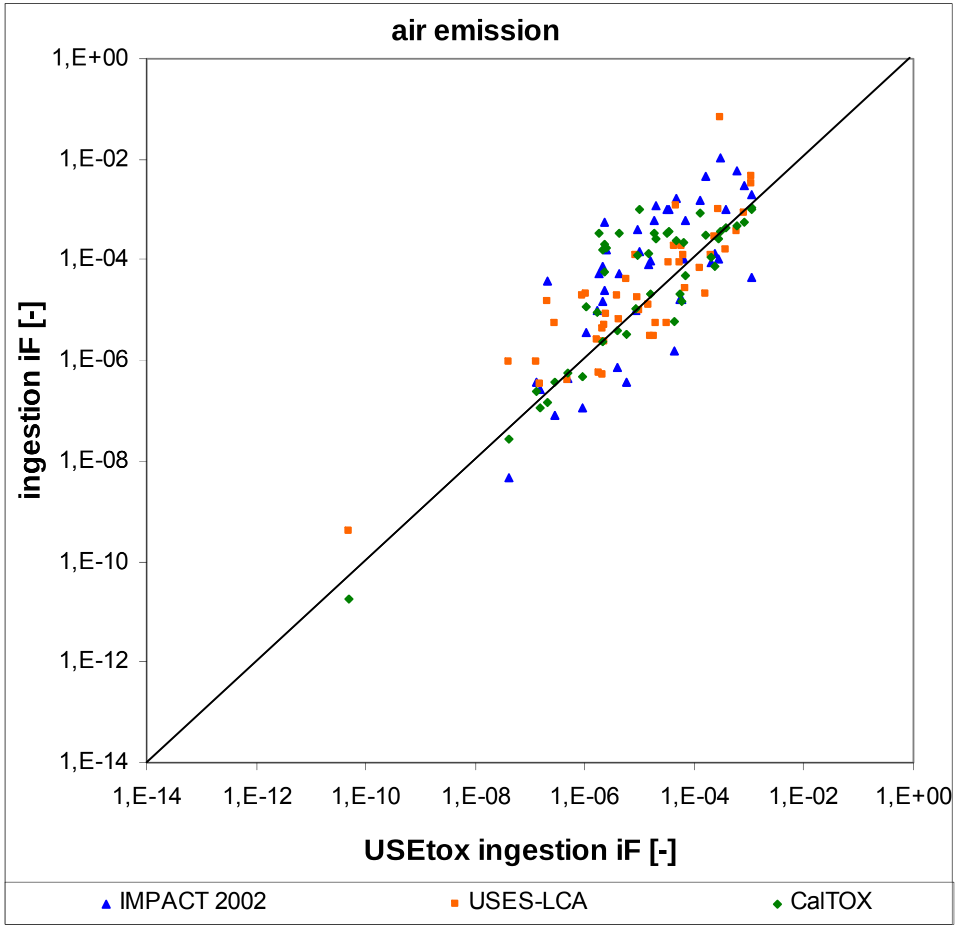
First workshop, Bilthoven

Final workshop, Montreal

IFs for ingestion

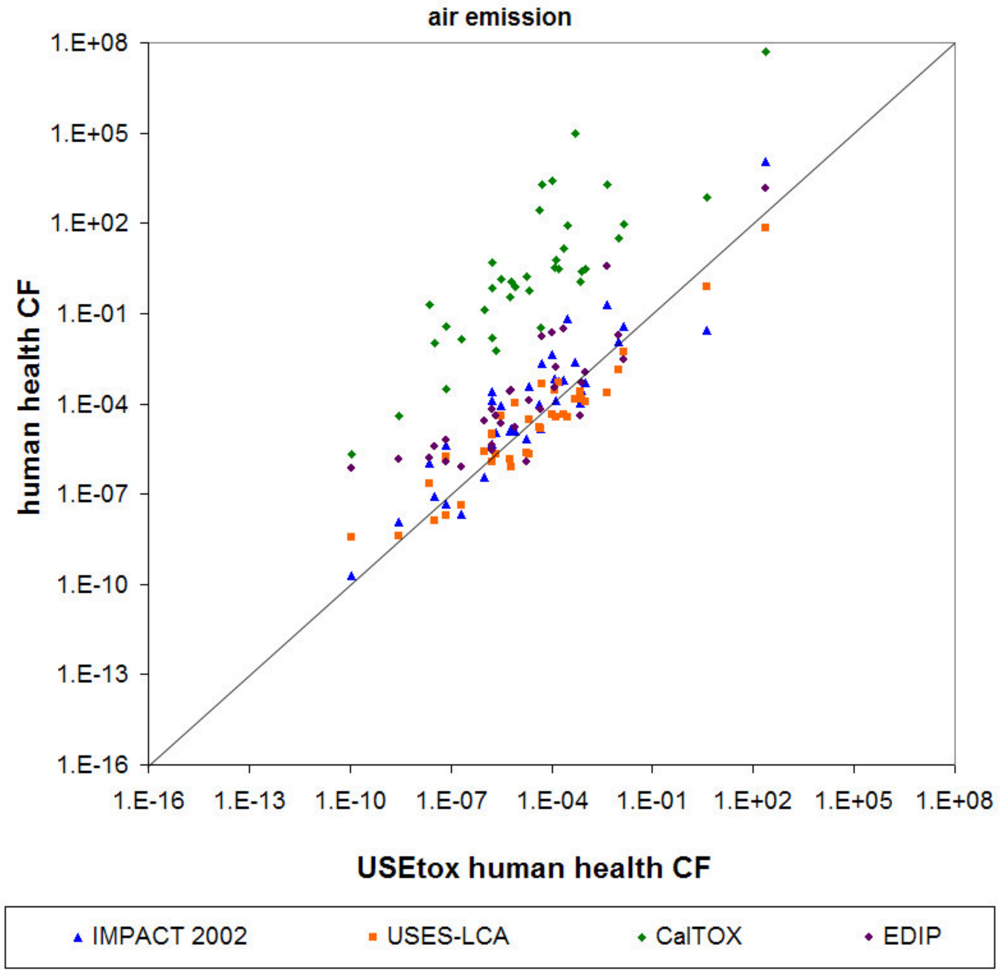


First workshop

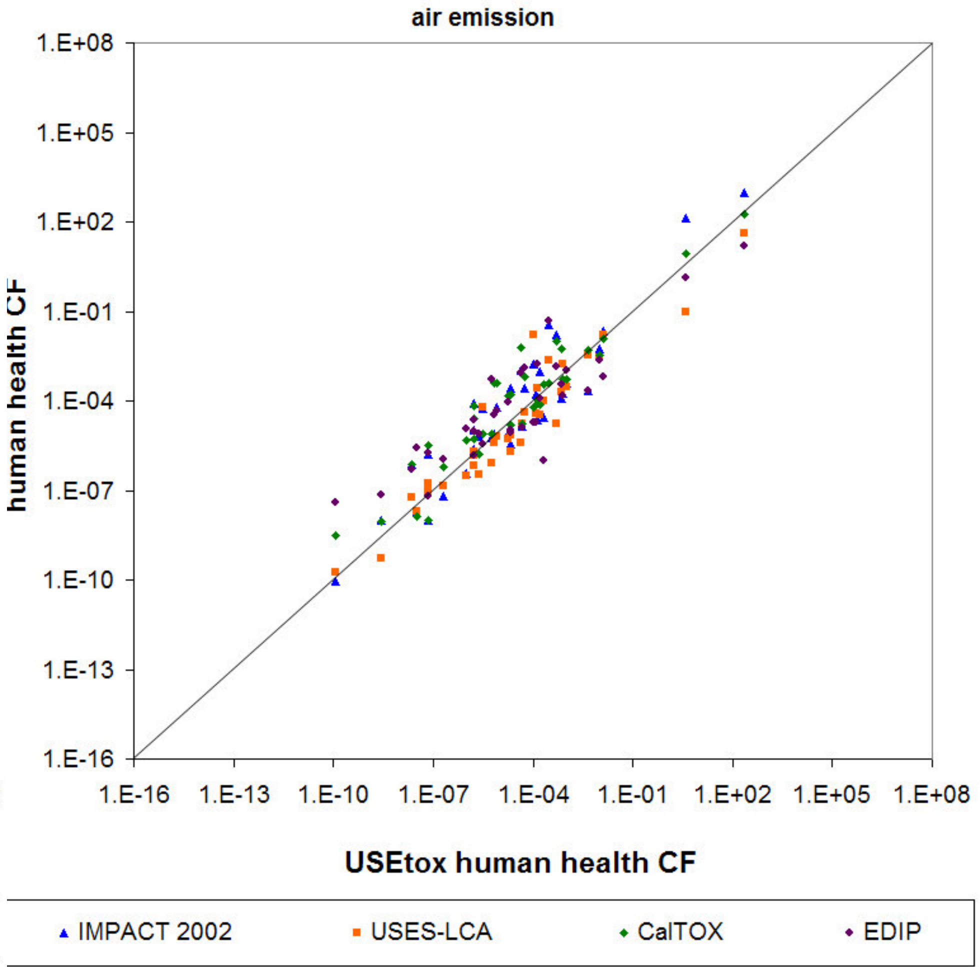


Final workshop

CFs Human health

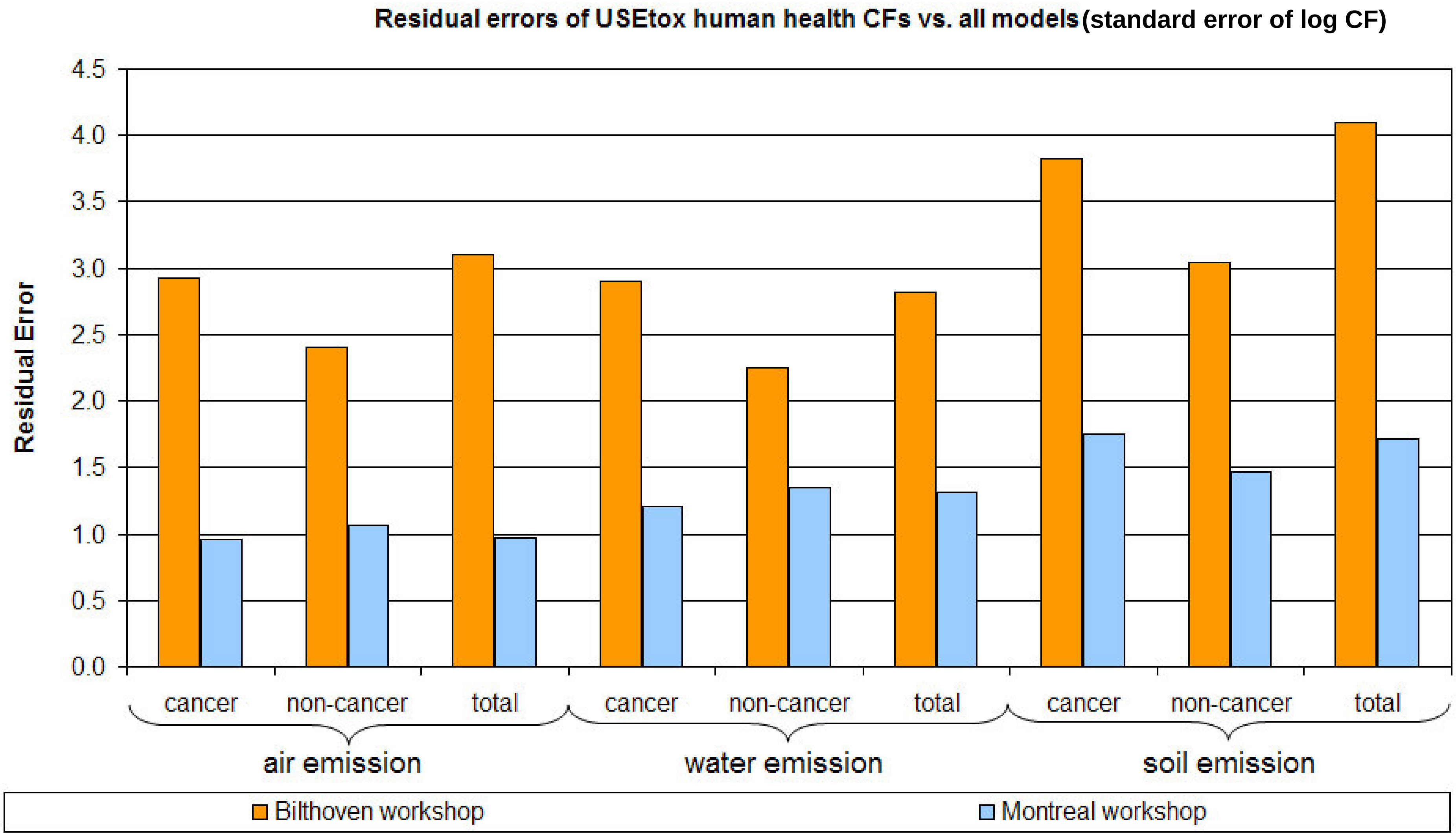


First workshop

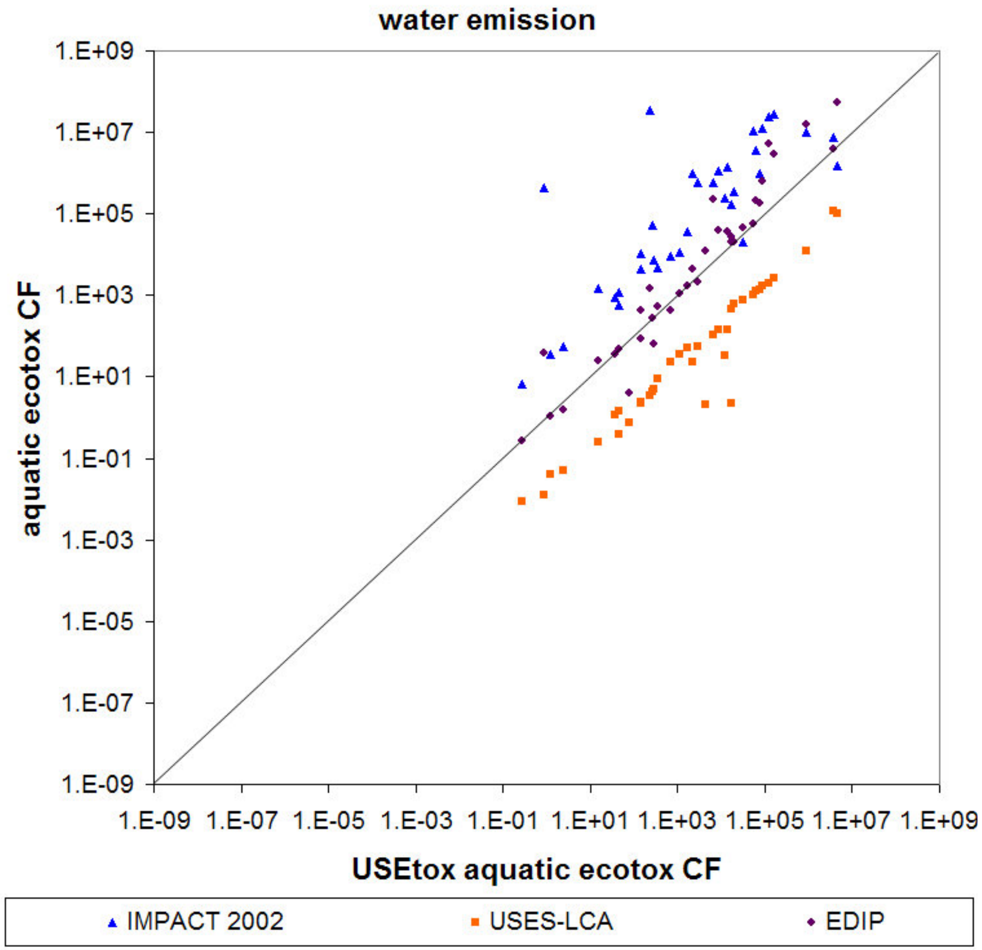


Final workshop

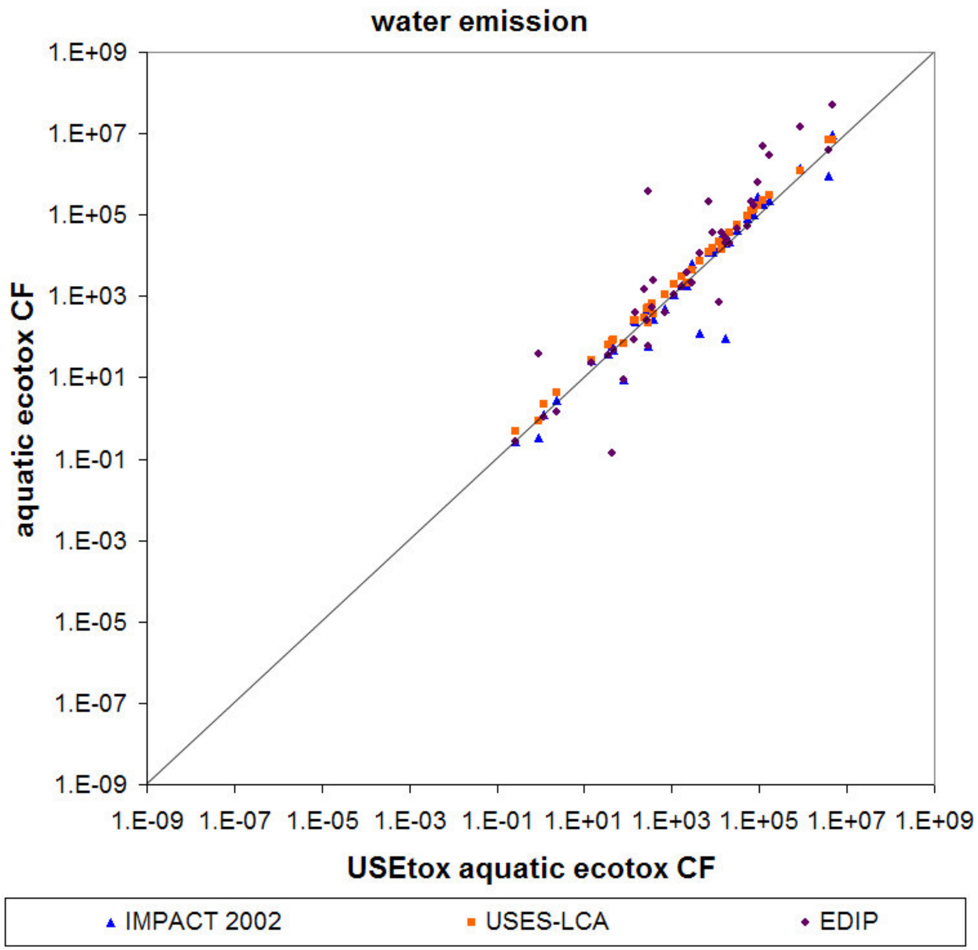
CFs Human toxicity



CFs Aquatic ecotoxicity

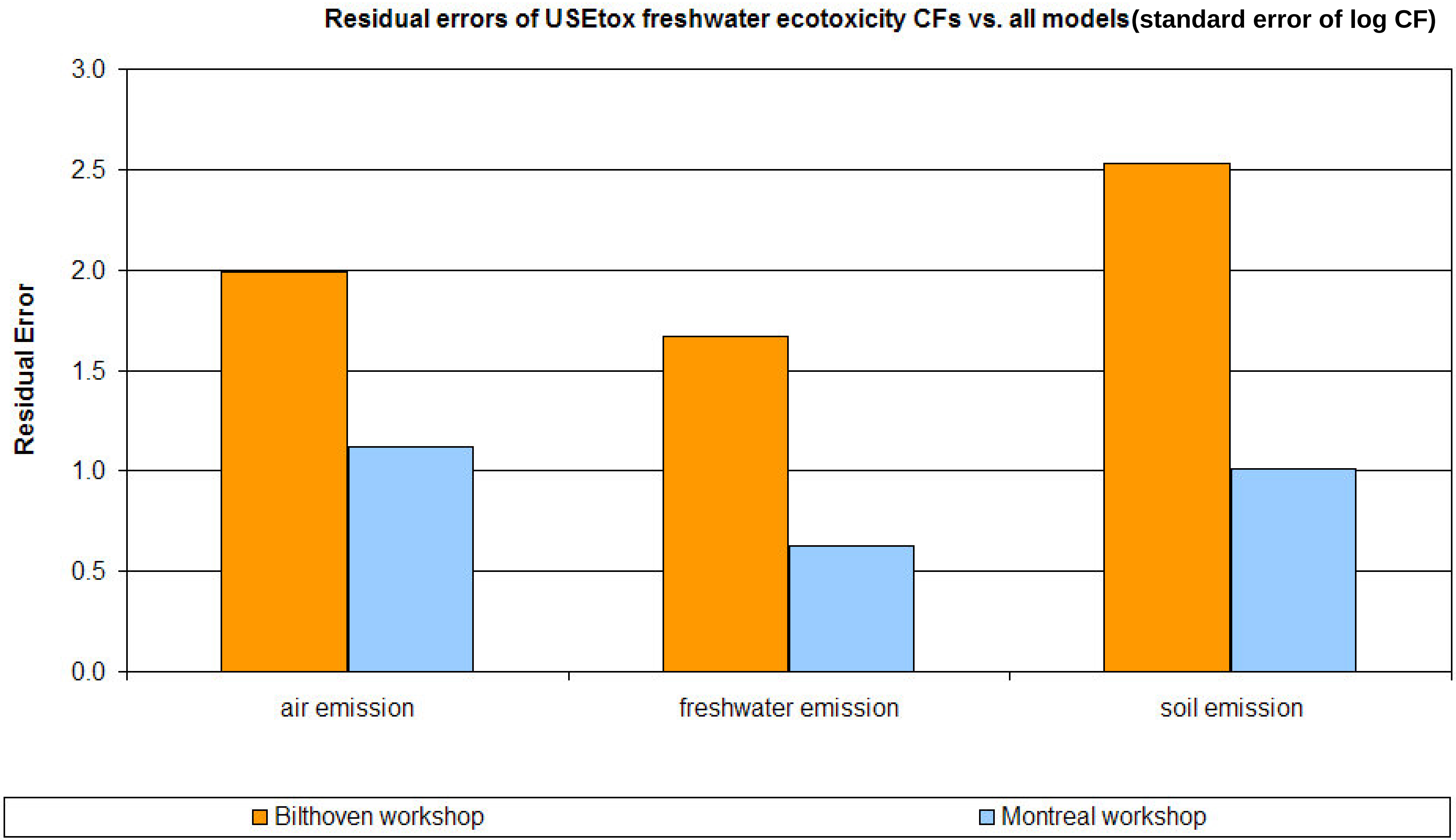


