

# Environmental Fate Modeling of Chemicals, Lecture 1:

## Motivation and Foundations

Martin Scheringer

RECETOX, Masaryk University, Czech Republic

ETH Zürich, Switzerland

Brno, September 19, 2025

# Introduction

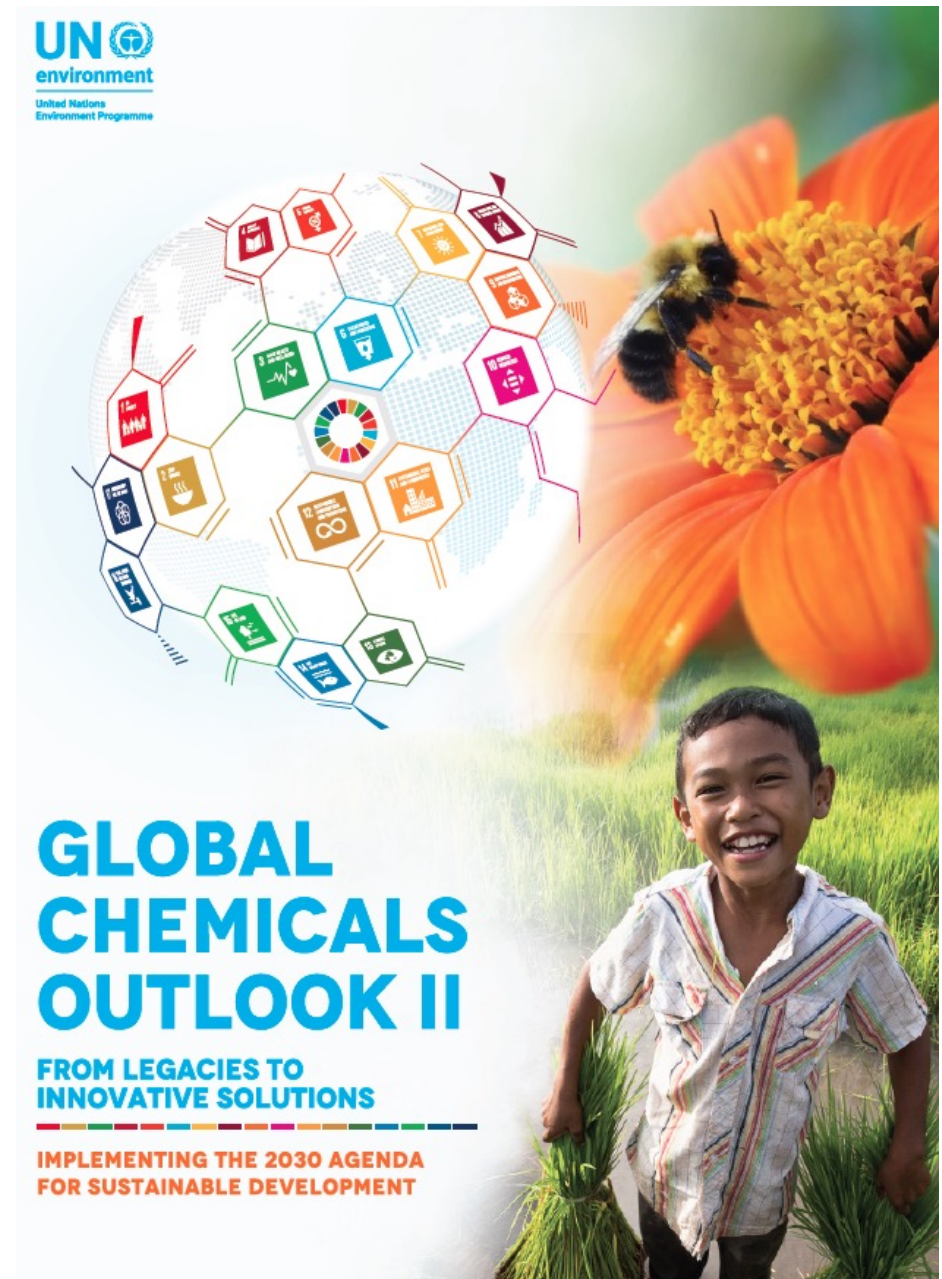
# Chemical Pollution as a Global Impact

“Findings of the GCO-II indicate that the sound management of chemicals and waste will not be achieved by 2020.

Trends data suggest that the doubling of the global chemicals market between 2017 and 2030 will increase global chemical releases, exposures, concentrations and adverse health and environmental impacts unless the sound management of chemicals and waste is achieved worldwide.

Business as usual is therefore not an option.”

From: key messages for policy makers



# Chemical Pollution as a Global Impact

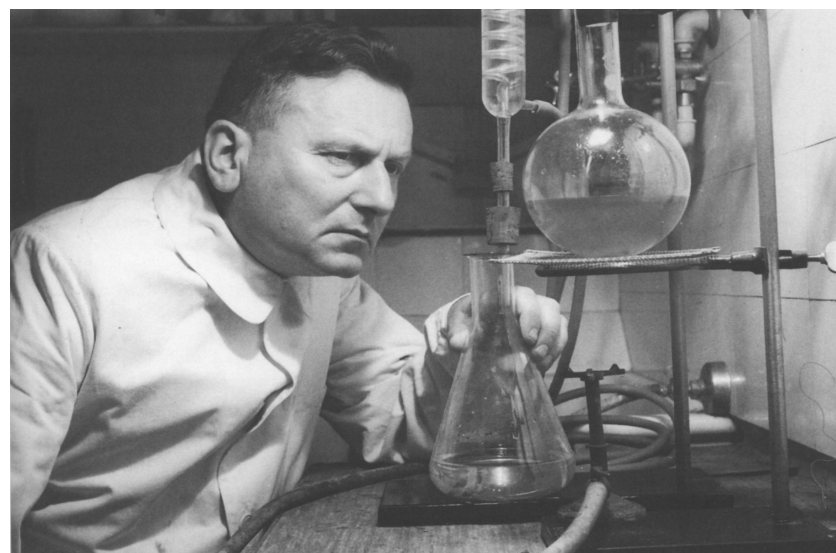
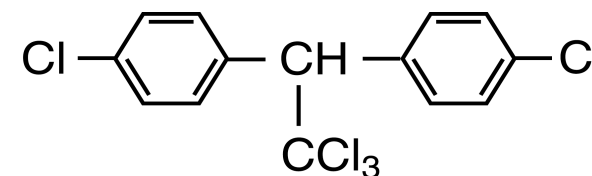
## Global Environment Outlook 6

Modern society is living in the most chemical-intensive era in human history, the pace of production of new chemicals largely surpasses the capacity to fully assess their potential adverse impacts on human health and ecosystems (...) and now chemical pollution is considered a global threat. (p. 76 and 88)



# 1940s: Discovery of DDT

- ◆ First synthesis in 1874 by O. Zeidler
- ◆ Insecticidal effect: discovered in 1938 by P. Müller, Geigy (Basel)
- ◆ First production: 1943, use in World War II against typhus, malaria
- ◆ DDT is the „ideal“ insecticide, 1948 Nobel Prize for P. Müller





# 1950s: Widespread Use of DDT



# Side Effects of DDT: Birds of Prey

- ◆ Population decline in, e.g., peregrine falcons
  - ➔ Eggshell thinning
  - ➔ Caused, among other chemicals, by DDT and its transformation product DDE
  - ➔ But: exact cause-effect relationship complicated

## The Case of the Thinning Eggshells

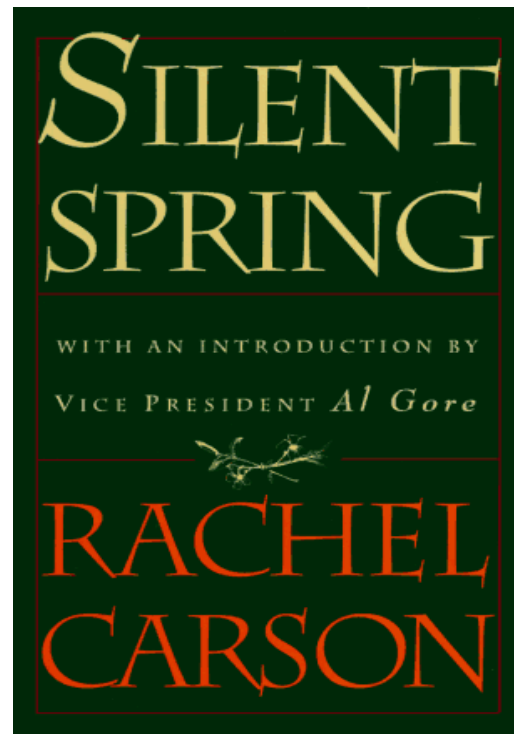
How the proliferation of pesticides like DDT almost undid the Peregrine falcon.



Peregrine Falcon, 1919 via Wikimedia Commons

# „*Silent Spring*“

- ◆ Rachel Carson publishes *Silent Spring* in 1962
  - ➔ Presents effects of pesticides on wildlife and **on humans**
  - ➔ Points out connection between research into DDT and chemical industry
  - ➔ Initiates heated debate, has long-term impacts





# Polychlorinated Biphenyls in Wildlife

NATURE VOL. 224 OCTOBER 18 1969

247

## DDT and PCB in Marine Animals from Swedish Waters

by

S. JENSEN

Institute of Analytical Chemistry,  
Stockholm

A. G. JOHNELS

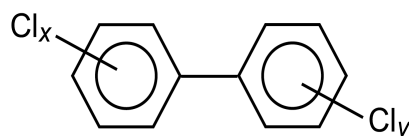
M. OLSSON

Swedish Museum of Natural History,  
Stockholm

G. OTTERLIND

Institute of Marine Research,  
Lysekil

Analyses of pesticide residues in a wide range of marine organisms from the coastal waters of Sweden show that there is a marked contamination in the Baltic. There are signs of an increase in polychlorinated biphenyls (PCB) from north to south in this area. Exceptionally large amounts of residues were found in white tailed eagles from the archipelago of Stockholm.



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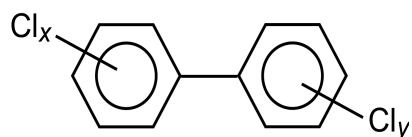
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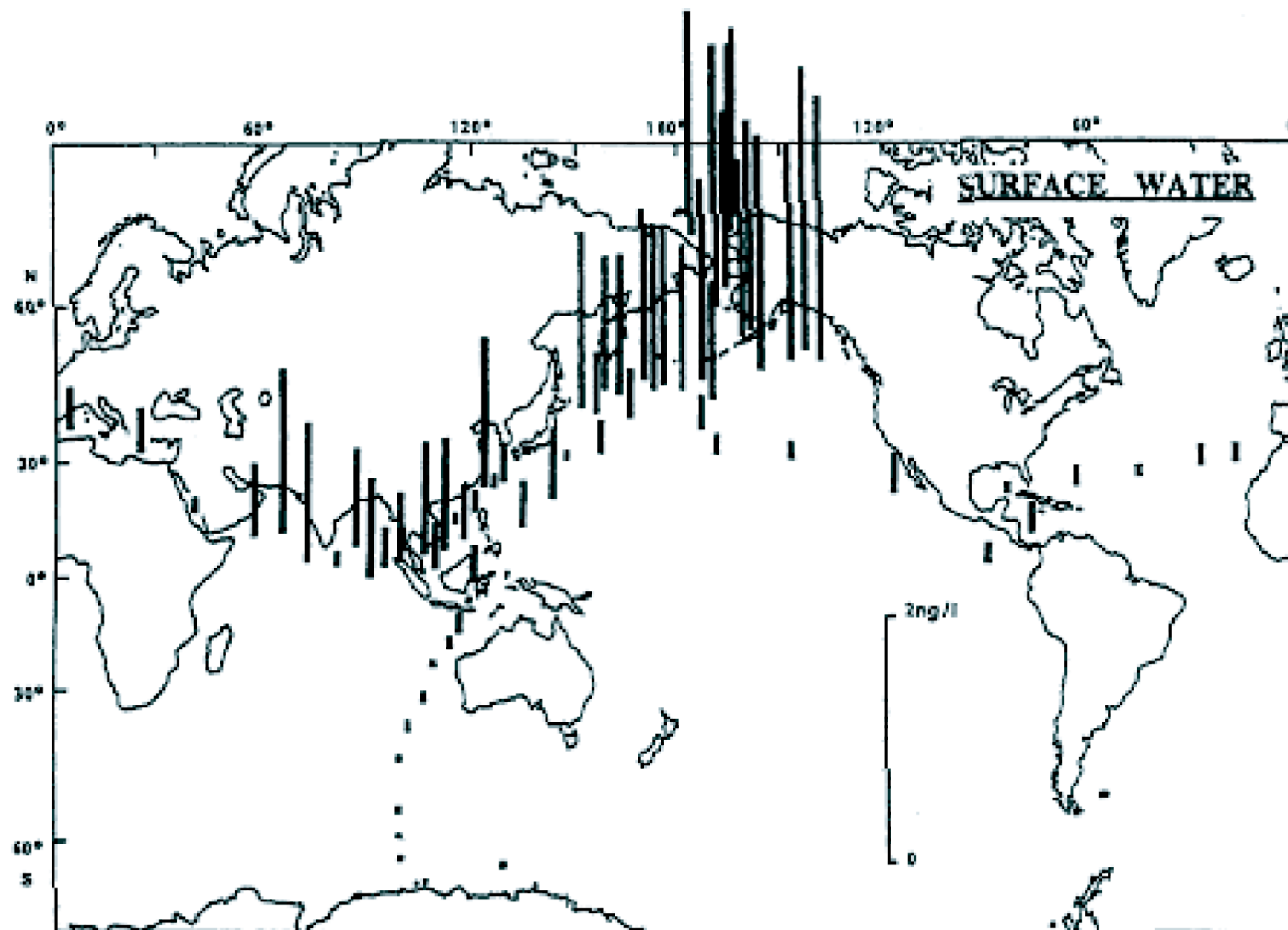
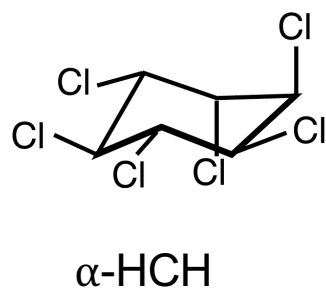
The New York State's 'eat none' advisory and the restriction on taking fish for this section of the Upper Hudson has been in place for 36 years.

<http://response.restoration.noaa.gov/about/media/pcbs-why-are-banned-chemicals-still-hurting-environment-today.html>



# The Global Presence of Chemicals

## ♦ alpha-HCH in the global oceans



# The Global Presence of Chemicals

## ANGEWANDTE CHEMIE

Volume 31 · Number 5

May 1992

Pages 487–664

International Edition in English

### Transport and Fate of Organic Compounds in the Global Environment

By Karlheinz Ballschmiter\*

*Dedicated to Professor Heinz Harnisch on the occasion of his 65th birthday*

The role of chemistry in our soon-to-be global industrial society requires a global perspective for the discussion of the uptake, transport, and conversion of chemical compounds in the environment. The fate of organic compounds in the volume flow of the atmosphere and hydrosphere can be categorized into transport pathways and adjustments of equilibria in the multiphase system atmosphere–oceans–land surface. The global volume flow in the atmosphere (wind, areas of high and low pressure) and in the hydrosphere (rivers, circulation of water in lakes, ocean currents) alone would account for the transport of organic compounds if they were stable and if all these

“During the last 50 years the prediction that many manmade chemicals would reach every corner of the global environment has become a reality.”  
(p. 512)



# The Global Presence of Chemicals

words,  $\text{MnO}_4^-$  abstracts  $\text{H}\cdot$  from toluene just as an oxygen radical would if it had a bond strength of  $83 \text{ kcal mol}^{-1}$ . This is true even though  $\text{MnO}_4^-$  is not a radical. Similar correlations have been found for oxidations of ethylbenzene by  $\text{RO}\cdot$  and  $\text{MnO}_4^-$  (6) and for oxidations of toluene, cyclohexane, and isobutane by  $\text{RO}\cdot$  and  $\text{CrO}_2\text{Cl}_2$  [on the basis of an estimated  $\text{CrO}-\text{H}$  bond strength (18, 19)]. The rate of toluene oxidation by  $\text{MnO}_4^-$  in water does not fit this relation because the mechanism is not  $\text{H}\cdot$  abstraction; rates of  $\text{H}\cdot$  transfer are essentially independent of solvent (25).

