Screening Tools for the Risk Assessment of Chemicals

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Brussels, 25 June 2003

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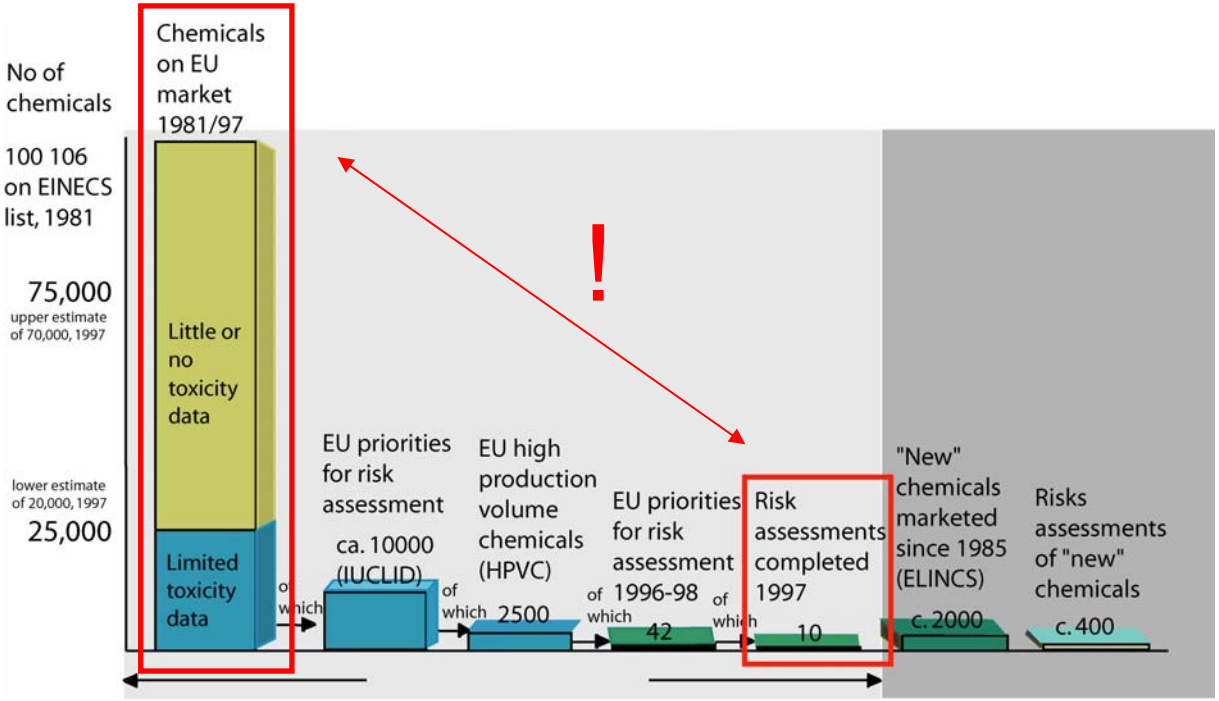
http://ltcmail.ethz.ch/hungerb/index.html

Overview

- **Risk assessment for chemicals: methodology and situation today**
- New screening approaches
  - Exposure-based hazard assessment (Approach 1)
    Models A, B, C
  - Scenario-based exposure assessment (Approach 2)
    Occupational exposure (A), Consumer exposure (B)
- Conclusions

Existing and New Chemicals in the EU



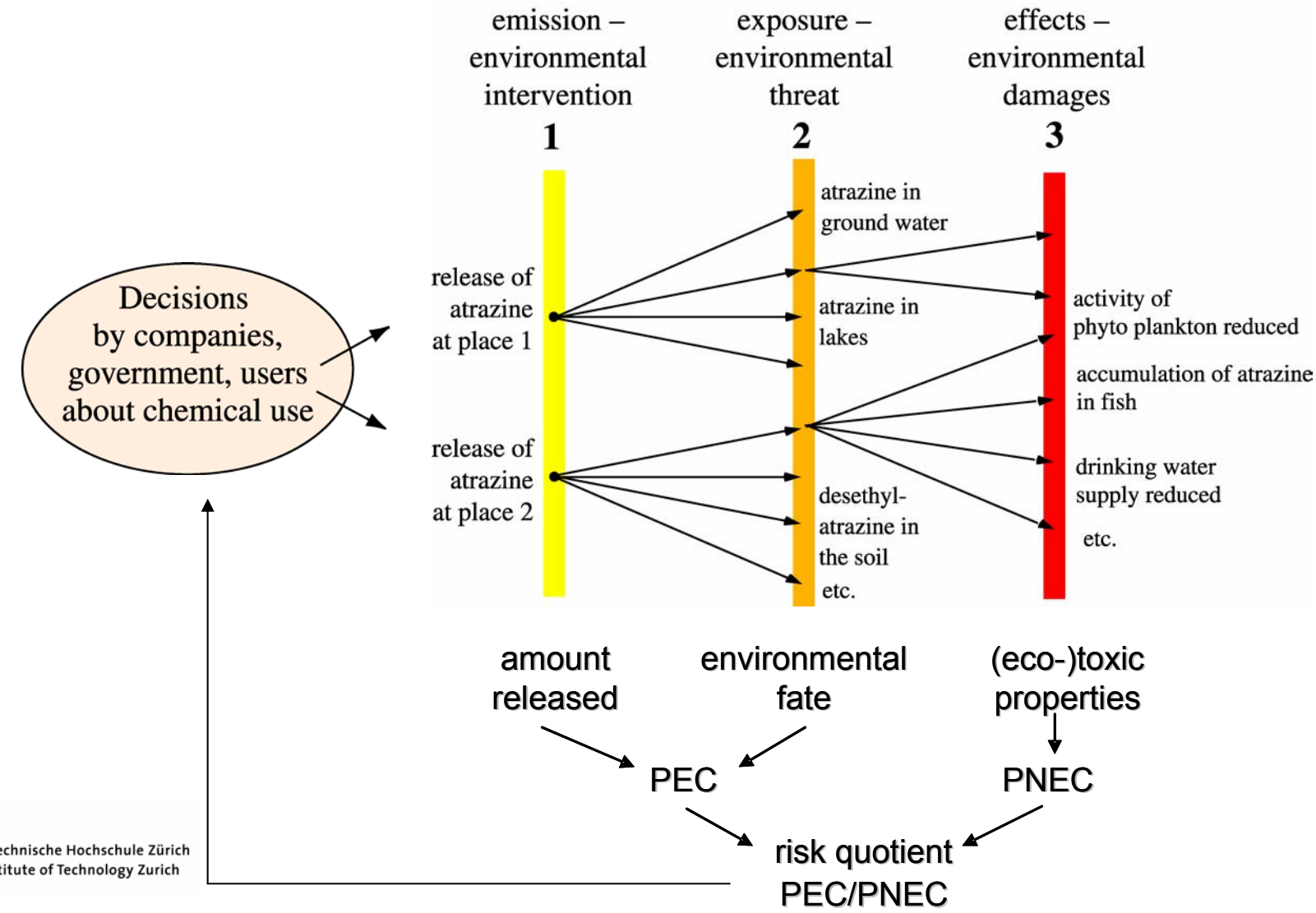
Implications:

- Additional criteria for prioritisation required,
- Methods for tiered assessments of chemicals desirabl (screening stage, in-depth stages)

Exposure, Effects, Risk, and Hazard

- EXPOSURE: presence of a chemical at a target, expressed in terms of concentration.
- EFFECT: toxic or ecotoxic impact caused by an exposure, characterised in terms of dose-reponse relationships (→ e.g. LC50).
- RISK: possibility of ocurrence of adverse effects to human health or the environment, expressed in terms of ratios of exposure levels to effect thresholds; depends on amount released.
- HAZARD: inherent potential of a chemical for effects, for bioaccumulation, or for widespread and long-lasting exposure; independent of amount released.

Methodology of Risk Assessment



Problems

- High number of chemicals and products containing chemicals
- Full risk assessments for environment and human health too expensive, too slow
- High complexity of environmental systems:
  - unknown effects
  - unpredictable behaviour of ecosystems
- High complexity of chemical use patterns; scenarios for consumer exposure often lacking

