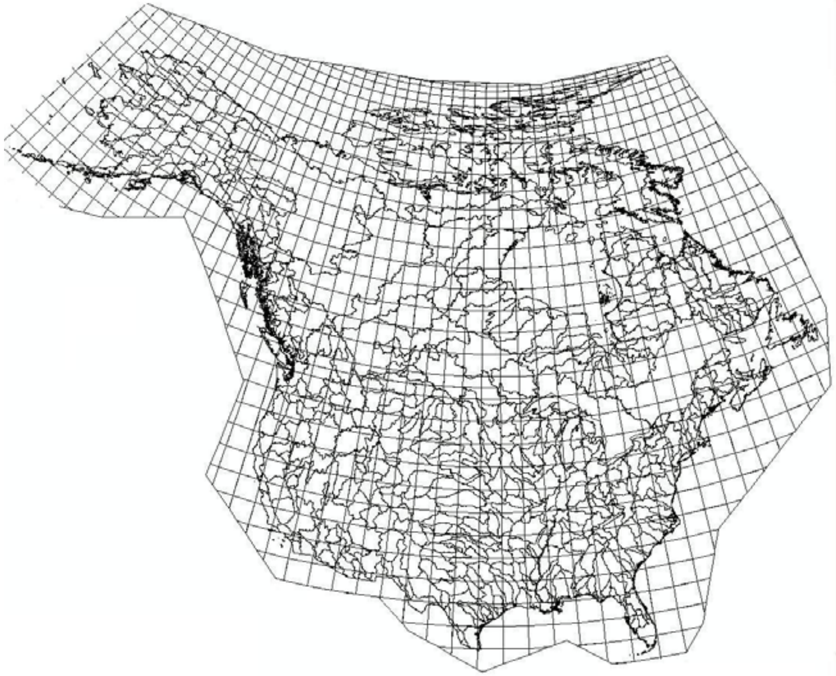
Multimedia Multipathway Modeling of Emissions to Impacts: screening with USEtox and advanced spatial modeling with IMPACT



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The USEtox team

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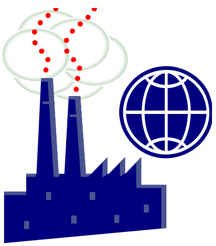
Framework: emission to Intake multimedia transport model

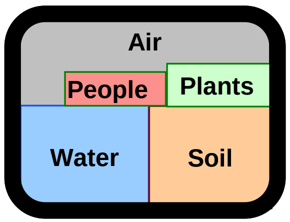
Bennett et al, ES&T 2002, 36, 207-212 A

$$iF = \frac{\text{intake of pollutant}\,[kg_{in}]}{\text{mass released into the environment}\,[kg_{emit}]}$$



Emissions to compartment *m* $[kg_{em}/yr]$

Env.Fate: $FF=k^{-1}$



Concentration & mass in compartment *n*

Exposure: XP

Dose taken in $[kg_{in}/yr]$

Intake fraction iF $[kg_{in}/kg_{em}]$

$iF=XP \cdot FF$

Dose-response

Damage to human health [DALYs/yr]

Matrix framework : from emission to damage

$\dot{\vec{S}}$	$\dot{\vec{M}}$	$\dot{\vec{I}}$	$\dot{\vec{N}}$
Emission flow (n_i) [*kg/day*]	Mass (n_i) [*kg*]	Intake flow (n_{xr}) [*kg/day*]	Impact flow (n_{ef}) [*cases/day*]
$\vec{S}$	$\int \vec{M}\,dt$	$\vec{I}$	$\vec{N}$
Mass emitted [*kg*]	Time integr. mass [*kg·day*]	Mass intake [*kg*]	Impact [*cases*]

$\overline{FF}$ ($n_i \times n_i$) [*day*] Fate matrix

$$\frac{\text{Mass}}{\text{Emission flow}}$$

$\overline{XR}$ ($n_{xr} \times n_i$) [*1/day*] Exposure matrix

$$\frac{\text{Intake flow}}{\text{Mass}}$$

$\overline{EF}$ ($n_{ef} \times n_{xr}$) [$cases/kg_{emitted}$] Effect matrix

$$\frac{\text{Risk of incidence}}{\text{Intake flow}}$$

$$\overline{iF} = \overline{XR} \cdot \overline{FF} = \frac{\text{Intake flow}}{\text{Emission flow}}$$

($n_{xr} \times n_i$) [$kg_{intake}/kg_{emitted}$]

Intake fraction matrix

Matrix format: Rosenbaum et al., Environment international, Vol. 33, 5, 624-634.

2. Screening: USETOX – the UNEP-SETAC toxicity model

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Obstacles/needs for use of comparative risks

- Too many competing methods (Life Cycle Impact Assessment, Risk Assessment
  → recommendations
- Too complex to understand and further explain
- → transparency, simplicity
- → need guidance to properly interpret
- Provide conflicting results → increase reliability
- Methods changes to quickly → stability
- 100,000 chemicals on the market
  → comprehensiveness

Make toxicity screening available for comparative risk: The USEtox core team

→ 3 comparison workshops with 5 teams, to identify most influential model components

TF3: 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.

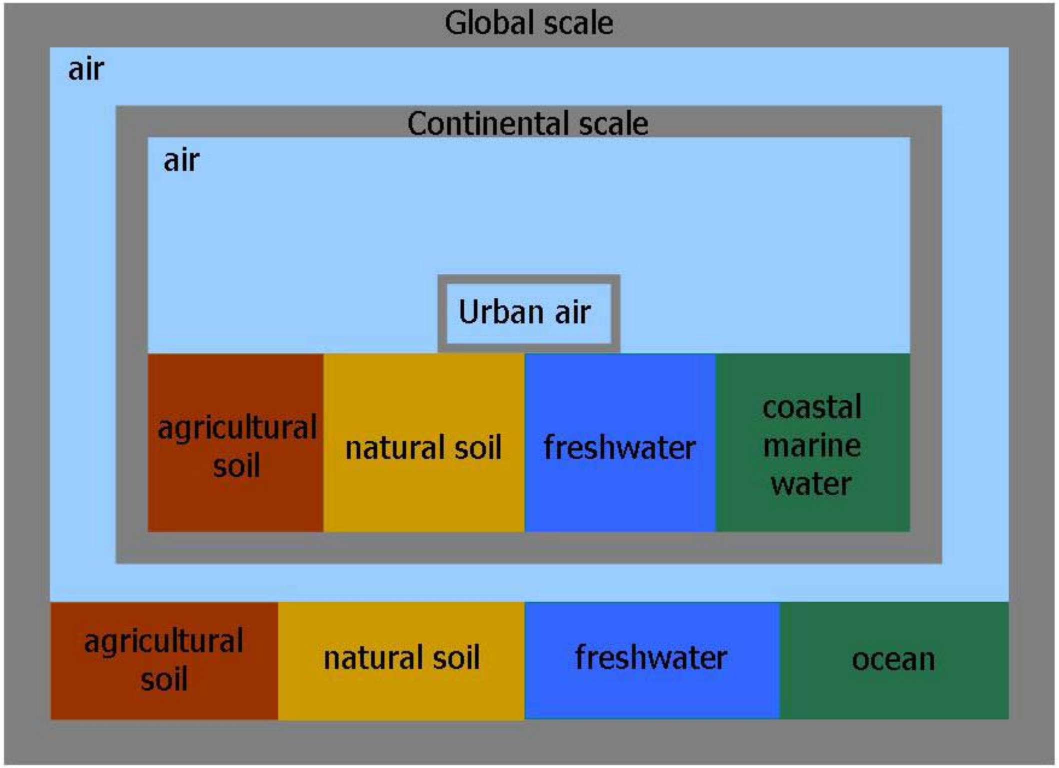
USEtox Consensus building process

Hauschild et al., 2008. The Search for Harmony and Parsimony. Environmental Science &Technology, 42(19), 7032-7036

- **4 expert review workshops to frame the field and define the useful metrics**
- **Compare existing models (also BETR)**
- **→ Identify main sources of difference, eliminate unintentional sources**
- **Construct a parsimonious UNEP/SETAC toxicity consensus model – USEtox**
- **Model evaluation, publication and expert review. Approval by International Life Cycle Panel**
- **Stakeholder evaluation (UNEP)**

USEtox: UNEP SETAC model for comparative TOXicity assessment

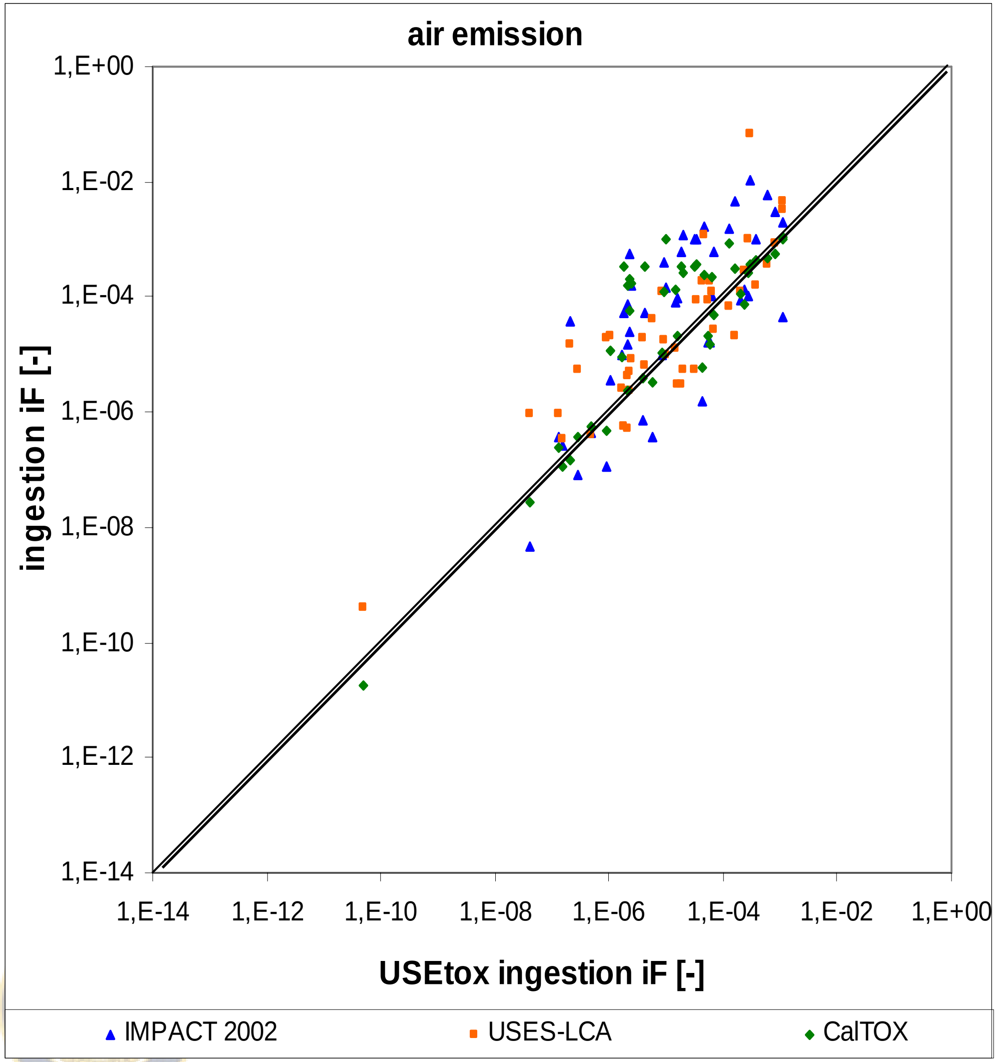
- **After 4 years effort: Build trust, highly motivated team → creation of a model prototype**



