Appendix 4: Proceedings of expert work-shop, 16 August 2005, EEA, Copenhagen

Contents

A4.1 Executive summary 1
A4.2 Introduction 2
A4.3 Summary of workshop discussions 3
A4.3.1 Is the 'toolbox' of models reviewed by the consultants complete? 4
A4.3.2 Feedback on the proposed strategy 4
A4.3.3 General discussion 6
A4.4 Workshop agenda 8
A4.5 Workshop delegates 9
A4.6 Workshop presentations 10

A4.1 Executive summary

This appendix provides copies of the expert presentations and a summary of the discussions that were used to inform revisions of the final report, contained in main report. To focus the discussions, delegates were asked to consider the following key issues as a framework for their deliberations:

1. Is the 'toolbox' of models reviewed by the consultants complete?
   Are the models adequately described?
   Which additional models are in use?
2. Feedback on the proposed strategy
   Is the approach realistic?
   What alternative approaches should be considered?
   What further recommendations are there?

The following key conclusions are drawn from the workshop discussions:

1. The consultant's report has included a comprehensive selection of appropriate models. The evaluation of the models reported in phase 1 of the feasibility study has been appropriate for the intended purposes of the work.
2. The staged approach underpinning the consultant's proposed strategy for the development of the work, based upon EUSES for screening to identify circumstances where more detailed modelling is required, is judged to be correct.
3. The study has shown that data on chemical releases available in EPER, along with other chemical properties, meteorological and geophysical data in publicly accessible sources can be used with the EUSES model to predict environmental concentrations of chemicals in various media on the regional, continental and global scales and so help to identify releases for which further detailed modelling is required.
4. For the impact of emissions on concentrations in the environment local to the emission source, information on the local dispersion following release has a major impact on the predicted local concentrations. This information (which includes details of stack height, plume buoyancy, dilution rates into water etc) is not generally accessible without detailed information from the facility operators. The use of default values for these parameters in EUSES results in unduly conservative predictions (at least for releases to air).
5. It is concluded that it is not possible to accurately model local environmental concentrations resulting from EPER emissions sources using publicly available input

data only: detailed release data would be required too and this is only available from the facility operators.

6. The strategy proposed an approach by which operators could be prompted to provide local concentration data on a voluntary basis through the publication of local screening predictions on a website, consultation and through seeking information from Integrated Pollution Prevention and Control (IPPC) permit applications held on the public record. The feedback received at the workshop indicates that this matter is likely to prove highly contentious with industry and local regulators. Further consideration of whether and how the EEA should seek to provide information on local concentrations of chemicals resulting from point source emissions requires further detailed consideration that is outside the scope of this feasibility study. Workshop participants suggested that all available European information sources, including existing substances risk assessment reports, should be used. Pilot studies should be undertaken to provide a more detailed assessment, based on selected regions where the national and local authorities are prepared to share information.
7. With the exception of that part of the part of the strategy concerned with the publication of screening modelling results on a public website to stimulate industry to provide estimates of local concentrations where detailed modelling cannot be undertaken due to the absence of discharge information, delegates endorsed the approach and strategy proposed in the consultant's draft final report.
8. A number of issues were raised for consideration in any follow up work and for possible inclusion in the revised final report of the feasibility study.

A4.2 Introduction

This document contains the presentations and summary of discussions at a workshop hosted by the European Environment Agency (EEA), Copenhagen, on 16th August 2005. The purpose of the workshop was to review the draft final report of a study contract undertaken for the EEA by AEA Technology Environment (UK), in association with RECETOX-TOCOEN (CR), entitled 'Feasibility study: Modelling environmental concentrations of chemicals from emission data'. The draft final project report, which had been reviewed at a summer school [1] on environmental chemistry and ecotoxicology held in Brno, Czech Republic, was circulated in advance to workshop delegates. The final report has been produced to take account of the revisions suggested at both the workshop and summer school. This document is Appendix 4 of the final report. It is presented as the second of the two reports that comprise the final project report. The main report provides full details of the purpose of the work, the methodology, findings and conclusions. It should be referred to for further information on the project.