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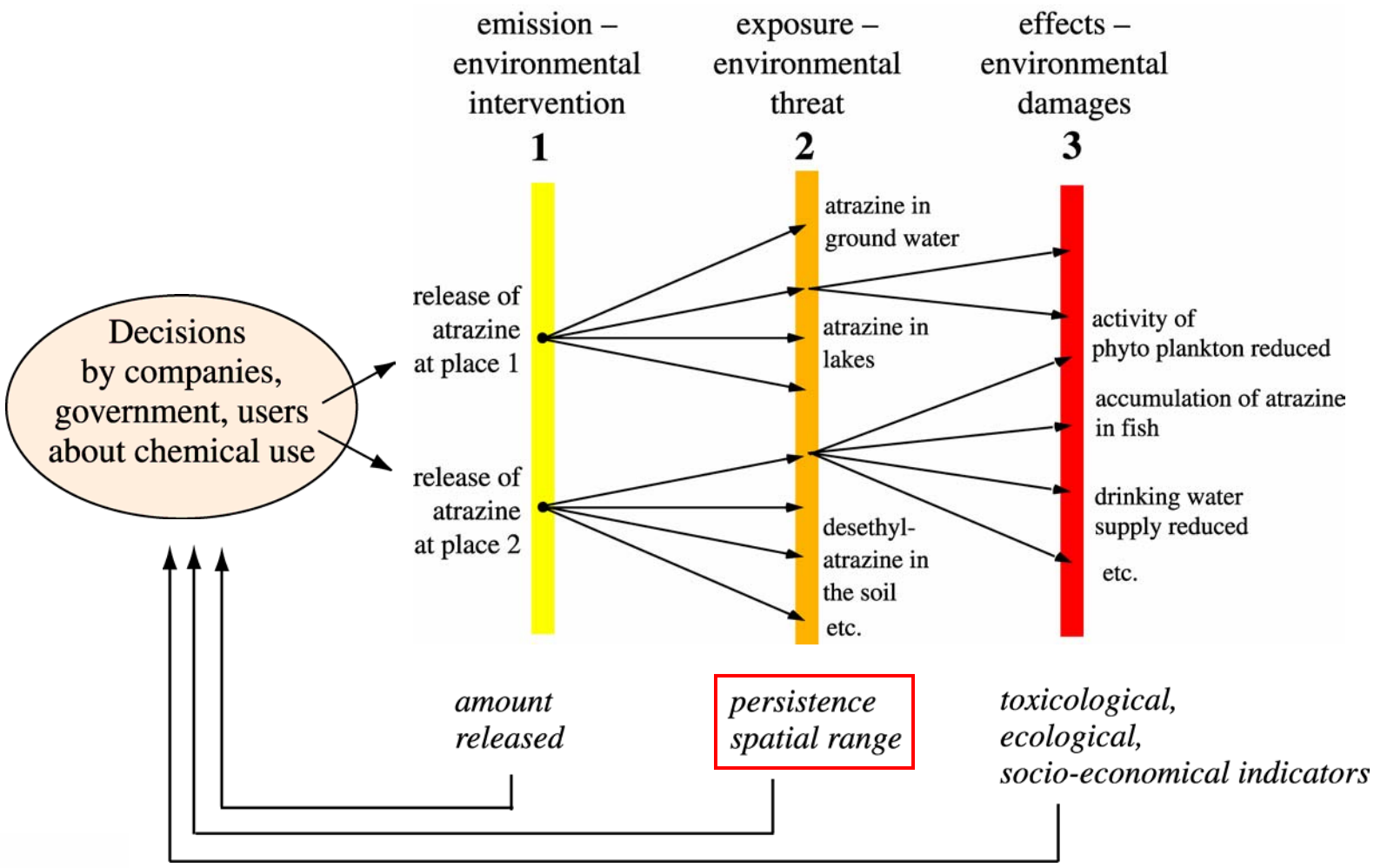
Exposure-based Hazard Assessment

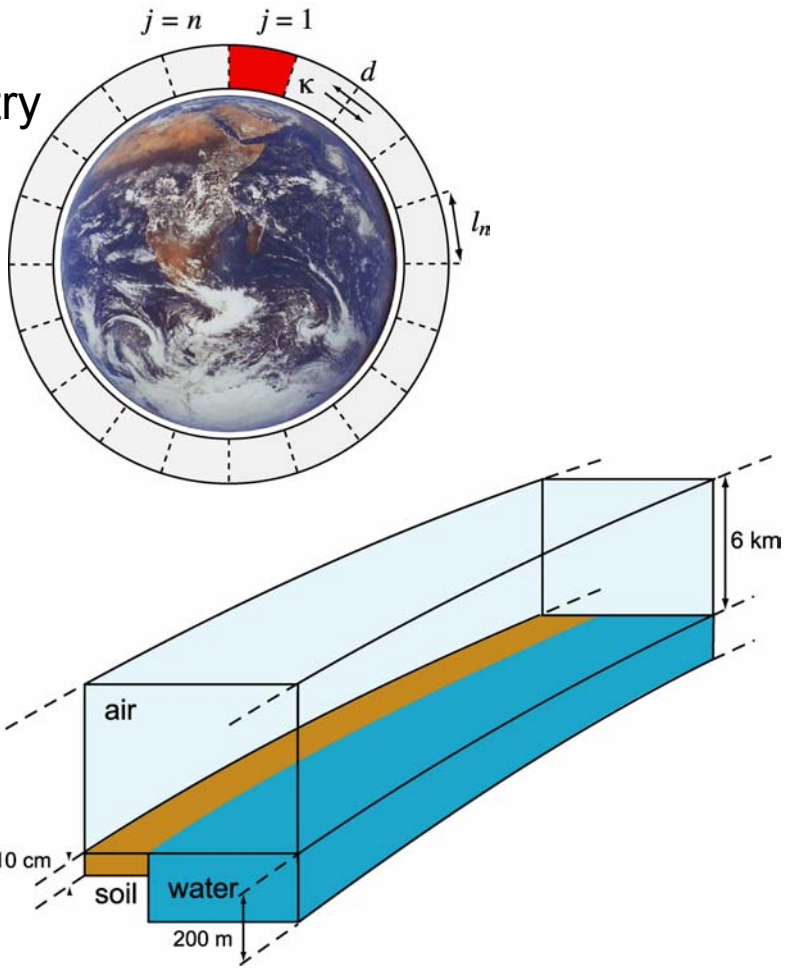


Persistence and Spatial Range

- Objective: to characterise the **duration** and **spatial extent** of a concentration pattern in the environment.
- Based on: information on **degradability & mobility** of chemicals in the environment.
- Information sources:
  - **Laboratory** experiments
  - **Field** measurements
  - **Model** calculations
- Here: model calculations with screening models of the environmental fate of chemicals.

Global Model »ChemRange«

Geometry



- Input parameters (from measurements):
  - degradation rate constants
  - partition coefficients
- Model results:
  - concentrations in soil, water, and air
  - persistence
  - spatial range

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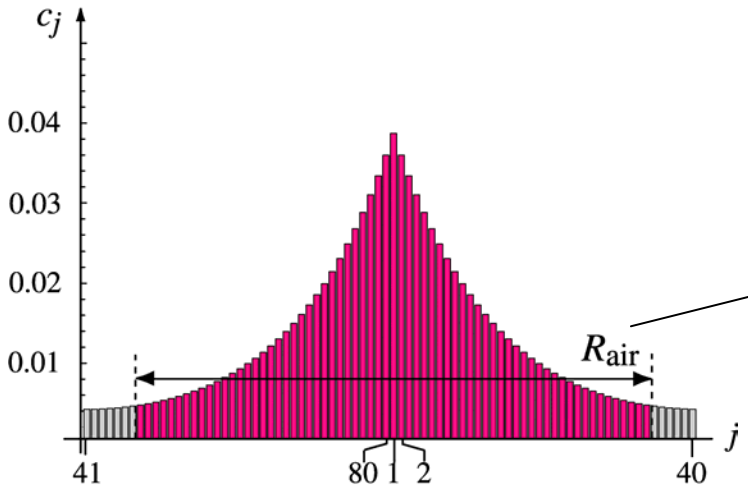
Model available at: http://ltcmail.ethz.ch/hungerb/research/product/chemrange.html

»Chemrange«: Results

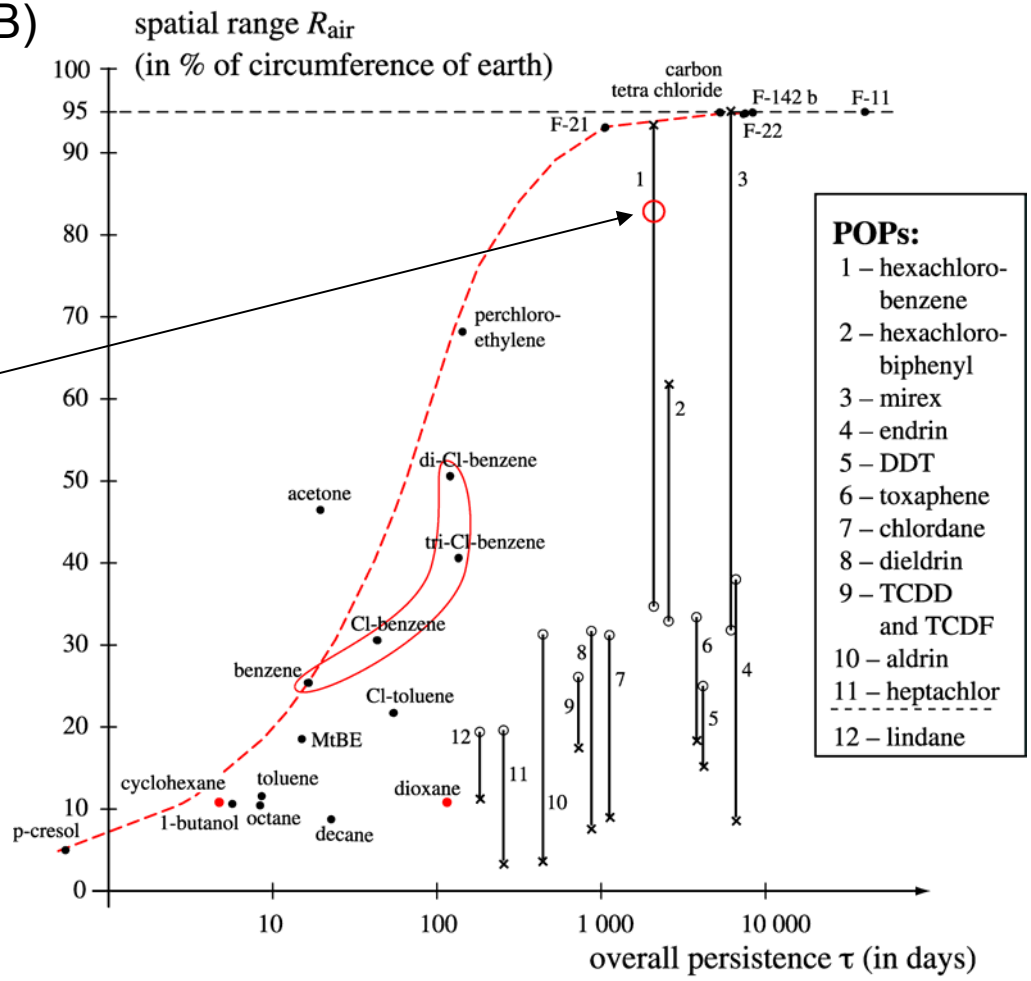
concentration in air (relative units)