Rosenbaum et al., 2008: USEtox factors for factors for human tox and freshwater ecotox, Int J LCA, 13(7)532-546.(http://dx.doi.org/10.1007/s11367-008-0038-4)

From emission to intake dose

Intake fraction: fraction of emission taken in by population

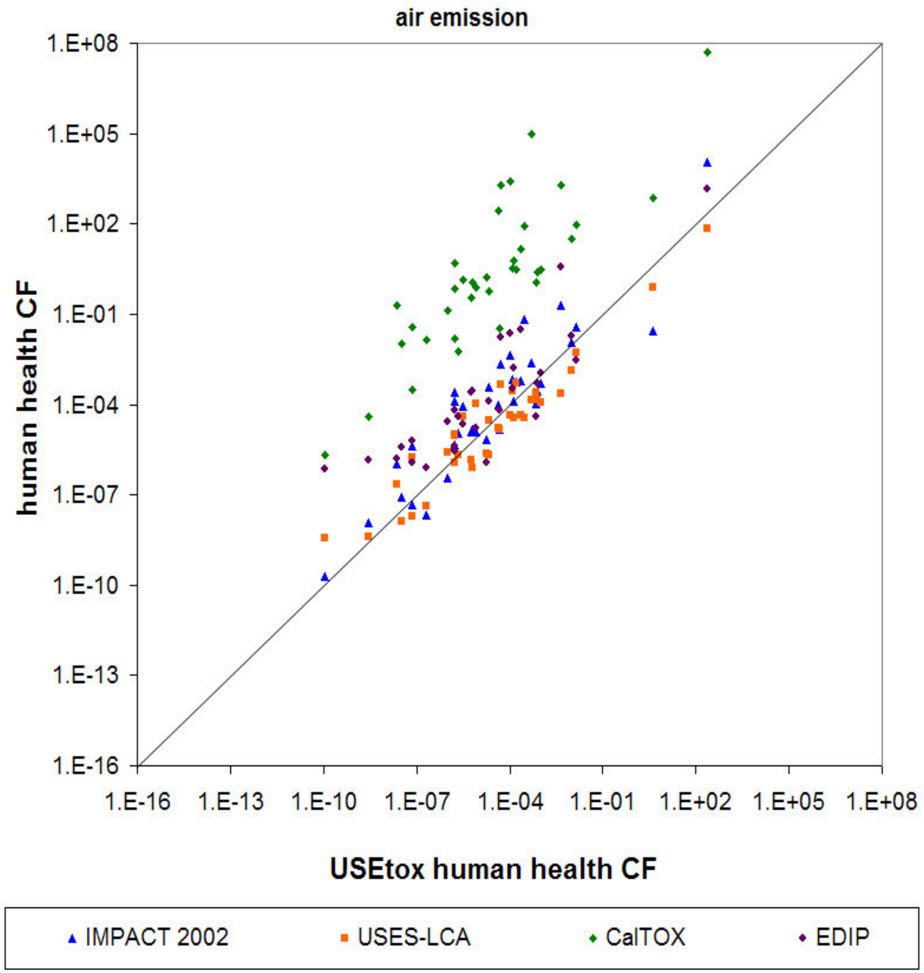


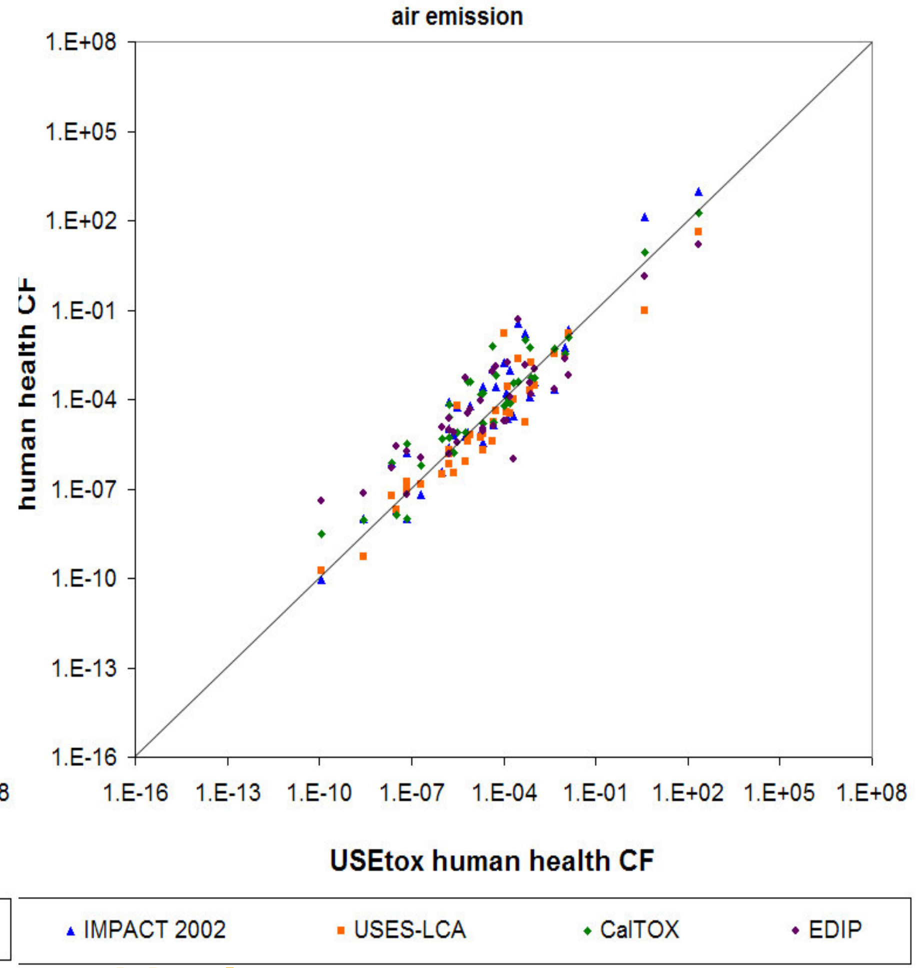
Comparison of iFs for ingestion
from 0.0001 to 10000 ppm

Dose-respose:
***0.5/ED50 for cancer based on Gold's Carcinogenic Potency Database,**
1600 substances tested, 60% positive

Non cancer: extrapolation of ED50 based on NOAEL and LOAEL: 400 substances

USEtox Characterization factors
Human health: *CF=iF * 0.5/ED50*



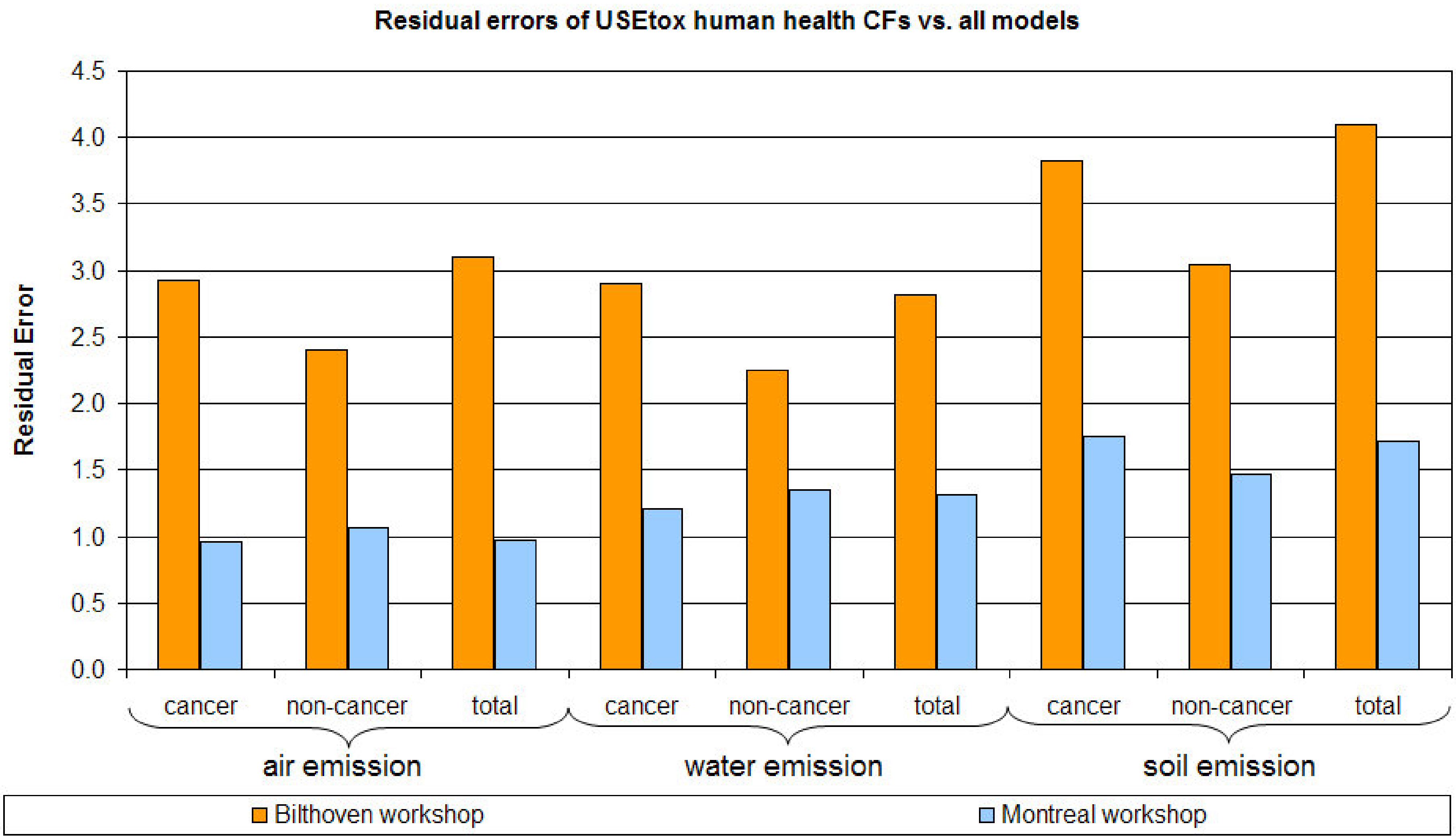


Initial
Bilthoven workshop

From factor 1000 residual error down to factor 10 to 100

Final
Montreal workshop

Change in residual error for human health model comparison



USEtox Deliverables

- **USEtox model**
  - Excel prototype, allows calculation of additional factors
  - USEtox simple matrices for Human Tox (HT) and ecotox (ET)
- **Substance database** with large chemical coverage
  - Referenced - but not quality self-assured data
- **Characterisation factors**
  - Recommended factors for 1000 HT and 1300 ET substances
  - Interim factors for 250+ substances HT and 1250 ET (incl. metals)
  - Model variability known from comparison
  - Stable: consensus model will only be updated after some years (new version)
  - Applicable for comparative purposes also outside LCA
- **Extension to respiratory inorganics, indoor emissions**