[1] Centre RECETOX, Masaryk University Brno, Czech Republic, EC DG Research Centre of Excellence for Environmental Chemistry and Ecotoxicology organized the Summer School of Environmental Chemistry and Ecotoxicology - Approaches to the study of relationships between environmental levels of chemicals and their biological effects with special attention to the persistent, toxic substances (9th – 16th July 2005). The summer school focused on experimental methods in environmental chemistry, ecotoxicology, ecological risk assessment, environmental monitoring, the study of exchange processes between environmental compartments, sampling procedures, collection of data for environmental modelling, field study of ecological stressors, focussing on integrated monitoring and modelling for POPs. Collaborating bodies included the European Commission DG Research, EMEP MSC East, Czech Ministry of Environment and Czech Hydrometeorological Institute with co-operation with international scientific association such as the SETAC (Society for Environmental Toxicology and Chemistry), the FECS (Federation of European Chemical Societies), Division of Environmental Chemistry and the SECOTOX (Society for Ecotoxicology and Environmental Safety). The lectures were given by leading scientists in the field of POPs. The summer school was organized as a contribution to the 25th Anniversary of the UNECE Convention on Long-range Transport of Air Pollution. http://recetox.chemi.muni.cz/coe/index.php?id=71.

Some 35 delegates drawn from the EEA's National Focal Point organisations in environmental policymaking and regulation, scientists and other experts attended the workshop.

Table 1 shows the workshop agenda. Professor Jacqueline McGlade, Executive Director of EEA, welcomed the participants and outlined the interests of the EEA in modelling and the different role the agency has in the field of chemicals as compared to other institutions such as the Commission, especially Eurostat, the JRC and the future Chemicals Agency. The focus of EEA is not on the risk assessment of single compounds, but on integrated assessments to identify fate and impacts of chemicals after they enter the environment and start circulating through ecosystems, whether they are accumulating as cocktails in water bodies, sediments or biota, or as single substances of concern. Professor McGlade referred to ongoing dialogue and discussions about targets for information flows and data interpretation amongst the EEA, the Commission, Eurostat and JRC, which is taking the lead in the area of chemicals. She invited the workshop participants to provide the EEA at, and potentially beyond, this meeting with focussed advice on how to use available models and ongoing research activities to support the EEA's integrated assessments.

Dr Gabriele Schöning (Chemicals project manager at the EEA) then presented the aims and overview of the study. This was followed by a presentation on the draft final project report by members of the consultant's team: Dr Keith Brown (the project manager) gave an overview of the project and the findings from the model evaluation undertaken in phase 1 of the work. Mr John Abbott then described the assessment of EUSES for modelling point sources and the strategic approach developed by the feasibility study. Professor Holoubek provided a summary of feedback on the draft final report from the Brno summer school. Presentations by leading experts were made on the role and requirements for detailed modelling (Dr Sergey Dutchak, MSC-E), research perspectives on modelling strategies (Dr Martin Scheringer, ETH, Zurich) and regulatory perspective on modelling strategies (Dr Jose Tarazona, INIA, Spain). Copies of the workshop presentations are given in Section A4.6 in this document. The following sections summarise the key points from the discussion sessions at the workshop.

A4.3 Summary of workshop discussions

Delegates were asked to consider the following key issues as a framework for their discussions:

1. Is the 'toolbox' of models reviewed by the consultants complete?
   Are the models adequately described?
   Which additional models are in use?
2. Feedback on the proposed strategy
   Is the approach realistic?
   What alternative approaches should be considered?
   What further recommendations are there?

These two main issues relate to phases 1 and 2 of the work described in the consultant's draft final report, circulated to delegates prior to the workshop and summarised in the consultants' presentation (by Keith Brown and John Abbott). In addition, a number of other issues were raised. The key points from the discussion are summarised below.

A4.3.1 Is the 'toolbox' of models reviewed by the consultants complete?

The overall impression from the delegates' discussions was that the project had succeeded in presenting a comprehensive selection of relevant and up-to-date models dealing with atmospheric dispersion and chemistry, surface water, sewage treatment and multimedia. A handful of potentially useful models that had not been included (including updates of existing models completed since the work under phase 1 of the study was completed) were also identified, and a number of delegates kindly offered to provide further details to the consultants so that any gaps could be filled in the final report. In addition, it was generally felt that the models had been appropriately and comprehensively reviewed.