Example: hexachlorobenzene (HCB)



Persistence: residence time in the model system, (HCB: 2100 days)

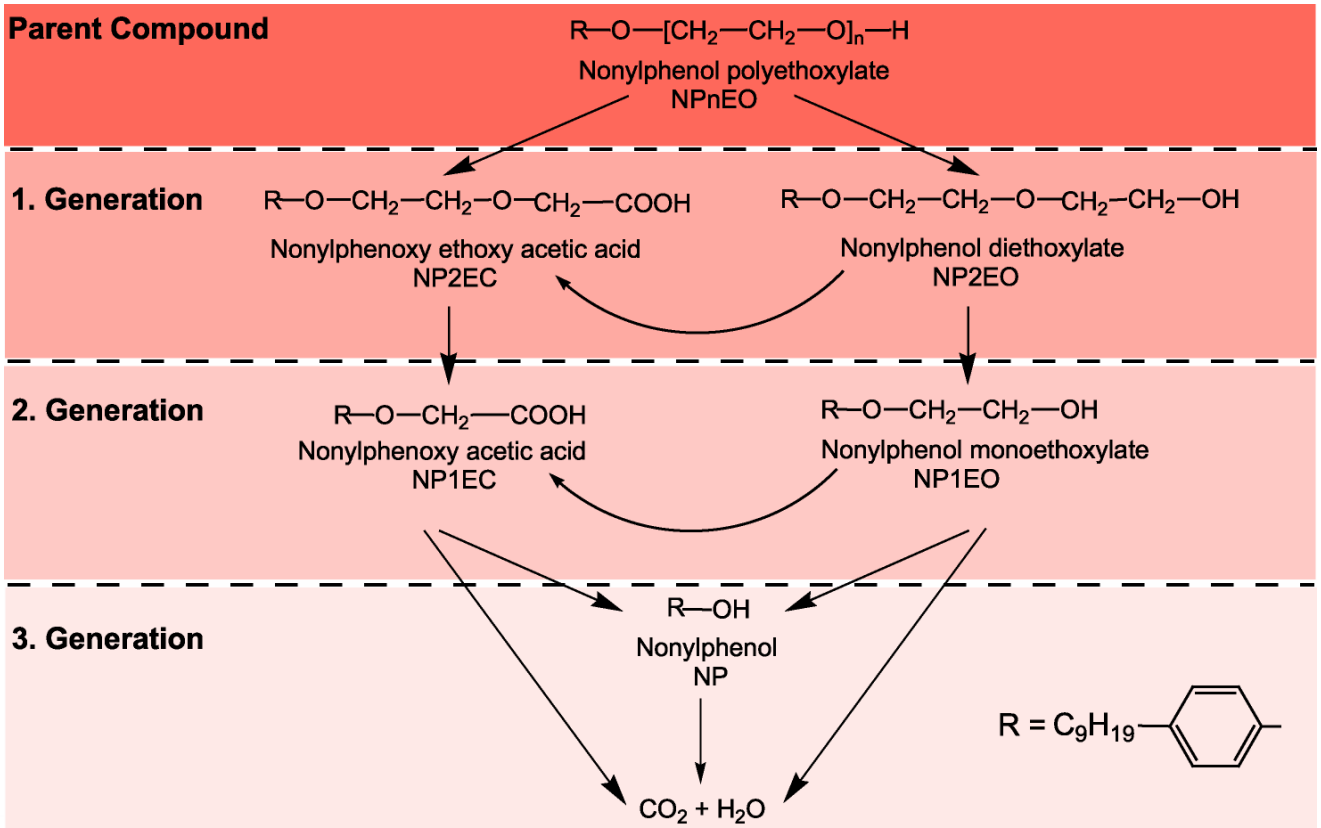
Spatial range: distance containing 95 % of the distribution (pink), (HCB: 83 % of circ. of earth)



Inclusion of Transformation Products

Transformation products:

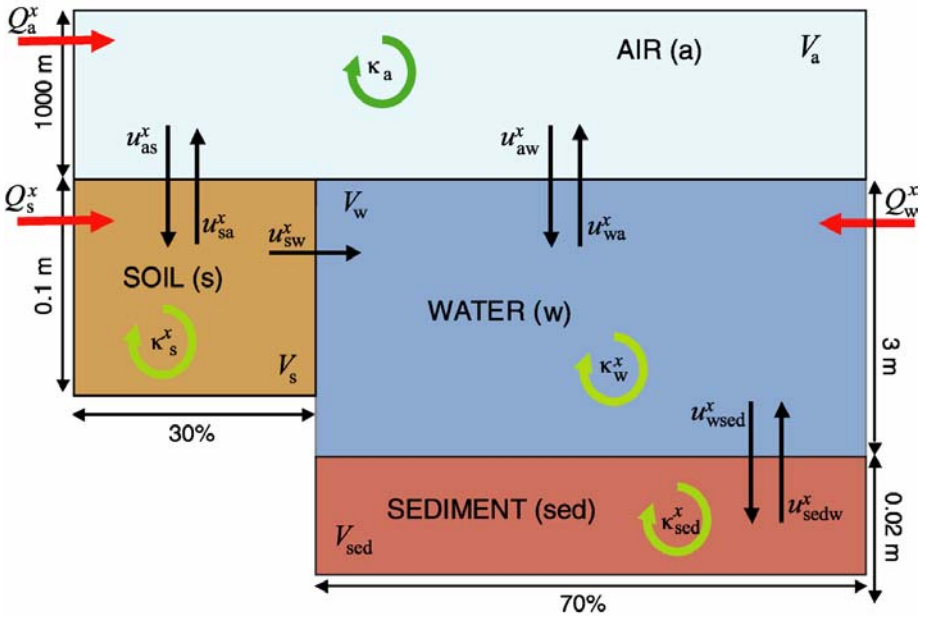
- Often neglected in risk assessments
- Can contribute significantly to exposure and effects



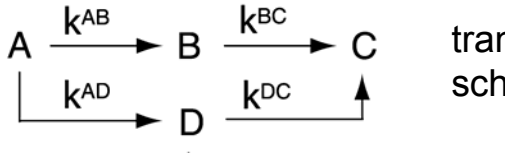
Example: Nonylphenol-polyethoxylates and their transformation products

Generic Model for Transformation Products

Simple four-compartment model



Model mathematics



transformation scheme

$$S = \begin{bmatrix} S^A & 0 & 0 & 0 \\ -K^{AB} & S^B & 0 & 0 \\ 0 & -K^{BC} & S^C & -K^{DC} \\ -K^{AD} & 0 & 0 & S^D \end{bmatrix}$$

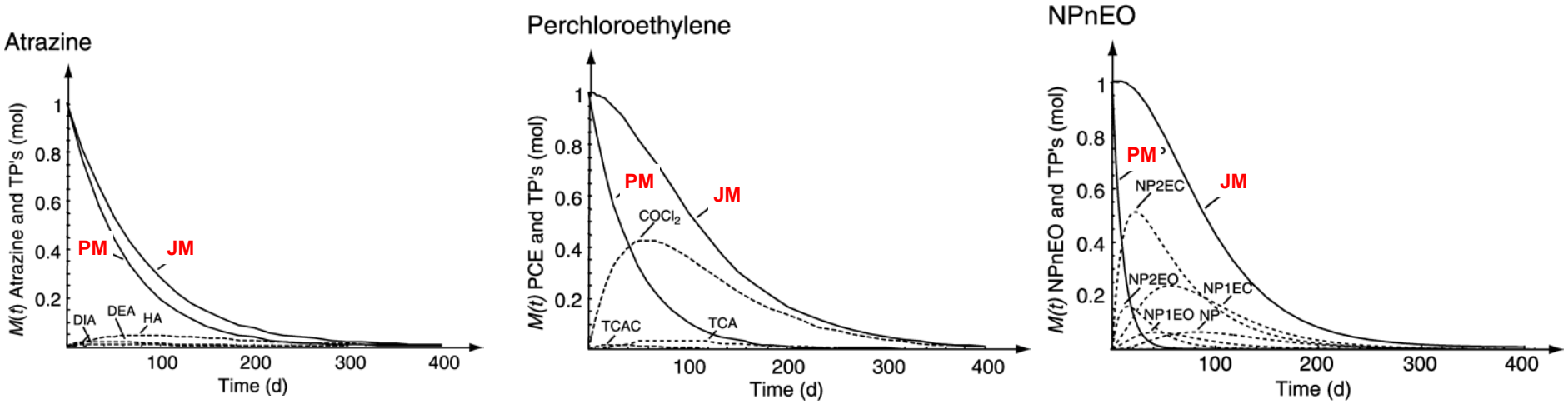
model matrix

$$\dot{c} = S \cdot c + q$$

mass balance equation, provides concentrations *c(t)*

Transformation Products: Results from Three Case Studies

Mass of chemicals in the model system as function of time
PM: primary mass profile, JM: joint mass profile