3. Spatially resolved model: IMPACT North America and IMPACT world

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Generic vs regionalized assessment

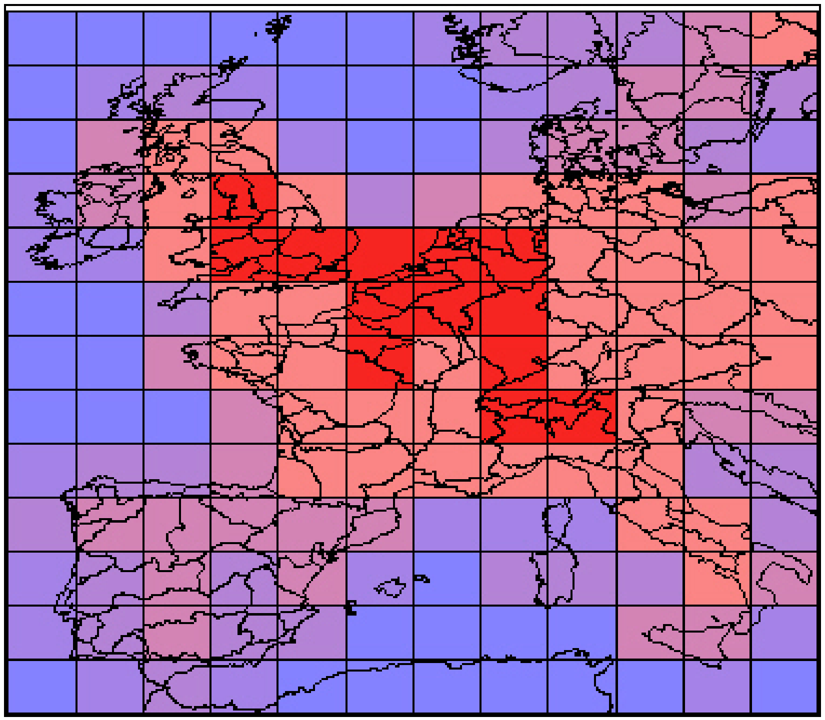
- Problems with generic characterization factors
  - disregard of spatial differences in fate, exposure, and effects
  - low acceptance for LCA results using generic data

- Increasing demand in methodologies
  - reflecting regional concerns
  - adapted to regional conditions

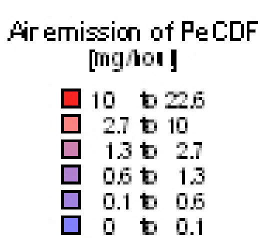
→ What really matters when spatially differentiating human toxicity in North America

Basis: spatial IMPACT model for Europe evaluated for PeCDF

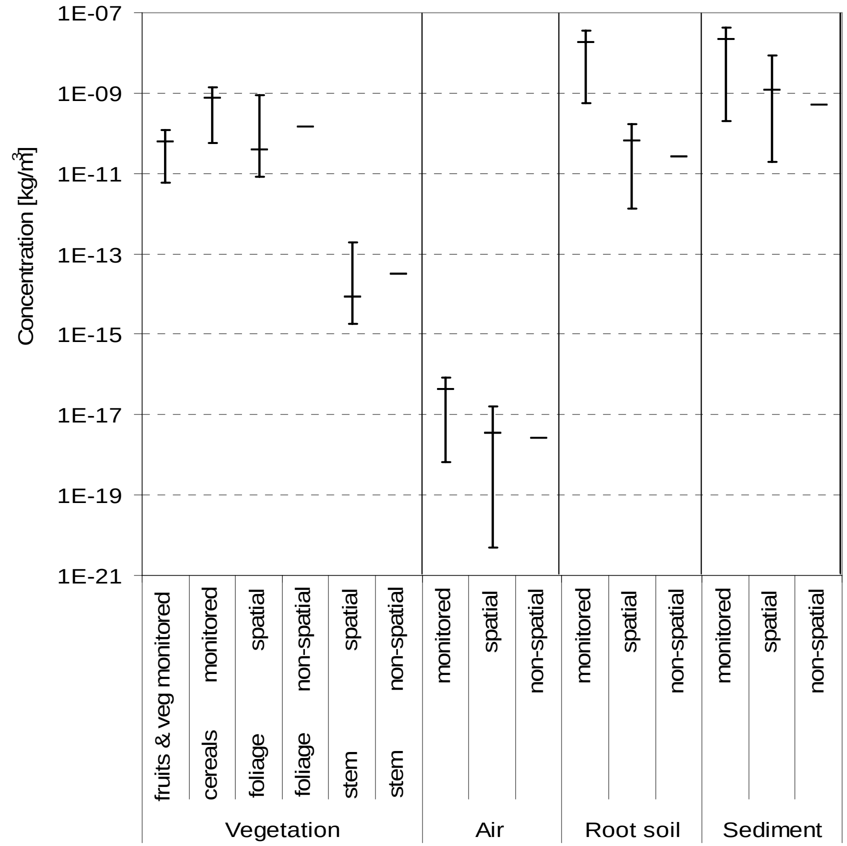
Pennington* et al., ES&T, 2005, *39, (4), 1119-1128



Emission of PeCDF in mg/hour



Environmental Pollution, vol. 128, (1-2), 263-277.

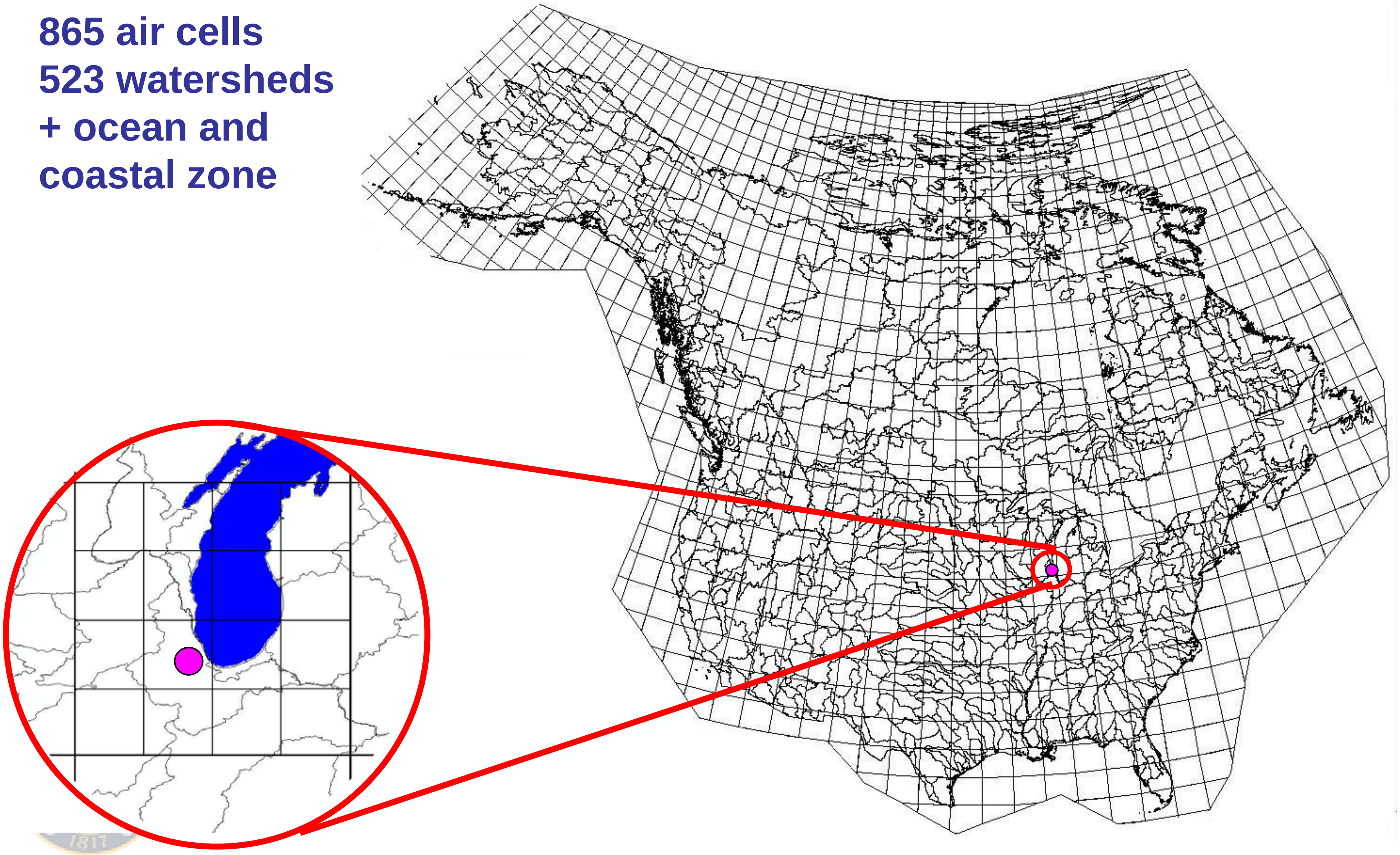


Measured iF=1.0E-2 (2E-3 to 5E-2)
Predicted iFspatial = 2.5E-2
Predicted iFnon-spatial = 1.0E-2

dioxin congener PeCDF (2,3,4,7,8-Pentachlorodibenzofuran; CAS# 39227-61-7)