A4.3.2 Feedback on the proposed strategy

There was a great deal of discussion on the strategy proposed by the consultants. This strategy in essence consists of the following key steps:

1. Use of EUSES with default input data to characterise releases and receiving environment to generate estimates of concentrations in environmental media, based on EPER emissions data. This would generate conservative estimates of environmental concentrations.
2. Substances where the predicted environmental concentrations derived from the first stage were above desired thresholds or other relevant criteria for the substance in question would be re-analysed using refined input data for EUSES (particularly to characterise local discharge characteristics). This information would be made publicly available on an internet site.
3. Industry may provide alternative information from measurement or modelling (for example, as used to support IPPC permit applications) to provide a more accurate figure for local concentrations to the conservative estimates generated by EUSES. Alternatively, the strategy considered the possibility of seeking this information from the public records, but the practicality of this is questionable. EPER does not currently contain the detailed information needed for local concentrations to be calculated accurately and so modelling at this scale can only be undertaken by those with access to this key input data – in other words, by installation operators, regulators or their agents.
4. On the regional or wider scale (continental, hemispheric or indeed global), operators will not usually have information on the concentrations produced by their emissions and at these scales the concentrations are much less dependent on the characteristics of the initial discharge. Detailed modelling at this scale (where the results from EUSES suggests that further investigation is needed) could therefore be undertaken with specialised models that do not require the discharge-specific information of local modelling. The stepwise approach of using EUSES as a screening tool to identify areas for more detailed assessment should allow future modelling activities to be undertaken in a more focused and cost-effective manner.

A number of delegates expressed their agreement with the principle of the staged approach outlined above, which forms the basis of the strategy developed by the consultants, and with the choice of EUSES as the screening tool. Because models of the EUSES/SimpleBox type are driven by air/water and solids/water partition coefficients, rather than by vapour pressures, solubilities and octanol-water partition coefficients (like many of the other multimedia fate models, often referred to as fugacity models), they allow modelling of non-hydrophobic chemicals (e.g. metals) for which intermedia partitioning cannot be easily predicted from the elementary physical-chemical properties.

The approach to providing EUSES with a spatial capability as described in the project report was widely considered to be a useful development. Others regarded it preferable to use spatially explicit models from the start. The JRC informed that they had also tested a specialised spatial EUSES version and were currently developing maps with locally specific environmental parameters on a 1 km² grid.

Delegates largely agreed that the staged approach would be a useful means of identifying chemicals where the concentration may give rise to concerns on the regional+ scale. The distribution of these chemicals could then be explored in detail using specialised models identified in the first phase of the study. Such detailed modelling is a highly complex and specialised task, requiring detailed input information and so the screening approach provides an appropriate way of identifying which substance the more detailed modelling should focus on. Some delegates mentioned the use of a nested modelling approach, following on from the initial stage, in which detailed transport and deposition models may be used to front-end multimedia models. Such an approach has proved useful in the case of modelling POPs distribution.

However, the issue of using the staged approach for local concentration modelling, and especially the publication of the outcome of such analysis was far more contentious. Industry would, it was said, be adamantly opposed to the publication of information on local concentrations due to its emissions listed in EPER if the results appeared to exceed limits agreed with the local regulatory authority. There was concern that this would undermine the regulatory process and lead to unwarranted concern by citizens and NGOs, especially if the predicted concentrations were unrealistically conservative, resulting in additional work for industry in countering claims for adverse local impacts. It was mentioned that NGOs could make these calculations now, based on EPER emissions data already in the public domain, resulting in similar issues arising. However, the extent to which it is appropriate for the EEA to undertake a similar 'blame and shame' role was questioned. Dr Schöning, for the EEA, stated that the Agency had no desire to interfere with local regulatory decisions or to undermine the permitting process.

Other delegates considered that the information should be made public, provided that its reliability and risk context were fully explained. The fact that such information is not readily available now already obstructs environmental research. Some delegates considered that Europe had much to learn from the United States, where local environmental quality data in the vicinity of emission sources is generally available to the public in a more harmonised style than in the various European countries. The issue of whether disclosure of such information into the public domain would be effective in prompting industry to provide less conservative estimates of local concentrations as envisaged as part of the consultant's strategy was not fully discussed. Similarly, the possible effectiveness of a more consultative approach with industry as an alternative to publication of screening model predictions of local concentrations to encourage the provision of better data was not further explored.
The strategy envisaged a possible alternative approach to gathering information on local environmental concentrations. This would entail inspection of IPPC permitting applications and supporting data that are, at least theoretically, held available for public inspection. There was general consent that this approach was not feasible on a European level. However, a proposal was made to consider pilot projects in some countries or regions where detailed knowledge of local conditions was available to test and fine-tune the strategy. Some member state representatives volunteered to go back to their national authorities to explore the potential for co-operation.