The correlation of rate with driving force provides insight into how a metal-containing active site can remove a hydrogen atom from an organic substrate. This correlation should apply not only to reagents such as permanganate but also to active sites in metalloenzymes and on metal oxide surfaces. The key feature of such an active site is not its radical character but its affinity for  $\text{H}\cdot$ . Understanding these reactions should be based primarily on the thermochemistry of the  $\text{H}\cdot$  abstraction step.

## REFERENCES AND NOTES

1. P. R. Ortiz de Montellano, Ed., *Cytochrome P-450: Structure, Mechanism, and Biochemistry* (Plenum, New York, 1985); Y. Watanabe and J. T. Groves, in *The Enzymes* (Academic Press, New York, ed. 3, 1992), vol. XX, pp. 405–452; A. C. Rosenzweig, C. A. Frederick, S. J. Lippard, P. Nordlund, *Nature* **366**, 537 (1993); J. C. Boyington, B. J. Gaffney, L. M. Amzel, *Science* **260**, 1482 (1993); L. C. Stewart and J. P. Klinman, *Ann. Rev. Biochem.* **57**, 551 (1988).
2. G. Centi, F. Trifiro, J. R. Ebner, V. M. Franchetti, *Chem. Rev.* **88**, 55 (1988); Y. Tong and J. H.

## Global Distribution of Persistent Organochlorine Compounds

Staci L. Simonich\* and Ronald A. Hites†

The global distribution of 22 potentially harmful organochlorine compounds was investigated in more than 200 tree bark samples from 90 sites worldwide. High concentrations of organochlorines were found not only in some developing countries but also in industrialized countries, which continue to be highly contaminated even though the use of many of these compounds is restricted. The distribution of relatively volatile organochlorine compounds (such as hexachlorobenzene) is dependent on latitude and demonstrates the global distillation effect, whereas less volatile organochlorine compounds (such as endosulfan) are not as effectively distilled and tend to remain in the region of use.

Researchers have long speculated that some organic pollutants move through the atmosphere from relatively warm source regions and condense at colder, higher latitudes onto vegetation, soil, and bodies of water. This process, known as the global distillation effect, could be the cause of the high concentrations of some pollutants found in Earth's arctic regions (1–5). Global distillation is driven by the change of a pollutant's subcooled liquid vapor pressure

with temperature, its environmental persistence, and its tendency to associate with lipids (1, 6). This effect appears to be most pronounced for organochlorine compounds of intermediate volatility, many of which are used as insecticides and fungicides. Some of these compounds are still in use throughout the world (for example, endosulfan), whereas others have been banned in almost all developed countries (for example, DDT). Understanding the environmental fate of these compounds is particularly important because some of them are carcinogens and some may be estrogen mimics (7).

These ubiquitous organochlorine pollutants have subcooled liquid vapor pressures of 0.1 to 0.001 Pa at 25°C (8). Although these vapor pressures are sufficient for all of

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# The Global Presence of Chemicals

## ◆ Results from an Africa-wide network of passive samplers

ENVIRONMENTAL  
Science & Technology

pubs.acs.org/est

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Article

### Temporal Trends of Persistent Organic Pollutants across Africa after a Decade of MONET Passive Air Sampling

Kevin B. White, Jiří Kalina, Martin Scheringer,\* Petra Příbylová, Petr Kukučka, Jiří Kohoutek, Roman Prokeš, and Jana Klánová\*



Cite This: *Environ. Sci. Technol.* 2021, 55, 9413–9424



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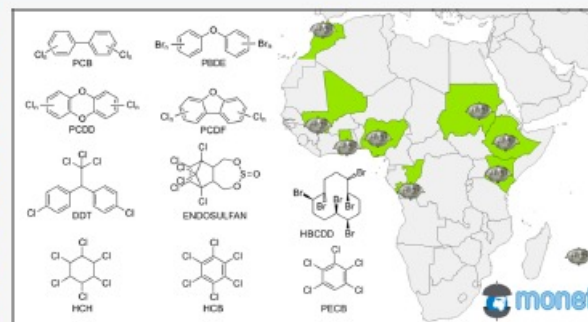
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**ABSTRACT:** The Global Monitoring Plan of the Stockholm Convention on Persistent Organic Pollutants (POPs) was established to generate long-term data necessary for evaluating the effectiveness of regulatory measures at a global scale. After a decade of passive air monitoring (2008–2019), MONET is the first network to produce sufficient data for the analysis of long-term temporal trends of POPs in the African atmosphere. This study reports concentrations of 20 POPs (aldrin, chlordane, chlordecone, DDT, dieldrin, endrin, endosulfan, HBCDD, HCB, HCHs, heptachlor, hexabromobiphenyl, mirex, PBDEs, PCBs, PCDDs, PCDFs, PeCB, PFOA, and PFOS) monitored in 9 countries (Congo, Ghana, Ethiopia, Kenya, Mali, Mauritius, Morocco, Nigeria, and Sudan). As of January 1, 2019,

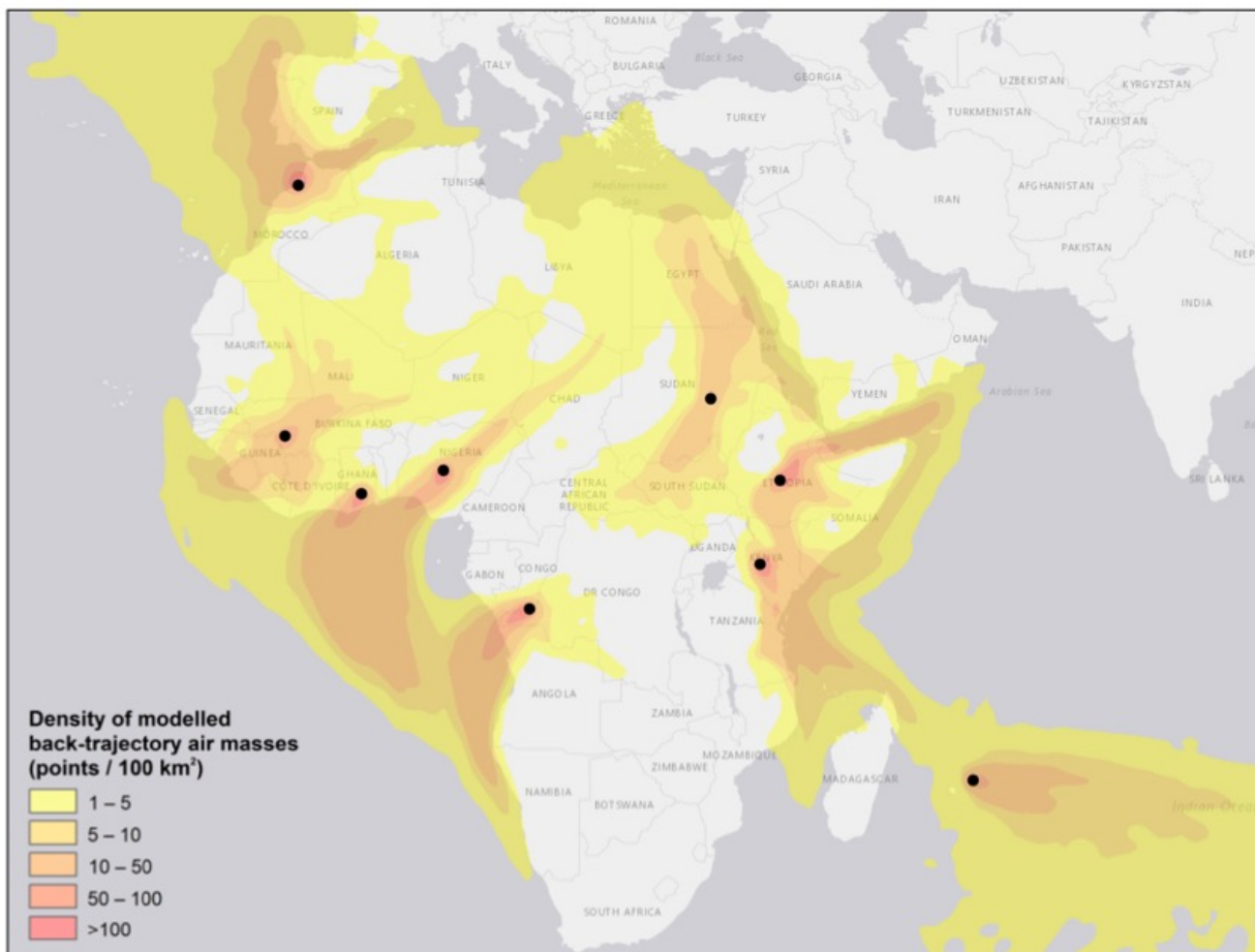


K. White et al. (2021)  
*Environ. Sci. Technol.* 55,  
9413–9424, <https://doi.org/10.1021/acs.est.0c03575>

# The Global Presence of Chemicals

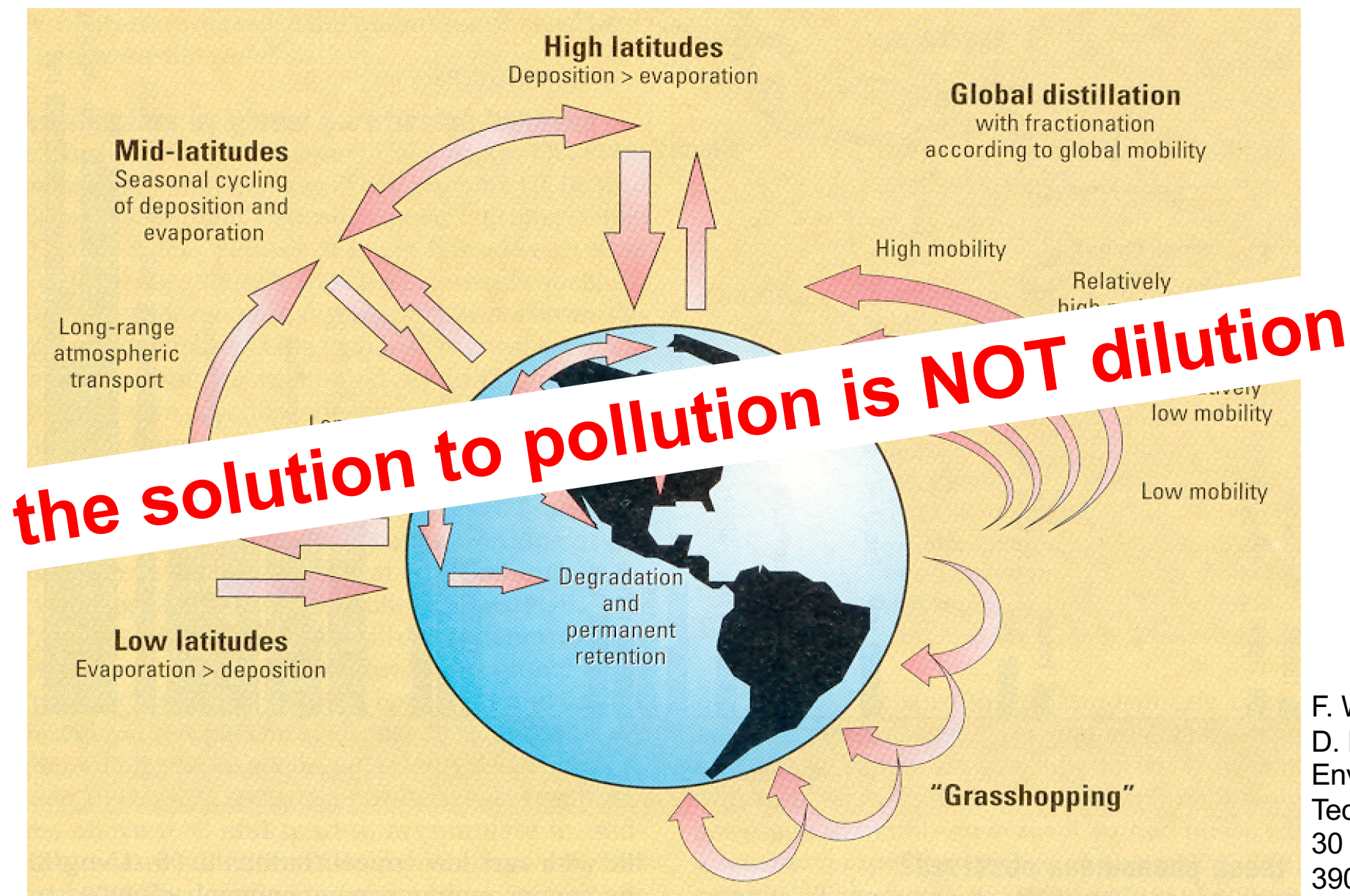
- ◆ Sampling locations in the African PAS network and their airflow patterns

K. White et al. (2021)  
*Environ. Sci. Technol.* 55,  
9413–9424, <https://doi.org/10.1021/acs.est.0c03575>





# The Global Presence of Chemicals



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



# Old Problems Come Back ...

♦ ... or, rather, have been with us all the time:



By Paul D. Jepson<sup>1</sup> and Robin J. Law<sup>1,2</sup>

**P**ersistent organic pollutants (POPs) are chemical substances that persist in the environment, accumulate in the

the Stockholm Convention committed more than 90 signatory countries to phasing out or eliminating large stocks or other sources of POPs, including PCBs (1). Yet, PCBs continue to threaten the survival of marine

centrations fell substantially from the 1960s and 1970s to 2010 (5, 7). Most avian marine apex predators, including herons, gulls, ospreys, petrels, and skuas, are no longer listed as threatened on the International Union for

REACTIVE

# Old Problems Come Back ...

- ♦ Orca whale with 950 mg/kg PCBs in blubber
- ♦ Accumulated over 22 years

UK killer whale died with extreme levels of toxic pollutants

Adult whale Lulu was one of UK's last resident pod and had never produced a calf, probably because pollutants in her blubber had caused infertility

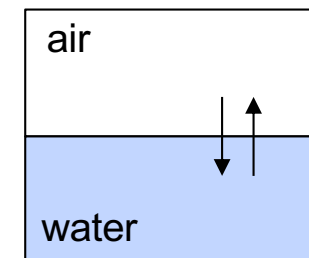


# Environmental Fate Modeling with Box Models: Concepts and a First Application

# Environmental Fate of Chemicals

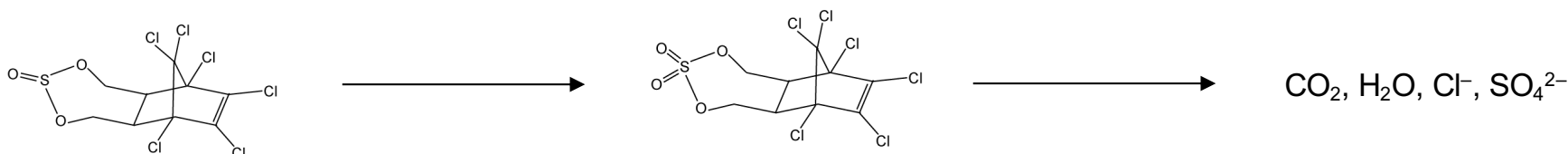
## ♦ Phase partitioning:

- ➔ distribution between air, water, soil, sediment, biota, ice/snow, ...