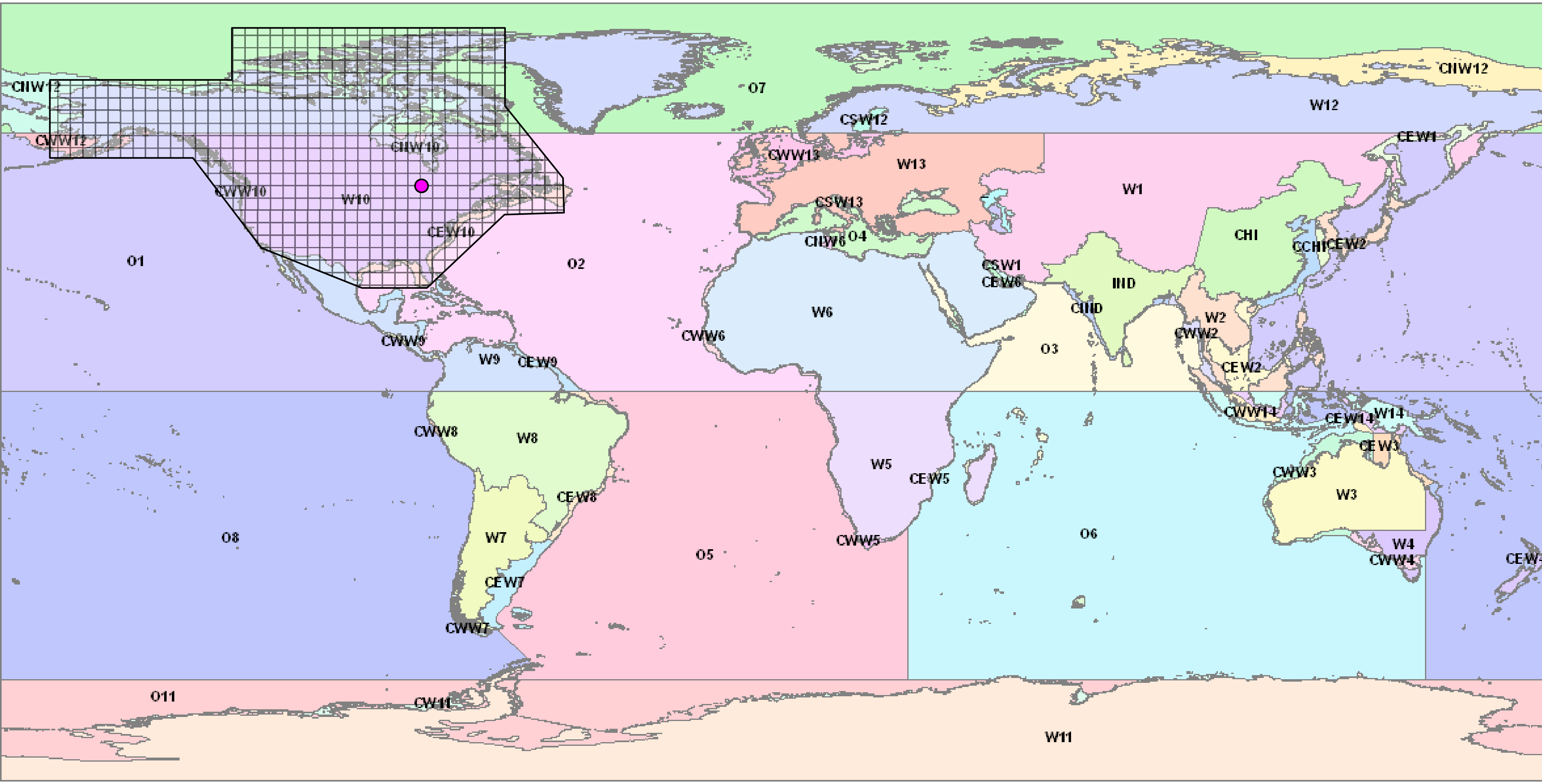
Airsheds (2°x2.5°) over watersheds

865 air cells
523 watersheds
+ ocean and coastal zone



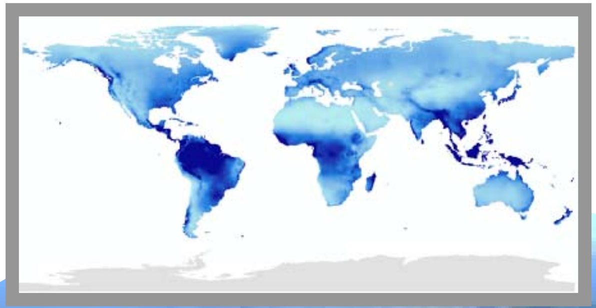
North American inserted in first World model with exposure

- Cells: 924 air, 540 watershed, 42 ocean/coast

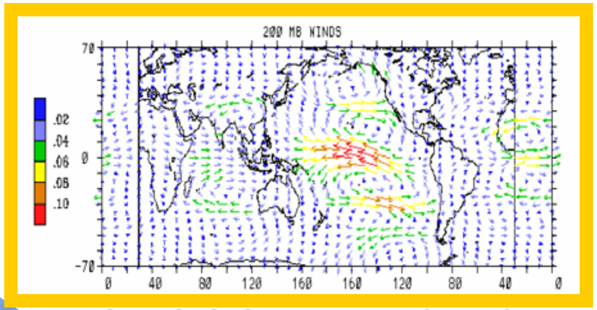


Important Multimedia Parameters: input from UNEP, UNECE

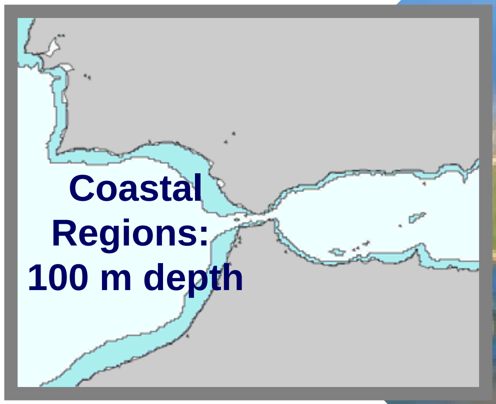
Rainfall Rate:
intermittent rain
Jolliet et al., 2005
ES&T, 2005,
39 (12), 4513-4522



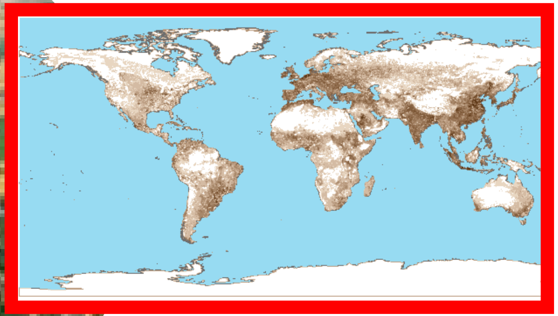
Wind



GEOSCHEM - 2 x 2.5

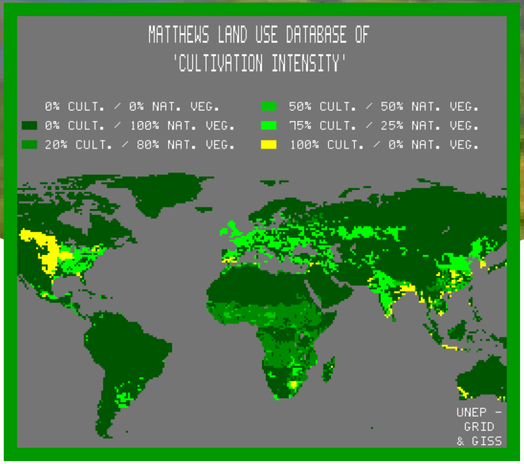


Coastal Regions: 100 m depth



Animal Production

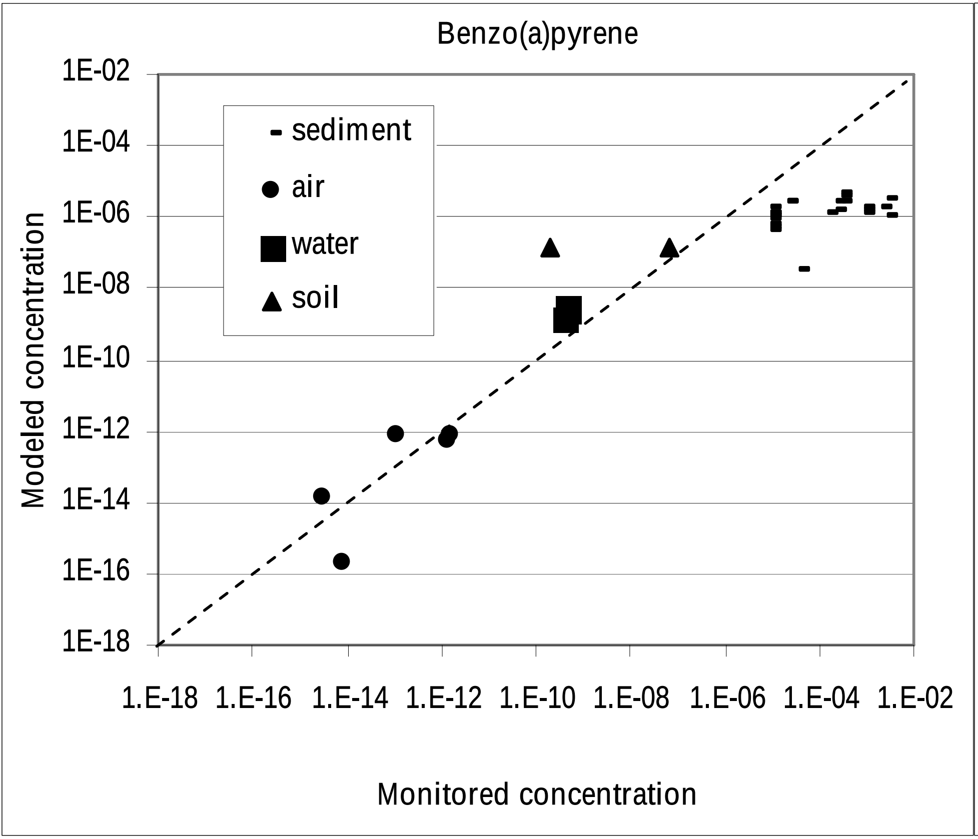
Coastal Area

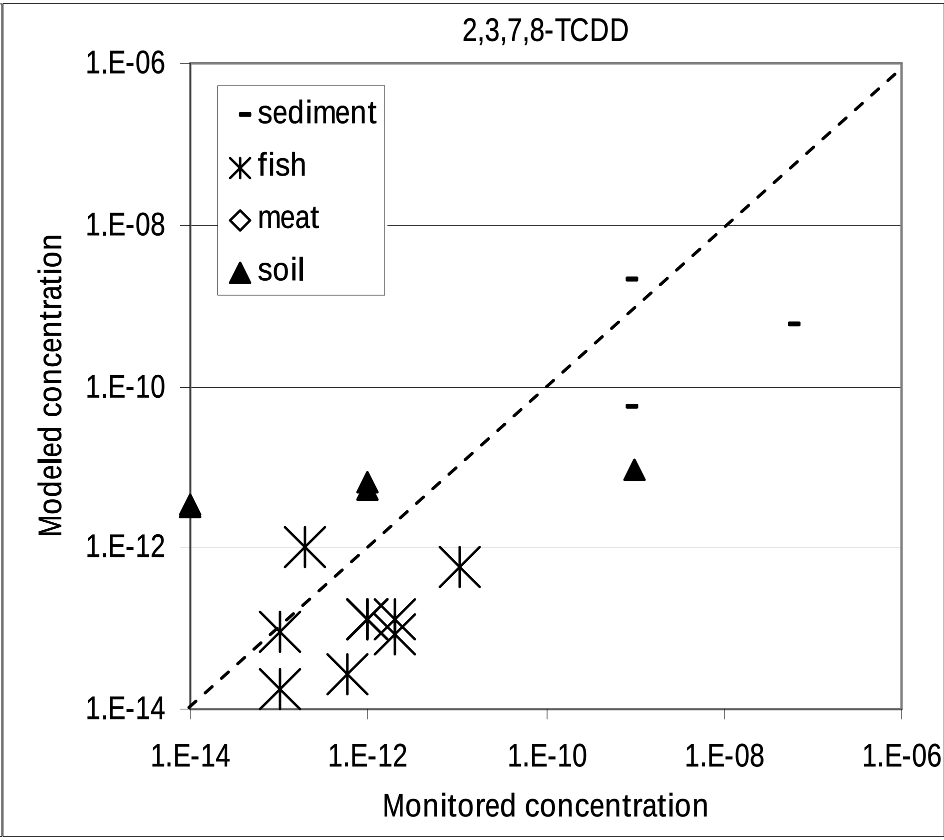


Vegetation fraction and production

FAO food balance data on production, human consumption import, exports, losses rice, cereals, beef, lamb, etc.

