Environmental Fate Modeling of Chemicals, Lecture 1:

Motivation and Foundations

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Brno, April 11, 2025

Introduction

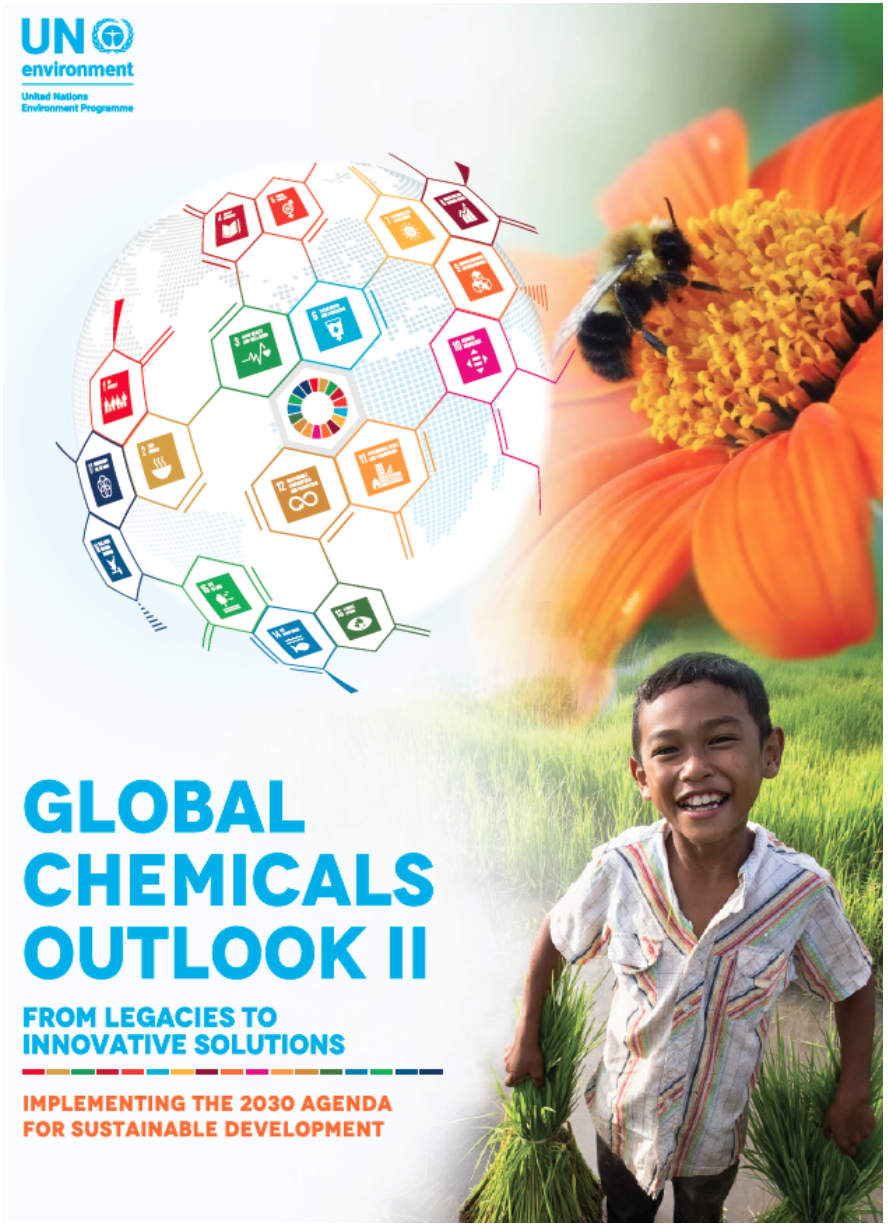
Chemical Pollution as a Global Impact

"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



https://www.unenvironment.org/explore-topics/chemicals-waste/what-we-do/policy-and-governance/global-chemicals-outlook

Chemical Pollution as a Global Impact

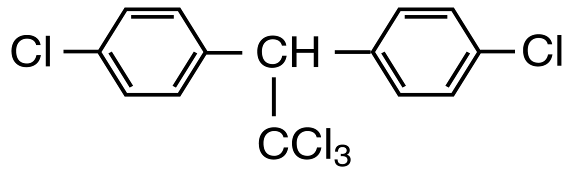
Global Environment Outlook 6

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)

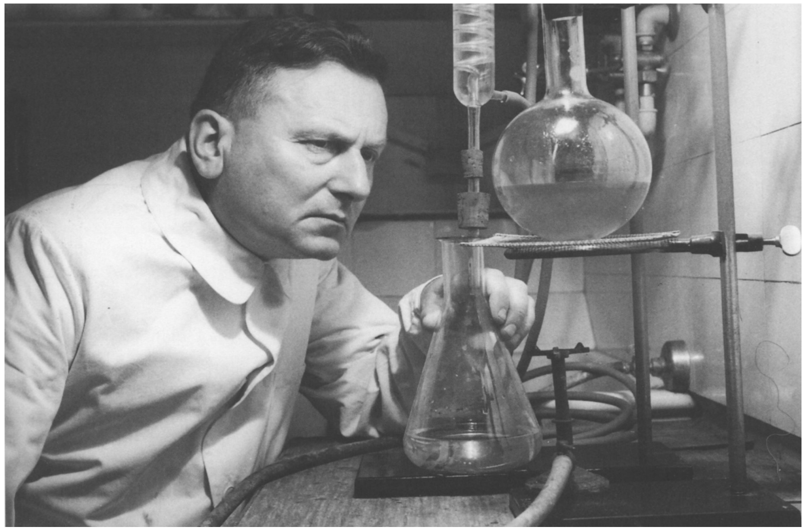
https://www.unep.org/resources/global-environment-outlook-6

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

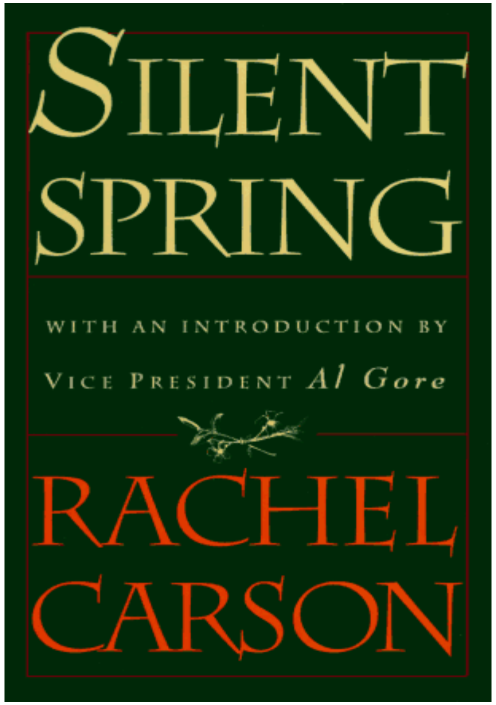
How the proliferation of pesticides like DDT almost undid the Peregrine falcon.

Peregrine Falcon, 1919 via Wikimedia Commons

https://daily.jstor.org/the-case-of-the-thinning-eggshells/

„*Silent Spring*“

- Rachel Carson publishes Silent Spring in 1962
  - Presents effects of pesticides on wildlife and **on humans**
  - Points out connection betweeen 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

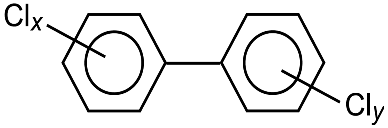
A. G. JOHNELS
M. OLSSON

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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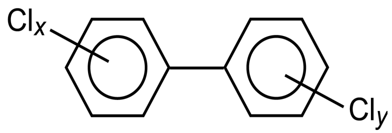
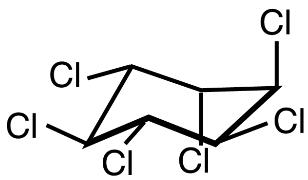


The New York State's 'eat none' advisory and the restriction on taking fish for this section of the Upper Hudson has been in place for 36 years.

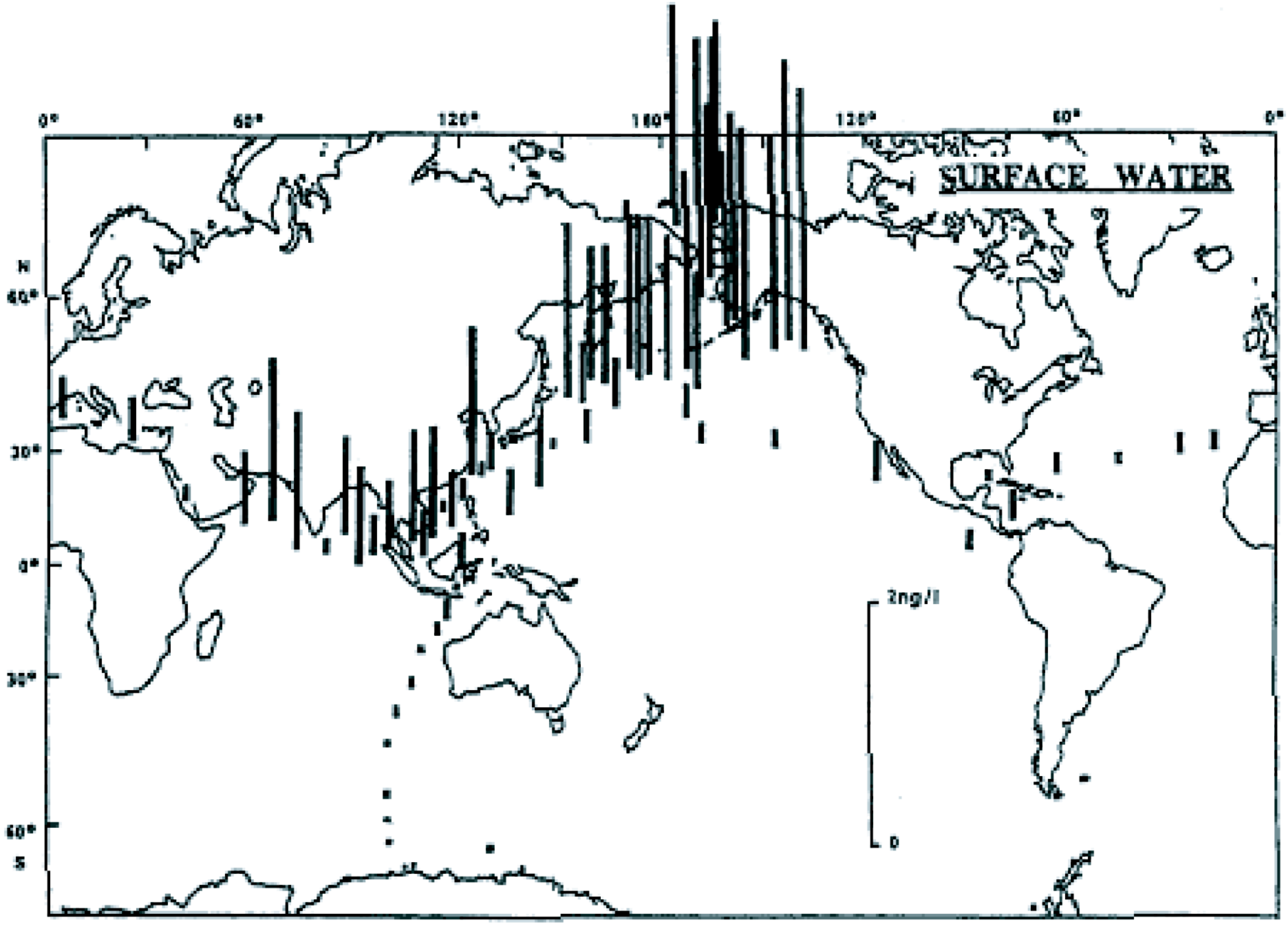
http://response.restoration.noaa.gov/about/media/pcbs-why-are-banned-chemicals-still-hurting-environment-today.html

The Global Presence of Chemicals

- alpha-HCH in the global oceans



α-HCH



Iwata, H.et al., *Environ. Sci. Technol*. 27 (1993), 1080–1098

The Global Presence of Chemicals

ANGEWANDTE CHEMIE

International Edition in English

Volume 31 · Number 5
May 1992
Pages 487–664

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)

https://doi.org/10.1002/anie.199204873

The Global Presence of Chemicals

words, MnO_4^- abstracts H· from toluene just as an oxygen radical would if it had a bond strength of 83 kcal mol^{-1}. This is true even though MnO_4^- is not a radical. Similar correlations have been found for oxidations of ethylbenzene by RO· and MnO_4^- (6) and for oxidations of toluene, cyclohexane, and isobutane by RO· and CrO_2Cl_2 [on the basis of an estimated CrO–H bond strength (*18*, *19*)]. The rate of toluene oxidation by MnO_4^- in water does not fit this relation because the mechanism is not H· abstraction; rates of H· 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 H·. Understanding these reactions should be based primarily on the thermochemistry of the H· abstraction step.