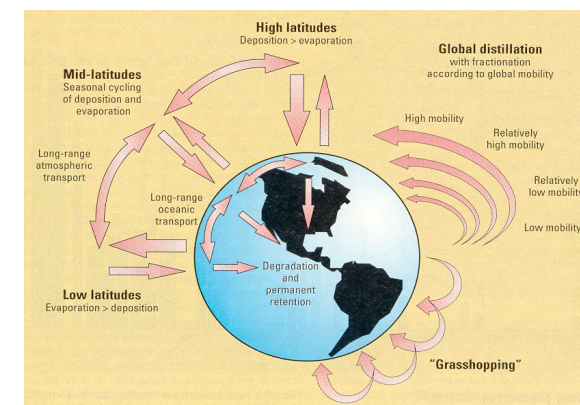
## ♦ Transformation and degradation:

- ➔ formation of transformation products; finally: mineralization



## ♦ Transport:

- ➔ movement of chemical with air and water;  
issue: long-range transport  
(Stockholm Convention)





# Why **Model** the Environmental Fate?

- ◆ We cannot measure everywhere:
  - ➔ interpolation
  - ➔ extrapolation:  
investigate problems before they become manifest
- ◆ Process understanding
- ◆ Uncertainty analysis
- ◆ Investigation of scenarios: warmer climate, ...
- ◆ Overall: models help create the big picture!

# What Is a Model?

## ♦ Selection of processes

- ➔ Considered **relevant** for the problem investigated:  
**here:** phase partitioning, degradation, transport
- ➔ Quantitatively described within a consistent **mathematical framework**  
**here:** mass balance equations for a chemical

## ♦ Solution of the model:

- ➔ Calculate masses of a chemical in all compartments of the model as function of time

## ♦ Purposes:

- ➔ „realistic“ description of the environment: **simulation models**
- ➔ Sketch of the environment: **evaluative models**.
  - Understanding of processes and their interplay;
  - Compare environmental fate of different compounds,
  - „screening“, „ranking“ of chemicals.

# Mechanistic Models

◆ Based on “laws of nature” ...

- ➡ conservation of mass
- ➡ laws of chemical thermodynamics
- ➡ laws of chemical kinetics, in particular: law of mass action
- ➡ laws of diffusion

◆ ... and on empirical data: rain rate, wind speed, chemical property data, etc.

# Multimedia Box Models

- ◆ Model types: there are many specific models for chemicals in
  - ➔ air
  - ➔ groundwater
  - ➔ soil
  - ➔ ...
- ◆ These different models are difficult to integrate into an overall picture of a chemical's fate.
- ◆ Multimedia box models:
  - ➔ **overall mass balance** of chemical in a system of several linked **environmental media** and **geographical regions**.
  - ➔ Often less highly resolved than media-specific models, but: overall picture, **consistent level of complexity**



# Multimedia Box Models

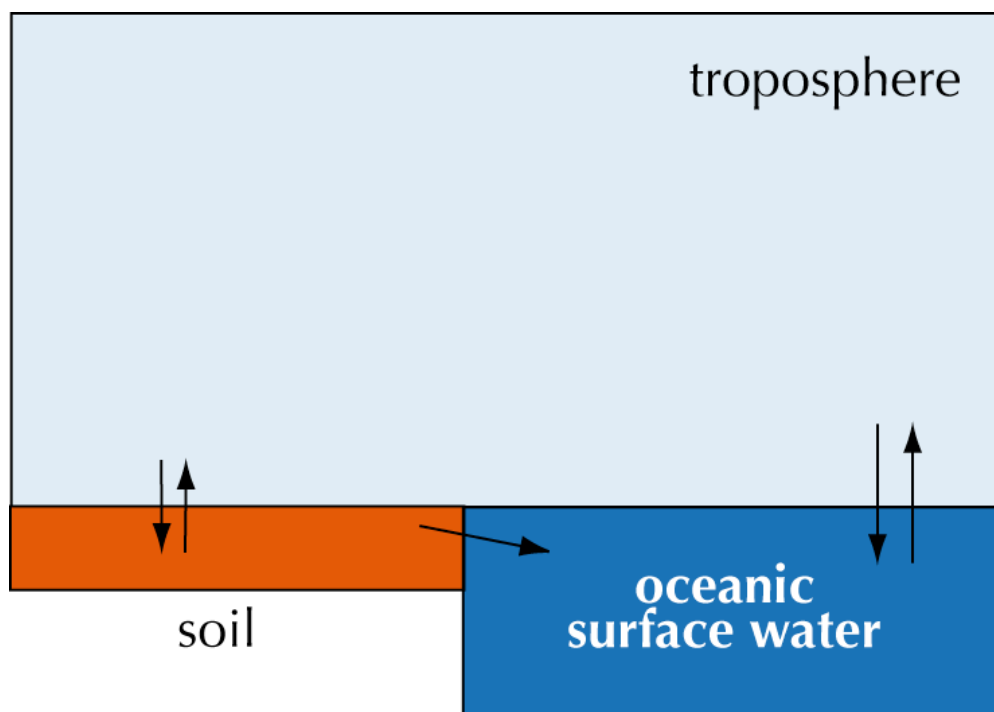
- ◆ Convenient analytical framework for investigating chemical fate in connected environmental media



Cover picture of Environ. Sci. Technol. **40**:  
issue on “Emerging Contaminants” (December 2006)

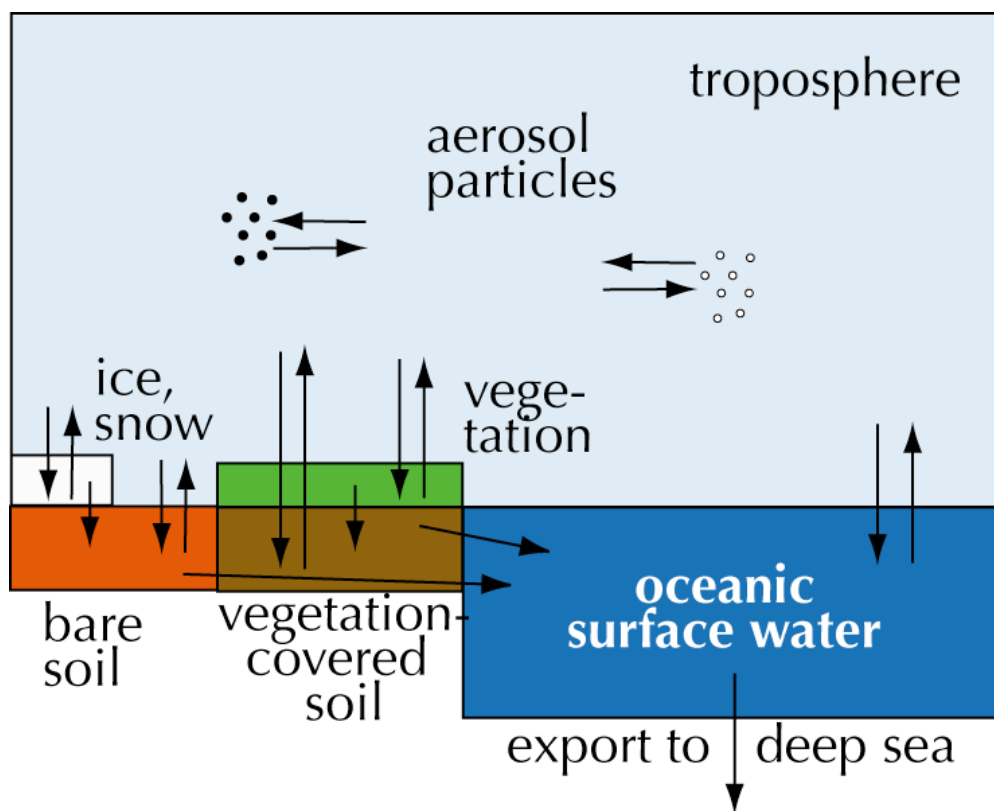
# Multimedia Box Models

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# Multimedia Box Models

- ◆ Convenient analytical framework for investigating chemical fate in connected environmental media



# A First Example: $\text{CCl}_4$ , Global

- ◆ Emission rate:  $E$  (kg/yr)
- ◆ Volume of air:  $V$  ( $\text{m}^3$ )
- ◆ Loss rate constant:  $k$  (1/yr)
- ◆ Concentration  
in air:  $c$  ( $\text{kg}/\text{m}^3$ )



- ◆ **Mass balance equation:**  $E = c \cdot V \cdot k$ 
  - ➡ estimate  $E$ ,  $V$ ,  $k$ ; solve for  $c$
  - ➡ estimate  $c$ ,  $V$ ,  $k$ ; solve for  $E$
  - ➡ estimate  $c$ ,  $V$ ,  $E$ ; solve for  $k$

# A First Example: CCl<sub>4</sub>, Global

◆ With actual data:

→  $E = 80 \text{ kt/yr} = 5.19 \cdot 10^8 \text{ mol/yr}$

→  $V = 5 \cdot 10^{18} \text{ m}^3$

→  $k = 1/30 \text{ yr} = 0.0333 \text{ yr}^{-1}$

→ this yields:

$$c = 3.1 \cdot 10^{-9} \text{ mol/m}^3 = 70 \text{ ppt}$$

→ measured concentration:

of CCl<sub>4</sub> in the troposphere:  $c = 90 \text{ ppt}$





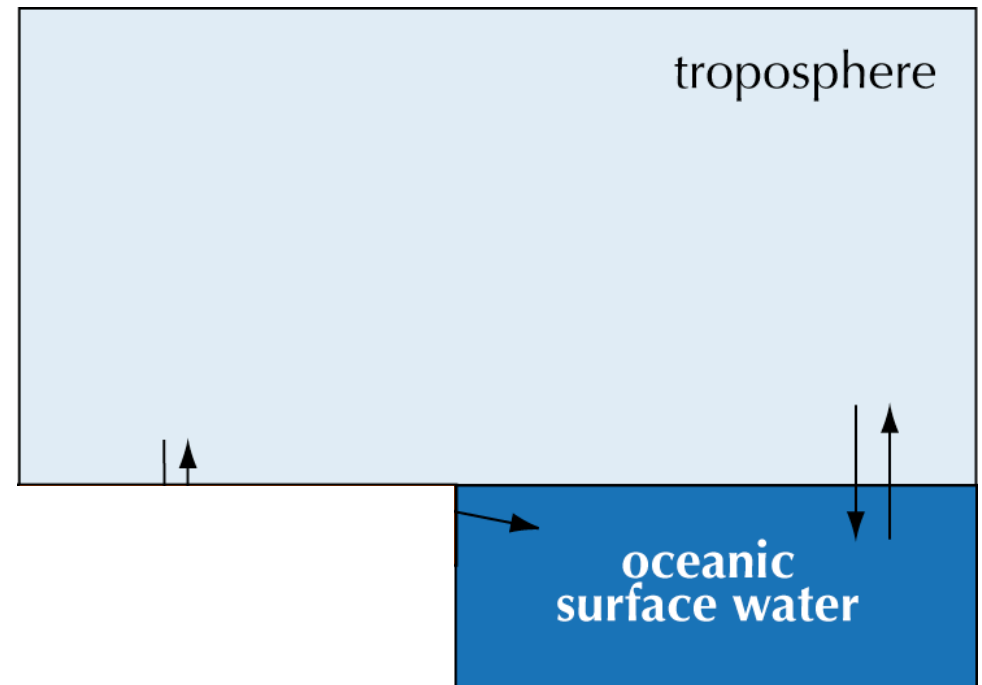
# Mass Balance Equation for Two Boxes

- ♦ air, a, and water, w
- ♦ mass-balance equation for one box:  $E = c \cdot V \cdot k$
- ♦ for two boxes:

$$E = c_a \cdot V_a \cdot k_a + c_w \cdot V_w \cdot k_w$$

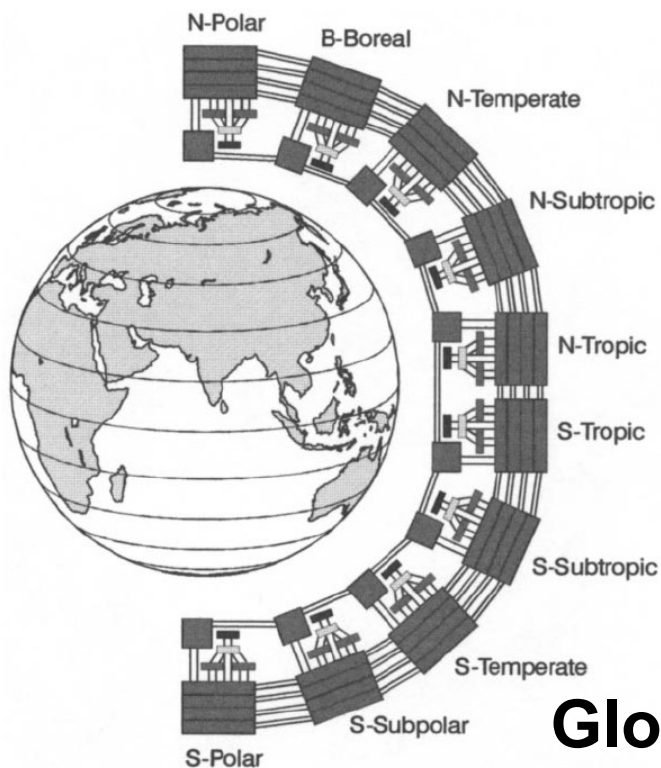
and

$$c_a/c_w = K_{aw}$$

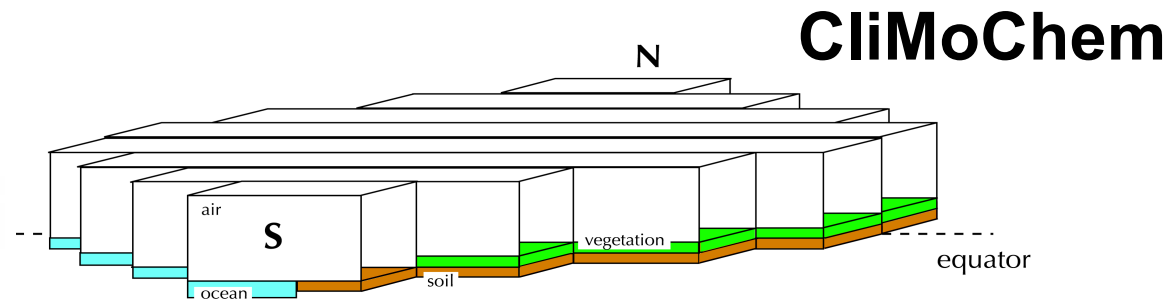


# Global Box Models

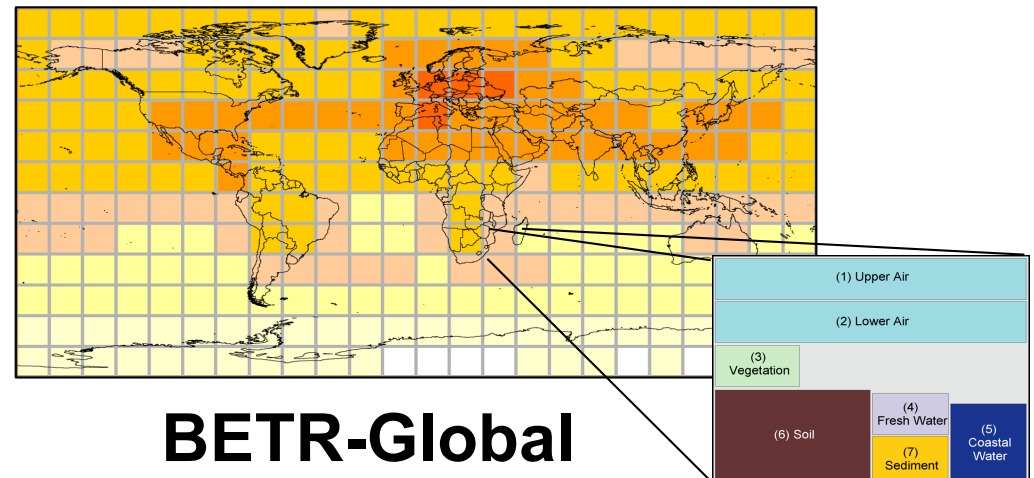
- ◆ Globo-POP (Wania, Mackay 1995)
- ◆ CliMoChem (Scheringer et al. 2000)
- ◆ BETR-Global (MacLeod et al. 2005)