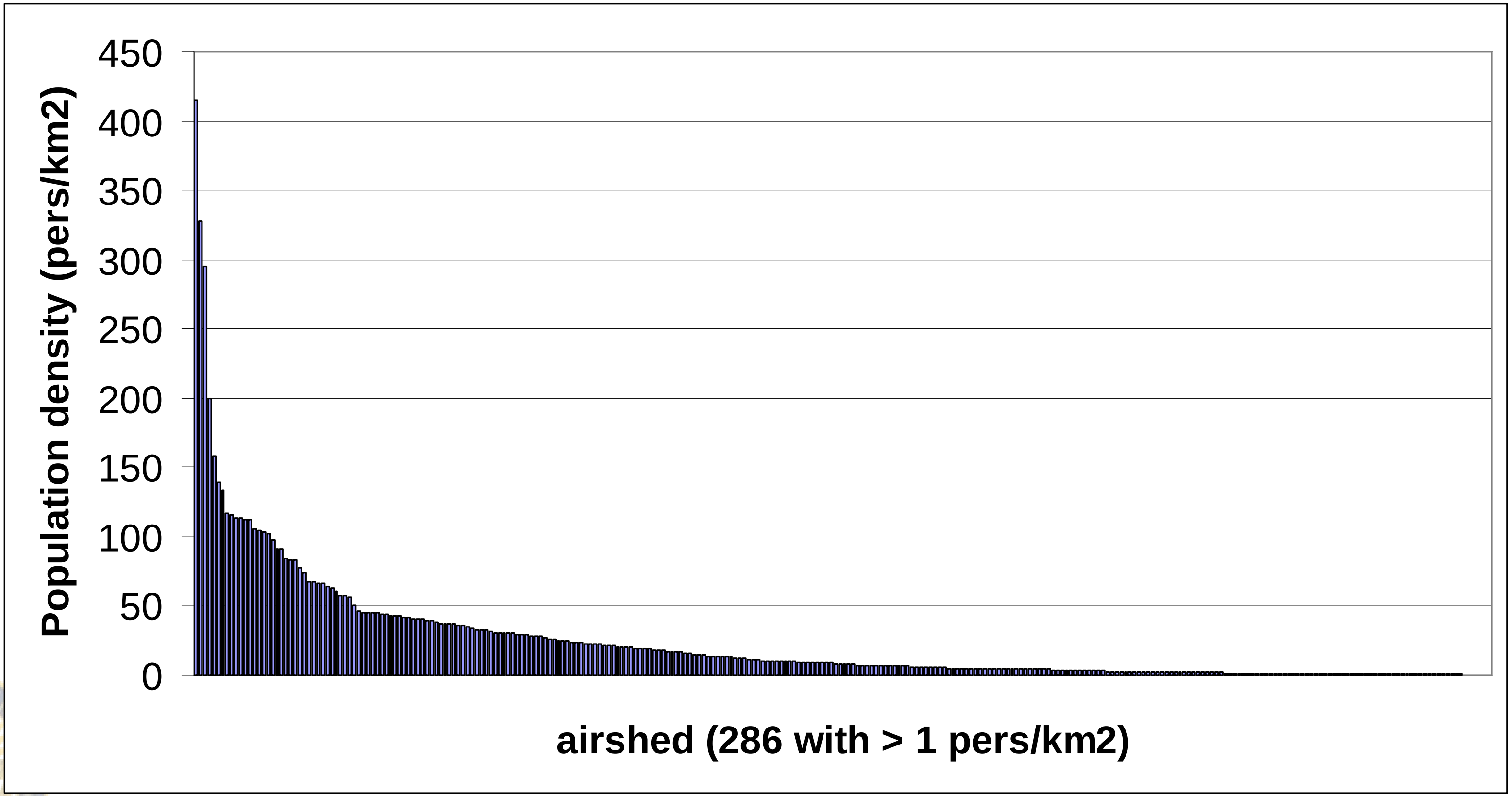
Model evaluation North America (BaP, TCDD)



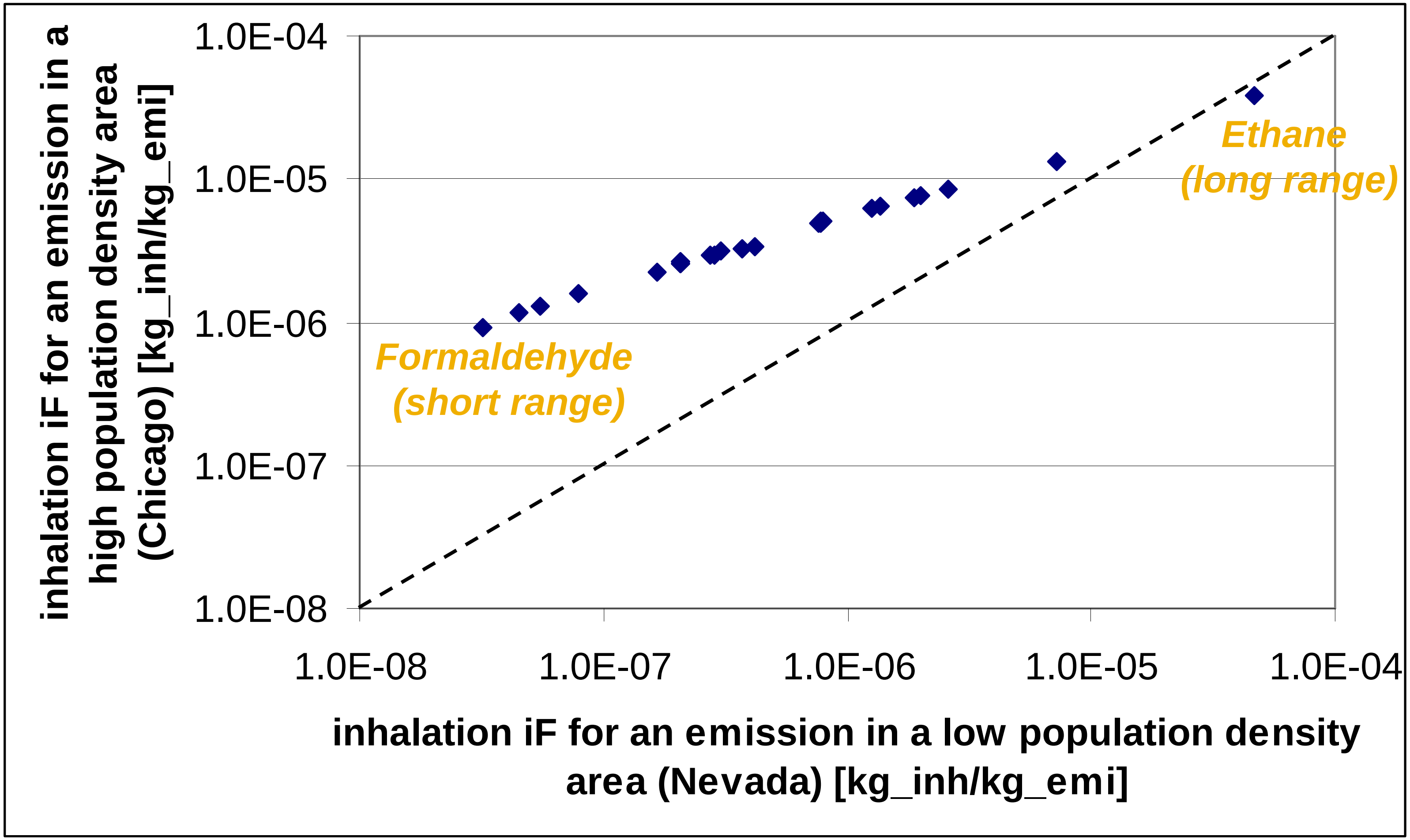


Variations in population density

- **Top 10 (> 100 pers/km²):**
  - **New-York, Washington, Boston, Chicago, Indianapolis, Milwaukee, East Los Angeles, West Los Angeles, Miami, San Francisco**



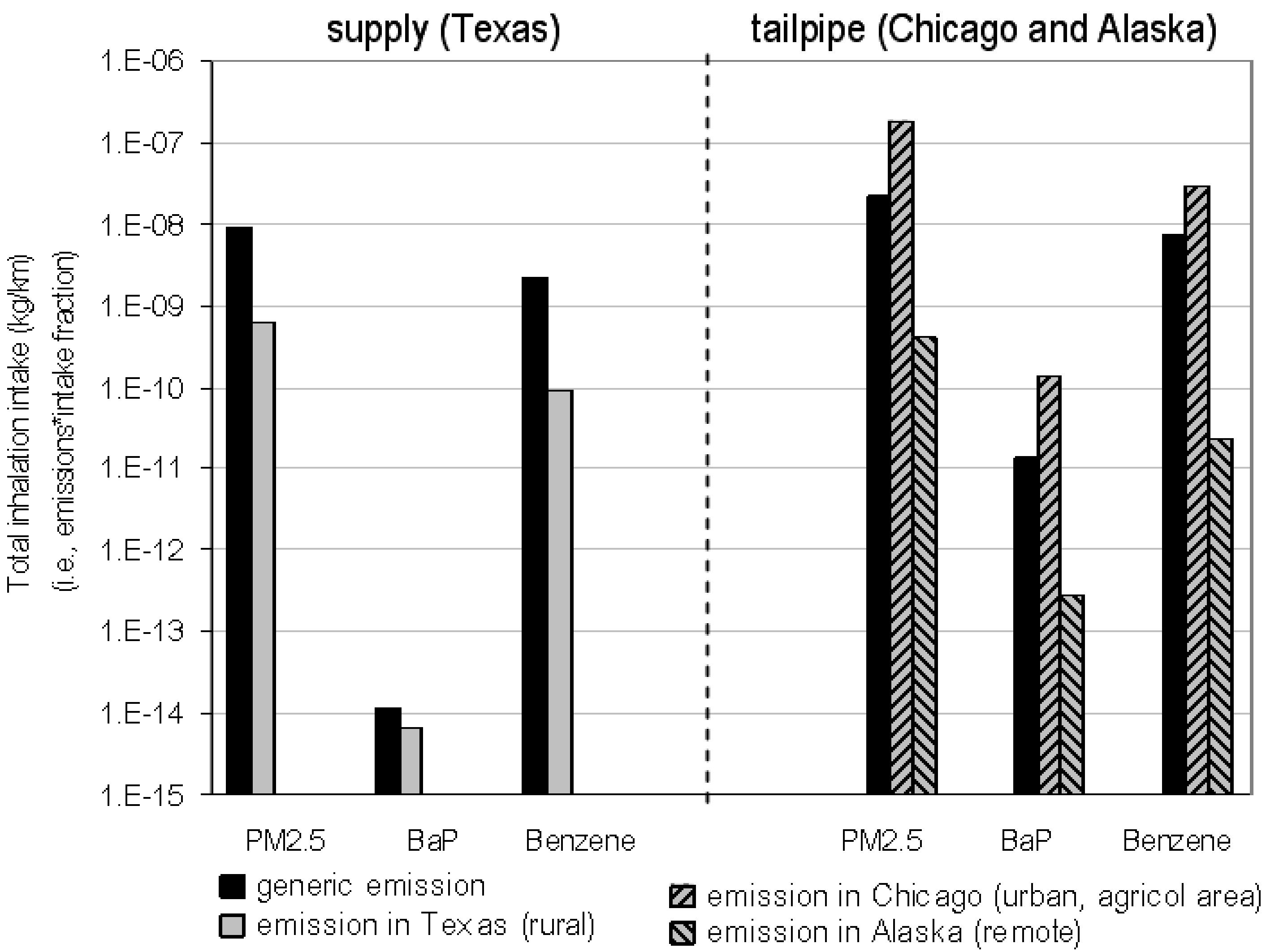
Variations in inhalation intake fraction as a function of location of emission