Notwithstanding the concerns expressed regarding the issue of local concentrations modelling, it appeared that most delegates supported the staged approach to modelling advocated by the consultant's strategy, subject to some modifications to address the issues raised above. A number of recommendations were also made for consideration in the preparation of the final report and for any follow up work arising from the study. These are as follows:

The option of running the EUSES screening model in a probabilistic manner, applying likely ranges to key input data, was proposed in order to predict likely uncertainty in the predicted concentrations should be explored, rather than staying with the 'reasonable worst case' approach.

Comparison of predicted concentrations from modelling should cover all sources – not just EPER sources – especially when these are of minor significance. As far as future modelling from EPER emissions data is concerned, this should focus on chemicals where EPER sources are the main source of release to the environment. It may also be useful to focus on those chemicals for which a risk assessment document is available, as this will provide useful background information for the modelling.

In presenting the results of such analysis, it would be important to ensure that concentrations resulting from various facilities are compared on a similar basis – for example, it could be problematic if concentrations calculated using default parameter values were presented along side those from other facilities where site-specific emission characteristics were used to derive concentrations, without a full explanation of the nature of the comparison. Indeed, it would be preferable not to show predicted local concentrations based on default input data at all. Further consideration should be given to the issues of defining the degree of exceedences that can be accepted in the comparison of screening results with criteria for further modelling – i.e. a normative step.

A4.3.3 General discussion

There was a high level of interest and general support for this EEA activity. While national regulators are already using chemical modelling as instrument to assess the current status of the environment (for exposure assessment, prioritisation of monitoring activities, and to cover spatial and temporal variation) and as a predictive tool, the experts identified a lack of a European wide strategy to assess effects of chemicals on the environment. Several delegates stated that they would welcome the development of an integrated strategy on chemicals risk management involving modelling and monitoring by the EEA, in co-operation with other players such as the European Chemicals Bureau and the Commission, if this approach were to be adopted.
A number of delegates, however, were unclear as to the precise objectives of the study. For example, was the ultimate goal to undertake some detailed integrated assessment modelling (for example, moving from simple concentration predictions to exposure assessment and economic valuation of impacts, single or multipollutant impacts etc)? Why was the focus on substances emitted from EPER point sources, which for many chemicals are minor compared with diffuse man-made or even natural sources of chemicals to the environment?

Dr Schöning recalled that the work presented at this stage is a feasibility study to explore what additional added value may be derived from the data in EPER in terms of predicting concentrations of chemicals in the environment (and their spatial and temporal distribution), and models represent the only means by which this added value may be realised.

Throughout the discussions the experts stressed that the successful development and application of models require a clear definition of the scope and reliable data for input, calibration and validation. The degree to which deviations will be tolerated as well as the resolution had to be defined beforehand. If the scope of further work was an integrated assessment of pressures/state/impact of chemicals – and not only an estimate of the added burden from EPER facilities – additional information was needed, for instance from monitoring or risk assessments under the existing substances regulation, to know the contributions from small point sources and diffuse sources. The proposal was made to start with pilot projects covering European regions where this information was available.

Several delegates offered their expertise as contribution to further EEA activities in the area of modelling of environmental concentrations of chemicals and some volunteered to explore whether authorities in their countries would be willing to share their data in the context of an EEA-project.

A4.4 Workshop agenda

09.30-10.00	Registration, coffee
10.00	Meeting starts
10.00-10.30	Welcome (Prof. Jacqueline McGlade) Overview of aims for the study (Dr. Gabriele Schöning)
10.30-11.30	Presentation of the project report – 'Feasibility study on modelling environmental concentrations of chemicals from emissions data'. Review of models, conclusions and proposed way forward (Dr Keith Brown & Mr John Abbott, AEA Technology)
11.30-12.00	Feedback on the report from the Brno modelling summer school (Prof Ivan Holoubek)
12.00-13.00	Discussion – Expert reflections on the models reviewed
13.00-14.00	Lunch
14.00-14.20	Role and requirements for detailed modelling (Dr Sergey Dutchak, MSC-E)
14.20-14.40	Research perspective on modelling strategies (Dr Martin Scheringer, ETH Zürich)
14.40-15.00	Coffee break
15.00-15.20	Regulatory perspective on modelling strategies (Dr Jose Tarazona, INIA, Spain)
15.20-16.30	General discussion
16.30	Meeting closes