**Globo-POP**



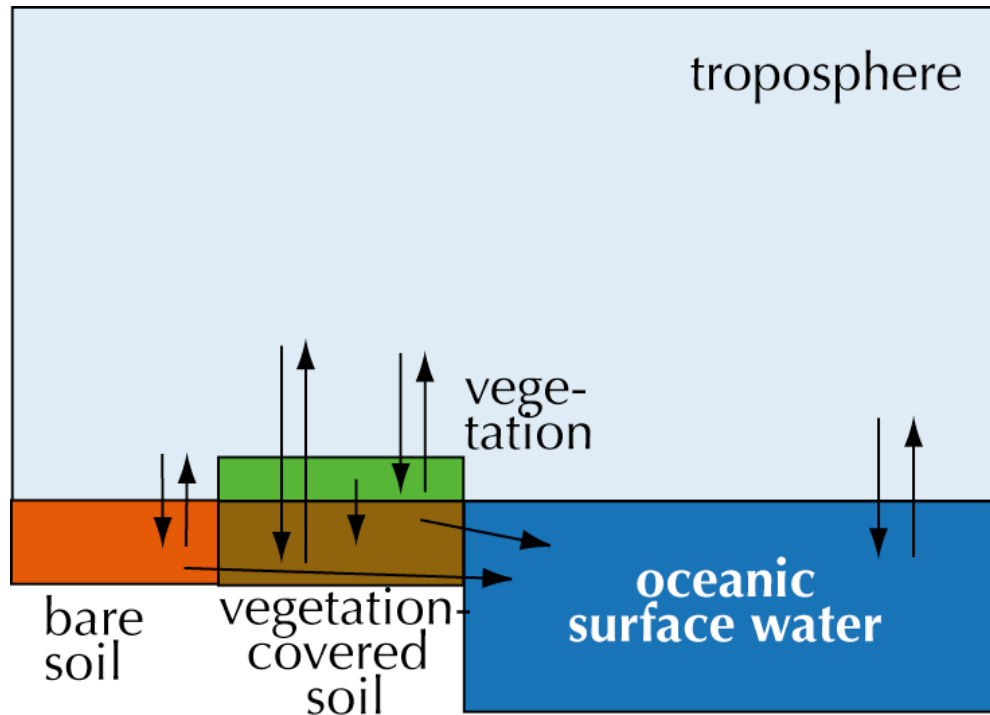
**CliMoChem**



**BETR-Global**

# General Approach: Mass Balances

- ♦ For all boxes, set up **mass-balance equations**



$$\frac{dm}{dt} = F_{\text{in}} - F_{\text{out}}$$

$F_{\text{in}}$ : emission sources and inflow from other boxes

$F_{\text{out}}$ : degradation and outflow to other boxes and out of the system

all fluxes:  $F = k \cdot m$

**needed:** rate constants,  $k$

# Parameter Requirements (I)

## ◆ Model parameters:

- ➔ **Chemical specific:** partition coefficients, degradation rate constants
- ➔ **Environmental parameters:** temperature, vegetation types, rain rate, aerosol concentrations, etc.

## ◆ Problems:

- ➔ Variability and uncertainty



# Parameter Requirements (I)

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## ♦ Problems:

- ➔ **Variability** and uncertainty

$k_s$

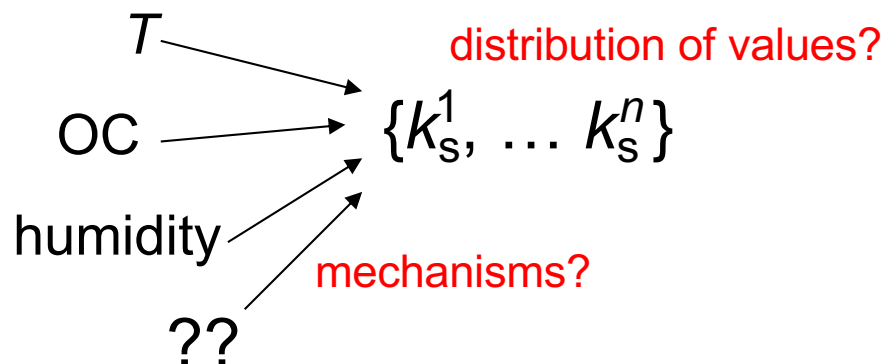
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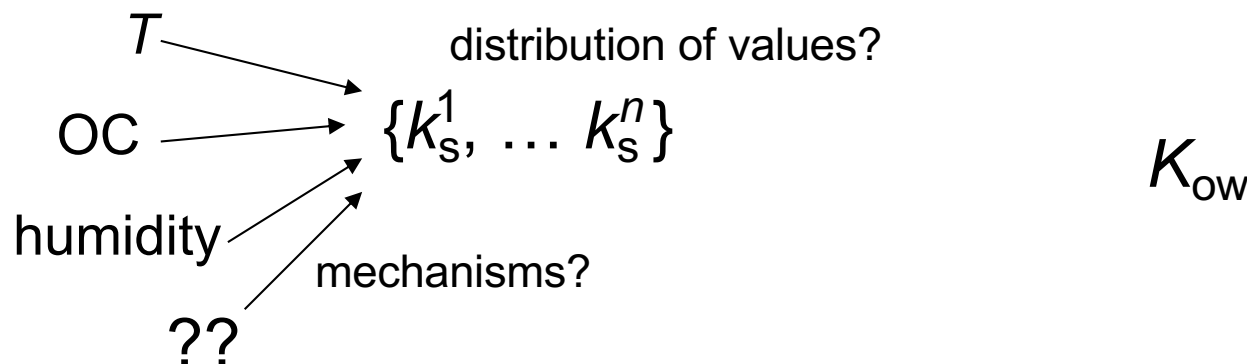
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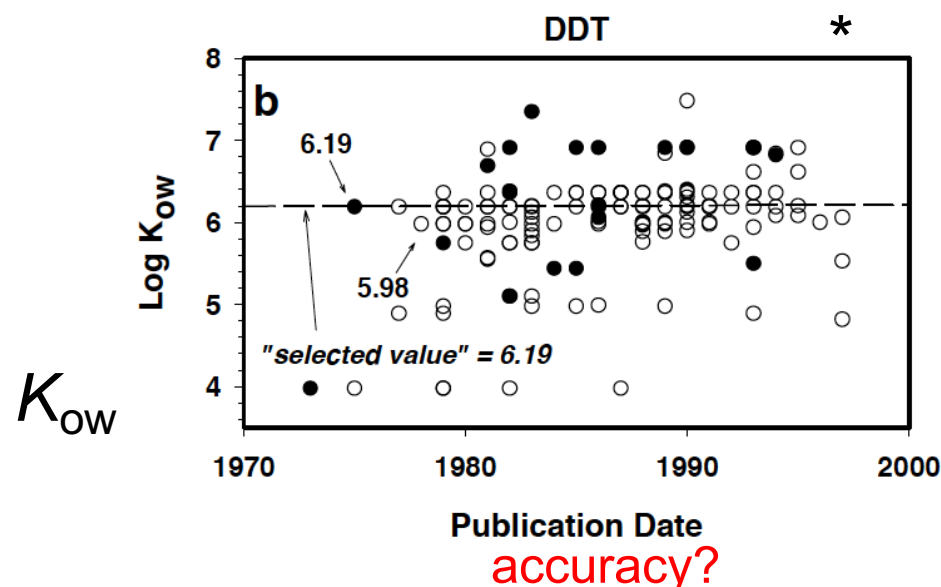
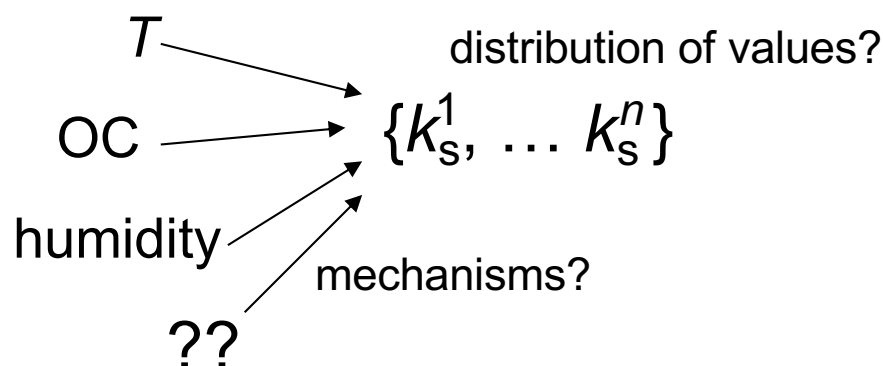
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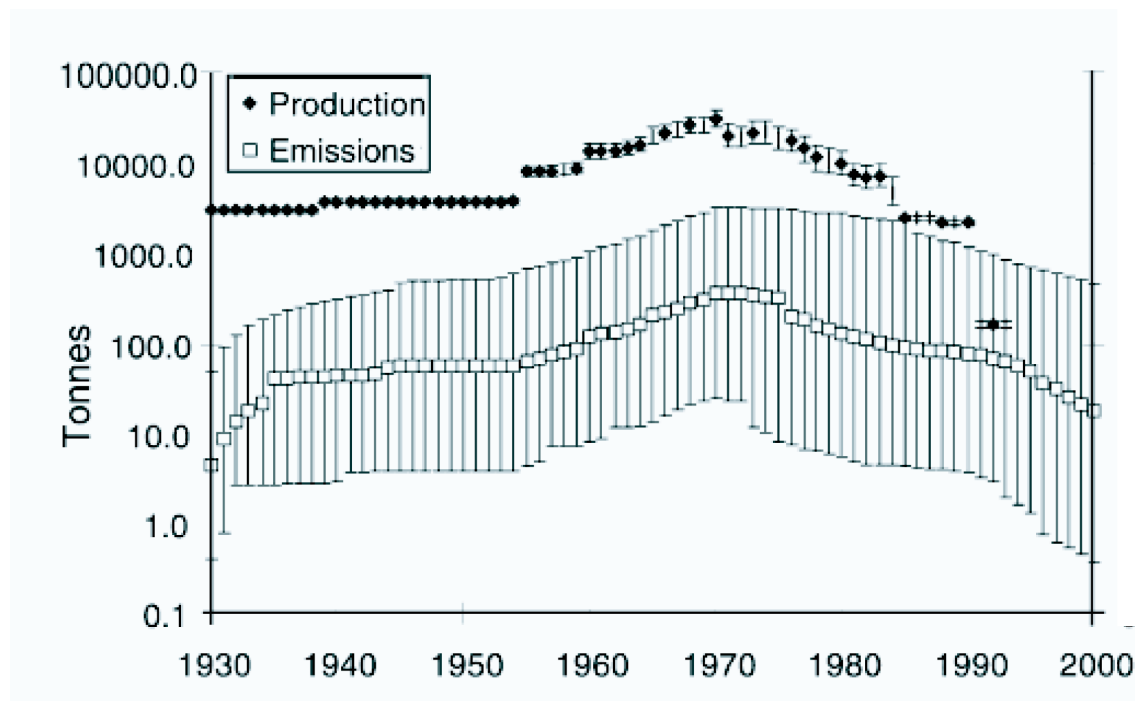
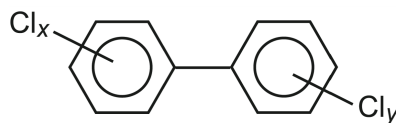




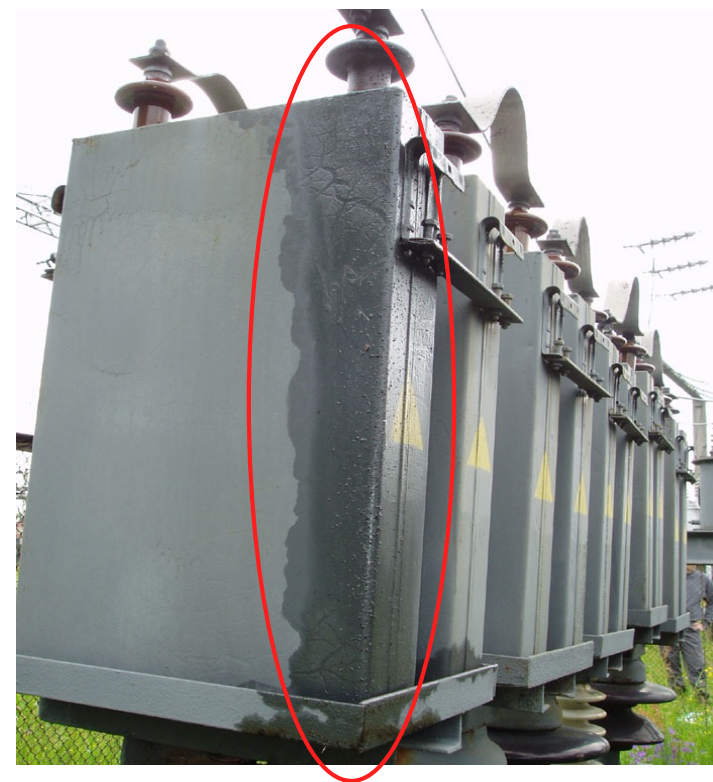
# Parameter Requirements: Emissions (I)

◆ Emission data: spatially and temporally resolved list of amounts of chemical released to the environment

◆ Example: PCBs



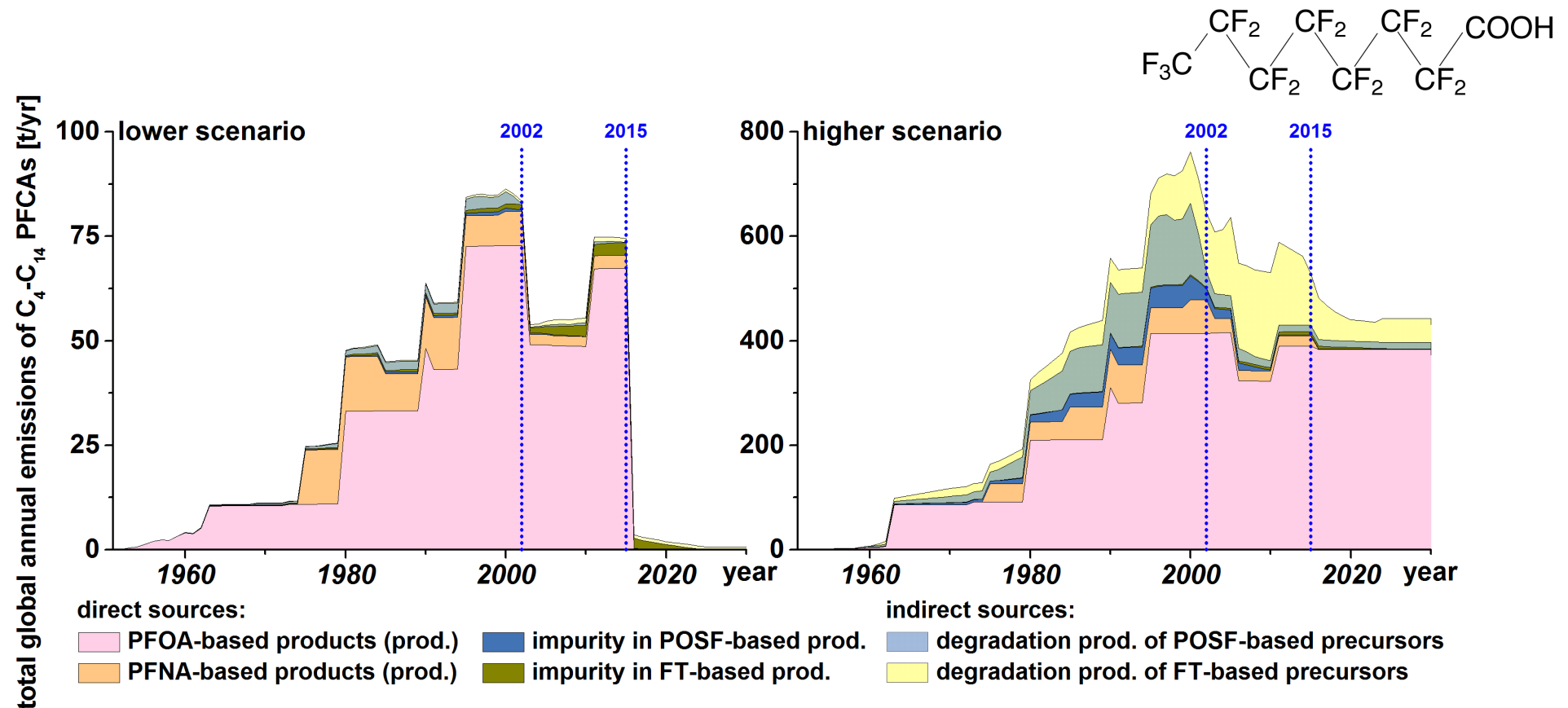
K. Breivik et al., *Sci Total Environ* **290** (2002) 199–224



source:  
Palina Tsytsik, Tamara Kukharchyk,  
Belarus

# Parameter Requirements: Emissions (II)

- ◆ Emissions peak only after 2000 (30 years after PCBs)
- ◆ Decrease after 2015: too optimistic estimate