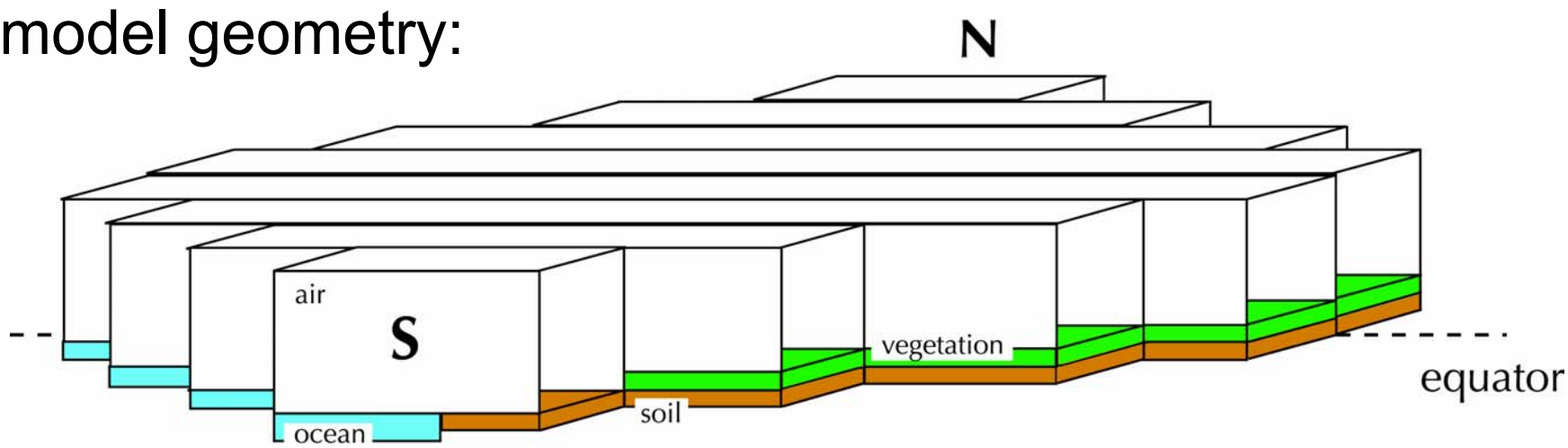
Case studies show: Joint exposure and persistence (including all transformation products) can be higher by a factor of 4.

Assessment of Persistent Organic Pollutants

- Problem: long-lasting contamination, accumulation in the food chain, in particular in polar regions. Addressed by the Stockholm Convention of 2001
- Effects of temperature:
  - Cold condensation
  - Global fractionation
- Influence of temperature requires a more complex model

Global Model »CliMoChem«

model geometry:

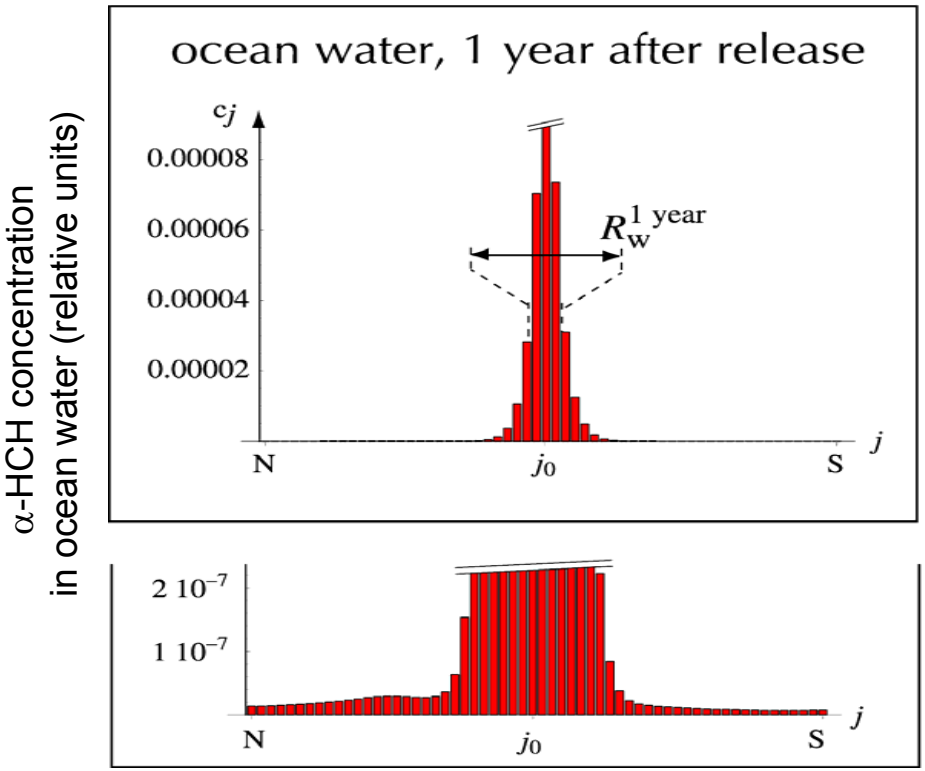


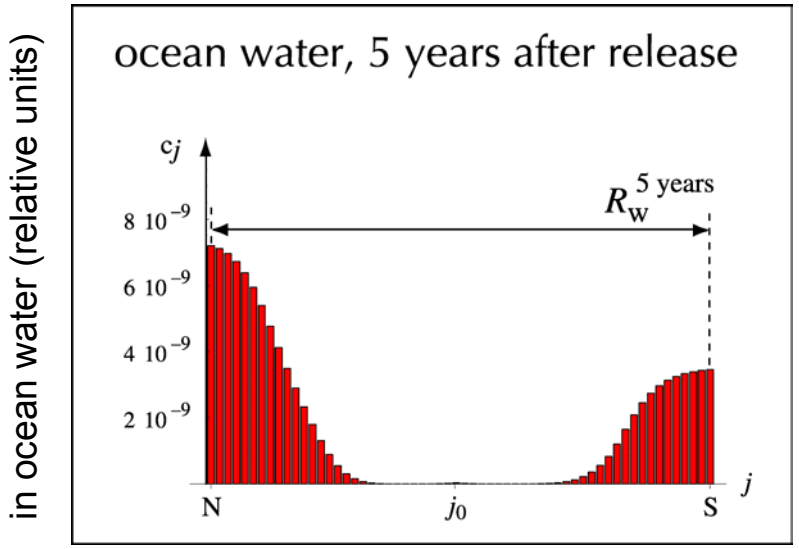
latitudinal zones with
– different temperatures
– different soil/water areas
and soil/vegetation types

model provides:
– concentrations, masses
– mass fluxes
in and between all media
of all zones
as functions of time.

Application of CliMoChem to α-HCH

- α-HCH: by-product of the insecticide γ-HCH (lindane)
- Model calculations with pulse release at the equator
- Enrichement in colder latitudes?