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2. G. Centi, F. Trifirò, 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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https://doi.org/10.1126/science.7569923

The Global Presence of Chemicals

- Results from an Africa-wide network of passive samplers

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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 Přibylová, Petr Kukučka, Jiří Kohoutek, Roman Prokeš, and Jana Klánová*

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

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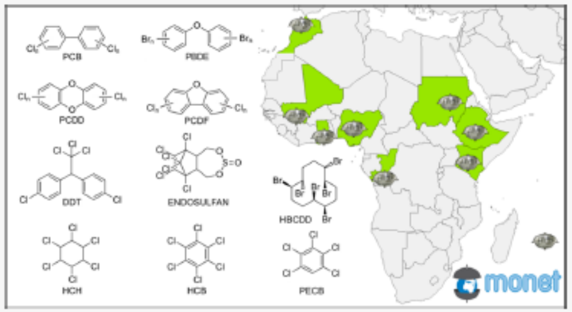
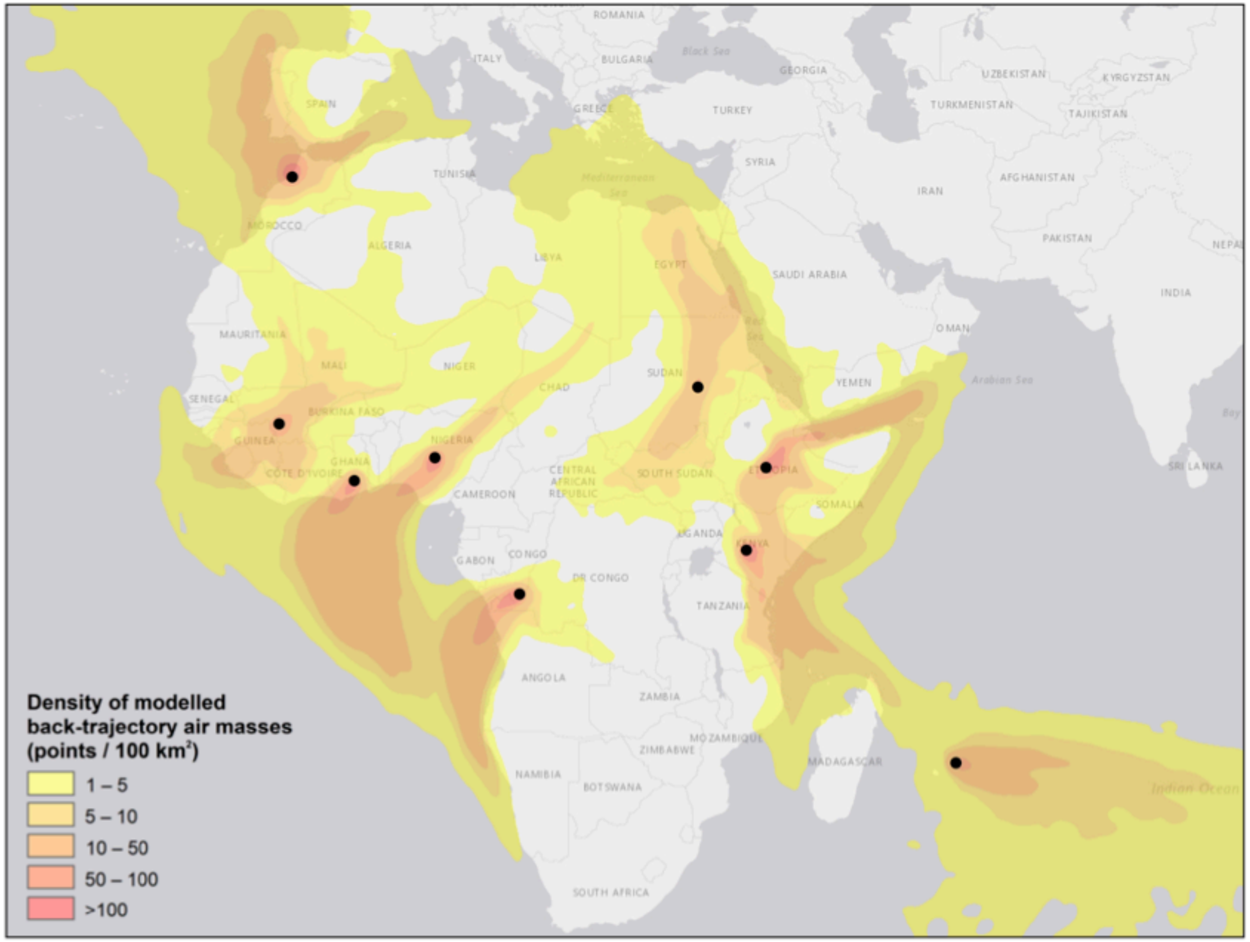
ABSTRACT: The Global Monitoring Plan of the Stockholm Convention on Persistent Organic Pollutants (POPs) was established to generate long-term data necessary for evaluating the effectiveness of regulatory measures at a global scale. After a decade of passive air monitoring (2008−2019), MONET is the first 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



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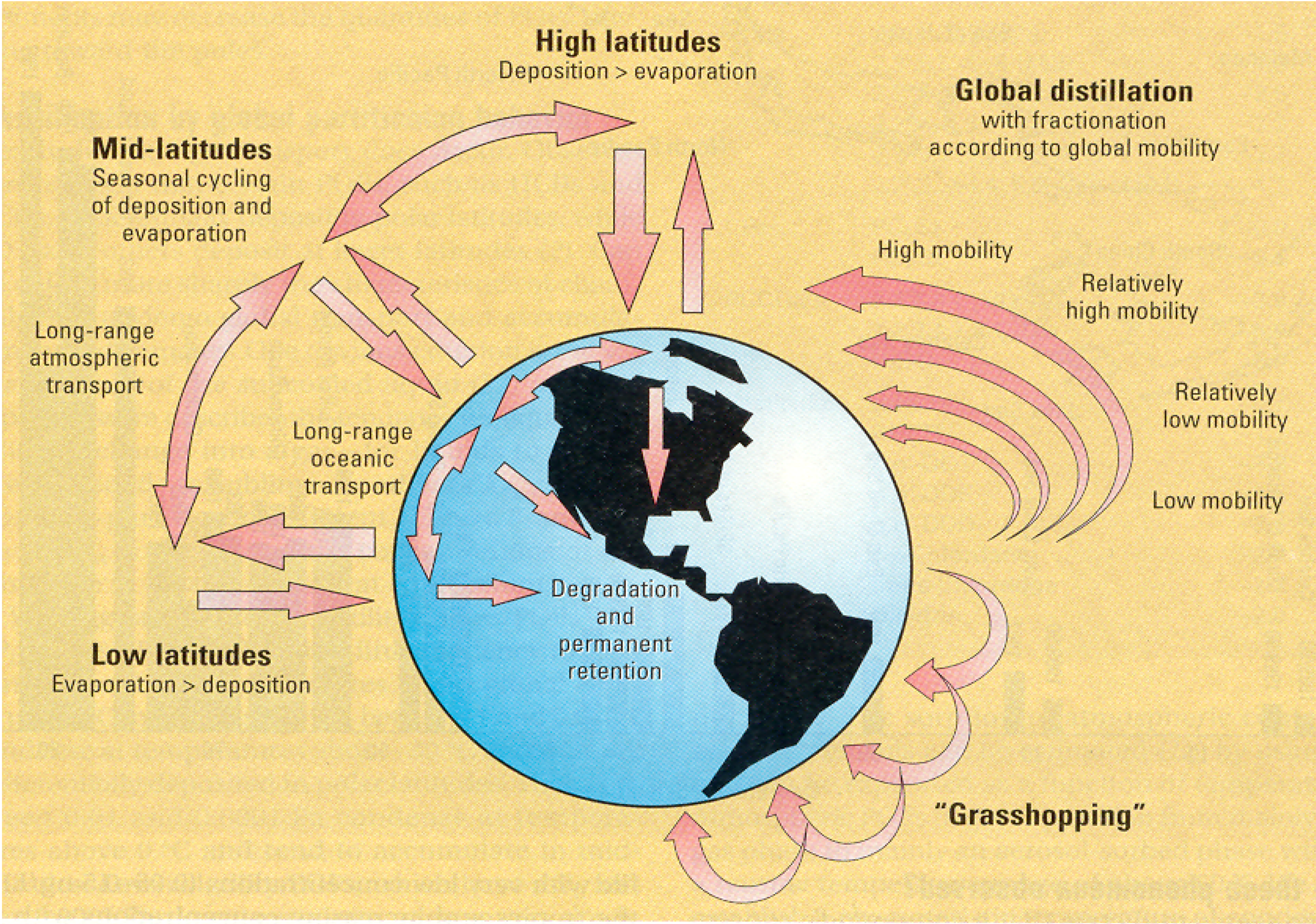
The Global Presence of Chemicals



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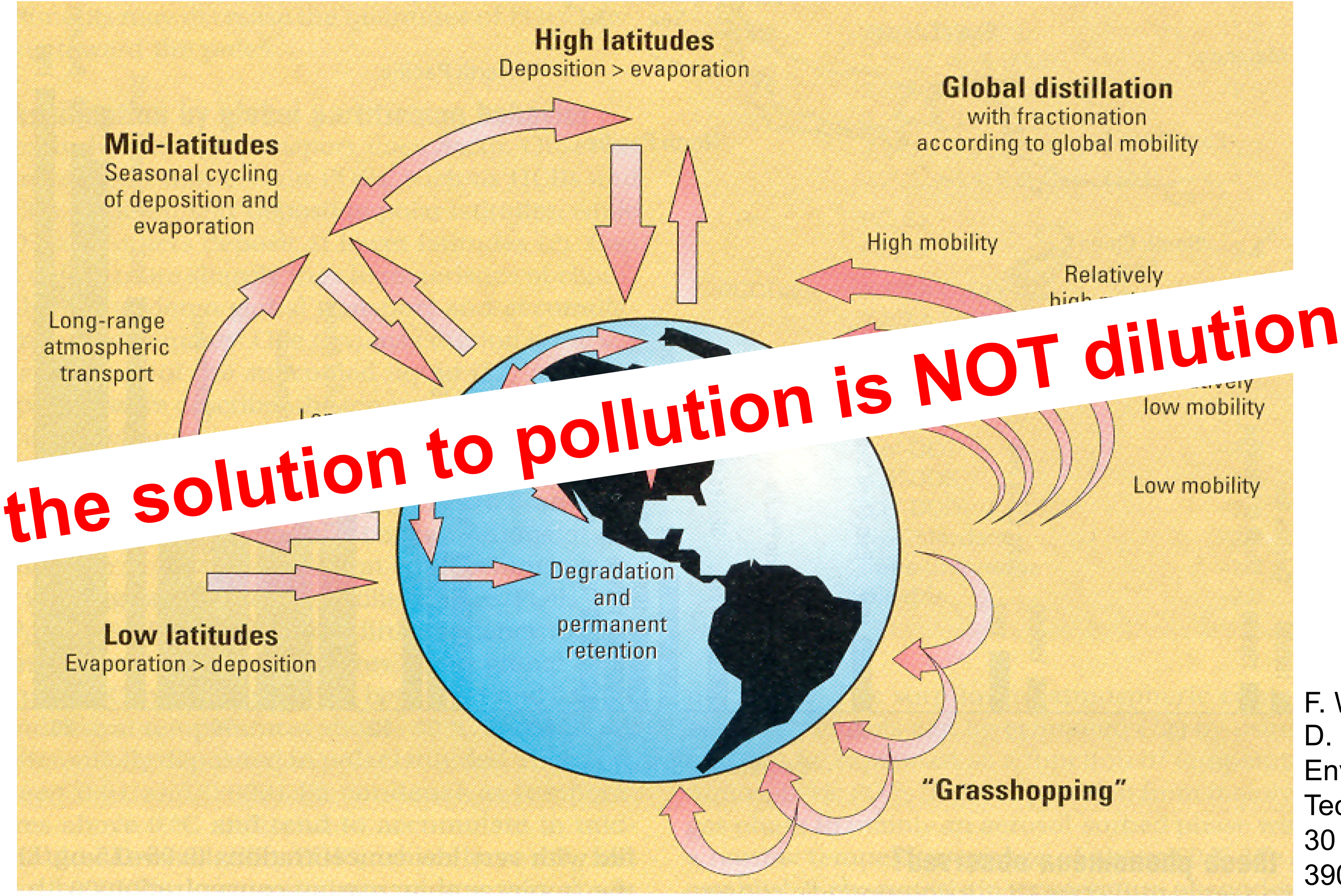
The Global Presence of Chemicals



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

Old Problems Come Back ...

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

Downloaded from http://science.sciencemag.org/ on June 16, 2016

By **Paul D. Jepson**[1] *and* **Robin J. Law**[1,2]

Persistent 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

Jepson and Law, *Science* 352 (2016)

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

MUNI | RECETOX

Source: The Guardian, May 2017

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

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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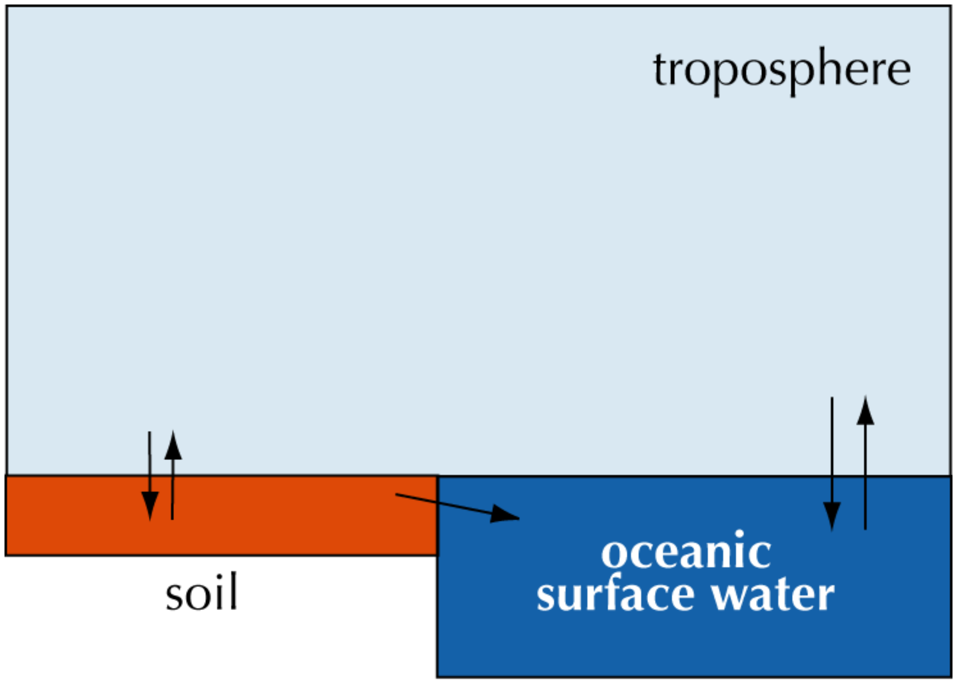