Z. Wang et al., *Environment International* 70 (2014), 62–75

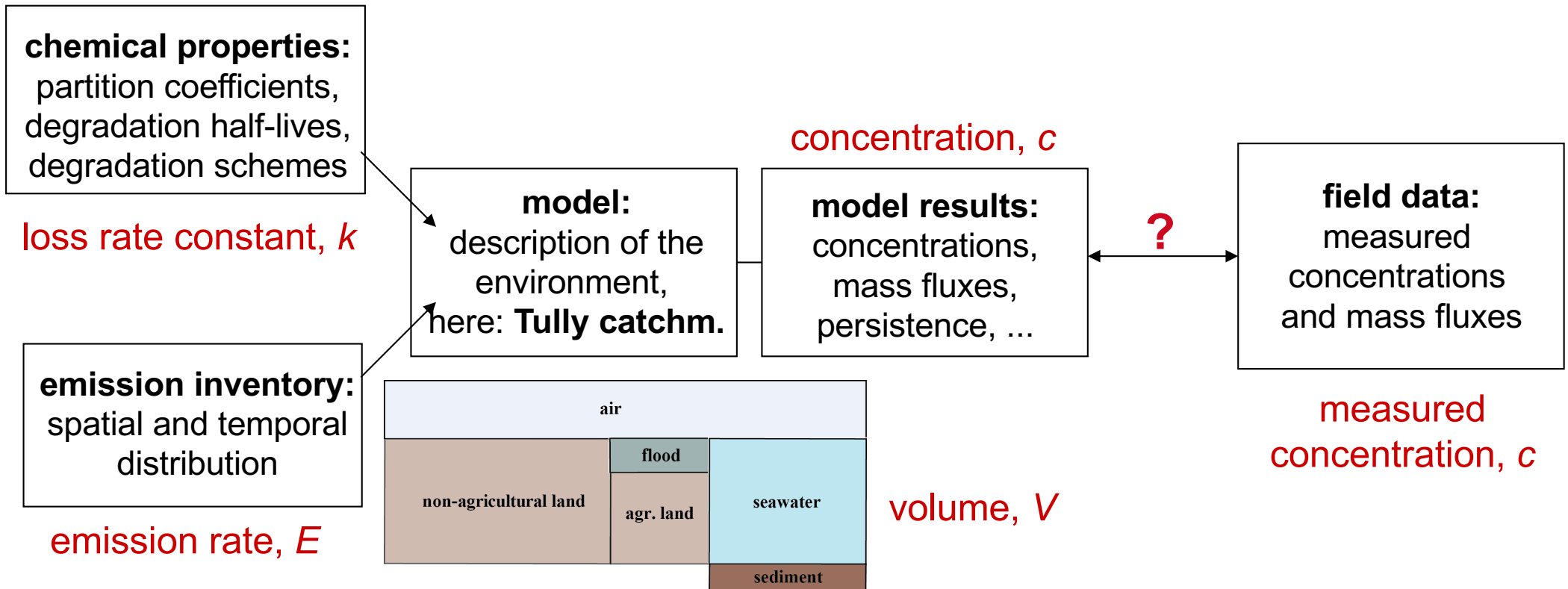
Z. Wang et al., *Environment International* 69 (2014), 166–176

# Environmental Fate Calculations with Box Models

## Regional Scale – Diuron in Queensland

# Environmental Fate Models as an “Integrative Platform”

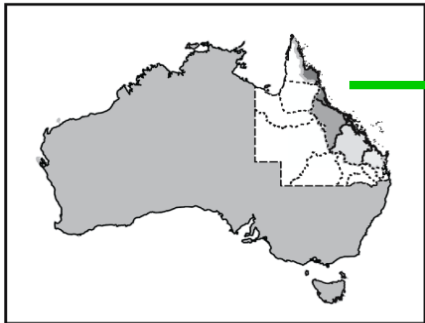
♦ Four main components:



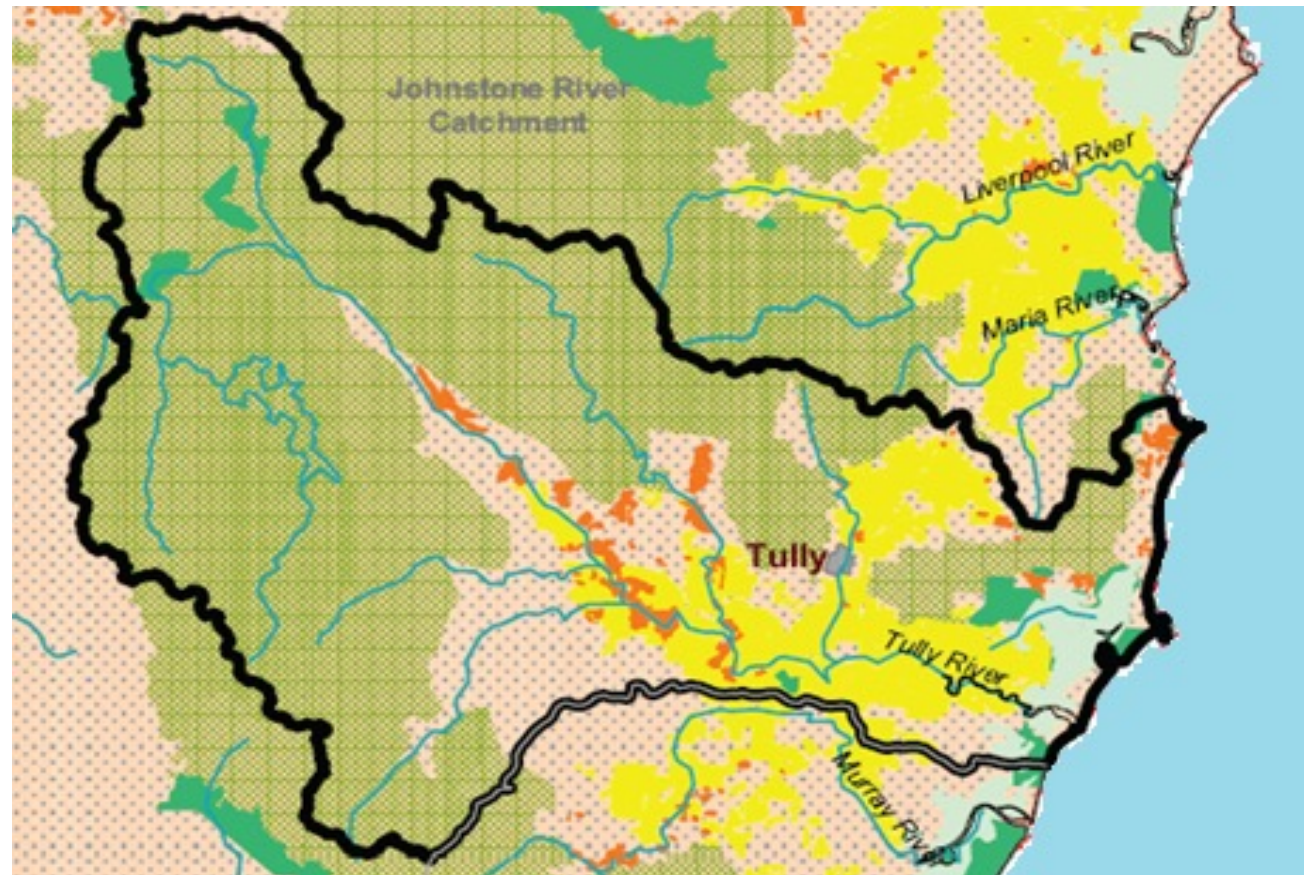


# A Less Persistent Chemical in a Small Region

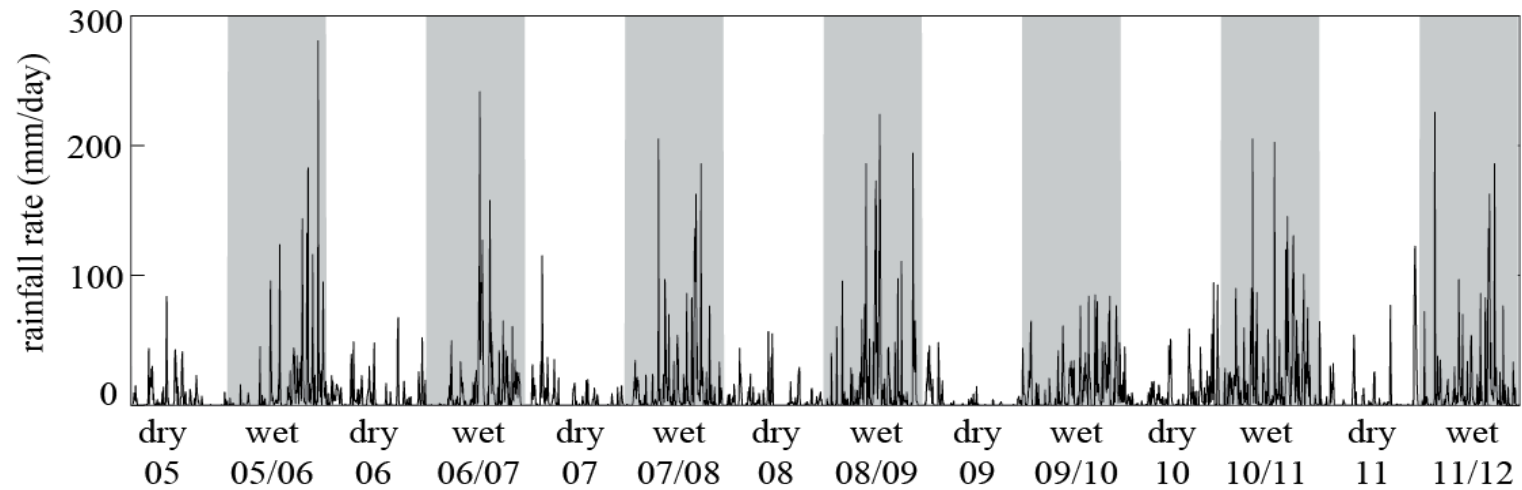
The Tully River Catchment, Queensland



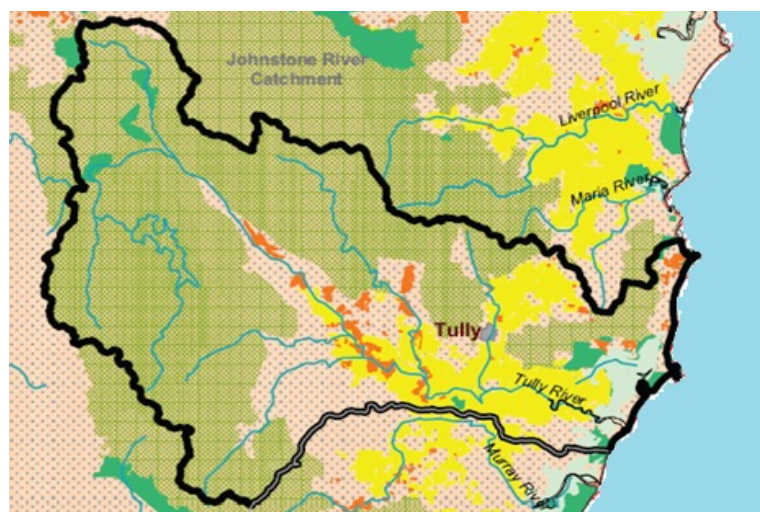
- State Forest
- Sugarcane
- Other Crops



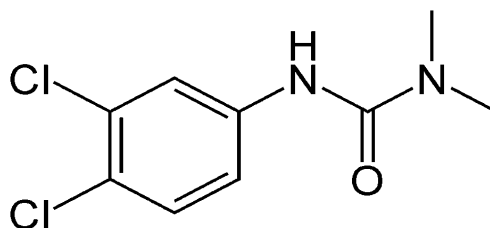
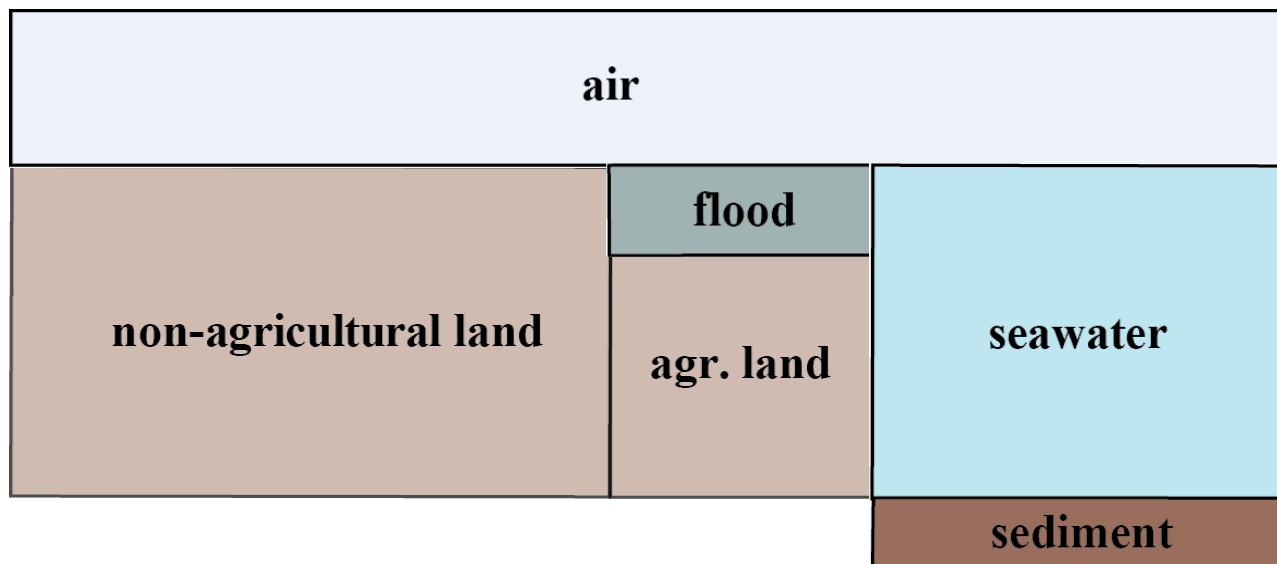
# Very Wet and Highly Dynamic



# Chemical and Model



diuron emissions  
derived from  
application to sugarcane:  
1.3 kg a.i. per ha and year



degradation half-lives  
and partition coefficients:

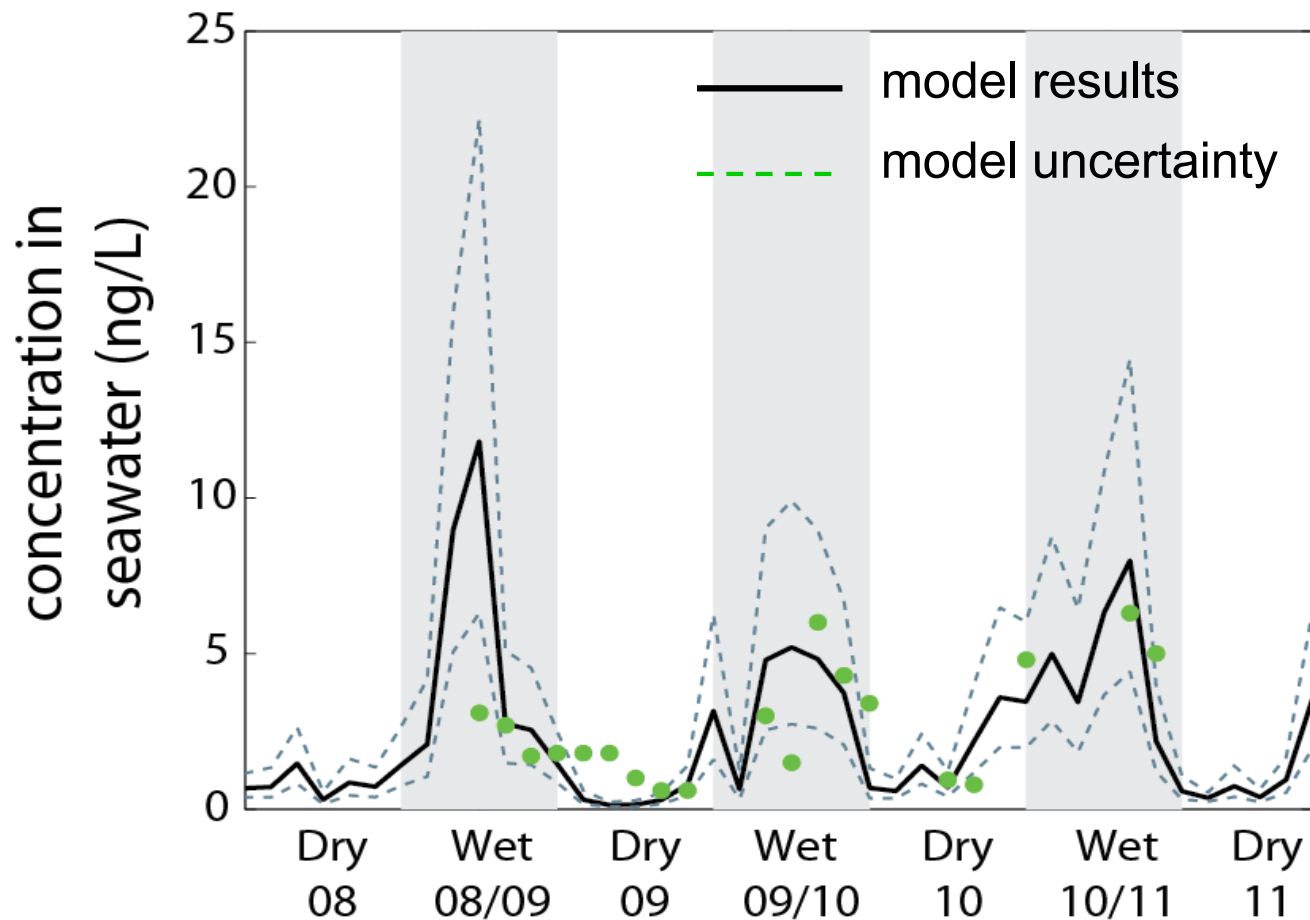
3 h (air)  
42 d (water),  
221 d (soil)

$\log K_{ow} = 2.7$

$\log K_{aw} = -7$

# Diuron Concentration in Seawater

Modeled and measured monthly-averaged diuron concentrations



L. Camenzuli, M. Scheringer et al. (2012)

Sci. Total Environ. 440 (2012), 178–185

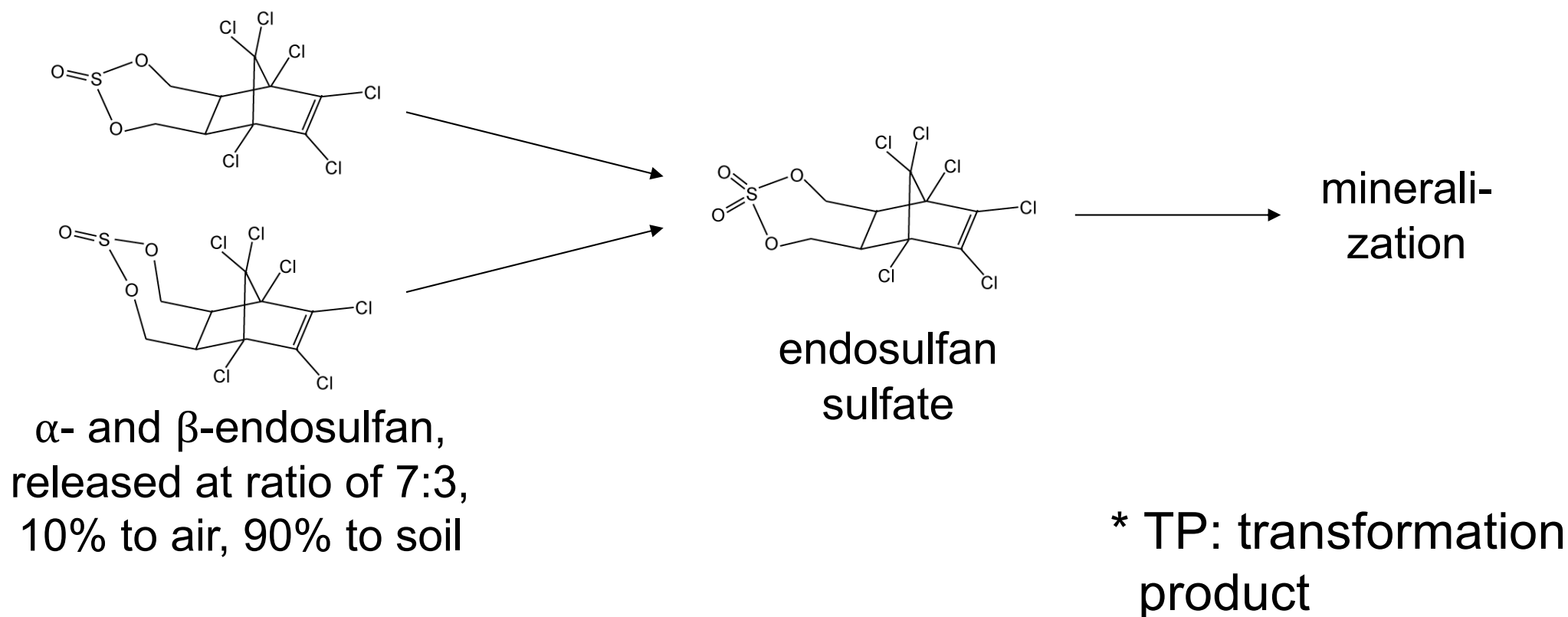
# Environmental Fate Calculations with Box Models

## Global Scale – Endosulfan in the Arctic



# Endosulfan: Two Isomers, One TP\*

- ◆ Endosulfan: insecticide, since 1950s, global pollutant
- ◆ Assessed under Stockholm Convention in 2009

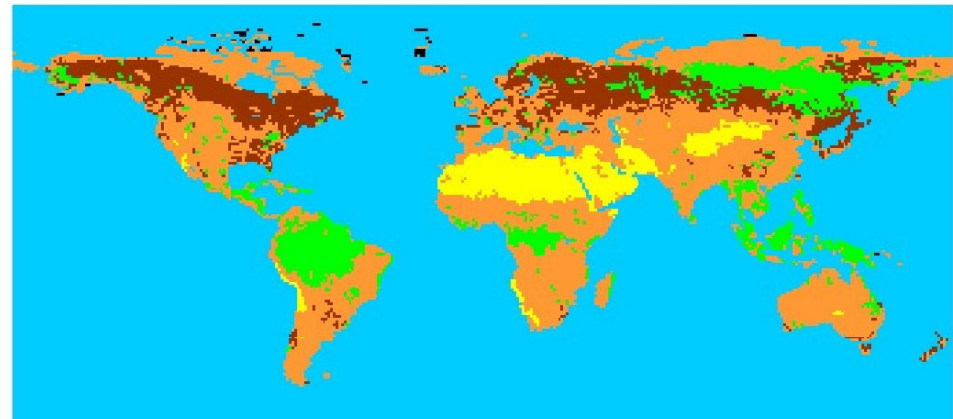


L. Becker, M. Scheringer, U. Schenker, K. Hungerbühler,  
Environ. Pollut. **159**, 1737–1743 (2011)

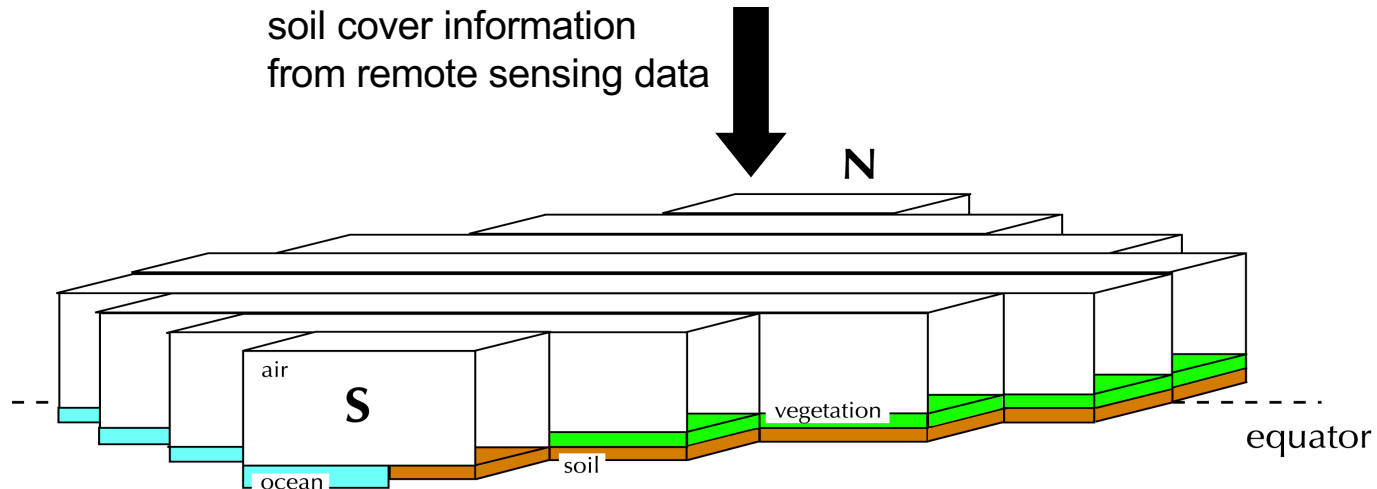
# Global Model “CliMoChem”

- ♦ Describes South-North transport of chemicals
- ♦ Well-mixed latitudinal zones
- ♦ Empirical information:
  - ➔ temperature
  - ➔ OH radicals
  - ➔ precipitation
  - ➔ soil composition
  - ➔ vegetation
  - ➔ and more ...

yellow: bare soil  
green: deciduous forests  
orange: grass land  
brown: coniferous forests



soil cover information  
from remote sensing data

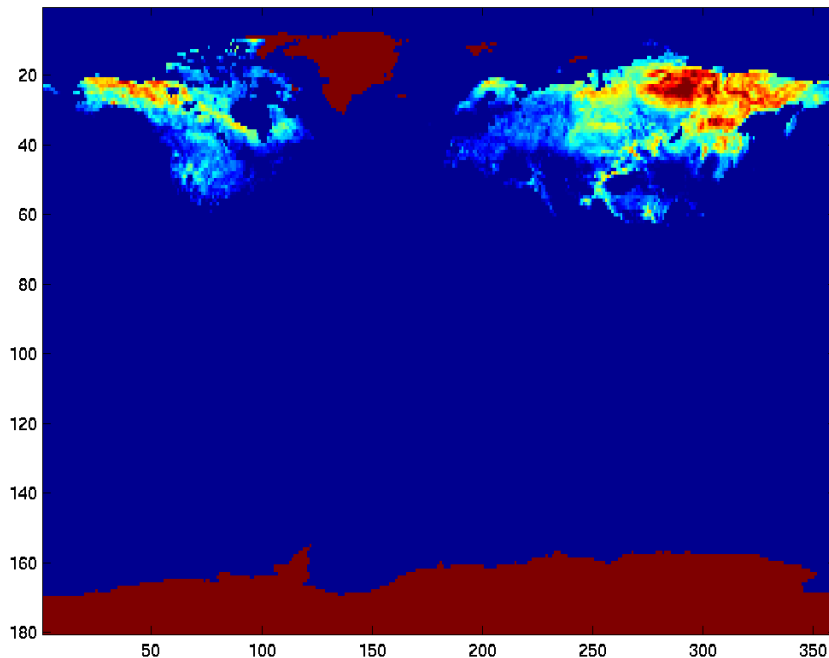


Scheringer, M., Wegmann, F., Fenner, K., Hungerbühler, K.  
*Environ. Sci. Technol.* 34 (2000), 1842–1850

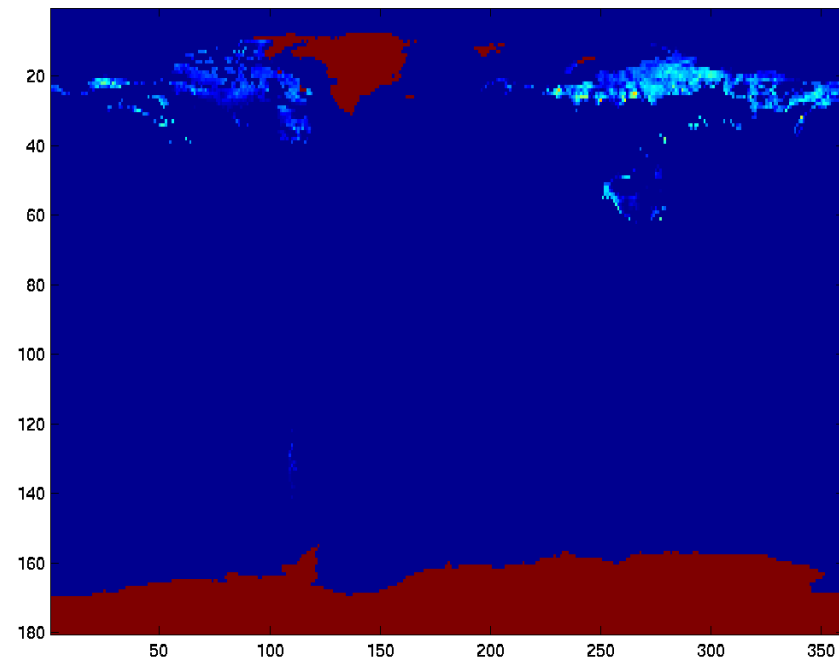
# Data for CliMoChem: Ice and Snow

## ◆ Snow depth from NASA EOS data

January



June



## ◆ Challenges:

- ➔ Changing snow density and water content
- ➔ Dynamics of snow melt
- ➔ Air-snow phase partitioning

# Model Inputs: Chemical Property Data

## ♦ Partition coefficients and degradation half-lives (days)

	$\alpha$ -endosulfan	$\beta$ -endosulfan	endosulfan sulfate
$\log K_{ow}$	4.93	4.78	3.71
$\log K_{aw}$	-3.56	-4.75	-4.78
$t_{1/2, \text{air}}$	6; 10; 18	4.4; 8; 13	4; 7; 12
$t_{1/2, \text{water}}$	12.6; 22; 38	17.4; 30; 52	58; 100; 173
$t_{1/2, \text{soil}}$	24; 42; 73	90; 156; 270	180; 312; 540