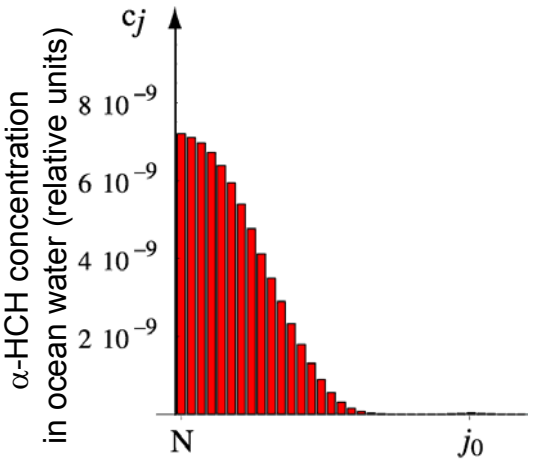




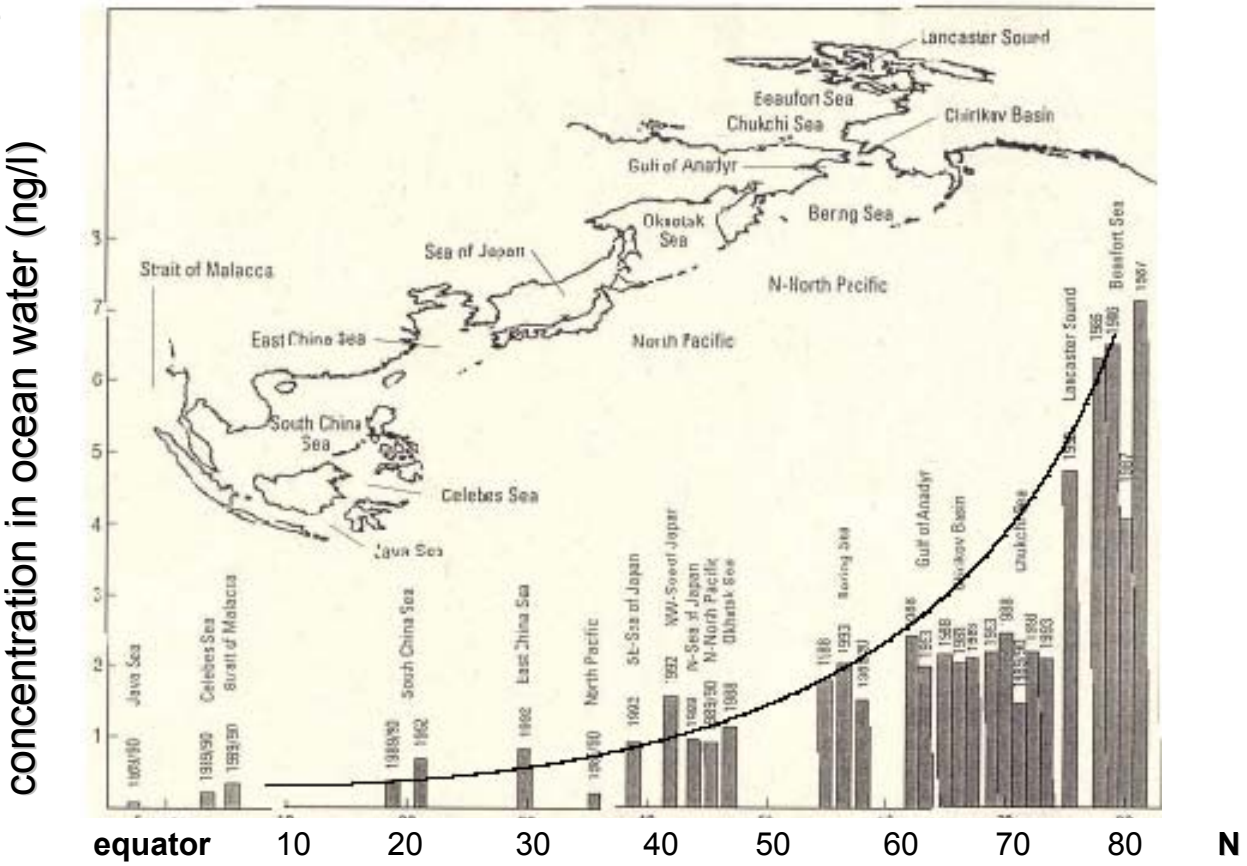
residues remain
in colder zones

Field Measurements for α-HCH

- Measured α-HCH concentrations in ocean water show a similar profile



CliMoChem results



From: Wania, F., Mackay, D., Environ. Sci. Technol. 30 (1996), 390A–396A

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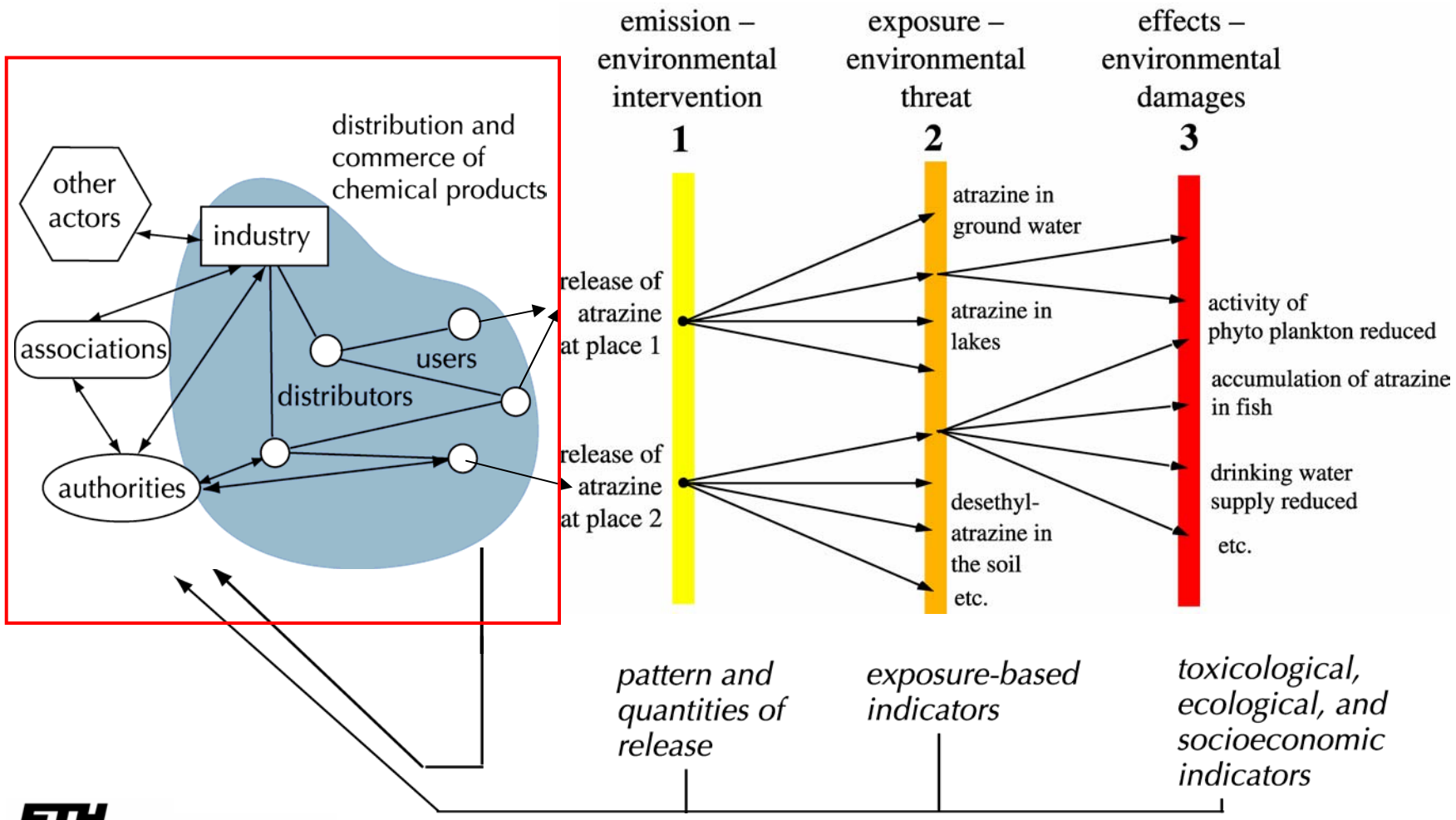
Distribution of Chemicals within the Technosphere



Scenario-Based Assessment of Occupational and Consumer Exposure

1) A set of scenarios can reflect highly variable exposure situations

2) Relatively few required parameters

3) Calculation of inhalative and dermal exposure

4) Combination with the number of exposed workers or consumers

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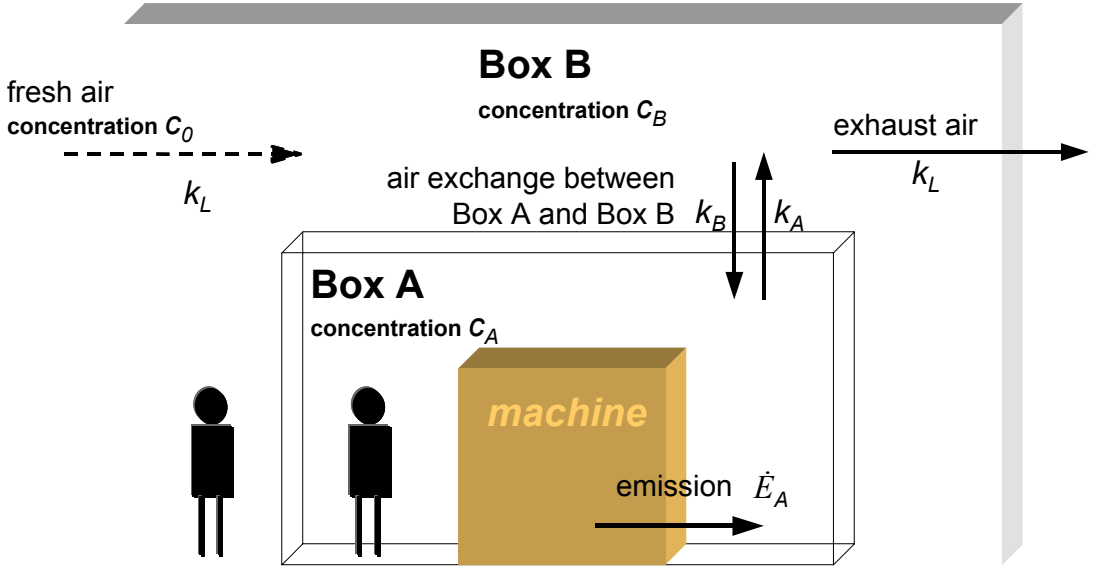
Occupational Exposure