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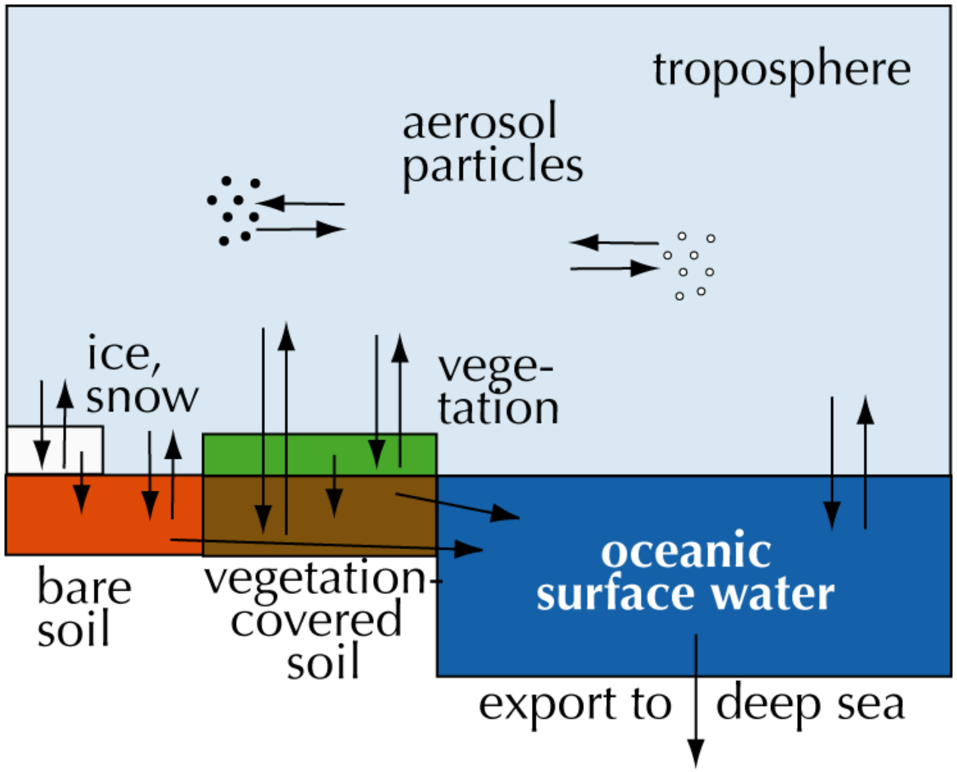


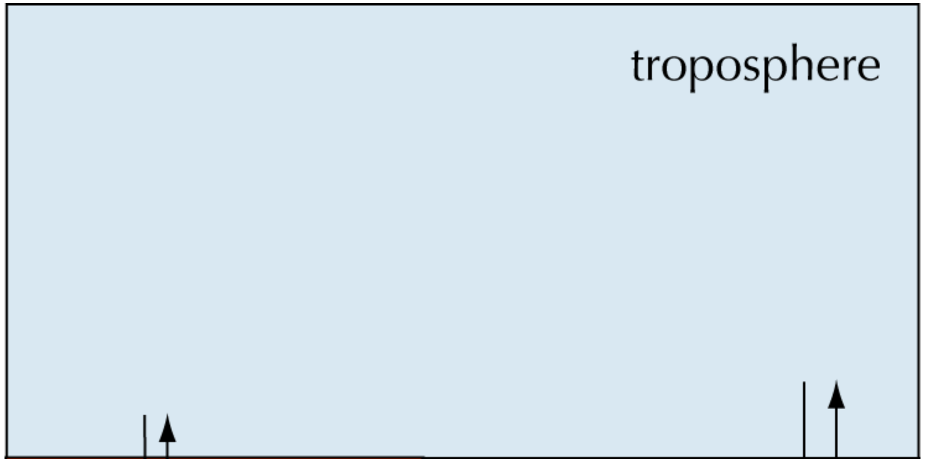
A First Example: CCl_4, Global

- Emission rate: *E* (kg/yr)
- Volume of air: *V* (m^3)
- Loss rate constant: *k* (1/yr)
- Concentration in air: *c* (kg/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_4, Global

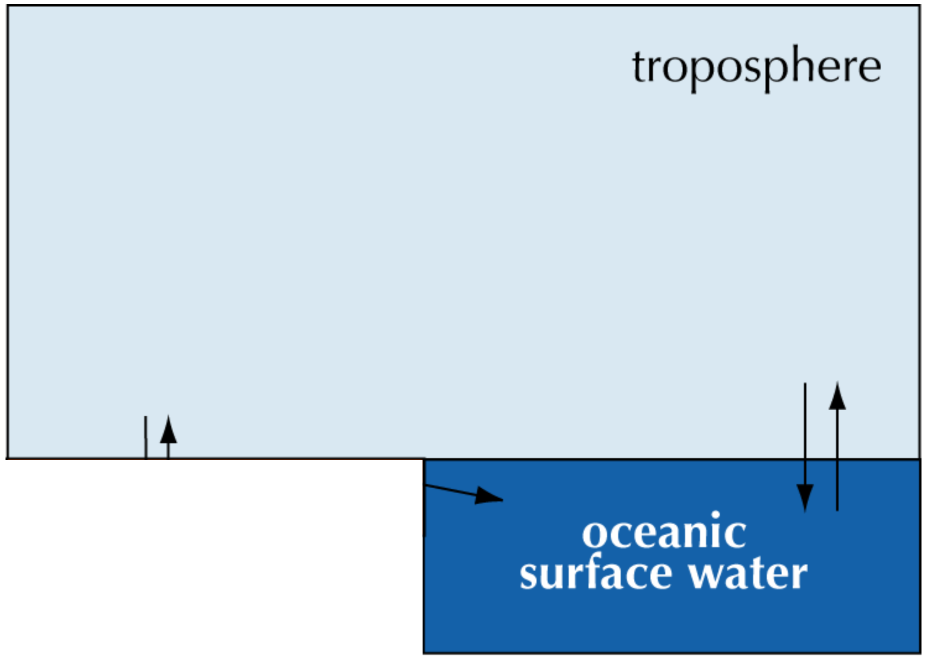
- With actual data:
  - E = 80 kt/yr = 5.19 $\cdot 10^8$ mol/yr
  - $V = 5 \cdot 10^{18}$ m^3
  - k = 1/30 yr = 0.0333 yr^{-1}



  - this yields:
    $c = 3.1 \cdot 10^{-9}$ mol/m^3 = 70 ppt
  - measured concentration:
    of CCl_4 in the troposphere: c = 90 ppt

Mass Balance Equation for Two Boxes

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



Mass Balance Equation for Two Boxes

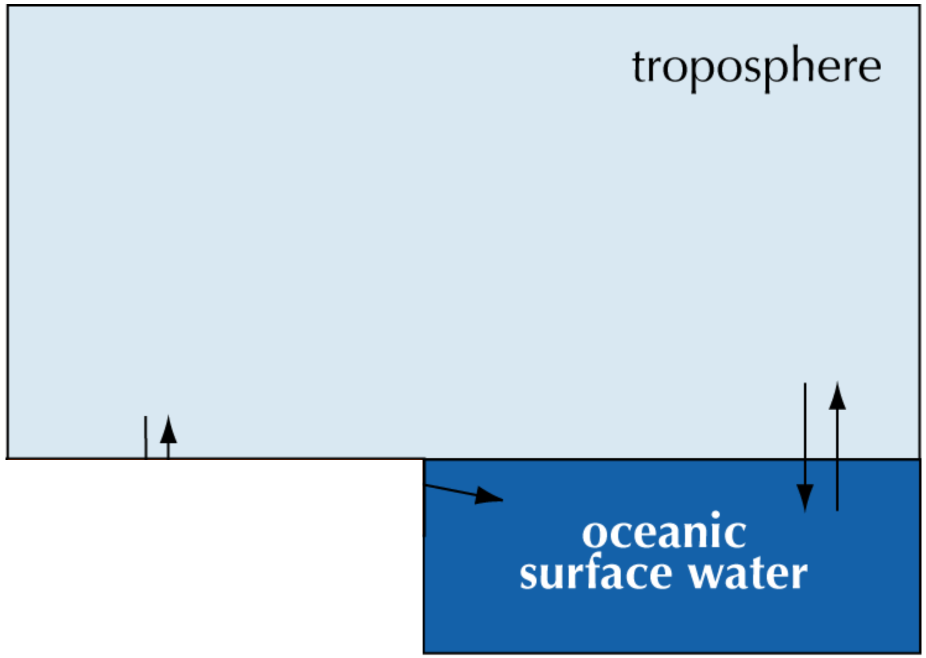
- air, a, and water, w
- mass-balance equation

  for one box: $E = c \cdot V \cdot k$
- for two boxes:

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

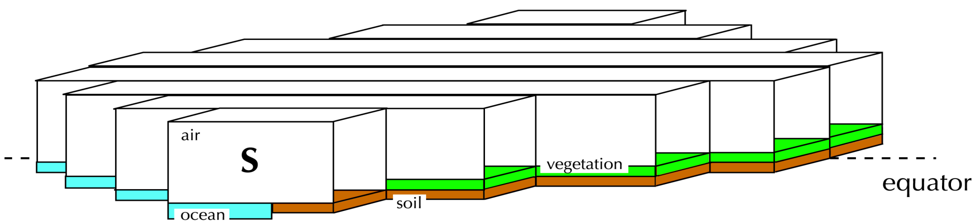
  and

  $c_a / c_w = K_{aw}$

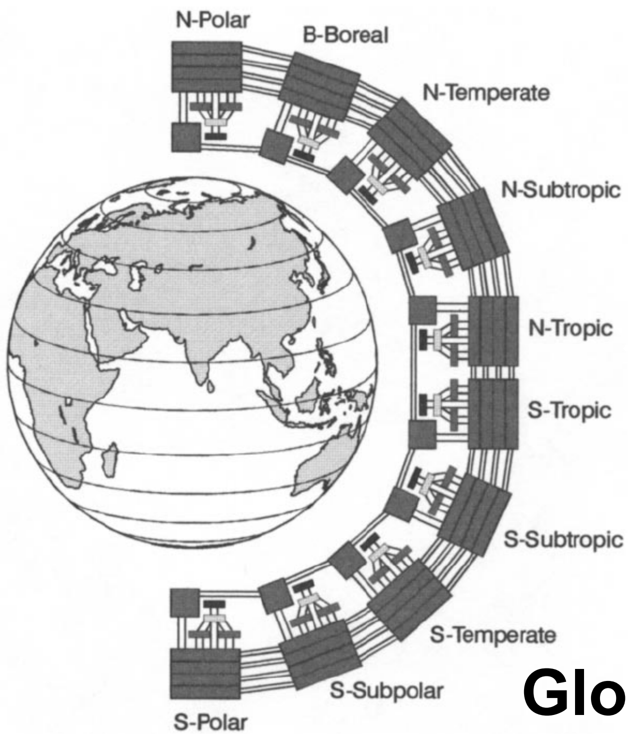


Global Box Models

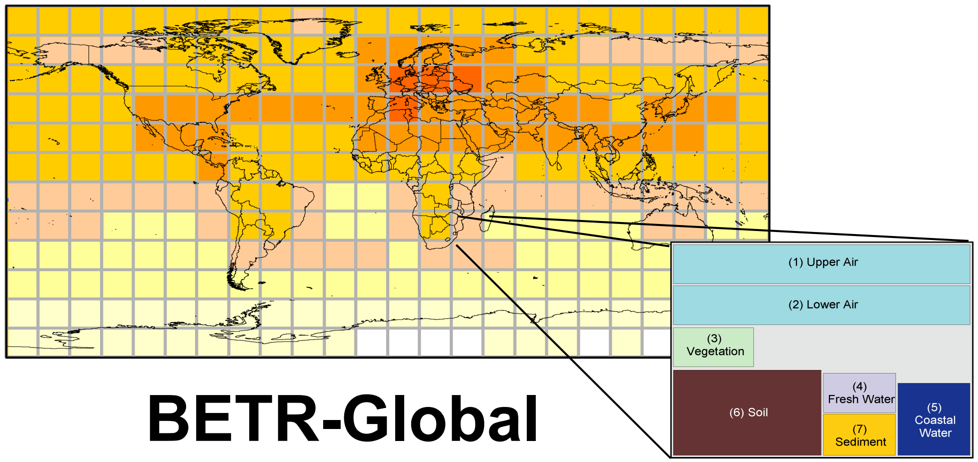
- ✦ Globo-POP (Wania, Mackay 1995)
- ✦ CliMoChem (Scheringer et al. 2000)
- ✦ BETR-Global (MacLeod et al. 2005)



CliMoChem



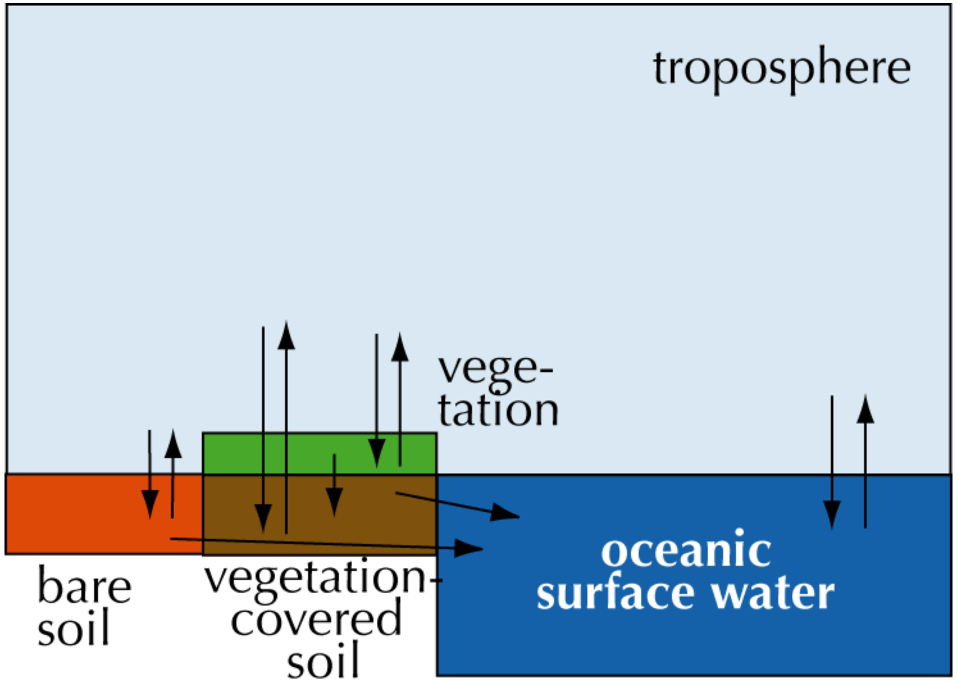
Globo-POP



BETR-Global

General Approach: Mass Balances

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



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

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

F_{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

k_s

Parameter Requirements (I)

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- Problems:
  - **Variability** and uncertainty

T

distribution of values?