➔ **For short range pollutants, location of emission is important.**

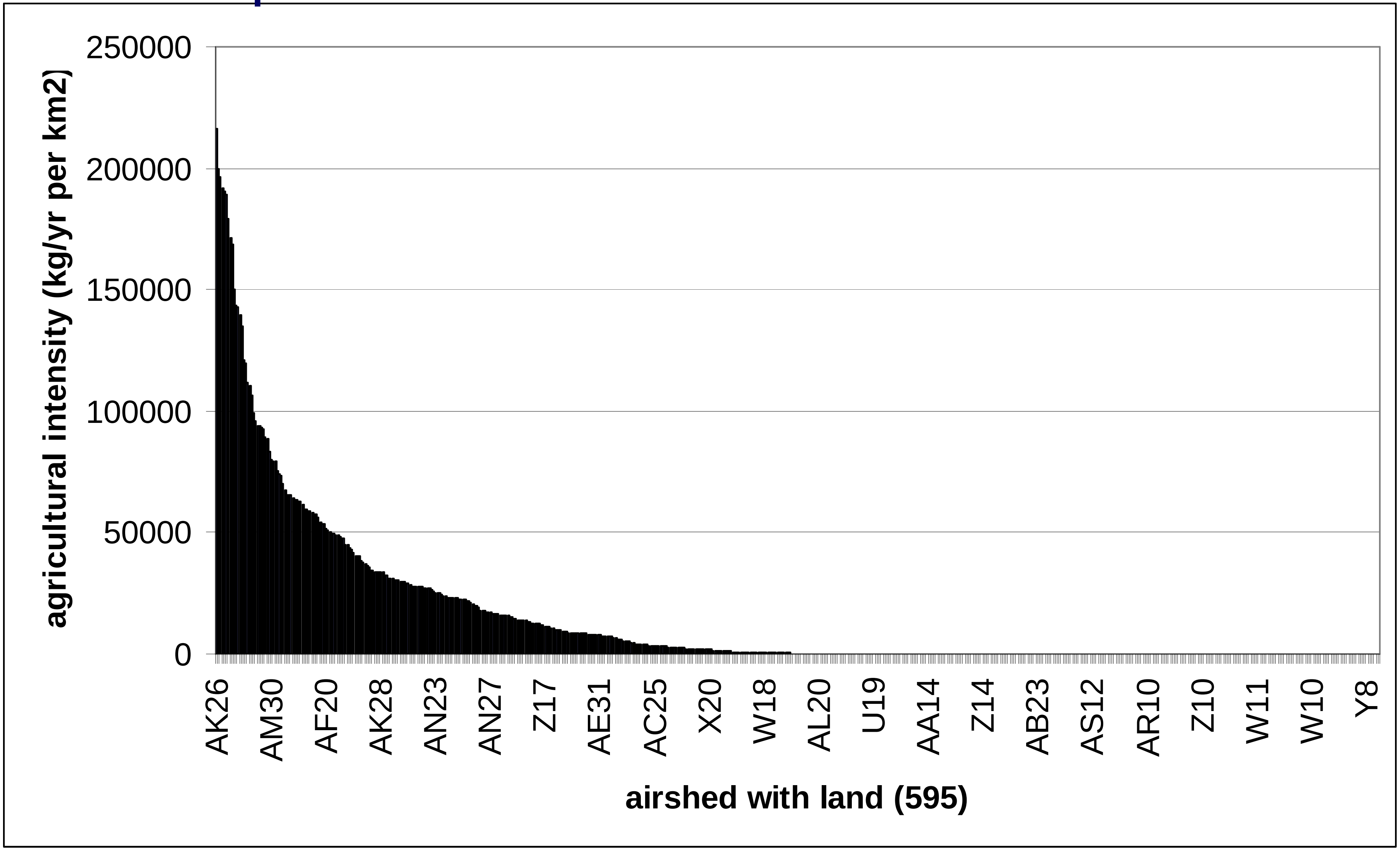
➔ **For long range pollutants (i.e. correlated with high inhalation iF), difference due to the location of emission becomes negligible.**

Inhalation Intake fractions from a diesel car for generic and regionalized models