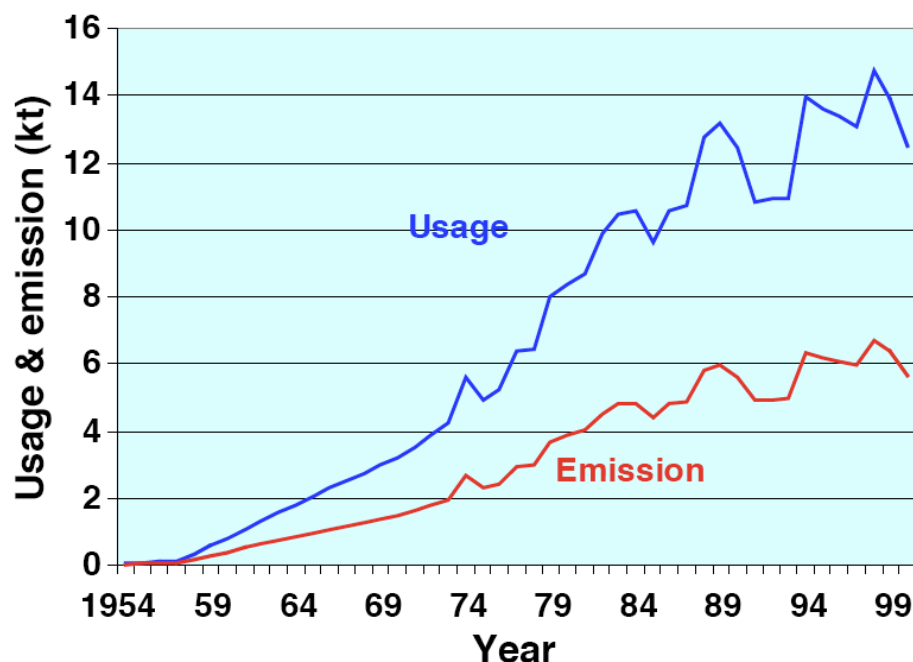
air: values based on measurements and AOPWIN

water: experimental data for hydrolysis in seawater

soil: selection based on assessment by US EPA R.E.D. (2002)

# Model Inputs: Emission Data (I)

- ◆ Overall historical emissions (global):<sup>1</sup>



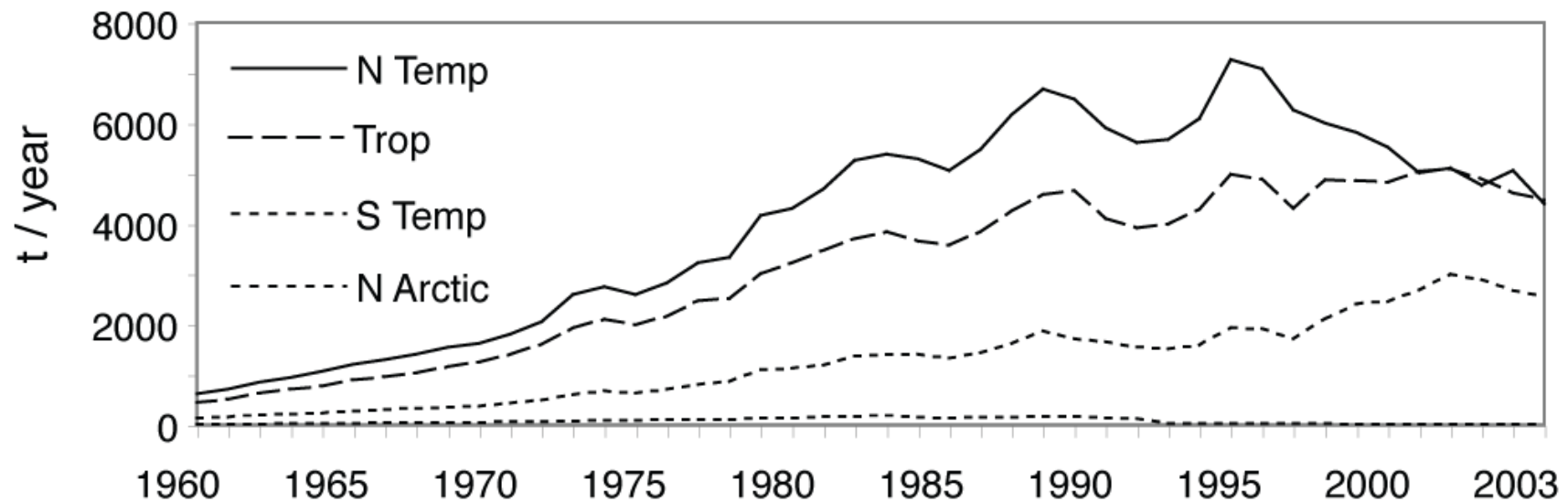
- ◆ Total historical usage (here assumed to be released): about 300 000 t

# Model Inputs: Emission Data (II)

## ♦ Contributions of latitudinal zones:<sup>1</sup>

➡ areas of crops under endosulfan treatment:  
cocoa, coffee, cotton, fruits, soy, tea, vegetables

## ♦ Model input:



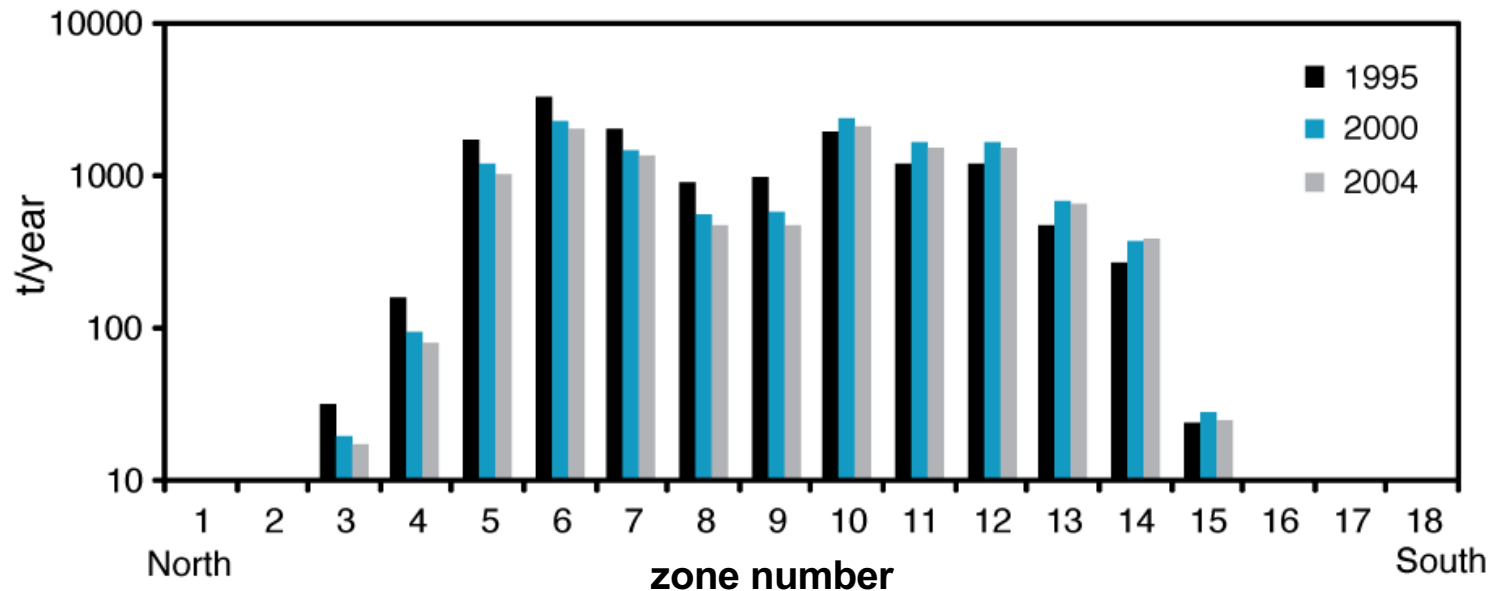


# Model Inputs: Emission Data (II)

## ♦ Contributions of latitudinal zones:<sup>1</sup>

➡ areas of crops under endosulfan treatment:  
cocoa, coffee, cotton, fruits, soy, tea, vegetables

## ♦ Model input:

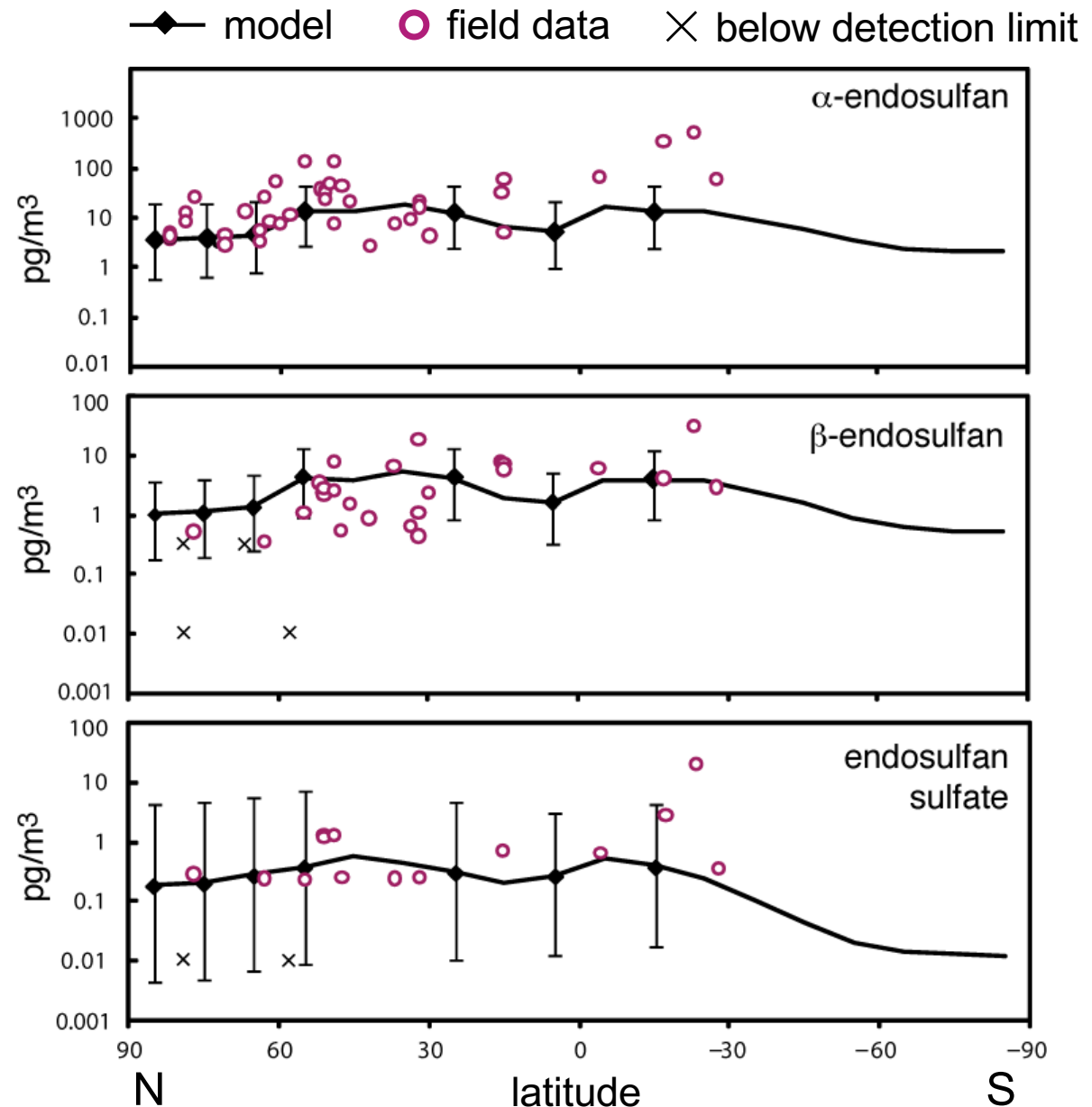


# Results: Concentrations in Air

◆ Good agreement  
for all three substances:

➡ latitudinal trend: ok

➡  $\alpha > \beta > \text{sulfate}$ : ok

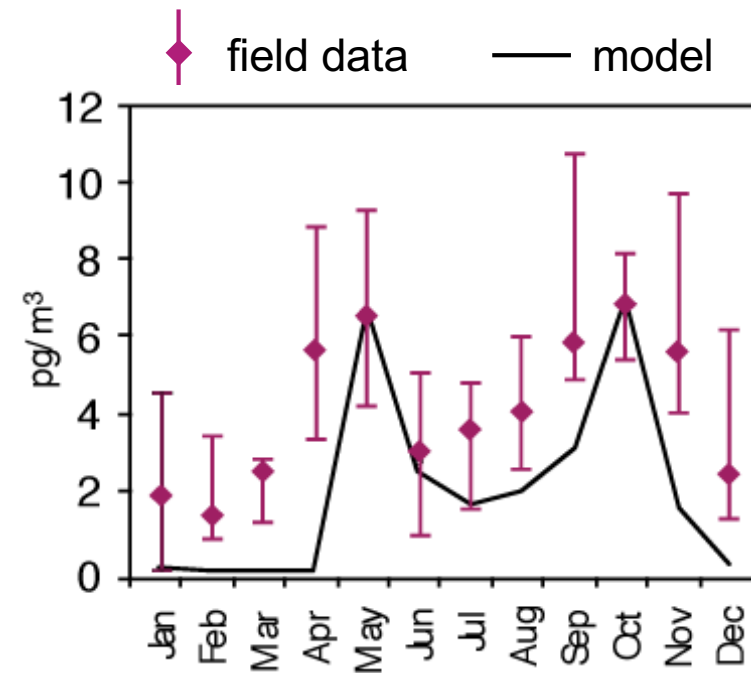


# Results: Time Trends in the Arctic

◆ concentrations of  $\alpha$ -endosulfan in Arctic air

➔ maximum in spring and fall

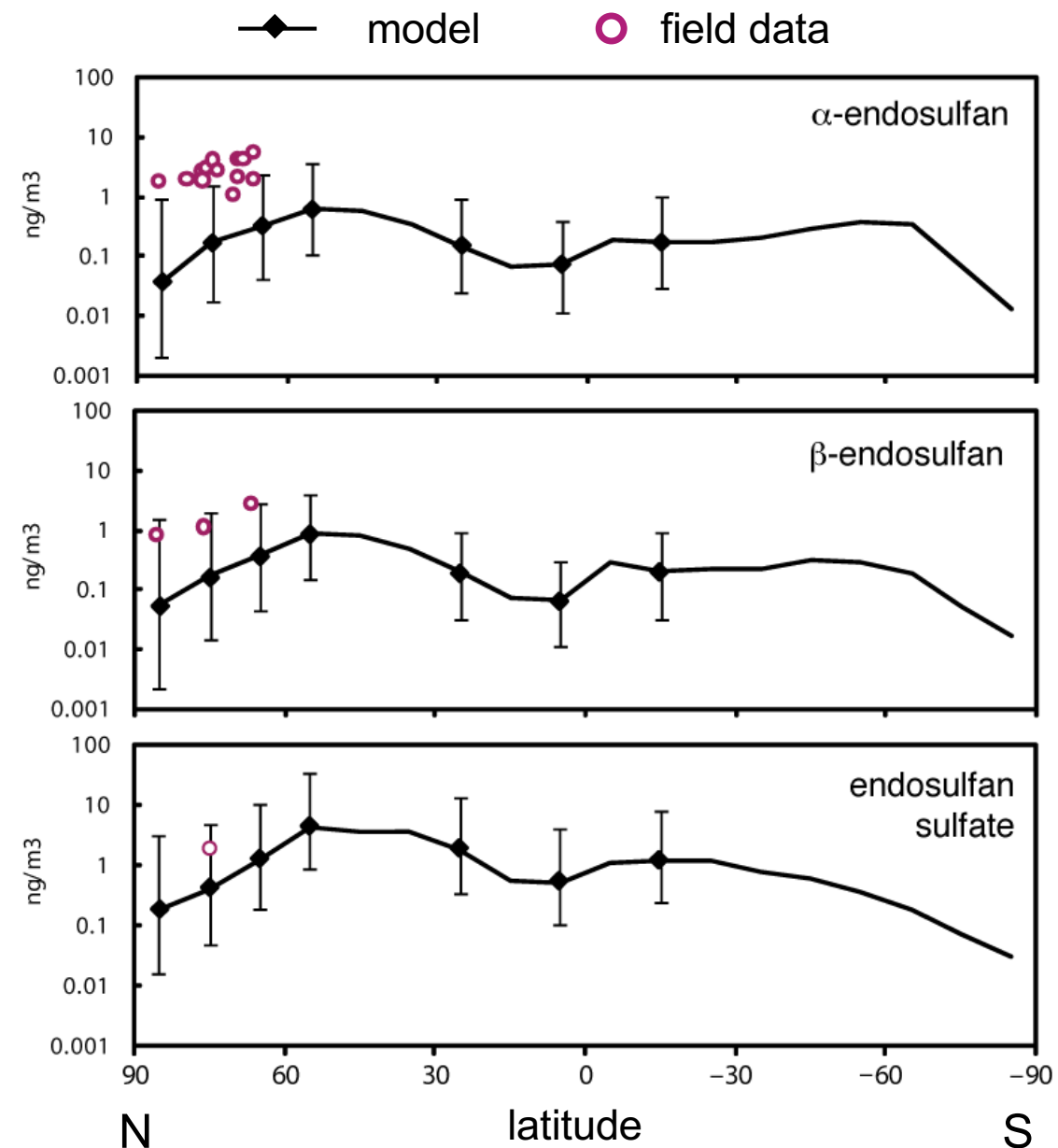
➔ why?