OC $\rightarrow$ $\{k_s^1, \ldots k_s^n\}$

humidity

mechanisms?

??

see: Fenner, K., Lanz, V., Scheringer, M., Borsuk, M. *Environ. Sci. Technol.* **41** (2007), 2840–2846

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OC

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??

$\{k_s^1, \ldots k_s^n\}$

mechanisms?

K_{ow}

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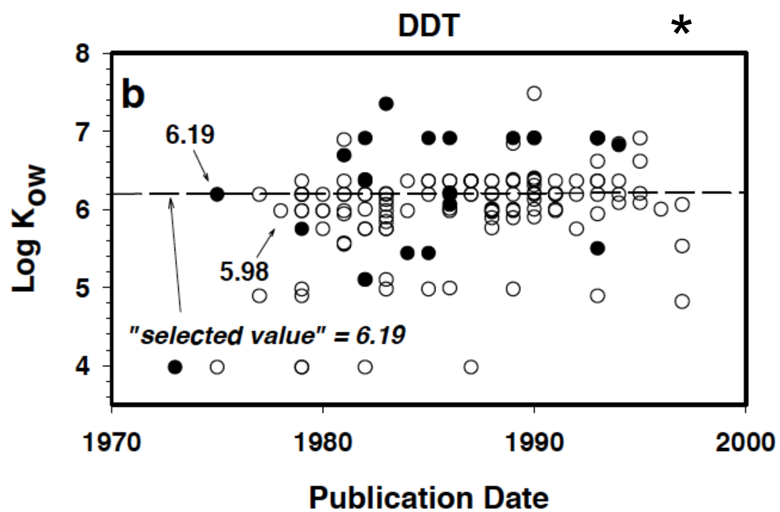
T, OC, humidity, ?? → $\{k_s^1, \ldots k_s^n\}$

distribution of values?

mechanisms?

K_{ow}

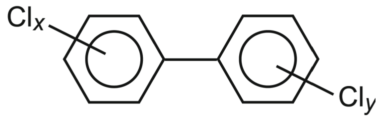


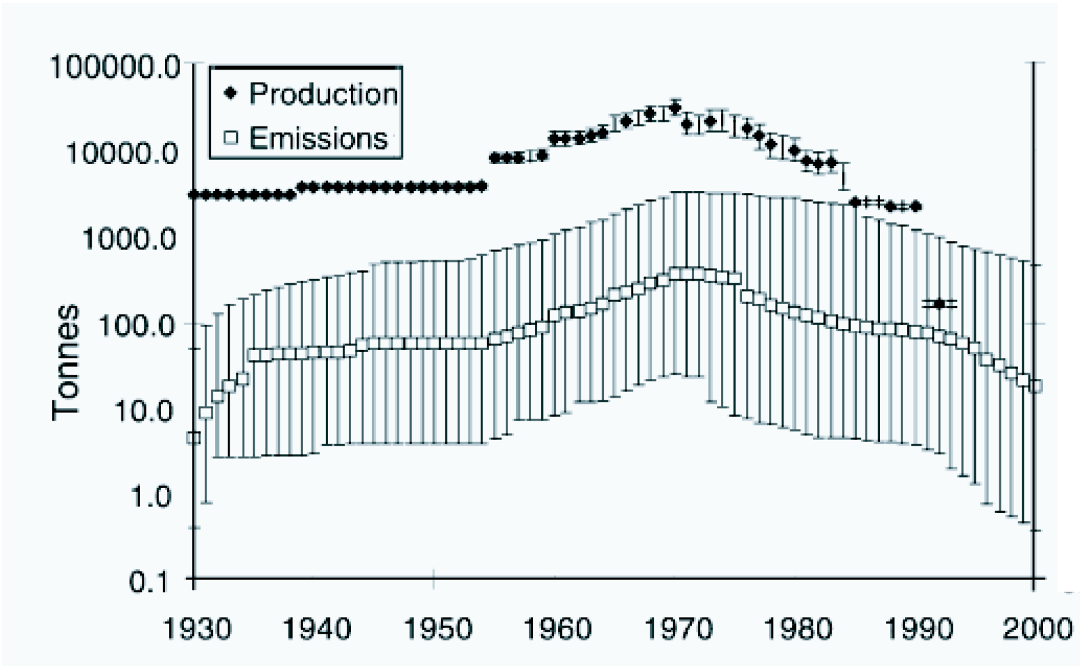
accuracy?

* from: J. Pontolillo, R. Eganhouse, USGS Report 01-4201 (2001)

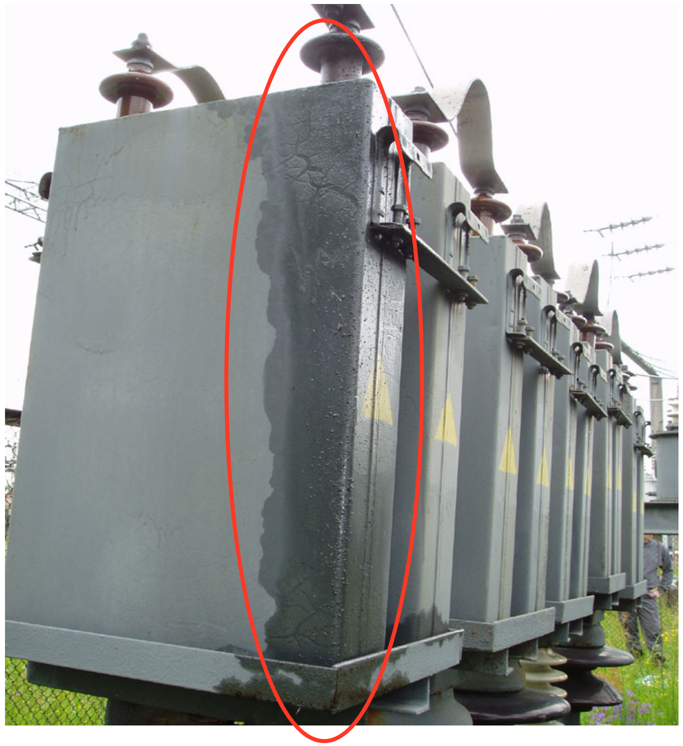
Parameter Requirements: Emissions (I)

- Emission data: spatially and temporally resolved list of amounts of chemical released to the environment
- Example: PCBs





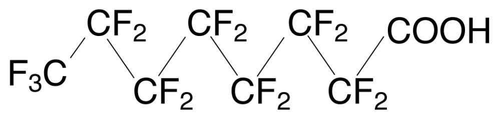
K. Breivik et al., *Sci Total Environ* **290** (2002) 199–224

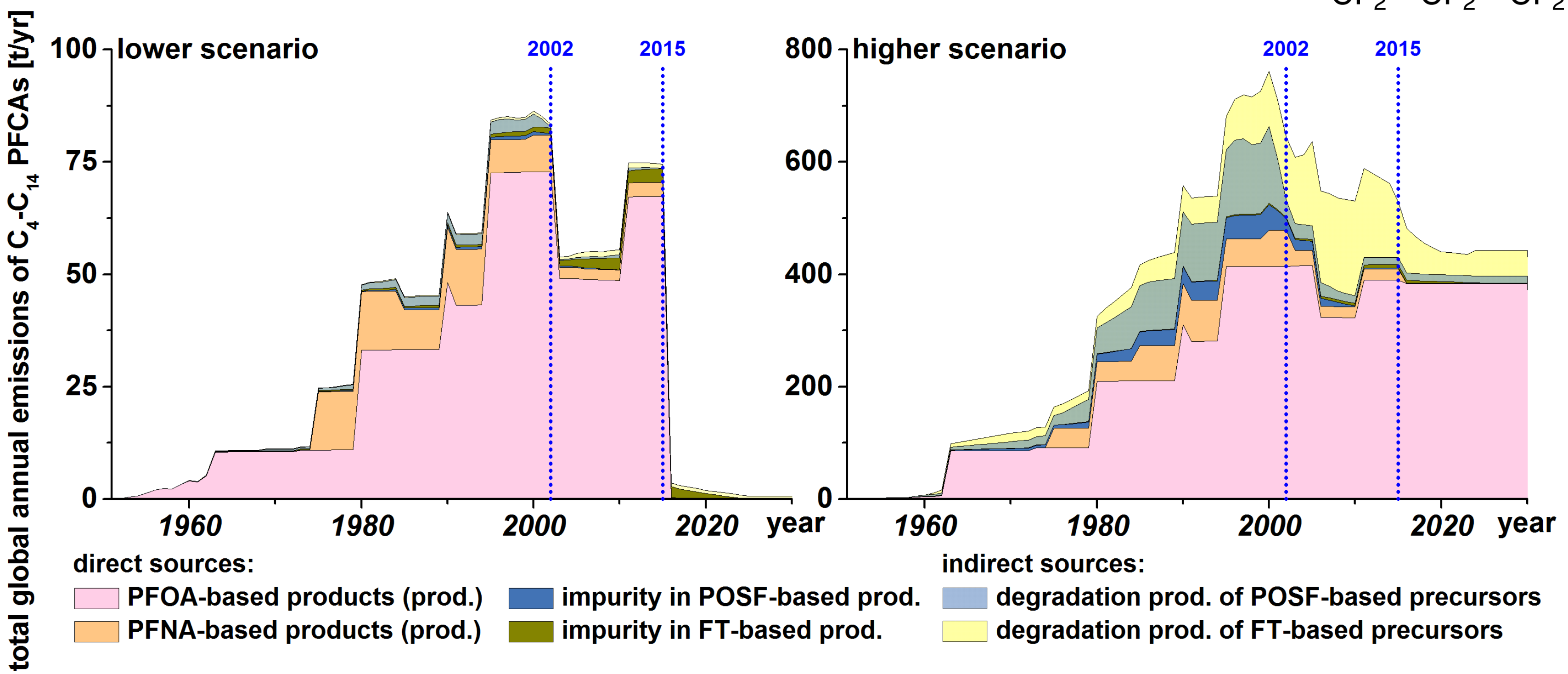


source:
Palina Tsytsik, Tamara Kukharchyk, Belarus

Parameter Requirements: Emissions (II)

- Emissions peak only after 2000 (30 years after PCBs)
- Decrease after 2015: 6oovoptimistic estimate



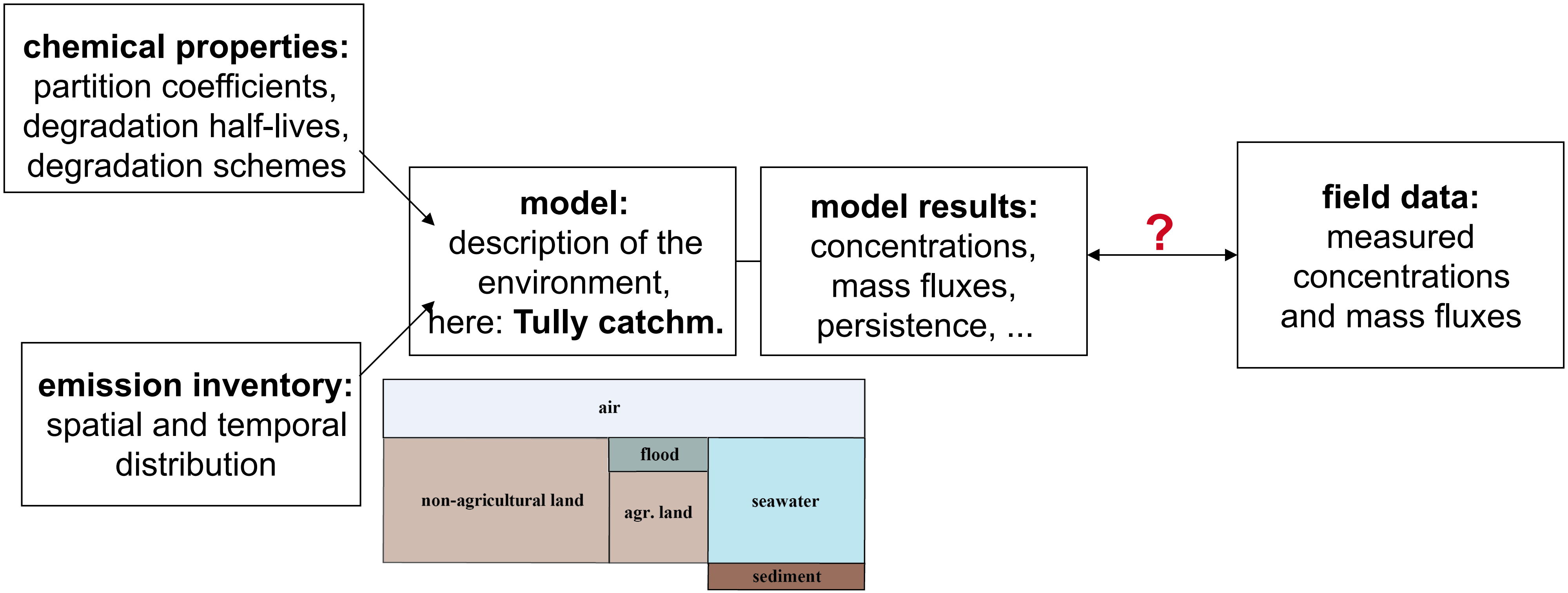


Z. Wang et al., *Environment International* 70 (2014), 62–75
Z. Wang et al., *Environment International* 69 (2014), 166–176