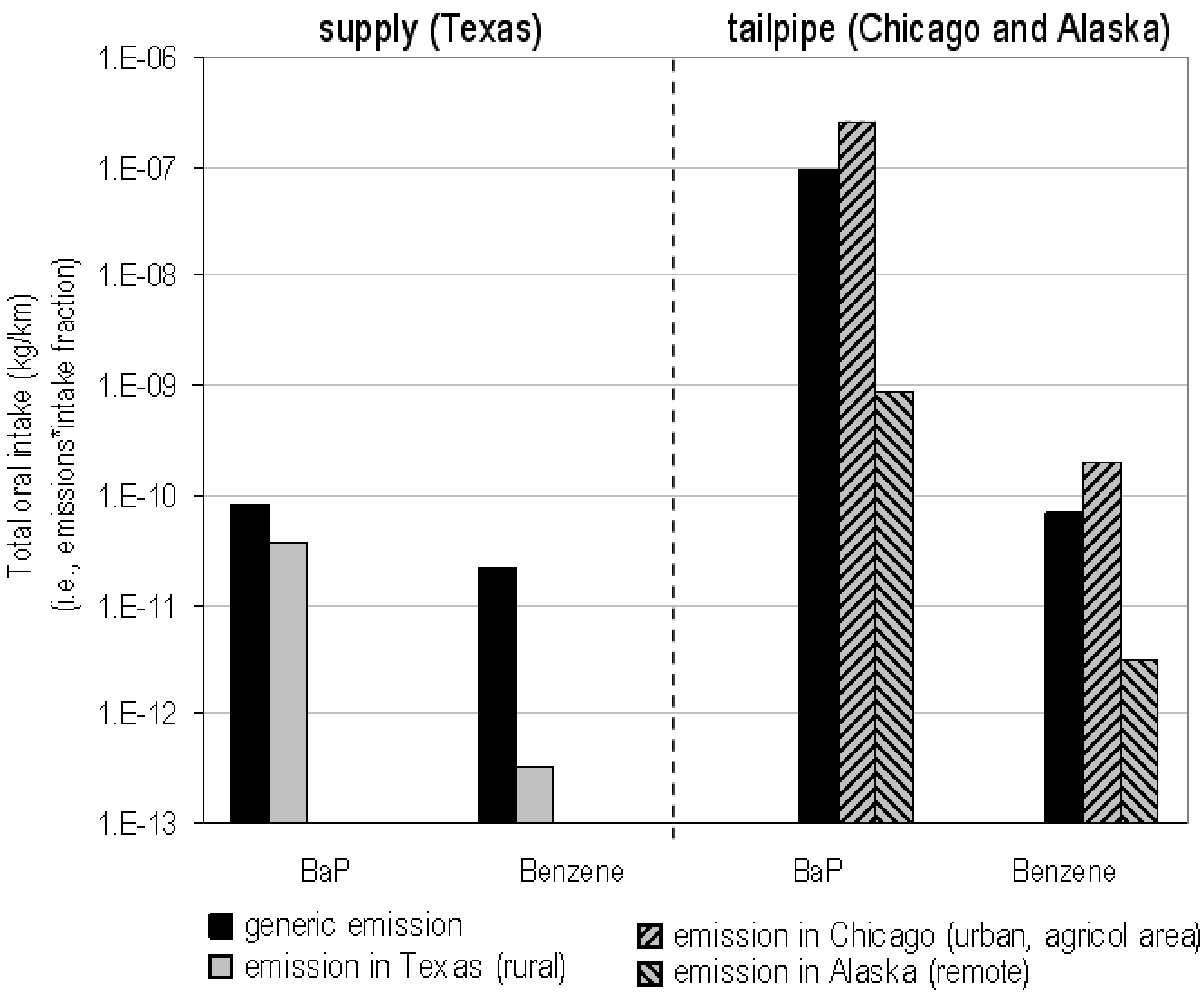


Variations in agricultural intensity

Top = Midwest

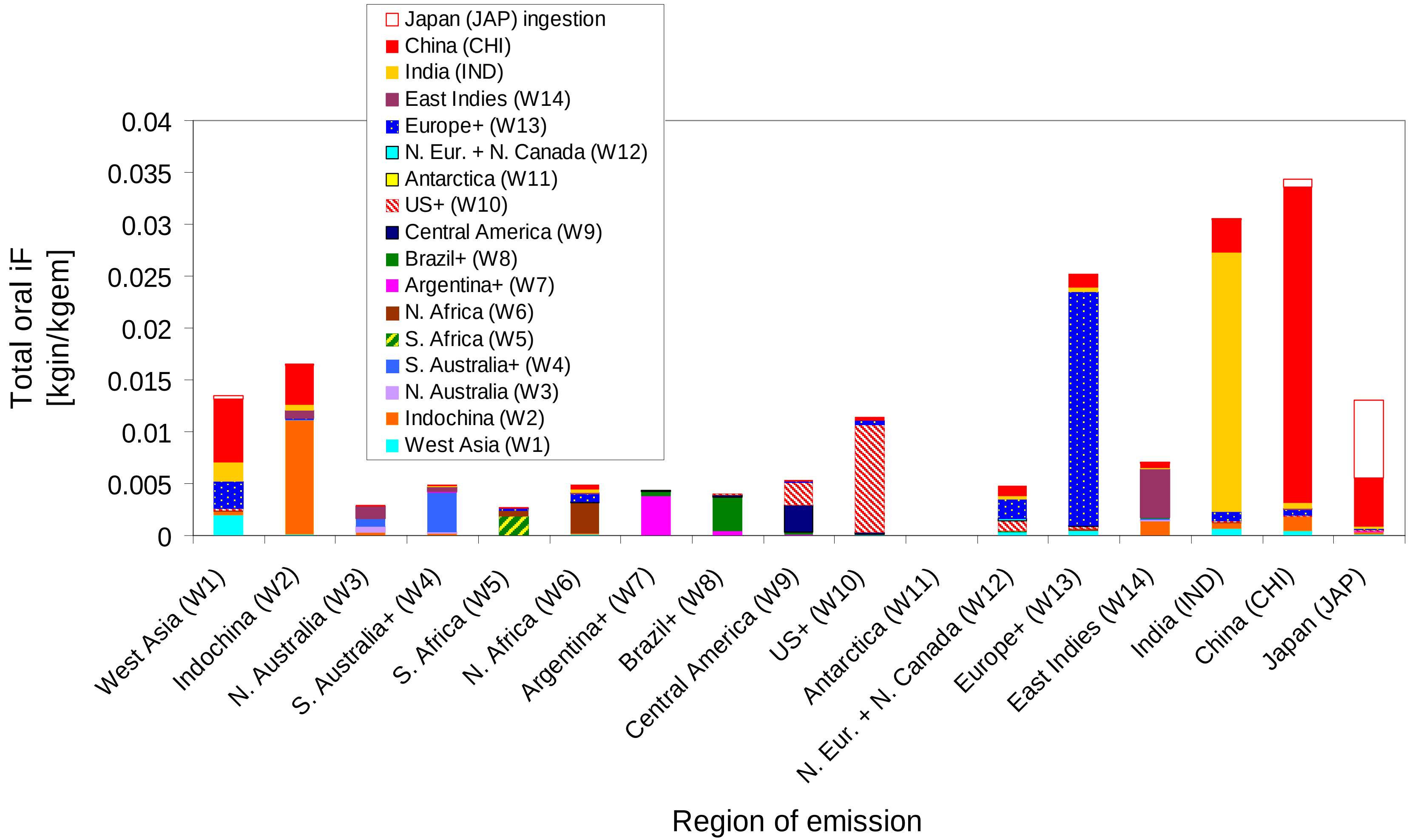


Ingestion Intake fractions from a diesel car for generic and regionalized models



Spatial oral intake fraction in the 17 world regions: Dioxin (2,3,7,8 TCDD)

- **So far, food produced in the region is consumed in the region!**



Accounting for truck transportation: fate in the economy

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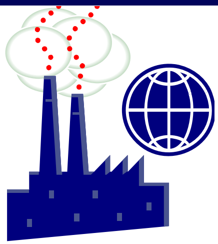
POPs spatial transfers in food imports and exports



Emissions to
compartment *m, region i*

[kg_{em}/yr]

Environmental fate:

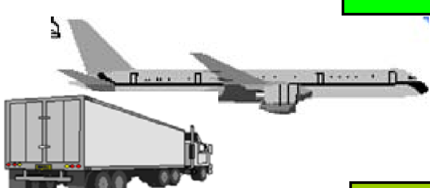
multi-compartmental and regional transport

Concentration & mass in
compartment *n, region k*

Exposure

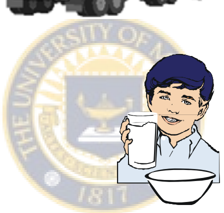
Dose in exposure product
in region k

[kg_{prod}/yr]



Economic fate:

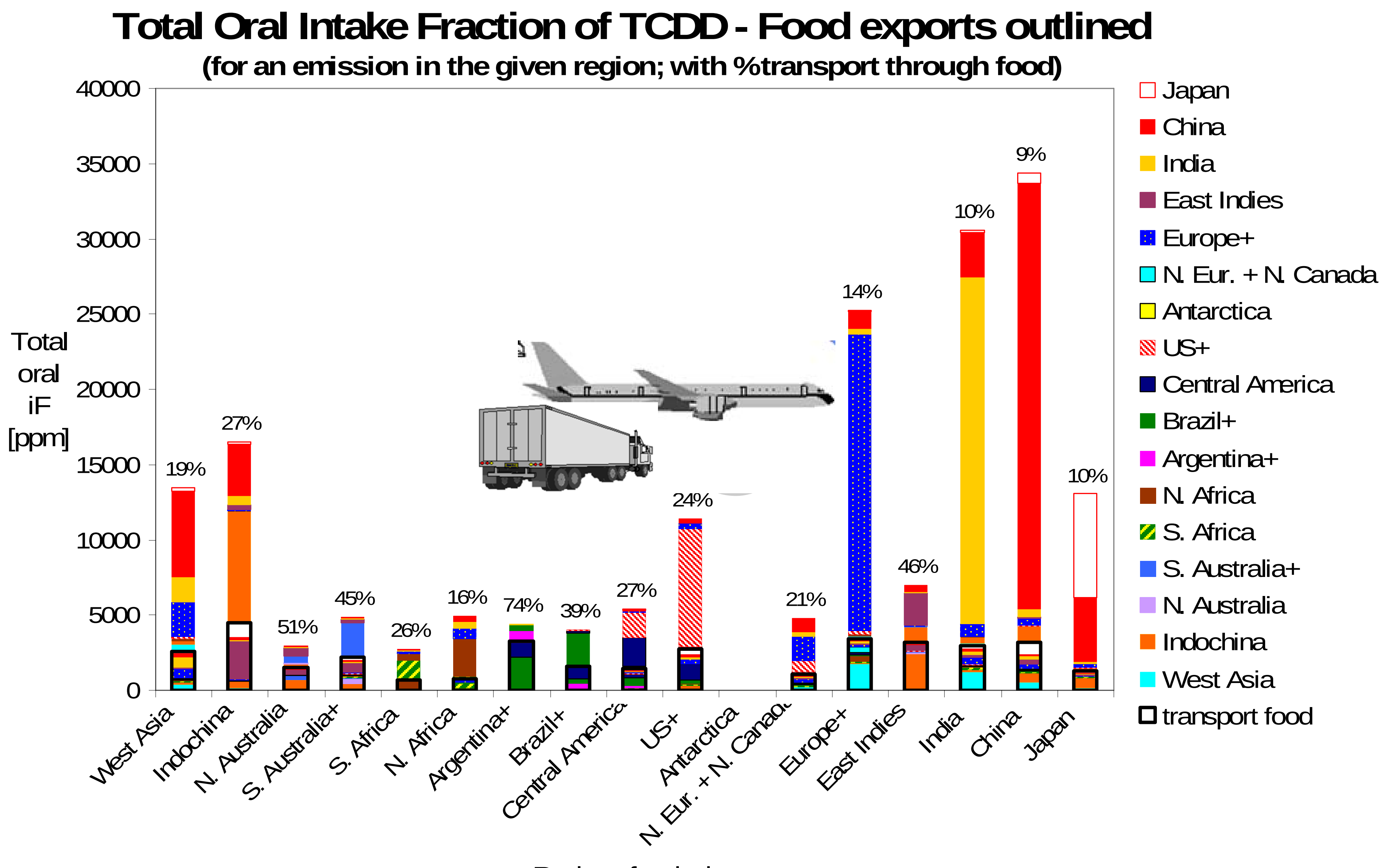
multi sectorial and regional trade



Dose taken in by humans
in region j

[kg_{in}/yr]

Food export doubles inter continental transfer: +24% (9%-74%) food export, 53%(18-99%) overall



Further developments and conclusions (multiscale, emissions to biomarkers)

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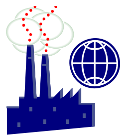
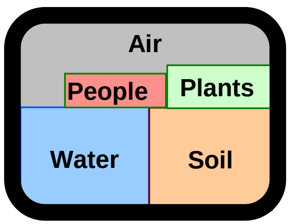
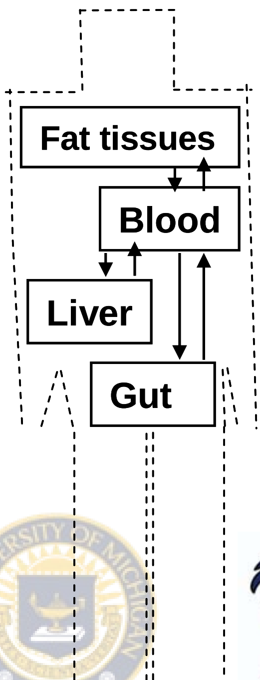
Emission source to biomarkers: combine iF with pharmacokinetic modeling (PBPK)







Emissions to compartment *m*

↓

Concentration & mass in compartment *n*

↓

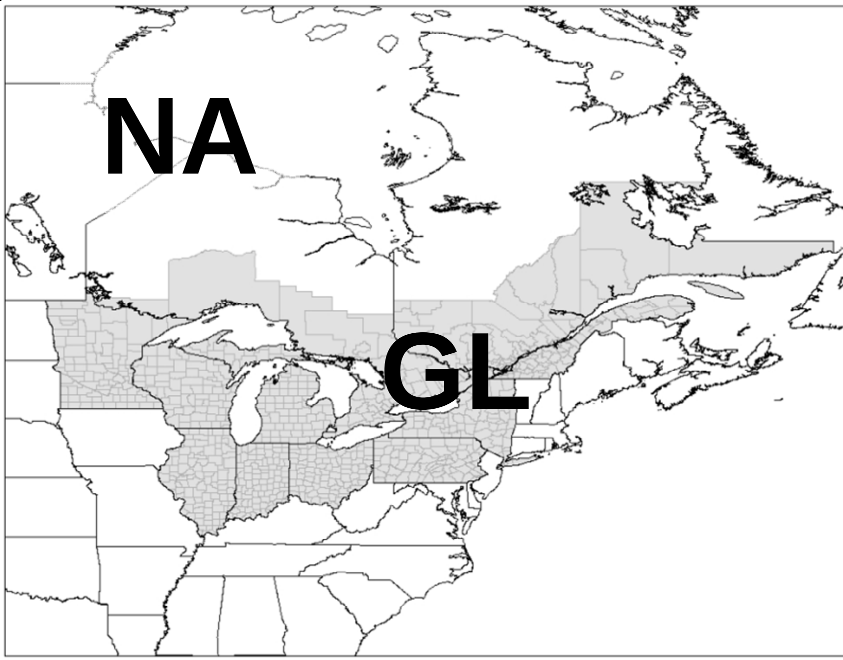
Dose taken in

↓

Concentration & mass in body & target organ

↓

Damage to human health



Compare with NHANES biomarker measurements: 300 substances for 2000 individuals every year