field data for Alert (82° N) from  
H. Hung, Environment Canada

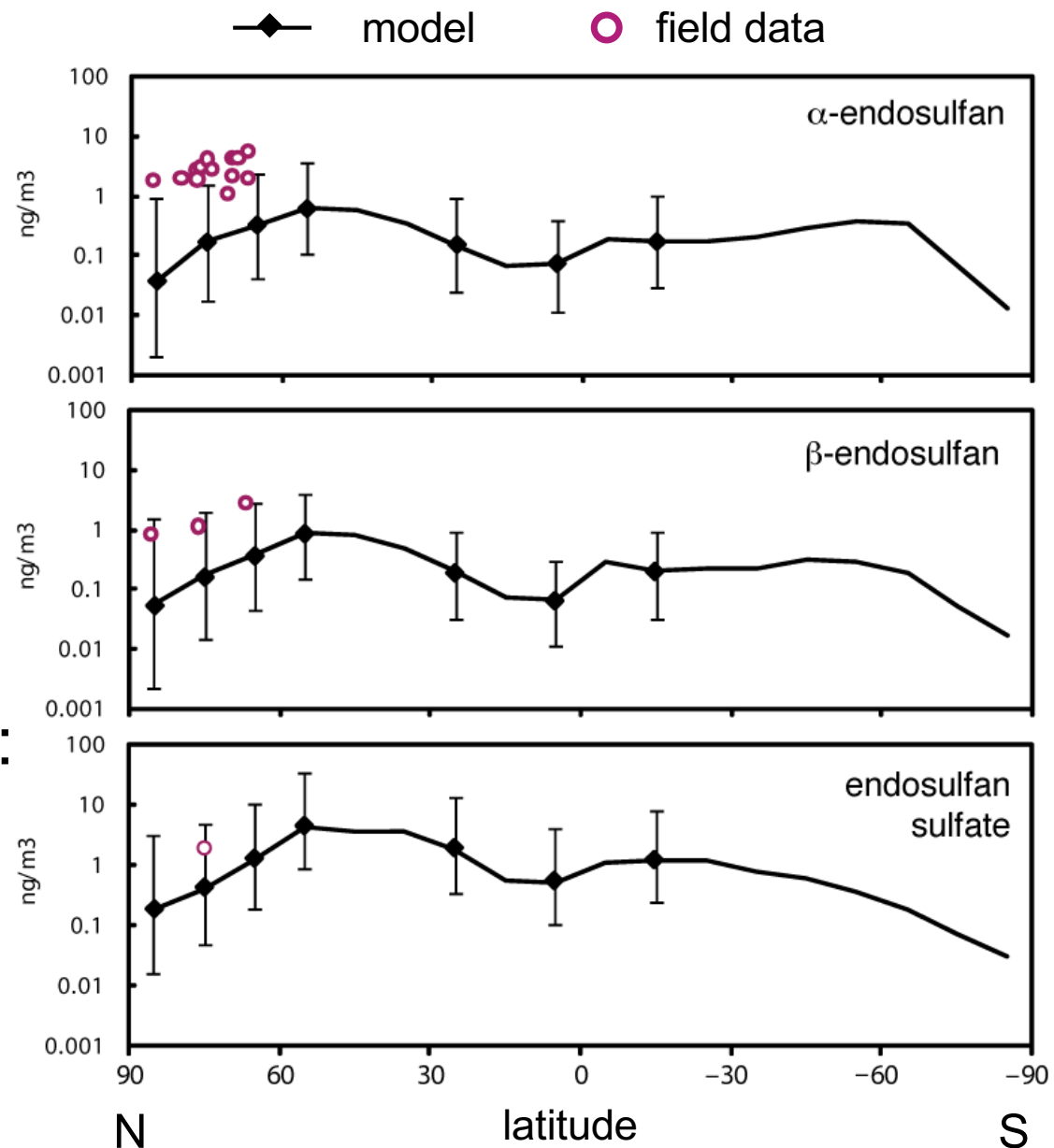
# Results: Concentrations in Ocean Water

- ♦ field data only north of 65° N
- ♦ sulfate >  $\alpha \approx \beta$ : ok
- ♦ all three substances: model by factor 10 too low



# Results: Concentrations in Ocean Water

- ♦ field data only north of 65° N
- ♦ sulfate >  $\alpha \approx \beta$ : ok
- ♦ all three substances: model by factor 10 too low
- ♦ most plausible explanation: **activation energy of hydrolysis too low**



# Results: Transfer to the Arctic

- ◆ What fraction of endosulfan in the Arctic stems from emissions in different latitudinal zones?

	N temperate (40–70 ° N)	N subtropic (20–40 ° N)	N tropic (0–20 ° N)
share of emissions in 2000	16%	33%	12%
transport distance to the Arctic (km)	2000	5000	8000
share of contribution to amount in Arctic seawater in 2000:			
$\alpha$ -endosulfan	57%	40%	2.5%
$\beta$ -endosulfan	66%	33%	1%
endosulfan sulfate	65%	34%	1%



# Other Applications ...

- ◆ Environmental fate of nanoparticles
- ◆ Chemicals in organisms: pharmacokinetic modeling

# Modeling Engineered Nanoparticles in the Environment

ENVIRONMENTAL  
Science & Technology


Article

pubs.acs.org/est

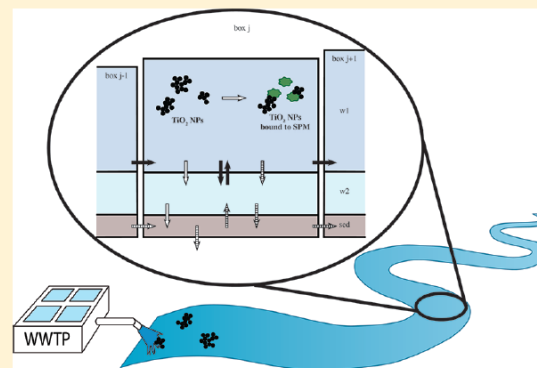
## Development of Environmental Fate Models for Engineered Nanoparticles—A Case Study of $\text{TiO}_2$ Nanoparticles in the Rhine River

Antonia Praetorius, Martin Scheringer,\* and Konrad Hungerbühler

Institute for Chemical and Bioengineering, ETH Zurich, Wolfgang-Pauli-Str. 10, 8093 Zurich, Switzerland

 Supporting Information

**ABSTRACT:** For a proactive risk assessment of engineered nanoparticles (ENPs) it is imperative to derive predicted environmental concentration (PEC) values for ENPs in different environmental compartments; PECs can then be compared to effect thresholds. From the basis of established multimedia environmental fate models for organic pollutants, we develop a new concept of environmental fate modeling for ENPs with process descriptions based on the specific properties of ENPs. Our new fate modeling framework is highly flexible and can be adjusted to different ENPs and various environmental settings. As a first case study, the fate and transport of  $\text{TiO}_2$  NPs in the Rhine River is investigated. Predicted  $\text{TiO}_2$  NP concentrations lie in the ng/L range in the water compartment and mg/kg in the sediment, which represents the main reservoir for the nanoparticles. We also find that a significant downstream transport of ENPs is possible. A fundamental process, the heteroaggregation between  $\text{TiO}_2$  NPs and suspended particulate matter (SPM), is analyzed in more detail. Our modeling results demonstrate the importance of both the SPM properties (concentration, size, density) as well as the affinity of  $\text{TiO}_2$  NPs and SPM, characterized by the attachment efficiency,  $\alpha_{\text{het-agg}}$ , on the transport potential of ENPs in a surface water system.



# Conclusions

- ◆ Multi-compartment models are highly flexible:
  - ◆ size and type of environmental system covered
  - ◆ temporal and spatial resolution
  - ◆ types of chemicals and processes covered
- ◆ Multi-compartment models make it possible to:
  - ➔ compare different processes
  - ➔ analyze importance of processes
  - ➔ integrate field data, chemical property data, and emission data

# Almost 40 Years of Contaminant Fate Models: from 1979 ...

Environmental Science & Technology Volume 13, Number 10, October 1979

## Finding fugacity feasible

*The fugacity approach can be used to gain insights into the likely behavior of toxic compounds. Widely used in describing chemical engineering operations, fugacity is a new and perhaps better way to quantify toxics transport and bioaccumulation in the air, water, and sediment*

---

**Donald Mackay**  
University of Toronto  
Toronto, Ontario, Canada

---

Considerable effort is currently being devoted to elucidating the mechanisms and rates by which toxic substances are transported and transformed in the environment. It is gen-

example, photolysis rate (kinetic) and aqueous solubility (equilibrium).

It is believed that the concept of fugacity can be potentially very useful in identifying the static and dynamic behavior of toxic substances in the environment. Phenomena such as bioaccumulation become readily understandable and predictable. The approach suggested here is capable of

elapsed so that all compartments are in equilibrium, then thermodynamics provides information about the nature of the partition. It is recognized that these assumptions are generally invalid because of in- and outflows of a physical, chemical, or biological nature, but interestingly they tend to be most valid for persistent substances that are often of greatest toxicological concern.

# ... to 2010

## ENVIRONMENTAL Science & Technology feature

*Environ. Sci. Technol.* **2010**, *44*, 8360–8364

### The State of Multimedia Mass-Balance Modeling in Environmental Science and Decision-Making

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THOMAS E. MCKONE  
*Lawrence Berkeley National Laboratory, University of  
California Berkeley, Berkeley, California*

KONRAD HUNGERBUHLER  
*ETH Zurich, Switzerland*

The multimedia mass-balance models advocated by these pioneers provided a powerful framework for understanding the behavior of chemicals in the environment. The mass-balance approach adopted from the field of chemical engineering focused attention on how chemical properties determine environmental behavior by requiring that air, water, soils, and even the tissues of animals be viewed only in terms of their capacity to hold a chemical pollutant. The description of the environment as a “unit world” made it clear that the environment is finite, and focused attention on how the properties of chemicals determine their behavior as environmental pollutants. Multimedia mass-balance models at different levels of detail provided a “tool box” that could be applied to different types of problems, and a logical and integrated framework for introducing environmental chemistry concepts to students. Therefore, it is not surprising that in subsequent decades these techniques proliferated and spawned an entire discipline dedicated to modeling environmental contaminants in multimedia environments (5).

In the ensuing three decades, multimedia mass-balance models played an important role in the scientific study of the behavior of chemicals in the environment. For example, the models supported the development of the concepts of persistence (P) and long-range transport (L RTP) that are now key hazard indicators used in chemical assessment (6). Models of the uptake of chemicals by fish from water and food were instrumental in elucidating the mechanisms of bioconcentration and biomagnification (7, 8). Global-scale multimedia models illustrated the potential that certain persistent pollutants could migrate to, and accumulate in, polar regions (9–11). Multimedia models provided a basis for quantifying cumulative, multipathway exposure to pollutants that originate from contaminated air, water, and soil (12). Mass-balance models were employed to characterize the relative importance of local and distant sources of

Are multimedia models dinosaurs in the modern world?





# ... and 2018

## Environmental Science Processes & Impacts



### CRITICAL REVIEW

[View Article Online](#)  
[View Journal](#)



Cite this: DOI: 10.1039/c7em00568g

## Environmental fate and exposure models: advances and challenges in 21<sup>st</sup> century chemical risk assessment

Antonio Di Guardo, <sup>a</sup> Todd Gouin, <sup>b</sup> Matthew MacLeod <sup>c</sup>  
and Martin Scheringer \*<sup>de</sup>

Environmental fate and exposure models are a powerful means to integrate information on chemicals, their partitioning and degradation behaviour, the environmental scenario and the emissions in order to compile a picture of chemical distribution and fluxes in the multimedia environment. A 1995 pioneering book, resulting from a series of workshops among model developers and users, reported the main advantages and identified needs for research in the field of multimedia fate models. Considerable efforts were



# Environmental Fate Modeling as a Technique

Integrated Environmental Assessment and Management — Volume xxx, Number xxx—pp. xxx–xxx  
© 2012 SETAC

1

## Good Modeling Practice Guidelines for Applying Multimedia Models in Chemical Assessments

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§Centre for Environmental Modeling and Chemistry, Trent University, Peterborough, Ontario, Canada

||Environment Canada, Ecological Assessment Division, Gatineau, Quebec, Canada

#DuPont Haskell Global Centers for Health and Environmental Sciences, Newark, Delaware, USA

††LimnoTech, Ann Arbor, Michigan, USA

(Submitted 30 September 2011; Returned for Revision 28 November 2011; Accepted 23 January 2012)

### ABSTRACT

Multimedia mass balance models of chemical fate in the environment have been used for over 3 decades in a regulatory context to assist decision making. As these models become more comprehensive, reliable, and accepted, there is a need to recognize and adopt principles of Good Modeling Practice (GMP) to ensure that multimedia models are applied with transparency and adherence to accepted scientific principles. We propose and discuss 6 principles of GMP for applying existing multimedia models in a decision-making context, namely 1) specification of the goals of the model assessment, 2) specification of the model used, 3) specification of the input data, 4) specification of the output data, 5) conduct of a sensitivity and possibly also uncertainty analysis, and finally 6) specification of the limitations and limits of applicability of the analysis. These principles are justified and discussed with a view to enhancing the transparency and quality of model-based assessments. Integr Environ Assess Manag 2012;xxx:xxx–xxx. © 2012 SETAC

**Keywords:** Modeling Good practice Hazard assessment Risk assessment Industrial chemicals  
Multimedia models Decision making

### INTRODUCTION

Multimedia mass balance models have been used to support environmental assessments of chemicals for over 3

output data, and 4) interpretation of model results. The results of multimedia modeling enable evaluation of human and ecological exposure to chemicals and provide insights into

A. Buser et al.,  
*Integrated  
Environmental  
Assessment &  
Management*  
8, 2012,  
703–708

Environmental Management