Environmental Fate Calculations with Box Models Regional Scale – Diuron in Queensland

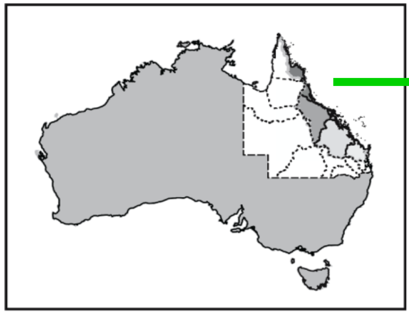
Environmental Fate Models as an "Integrative Platform"

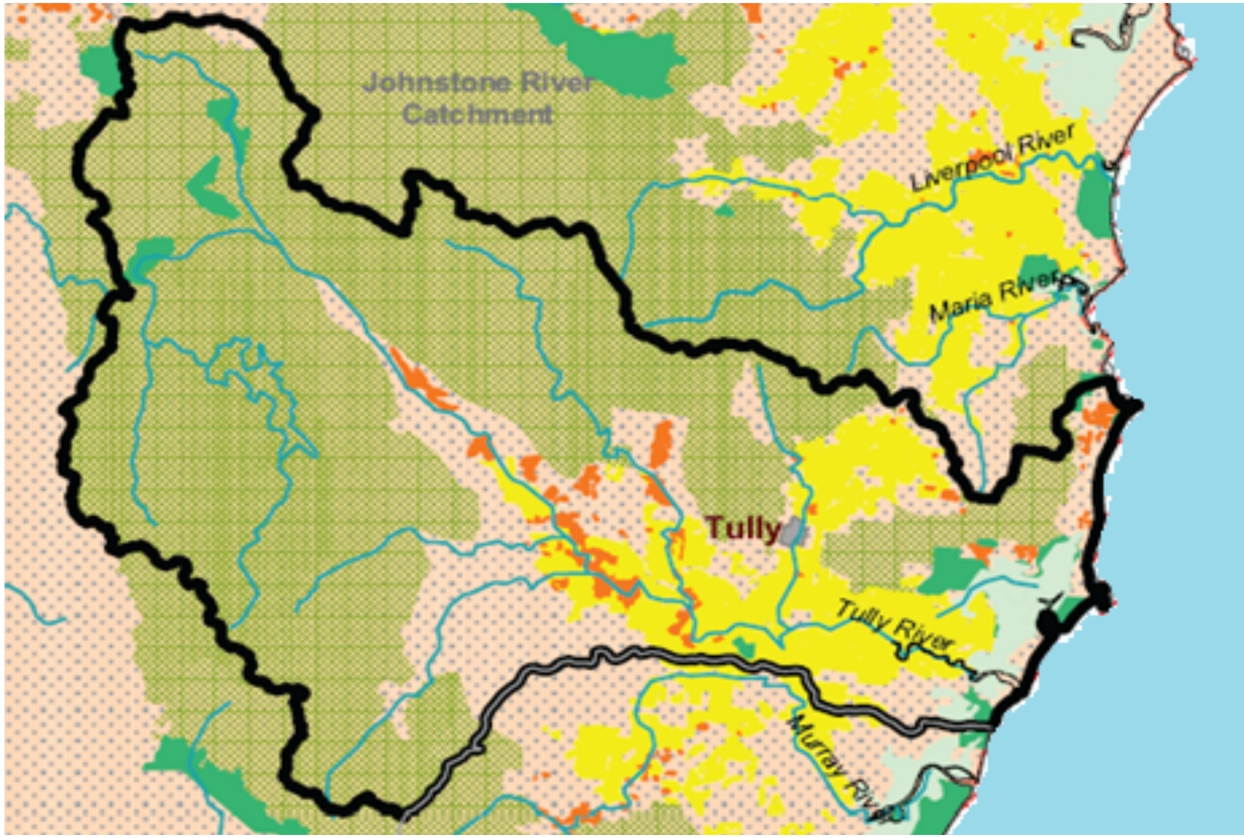
- Four main components:



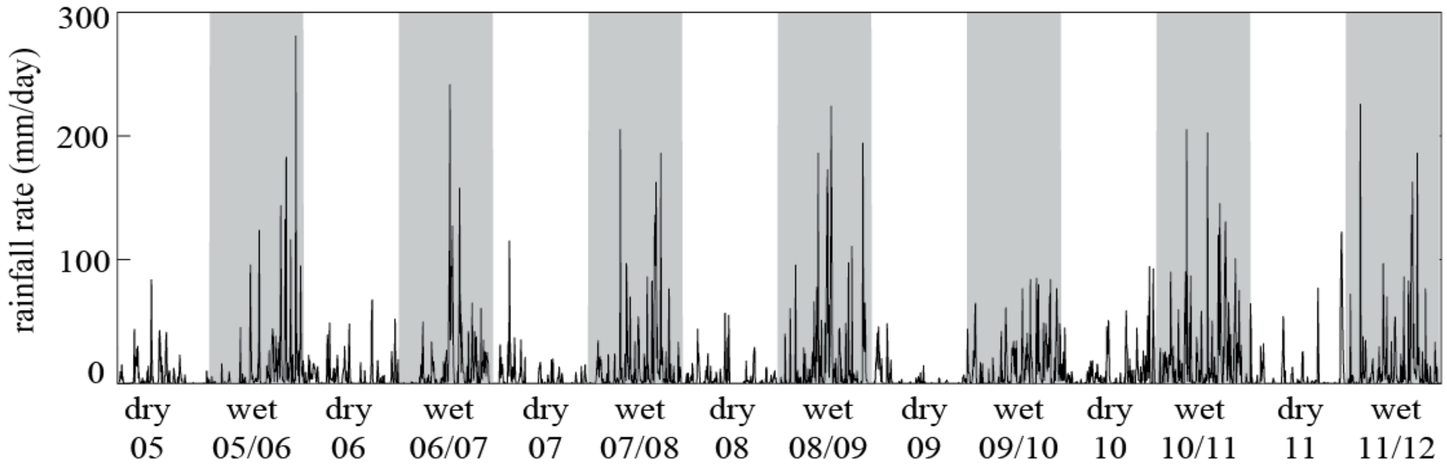
A Less Persistent Chemical in a Small Region

The Tully River Catchment, Queensland



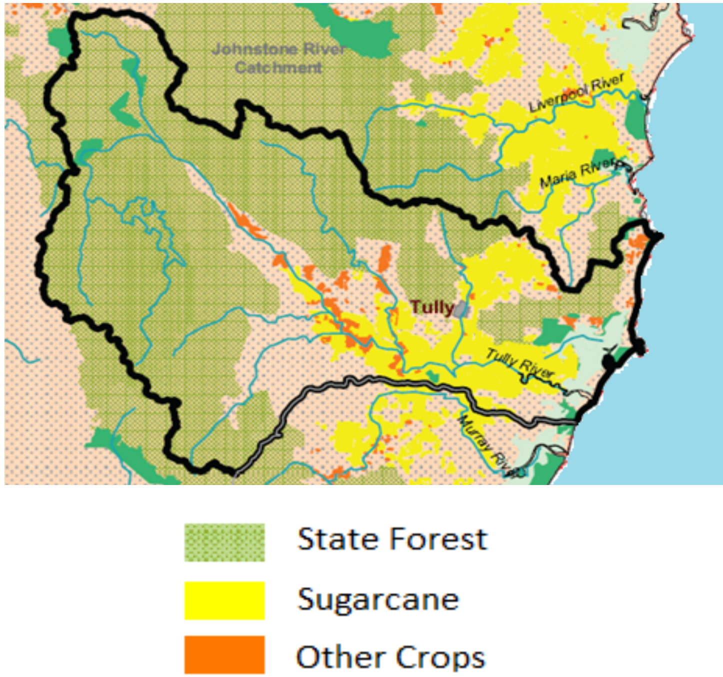


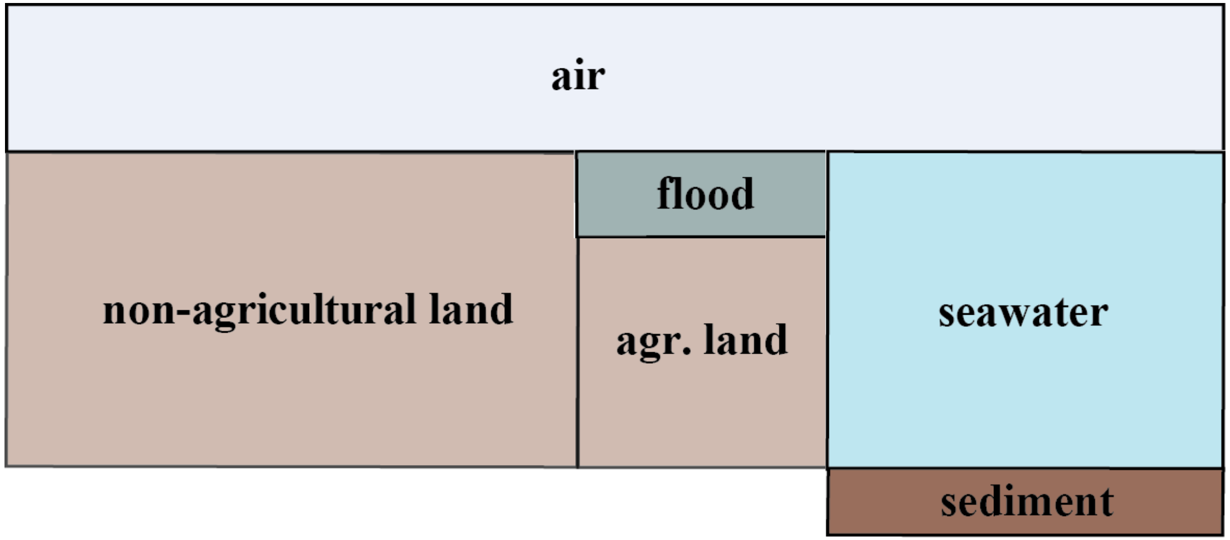
Very Wet and Highly Dynamic



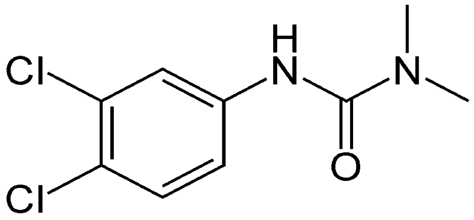
Australian Bureau of Meteorology

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),

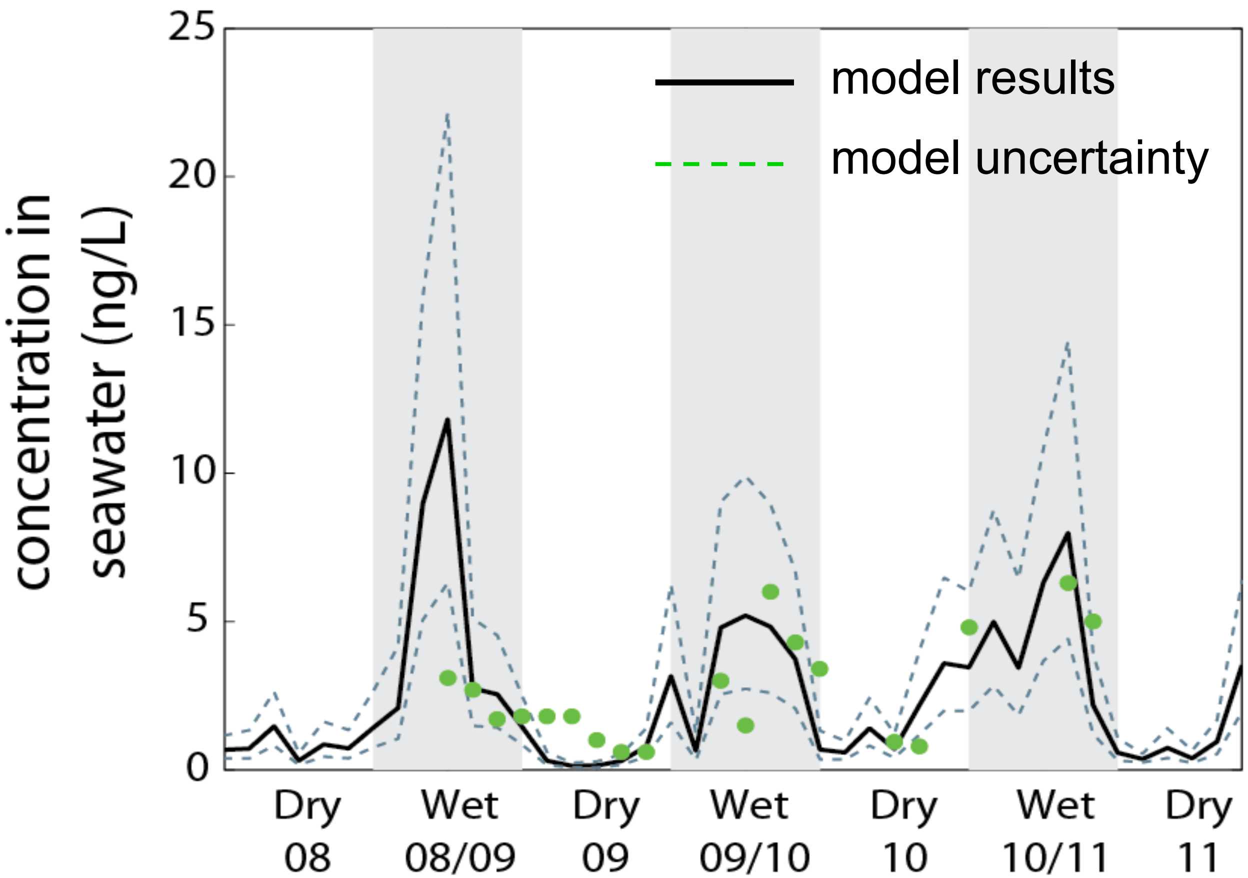
221 d (soil)