First workshop



Final workshop

CFs Aquatic ecotoxicity



Conclusions

Harmonisation eliminates unintentional differences and considerably reduces variation between models.

Characterisation factors calculated with USEtox™ fall within range of the other models, even after their harmonisation.

Relative accuracy (model variability) of the new CFs is within a factor of

- 100-1000 for human health and
- 10-100 for freshwater ecotoxicity
- compared to 12 orders of magnitude variation between CFs.

CFs calculated with USEtox™:

- *recommended* factors for 1000 substances for human toxicity and 1300 substances for freshwater ecotoxic impacts
- *interim* factors for additionally 350 substances for human toxicity and 1250 substances (including metals) for freshwater ecotoxic impacts.

Outlook

USEtox™ and recommended CFs will be stable for at least 3-5 years though the other characterization models change.

Results are applicable to comparative chemical assessments also outside Life Cycle Impact Assessment, e.g.

- Ranking and prioritization of chemicals
- Chemical substitutions

Second phase of UNEP-SETAC Life Cycle Initiative (on-going):

- Metals targeted (freshwater, soil) to give realistic CFs
- USEtox™ will be made available in user-friendly version
- Substance data will be quality assured and parameter uncertainty estimated
- Case studies will be developed with chemical industry partners

Collaboration

The USEtox™ team invites partners from industry to collaborate on:

- Workshops to introduce and train the participants in use of the USEtox model
- Calculation of characterisation factors for other substances
- Development of cases demonstrating the relevance of:
  - looking at chemicals in life cycle perspective (e.g. chemical substitution)
  - including chemical impacts in life cycle assessments (*"carbon footprint does not say it all"*)

Please contact:

Michael Hauschild, USEtox™ project leader Europe mic@man.dtu.dk

Olivier Jolliet USEtox™ project leader North America ojolliet@umich.edu

More information

Hauschild, M.Z., Huijbregts, M., Jolliet, O., MacLeod, M., Margni, M., van de Meent, D., Rosenbaum, R.K. and McKone, T.: **Building a model based on scientific consensus for Life Cycle Impact Assessment of chemicals: the Search for Harmony and Parsimony.** *Environmental Science and Technology, 42(19), 7032-7037, 2008.*

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www.usetox.org (under construction)