Multiscale multimedia source to intake - biomarker modeling

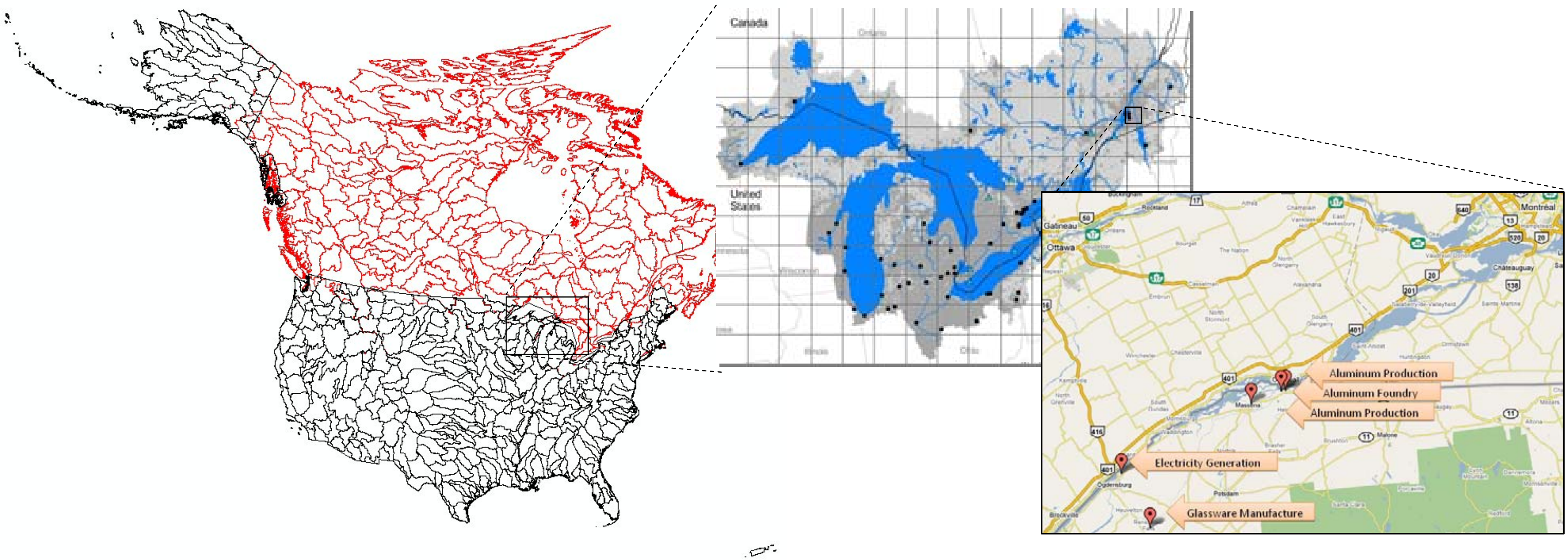
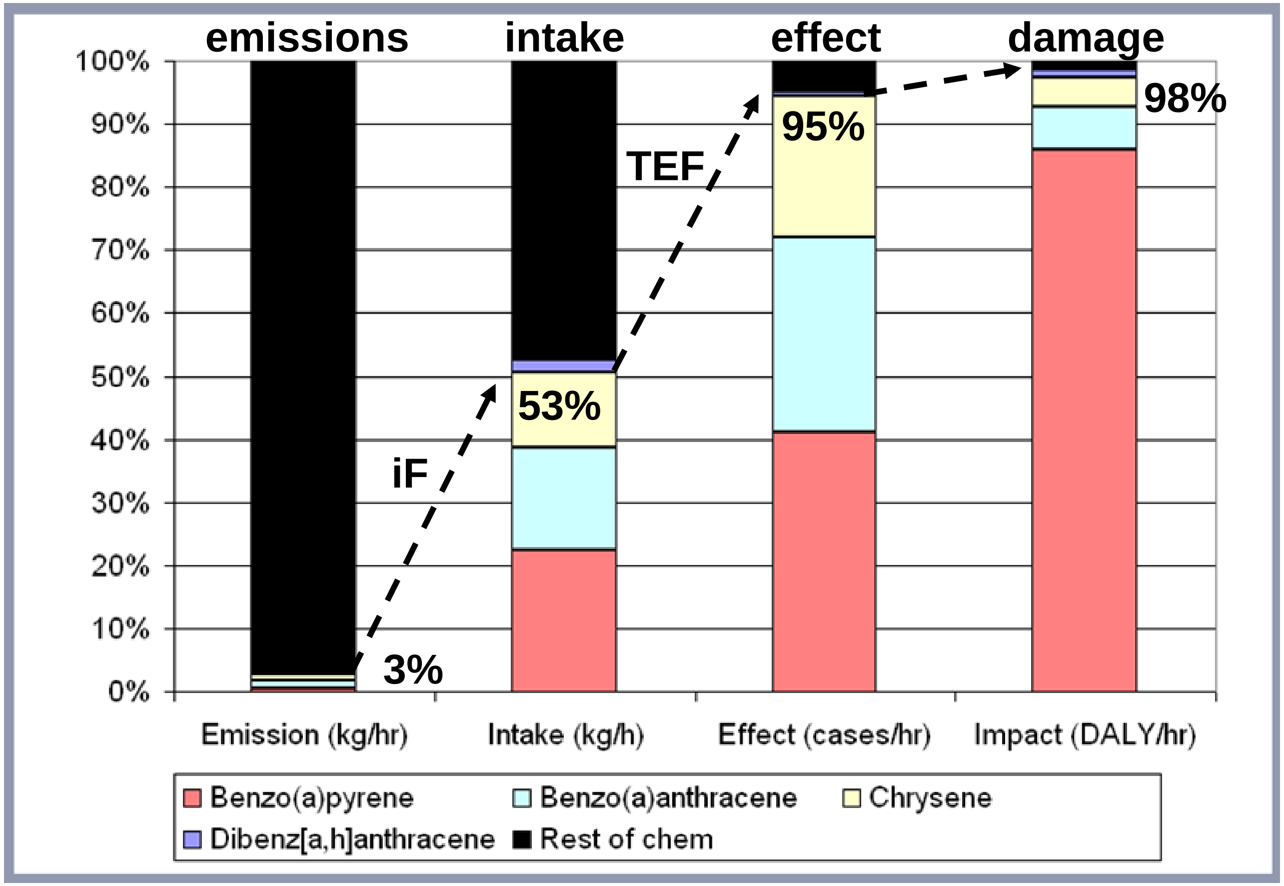


Figure 1. Schematic description of the multiscale multimedia model

e.g.
- Study the local vs long range impact of an incinerator
- Create policy-relevant source apportionment maps: which sources are responsible for which exposure and health impact

Comparative assessment of PAH from emission to damage



- To assess PAH **intake,** Toxic Equivalency Factor:TEF but not for emissions or blood

- To assess PAH **emissions**, Emission Equivalency factors: EEF=iF * TEF, (iF= Intake fraction)

Emissions, intakes and effects of 16 PAH emissions

3% of emissions correspond to 53% of intake which account for 98% of impact

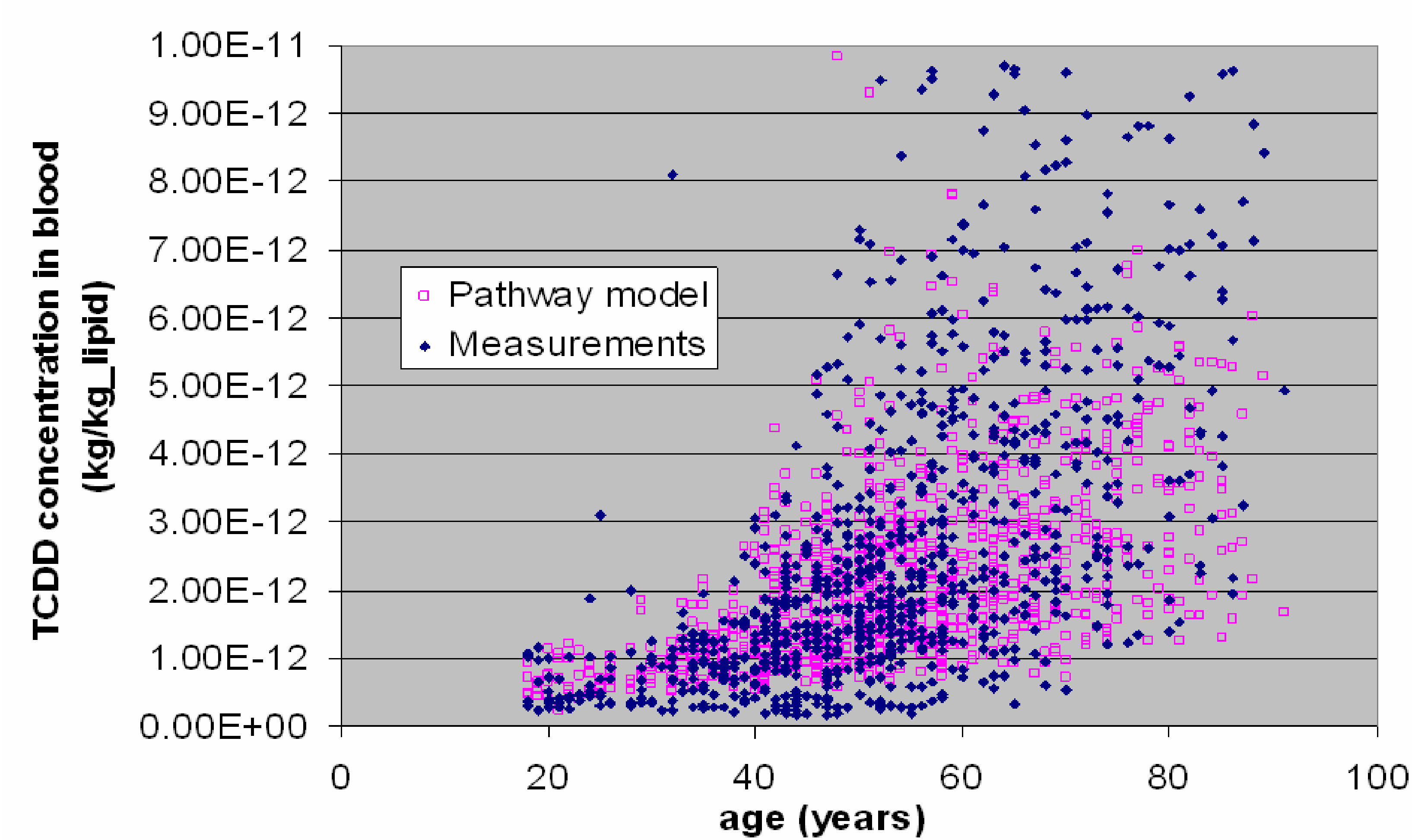
Conclusions

- The USEtox tool built on parsimony and intense collaboration is a useful tool for chemical screening from emission to impacts
- The IMPACT models provides regionalized exposures in North America and worldwide
- Import - exports of POPs in food do matter and are as important as long range environmental transport. The developed framework enables to model the fate in the economy in a similar way to the fate in the environment

→ Extension to local multiscale and biomarkers

→ Further study uncertainty and input data quality (half-lives, biocincnetration factors, etc.)

Predicted versus monitored TCDD Blood concentrations for 942 individuals as a function of age diet survey: R^2=0.42



University of Michigan Dioxin Exposure Study