log K_{ow} = 2.7

log K_{aw} = –7

Diuron Concentration in Seawater

Modeled and measured monthly-averaged diuron concentrations

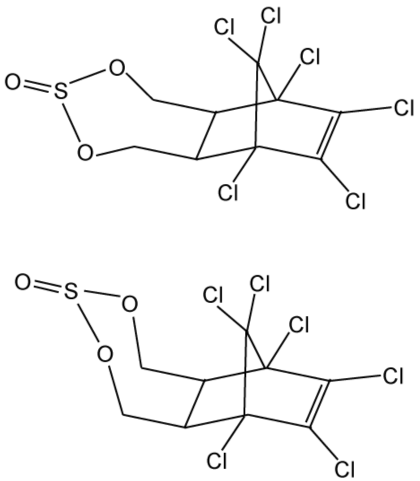


L. Camenzuli, M. Scheringer et al. (2012)
Sci. Total Environ. 440 (2012), 178–185

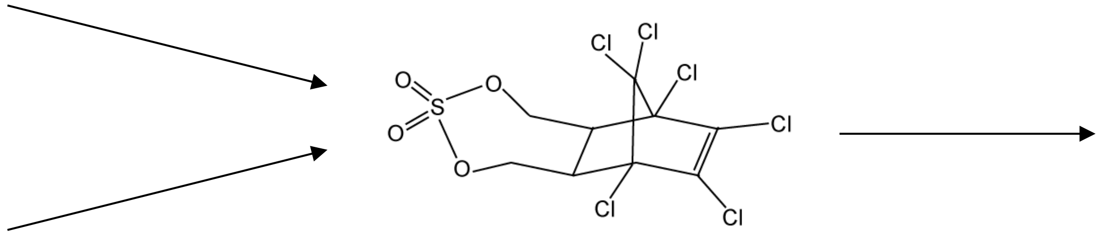
Environmental Fate Calculations with Box Models
Global Scale – Endosulfan in the Arctic

Endosulfan: Two Isomers, One TP*

- Endosulfan: insecticide, since 1950s, global pollutant



α- and β-endosulfan,
released at ratio of 7:3,
10% to air, 90% to soil



endosulfan
sulfate

minerali-
zation

* TP: transformation
product

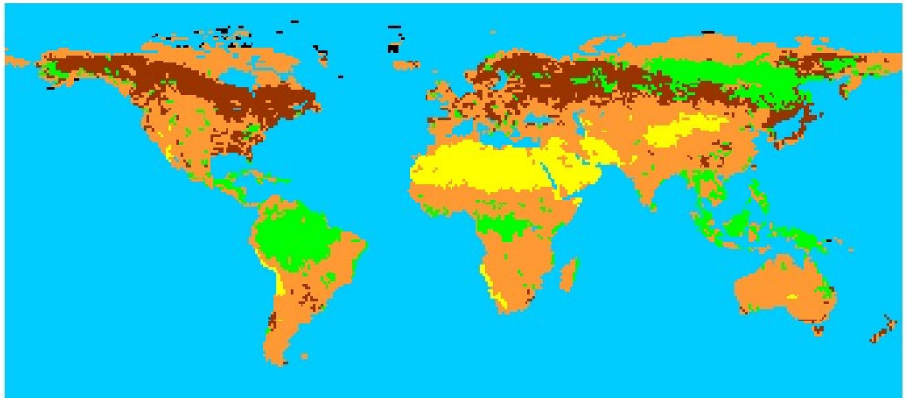
L. Becker, M. Scheringer, U. Schenker, K. Hungerbühler,
Environ. Pollut. **159**, 1737–1743 (2011)

MUNI | RECETOX

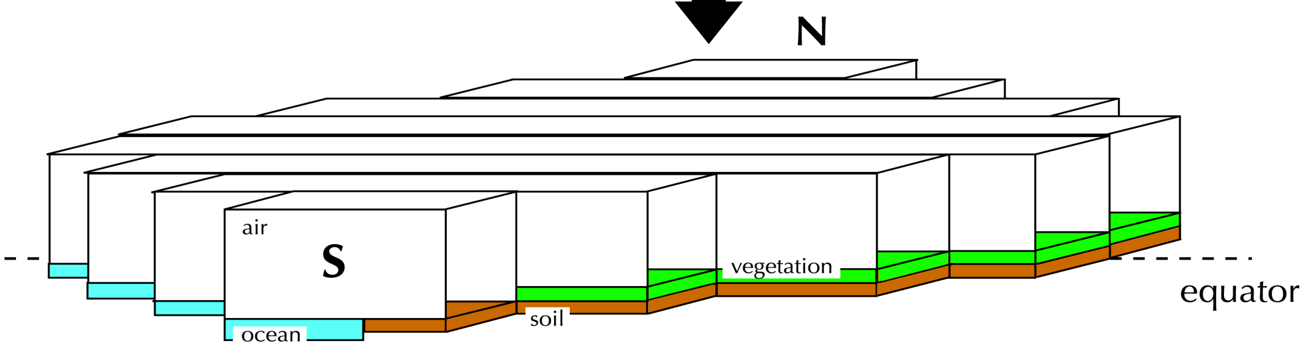
Global Model “CliMoChem”

- 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

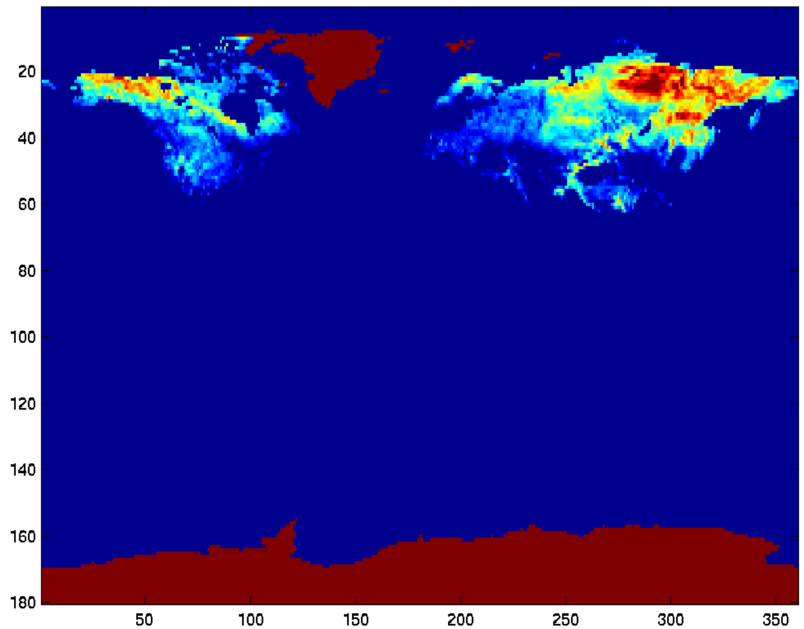


Scheringer, M., Wegmann, F., Fenner, K., Hungerbühler, K.
Environ. Sci. Technol. 34 (2000), 1842–1850

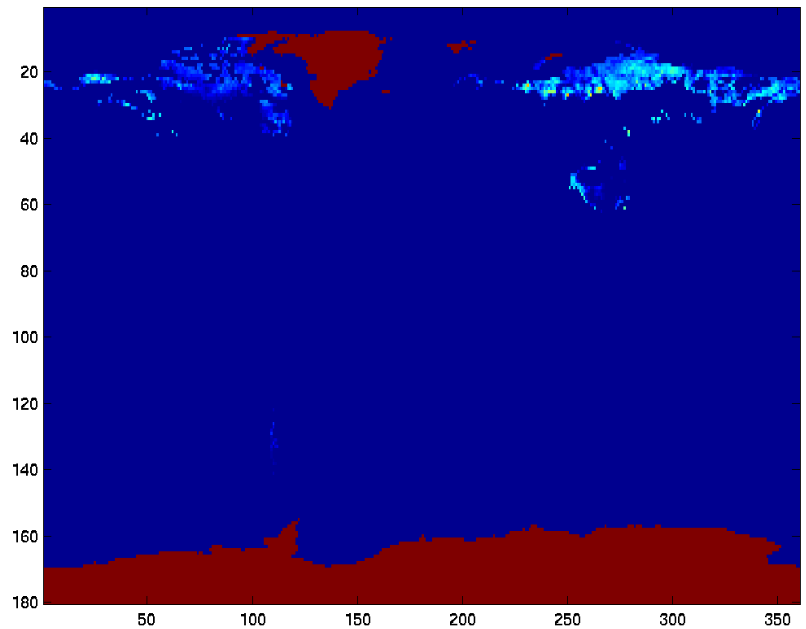
Data for CliMoChem: Ice and Snow

- Snow depth from NASA EOS data

January



June



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

MUNI | RECETOX

J. Stocker, M. Scheringer, F. Wegmann, K. Hungerbühler
Environ. Sci. Technol. 41 (2007), 6192–6198

Model Inputs: Chemical Property Data

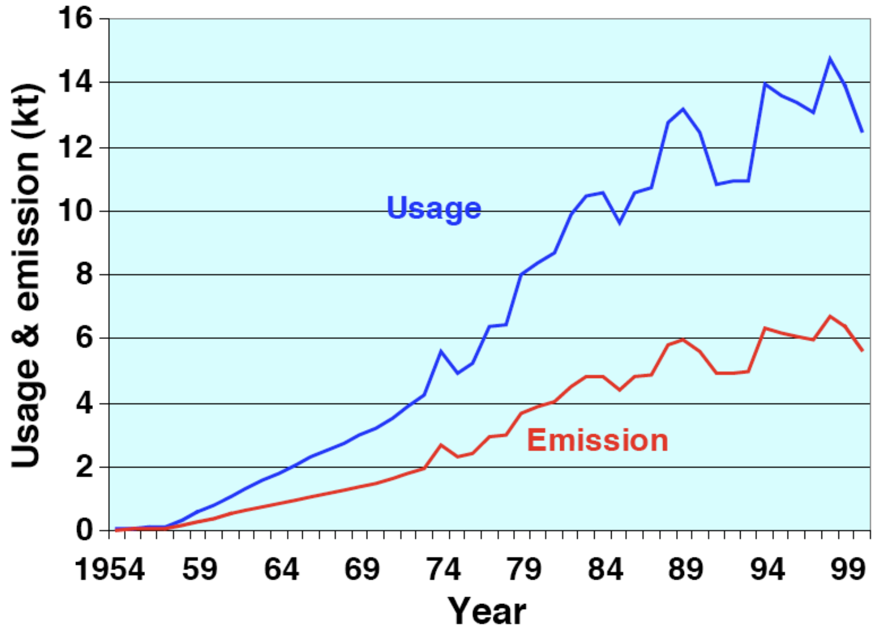
- Partition coefficients and degradation half-lives (days)

	α-endosulfan	β-endosulfan	endosulfan sulfate
log K_{ow}	4.93	4.78	3.71
log K_{aw}	–3.56	–4.75	–4.78
$t_{1/2,\ air}$	6; 10; 18	4.4; 8; 13	4; 7; 12
$t_{1/2,\ water}$	12.6; 22; 38	17.4; 30; 52	58; 100; 173
$t_{1/2,\ soil}$	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):[1]

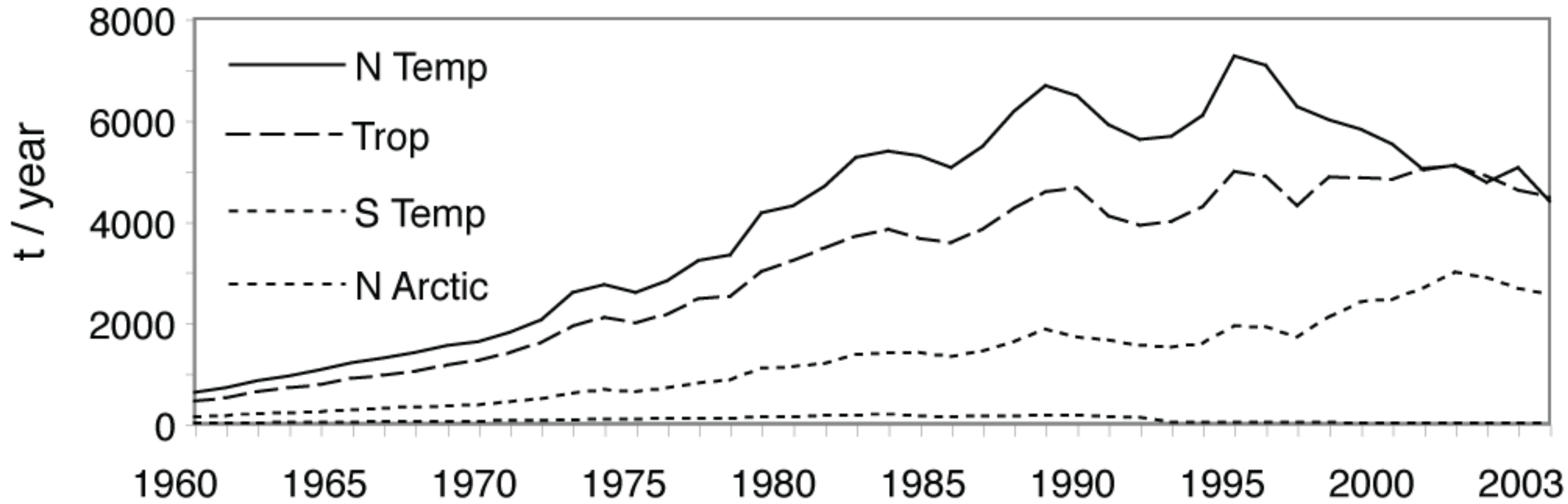


- Total historical usage (here assumed to be released): about 300 000 t

1: Li and Macdonald, Sci. Total Environ. 342 (2005), 87–106

Model Inputs: Emission Data (II)