A4.5 Workshop delegates

Name	Organisation	Email
John Abbott	AEAT	John.abbott@aeat.co.uk
Till Bachmann	IER-Stuttgart University	TB@ier.uni-stuttgart.de
Andreas Barkman	EEA and UNECE Task Force on Emission Inventories and Projections (TFEIP)	Andreas.barkman@eea.europa.eu
Keith Brown	AEAT (project manager)	Keith.brown@aeat.co.uk
Jasmina Comic	CETEOR Sarajevo	ceteor2@pksa.com.ba
Bert Droste-Franke	IER-Stuttgart University	bd@ier.uni-stuttgart.de
Sergey Dutchak	Director, MSC-EAST	sergey.dutchak@msceast.org
Ozlem Esengin	Ministry of Environment and Forest, Turkey	ozlemesengin@yahoo.com
Sigurður B. Finnsson	Environment and Food Agency of Iceland	sigurdurb@ust.is
Stellen Fischer	Swedish Chemicals Inspectorate	Stellan.Fischer@kemi.se
Juris Fridmanis	Environment, Geology and Meteorology Agency, Latvia	Juris.Fridmanis@lvgma.gov.lv
Britta Hedlund	Swedish EPA	Britta.Hedlund@naturvardsverket.se
Ivan Holoubek	TOCOEN	holoubek@recetox.muni.cz
Martin Holt	ECETOC	MARTIN.HOLT@ecetoc.org
Sergio Cuadrado Iglesias	Spanish Environmental Ministry	sgiaprat05@mma.es
Allan Astrup Jensen	Force Technology (associated Danish Ministry of Science, Technology and Innovation)	aaj@force.dk
Gulsen Kaybal	Ministry of Environment and Forest, Turkey	gkaybal66@yahoo.com
Juliana Knazovicka	Slovak Environmental Agency	knazovic@sazp.sk
Nataša Kovač	Environmental Agency of the Republic of Slovenia	Natasa.Kovac@gov.si
Gerhard Lammel	Max Planck Institute for Meteorology	lammel@dkrz.de
Aleksandra Nestorovska-Krsteska	Ministry of Environment and Physical Plannin, Republic of Macedonia	A.Krsteska@moepp.gov.mk
Violeta Pisljagic	Austria	ciara8@gmx.at
Alberto Pistocchi	EC JRC	alberto.pistocchi@jrc.it
Nebojsa Redzic	Environmental Protection Agency, Serbia and Montenegro	nebojsa.redzic@sepa.sr.gov.yu
Pete Roberts	Shell Global Solutions	Pete.roberts@shell.com
Bernd Scharenberg	Federal Environmental Agency (Germany)	bernd.scharenberg@uba.de
Martin Scheringer	Institute for Chemical and Bioengineering, ETH Zürich	scheringer@chem.ethz.ch
Gabriele Schöning	EEA (project manager 'Chemicals')	Gabi.Schoening@eea.europa.eu
Olav Skogesal	SFT	olav.skogesal@sft.no
Joseph V. Spadaro	Ecole des Mines, Paris	JAASSPADARO@aol.com
Jose Tarazona	INIA, Spain	tarazona@inia.es
Dirk van de Meent	RIVM, Laboratory for Ecological Risk Assessment, Netherlands	D.van.de.Meent@rivm.nl
Matti Verta	Finnish Environment Institute	matti.verta@ymparisto.fi
Yavor Yordanov	Executive Environment Agency, Bulgaria	landmon@nfp-bg.eionet.eu.int
Josema Zaldivar	EC JRC	jose.zaldivar-comenges@jrc.it

A4.6 Workshop presentations

Overview of the study (Dr Gabriele Schöning)

Presentation of the project report Feasibility study: modelling environmental concentrations of chemicals from emission data
(Dr Keith Brown and Mr John Abbott)

Feedback report from the Brno modelling summer school
(Prof Ivan Holoubek)