Case Study: Dry Cleaning with Perchloroethylene

2-Box Model



Mass balance equations:

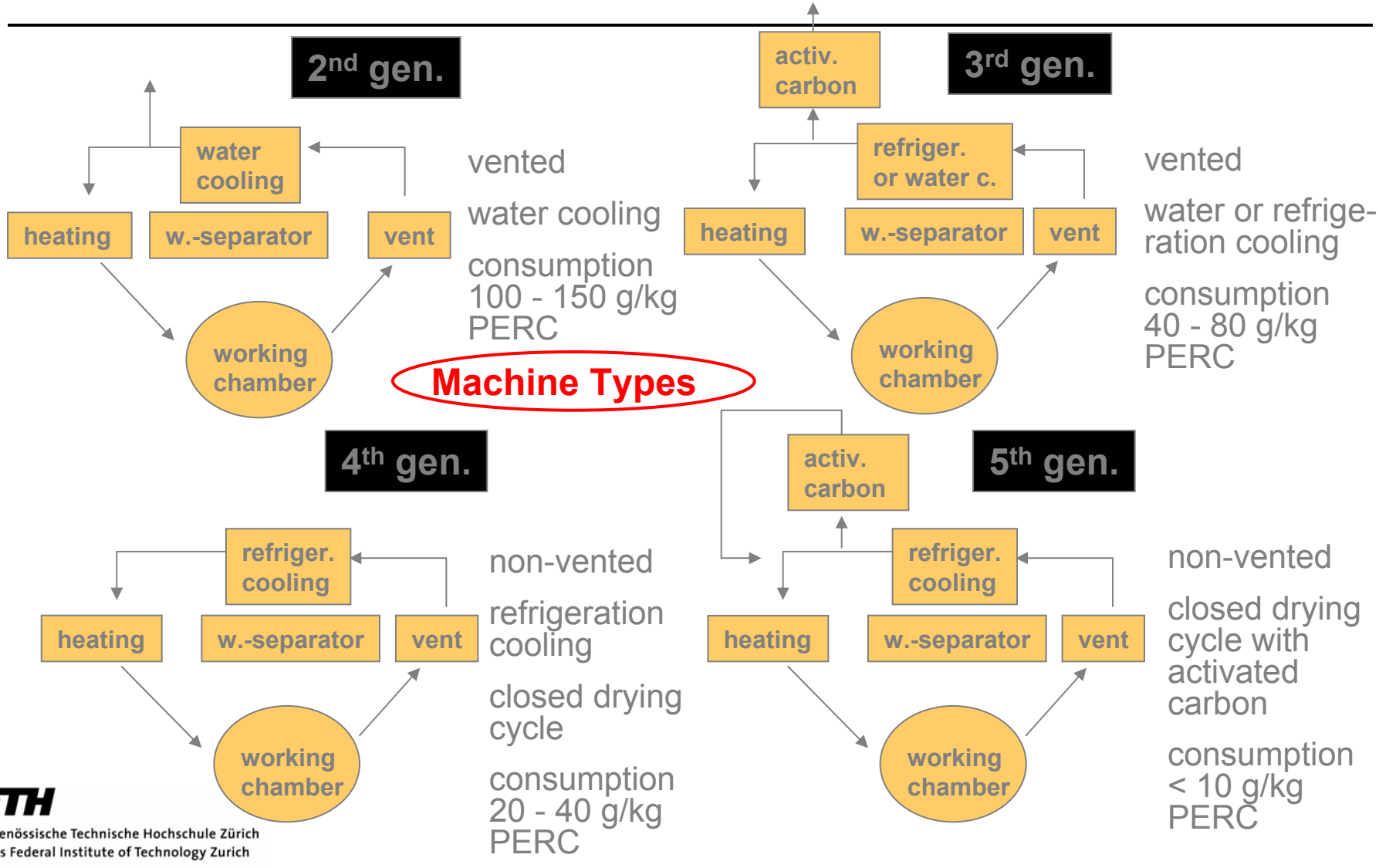
V_A = volume box A
V_B = volume box B
t = working time 8h
$\dot{E}_A$ = emission rate into box A

$$\frac{dC_A}{dt} = \frac{\dot{E}_A}{V_A} - C_A \cdot k_A + C_B \cdot \frac{V_B}{V_A} \cdot k_B$$

$$\frac{dC_B}{dt} = C_A \cdot \frac{V_A}{V_B} \cdot k_A - C_B \cdot (k_L + k_B)$$

C_A = airborne concentration box A
C_B = airborne concentration box B
k_L = air exchange environ. → box B
k_A = air exchange box A → box B
k_B = air exchange box B → box A

Machine Types in Dry Cleaning (Germany, 1960-2000)



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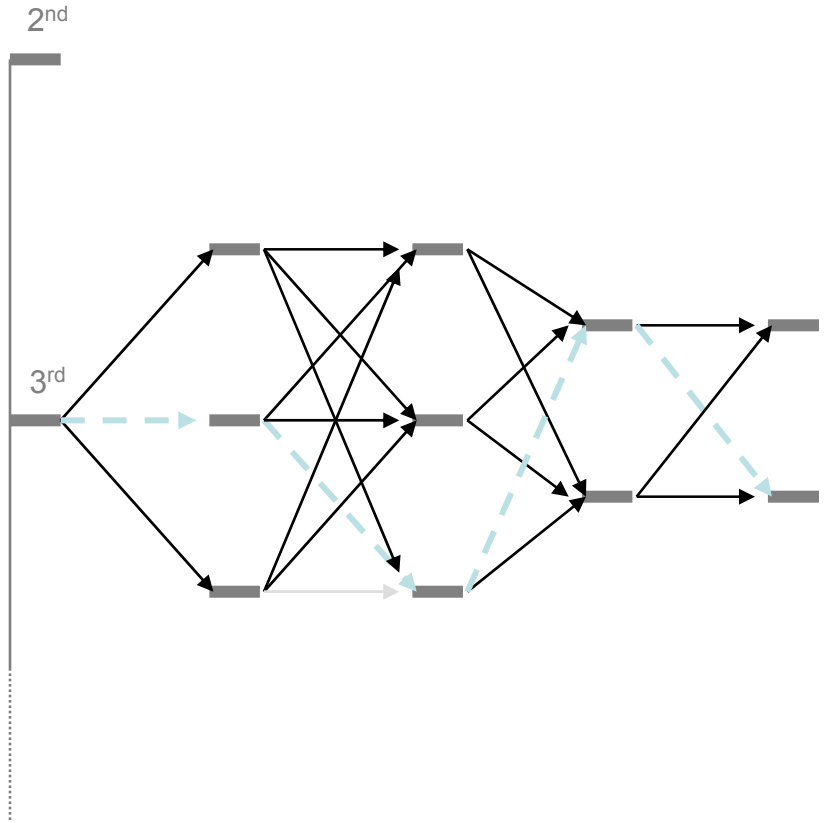
Scenario Generation: Combination of Input Parameters

Parameter Combination

machine generations	$\dot{E}_{c1}$ $\dot{E}_{c2}$ t_b	E_p	$V = V_A+V_B$	k_A k_B



E_{c1} = continuous diffuse emissions

E_{c2} = continuous emissions from textiles

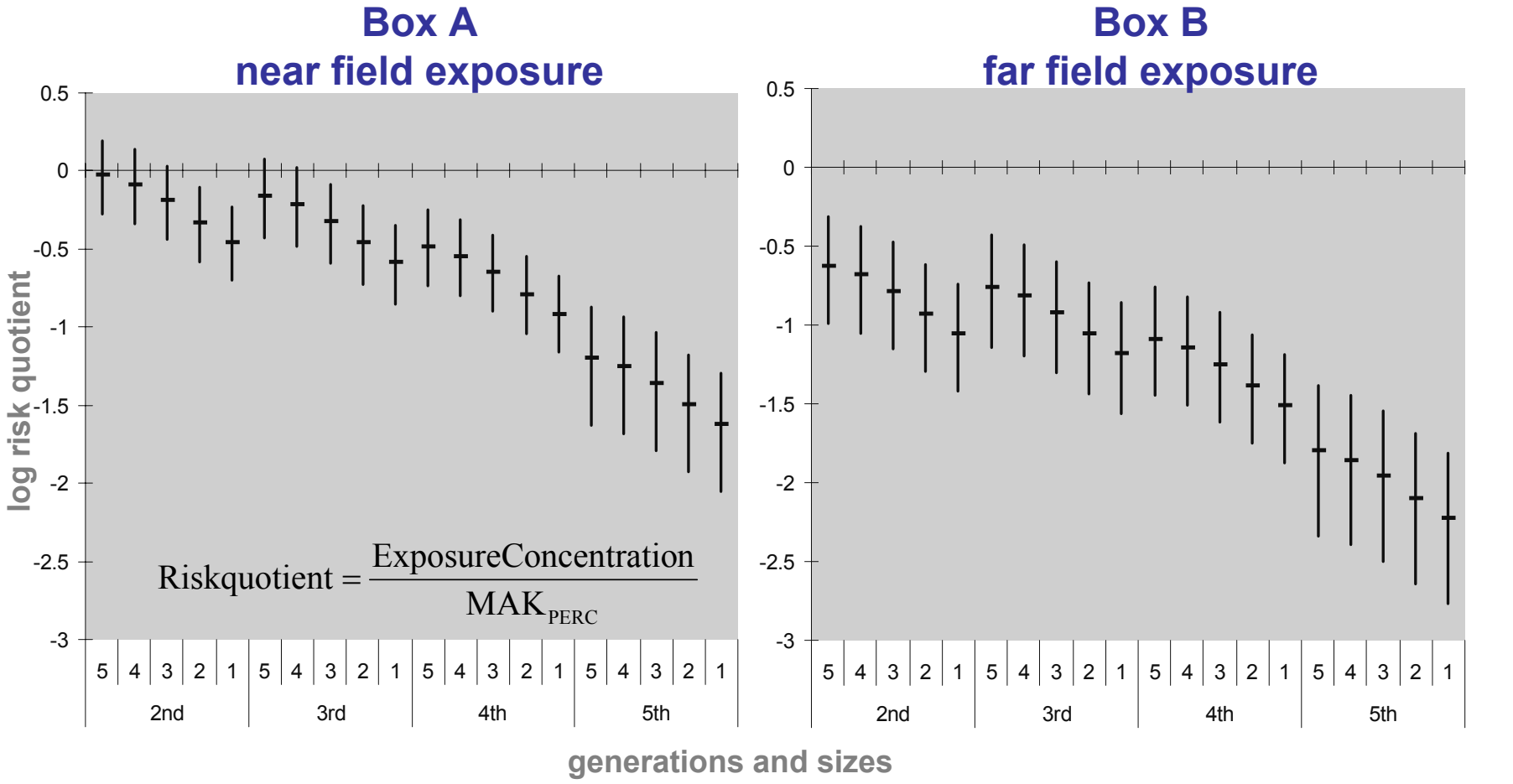
E_p = periodic emission during unloading