- Contributions of latitudinal zones:[1]
  - areas of crops under endosulfan treatment:
    cocoa, coffee, cotton, fruits, soy, tea, vegetables
- Model input:



1: data from FAO; Bayer Crop Sciences

Model Inputs: Emission Data (II)

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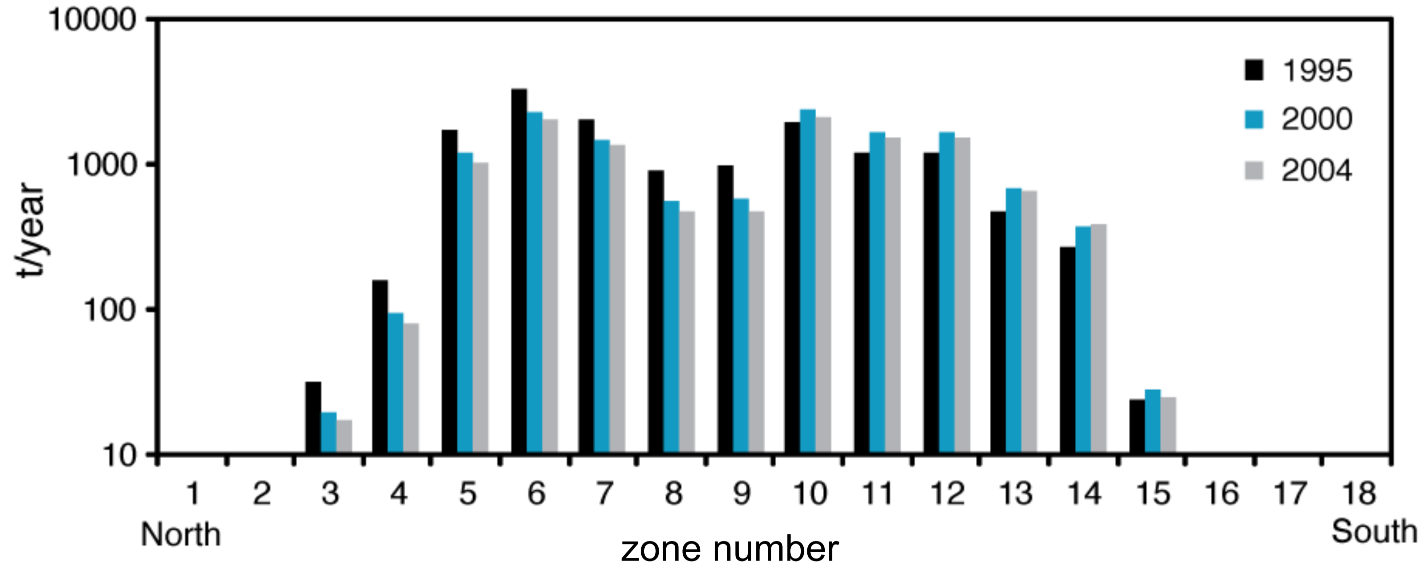
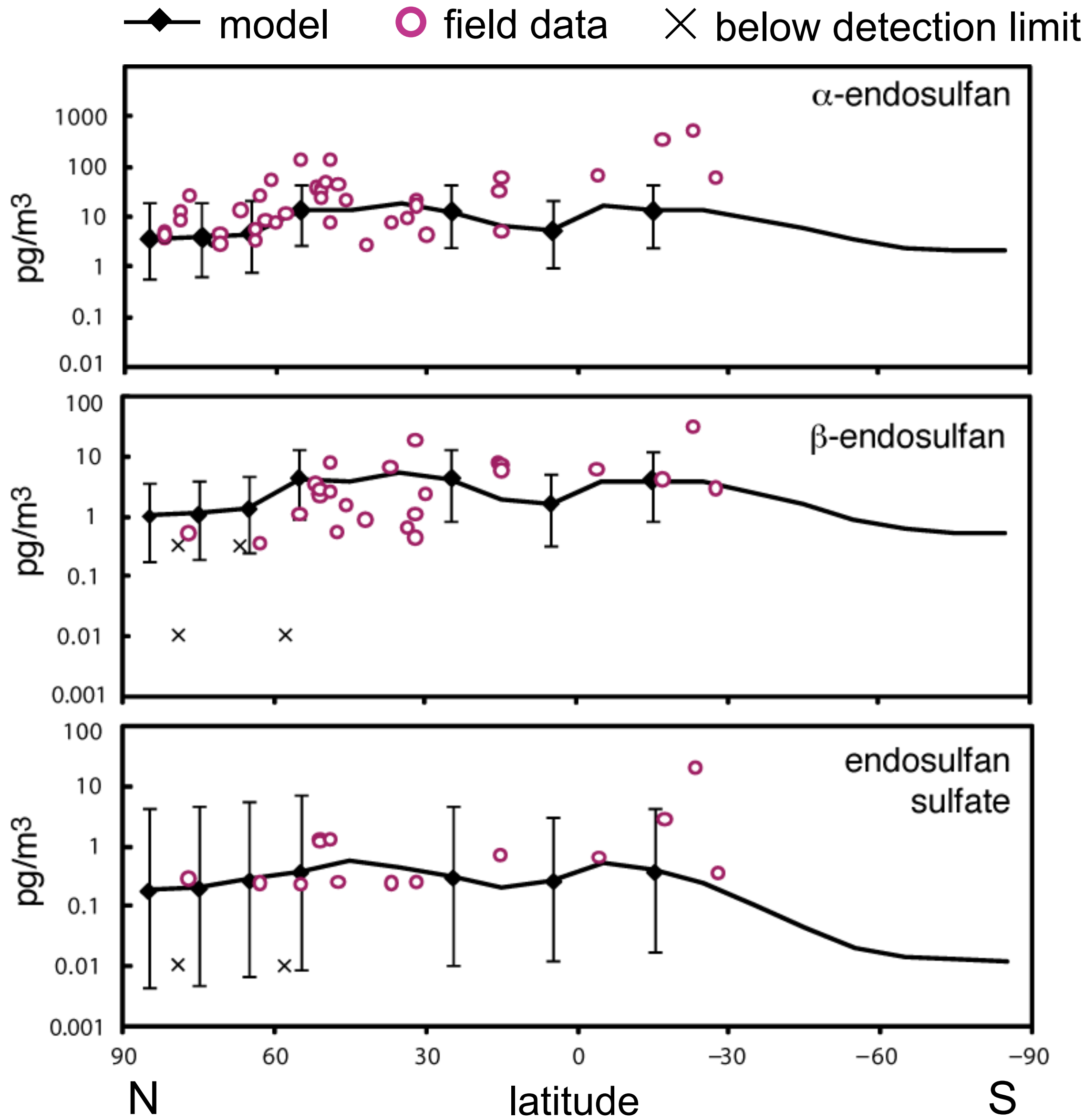


1: data from FAO; Bayer Crop Sciences

Results: Concentrations in Air

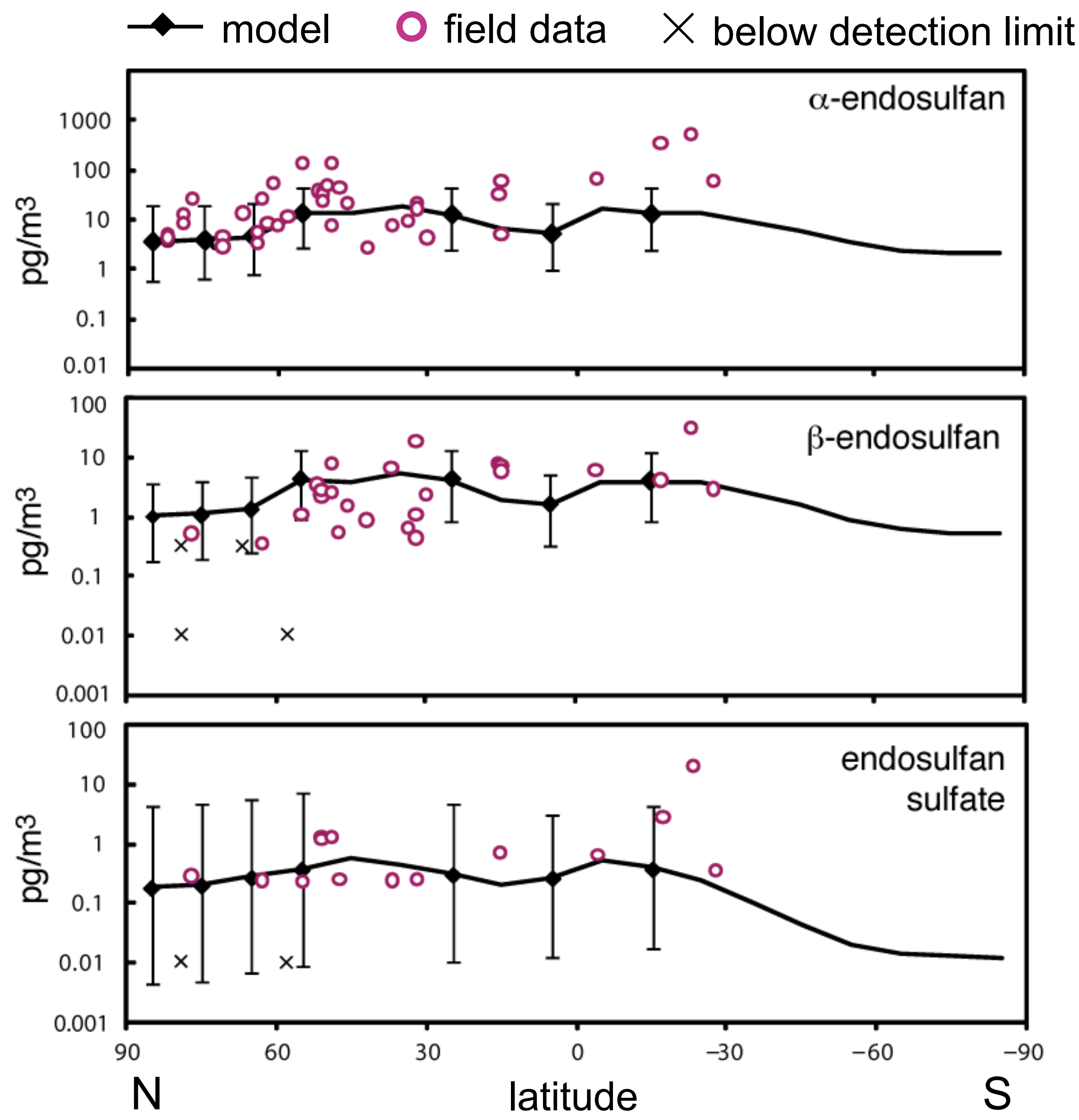
- Agreement?



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

Results: Concentrations in Air

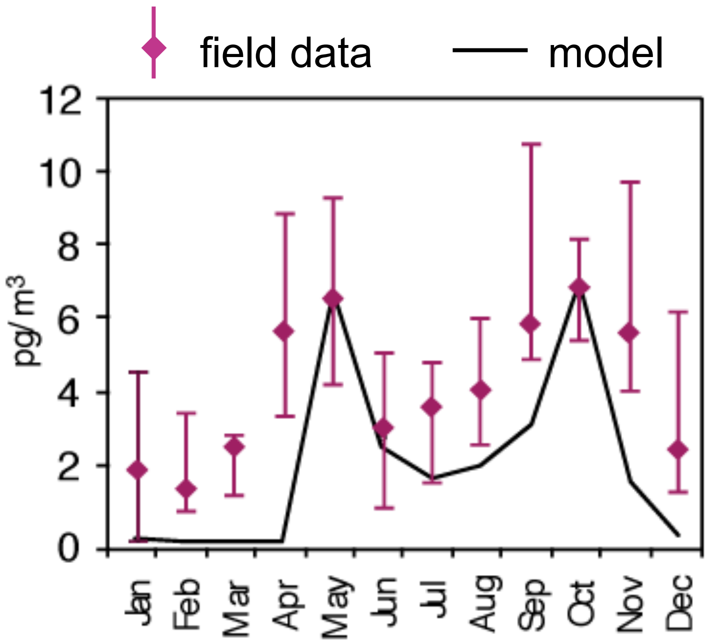
- ✦ Good agreement for all three substances:
  - ➡ latitudinal trend: ok
  - ➡ $\alpha > \beta >$ sulfate: ok



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

Results: Time Trends in the Arctic

- concentrations of α-endosulfan in Arctic air
  - maximum in spring and fall
  - why?

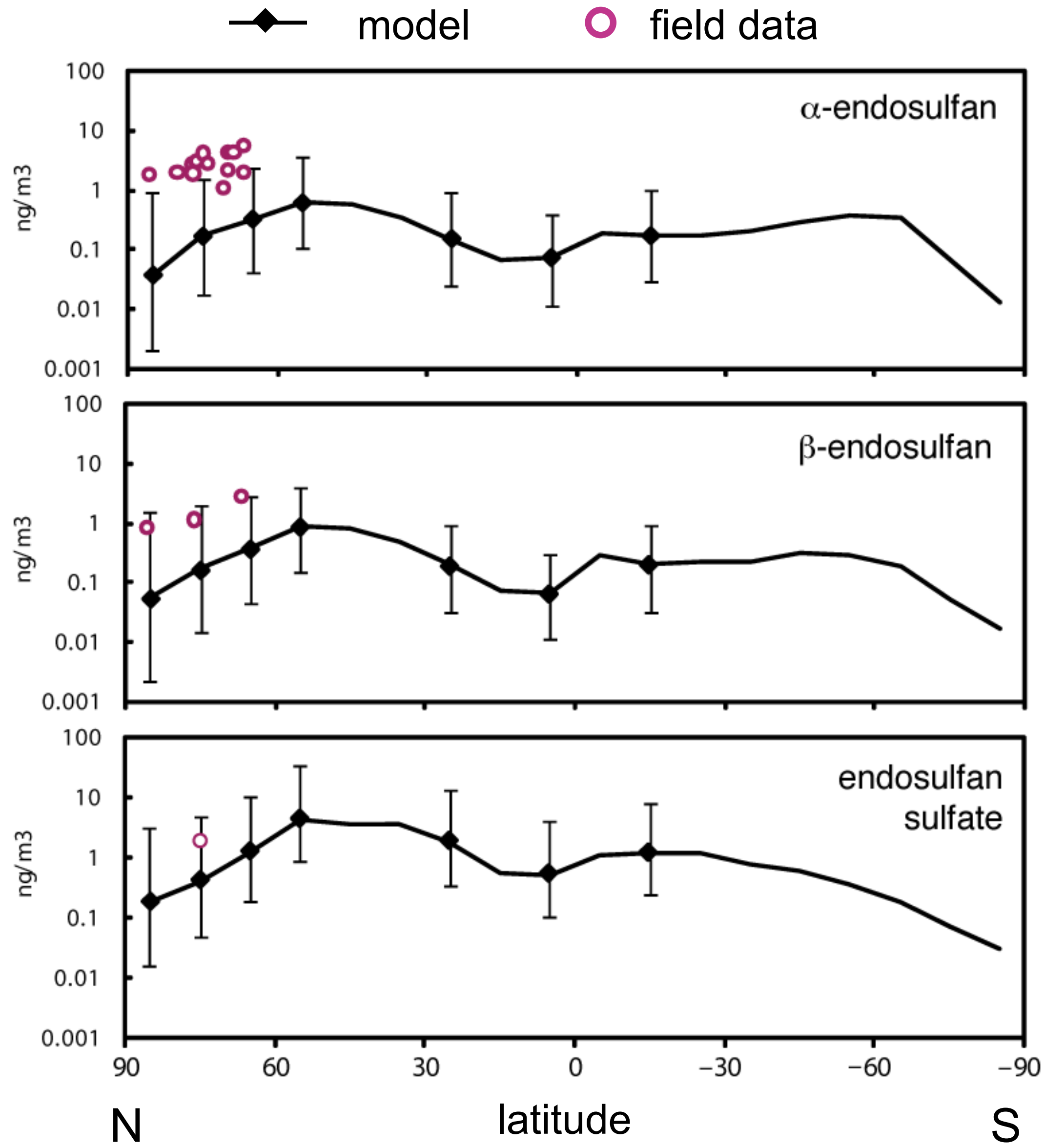


field data for Alert (82°N) from
H. Hung, Environment Canada

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

Results: Concentrations in Ocean Water

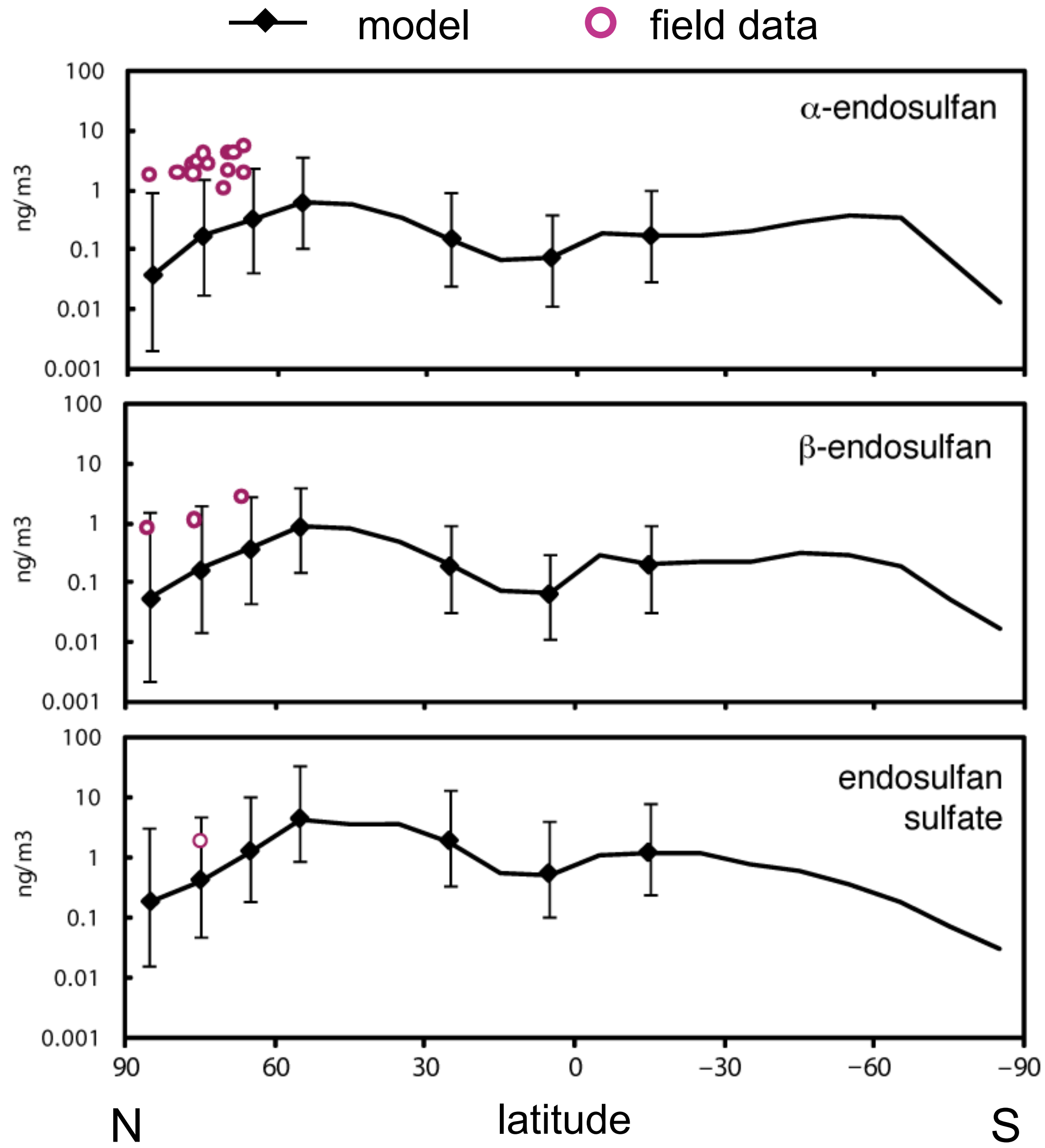
- field data only north of 65° N
- sulfate > $\alpha \approx \beta$: ok



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

Results: Concentrations in Ocean Water

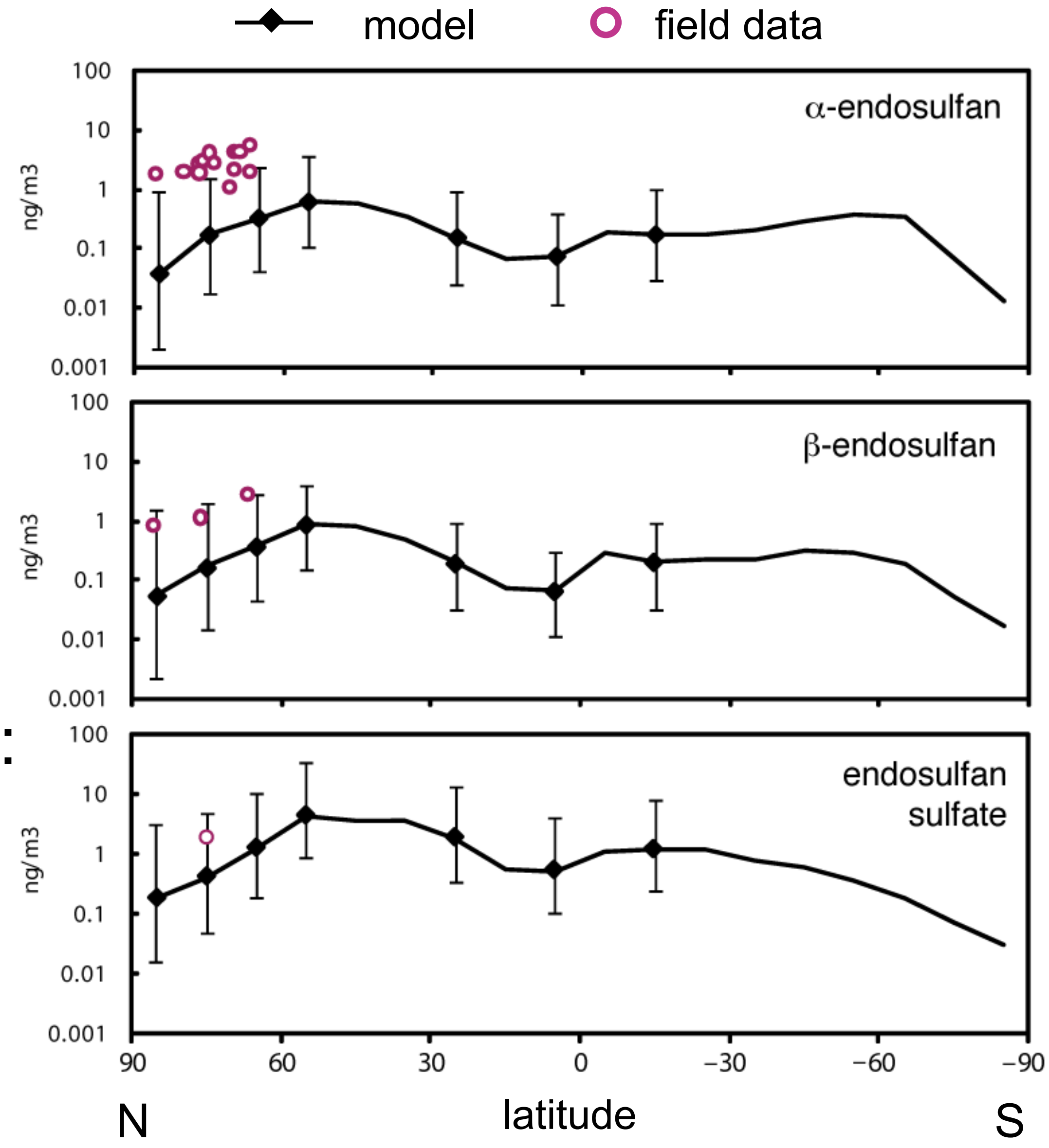
- field data only north of 65° N
- sulfate > α ≈ β: ok
- all three substances: model by factor 10 too low



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

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



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

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:			
α-endosulfan	57%	40%	2.5%
β-endosulfan	66%	33%	1%
endosulfan sulfate	65%	34%	1%

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

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

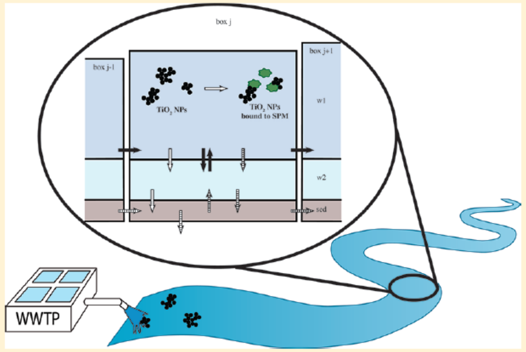
Development of Environmental Fate Models for Engineered Nanoparticles—A Case Study of TiO_2 Nanoparticles in the Rhine River

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 TiO_2 NPs in the Rhine River is investigated. Predicted 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 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 TiO_2 NPs and SPM, characterized by the attachment efficiency, $\alpha_{het\text{-}agg}$, on the transport potential of ENPs in a surface water system.



Environ. Sci. Technol. **46** (2012), 6705–6713, dx.doi.org/10.1021/es204530n

Conclusions

- Multi-compartment models highly flexible
- 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 persistant substances that are often of greatest toxicological concern.

... to 2010

M. MacLeod et al., *Environ. Sci. Technol*. **44**, 2010, 8360–8364

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

Environmental Science & Technology feature

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

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THOMAS E. MCKONE
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KONRAD HUNGERBUHLER
ETH Zurich, Switzerland

Are multimedia models dinosaurs in the modern world?

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 (LRTP) 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

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CRITICAL REVIEW

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Cite this: DOI: 10.1039/c7em00568g

Environmental fate and exposure models: advances and challenges in 21st century chemical risk assessment

Antonio Di Guardo,[a] Todd Gouin,[b] Matthew MacLeod[c] and Martin Scheringer*[de]

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

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

Integrated Environmental Assessment and Management — Volume xxx, Number xxx—pp. xxx–xxx
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Good Modeling Practice Guidelines for Applying Multimedia Models in Chemical Assessments

Andreas M Buser,† Matthew MacLeod,‡ Martin Scheringer,† Don Mackay,§ Mark Bonnell,|| Mark H Russell,# Joseph V DePinto,†† and Konrad Hungerbühler†*

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‡Department of Applied Environmental Science, Stockholm University, SE 106 91 Stockholm, Sweden
§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

Environmental Management

INTRODUCTION

Multimedia mass balance models have been used to

output data, and 4) interpretation of model results. The results of multimedia modeling enable evaluation of human