t_b = batch time

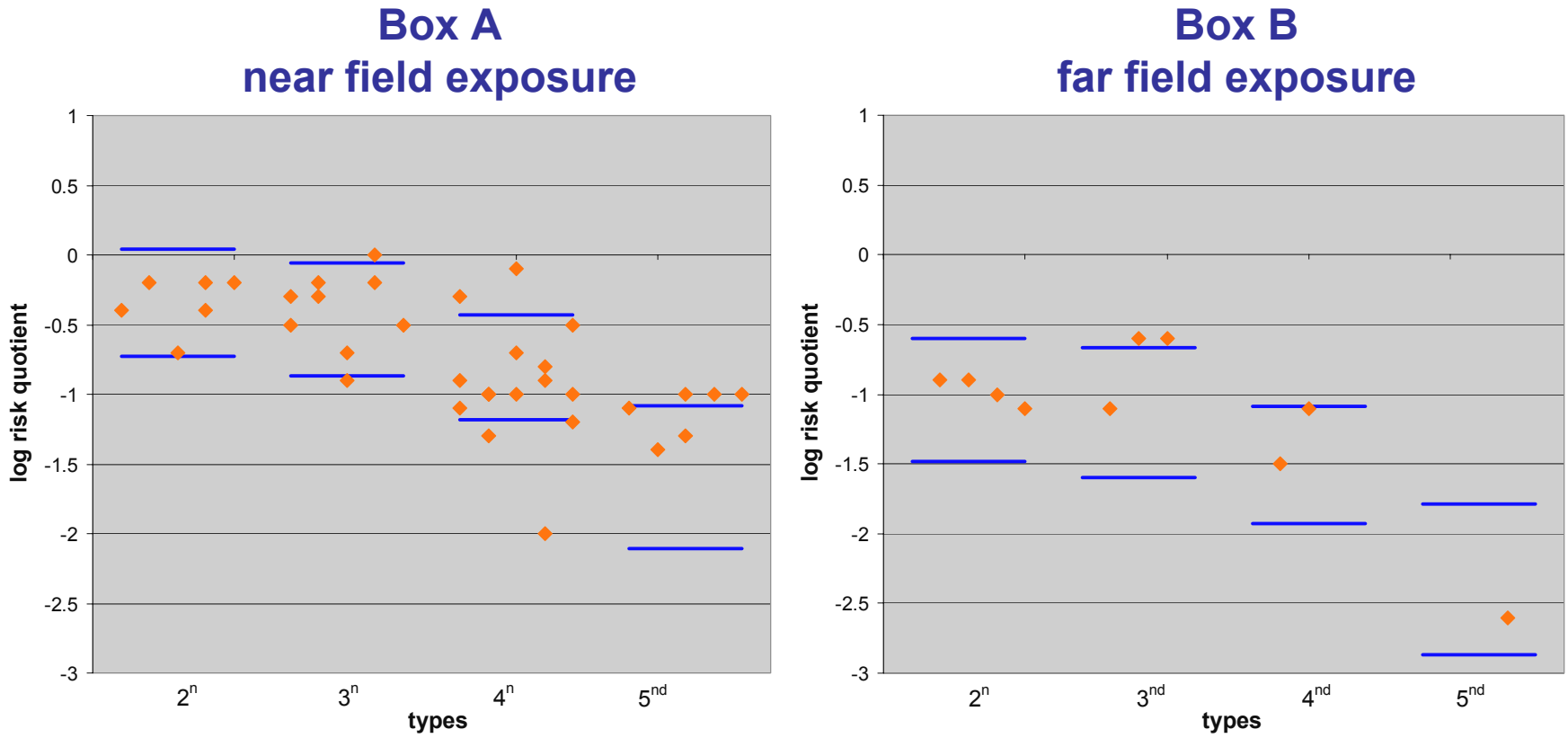
V = total box volume (V_A +V_B)

k_A and k_B = air exchange rates

Results (I): Comparison of Different Machine Generations



Results (II): Validation of the Model



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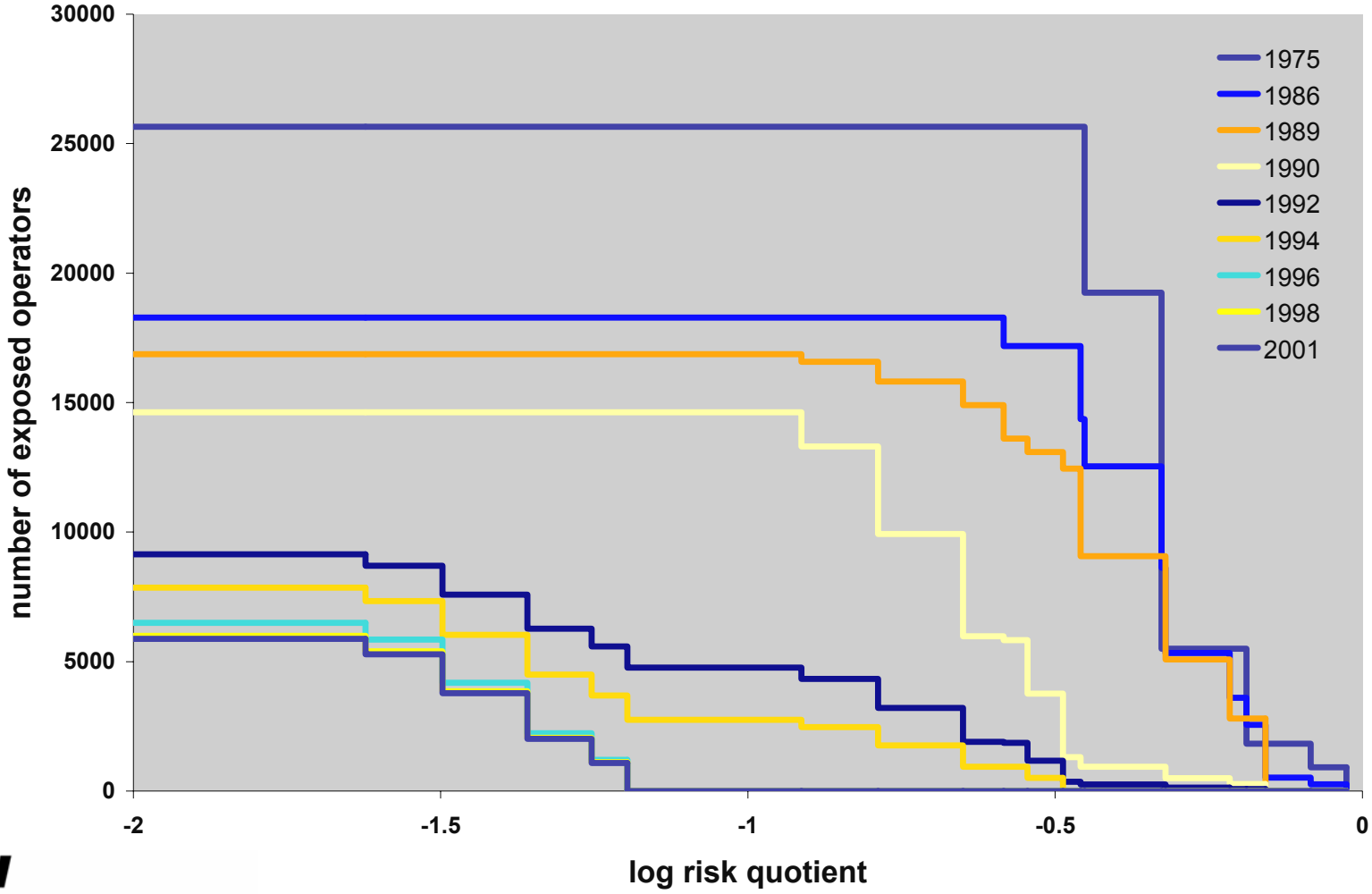
Approach 2, Model A

Results (III): Near-field Exposure for Operators in German Dry Cleaning Facilities Since 1975



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Scenario-Based Exposure Assessment

Focus on **POLYCYCLIC MUSK FRAGRANCES** in personal care Products

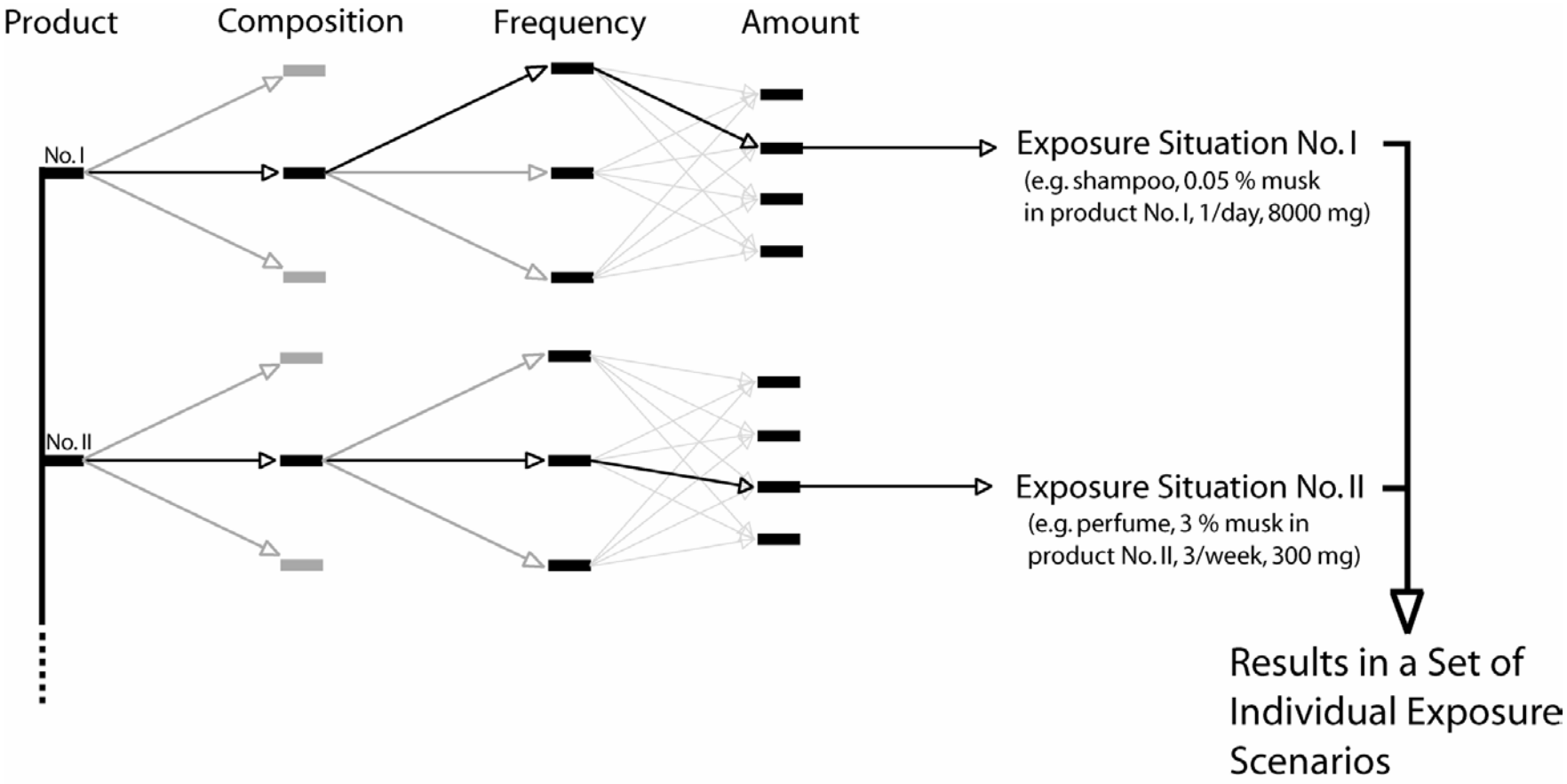
(Dermal uptake ≈ 2 % for AHTN, ≈ 0.1 % for HHCB (SCCNFP 2002))

Related problems:

- great product variety on the market,
- broad spectrum of chemical ingredients (e.g. Fragrance compounds, solvents, etc.)
- strongly variable use patterns / consumer behaviour
- few systematic investigations of the consumer behaviour

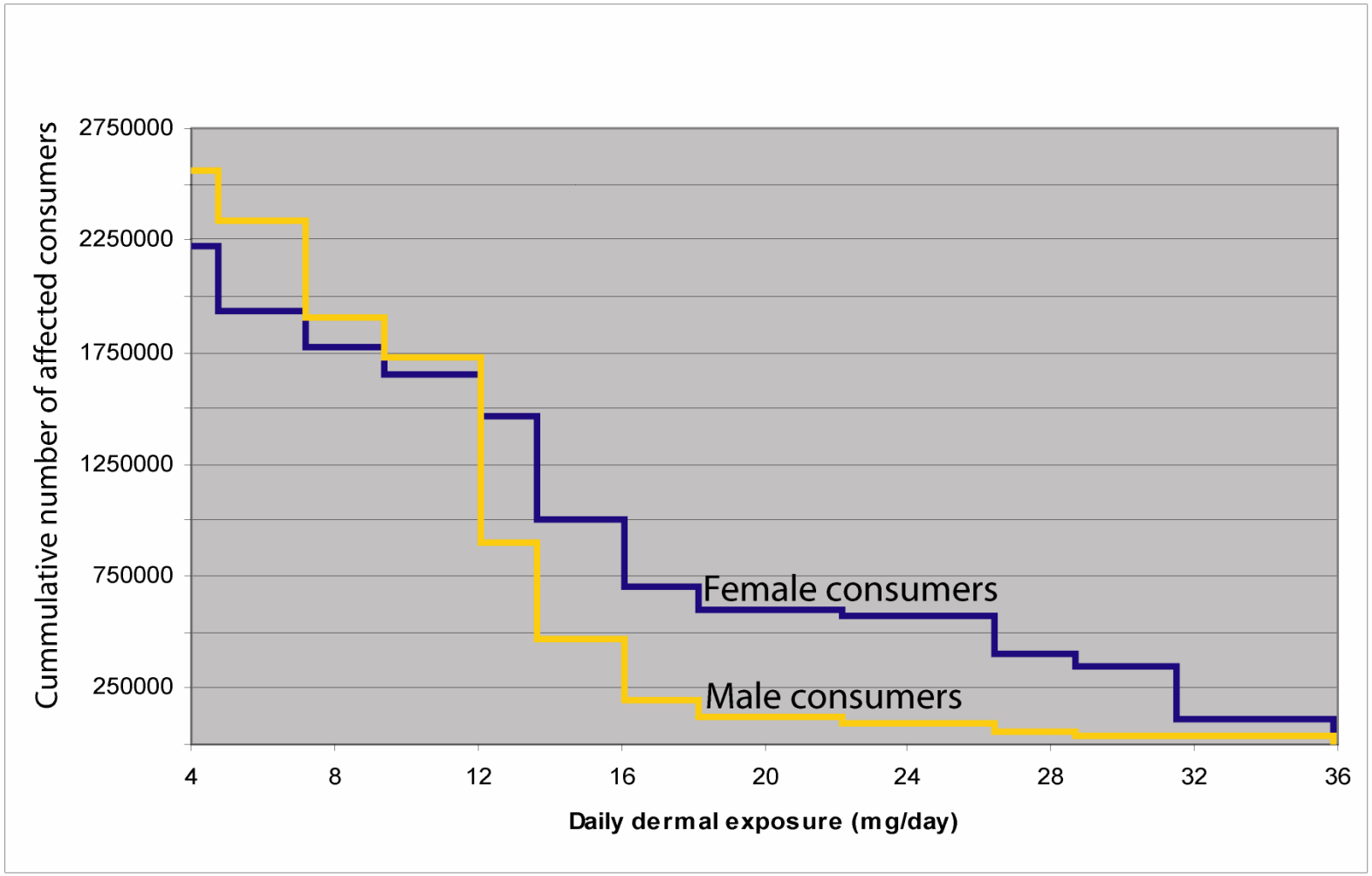
Approach 2, Model B

Systematic Generation of Individual Exposure Scenarios for Multi-Product Use



Approach 2, Model B

Results: Daily Dermal Exposure to AHTN and Number of Exposed Individuals



Dermal exposure model of SCCNFP; assumption: 12% AHTN in fragrance compound

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Conclusions

- Objective for screening methods:
  - limited data requirements
  - applicable to many chemicals
- Development of screening methods requires simplification of more complex models
- Development of simple methods is not a simple task
- Output from screening methods could be used by legislative frameworks to deal with the actual chemicals assessment problem