Role and requirements for detailed modelling
(Dr Sergey Dutchak)

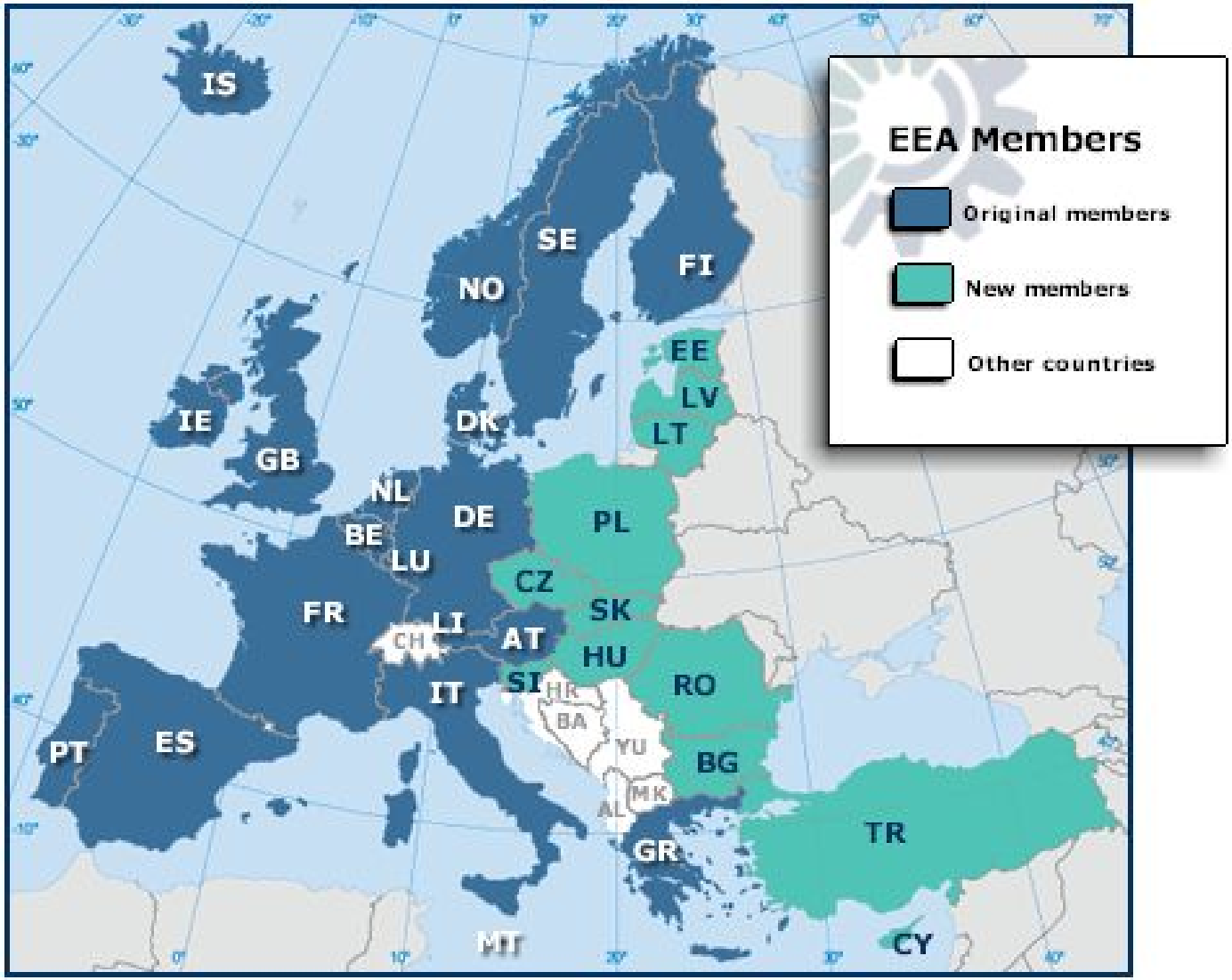
Research perspectives for detailed modelling
(Dr Martin Scheringer)

Regulatory perspective on modelling strategies
(Dr Jose Tarazona, INIA)

Feasibility study: Modelling environmental concentrations of chemicals from emission data

EEA Study contract REF No 34442/B2004.EEA.51980

EEA Member and Participating Countries

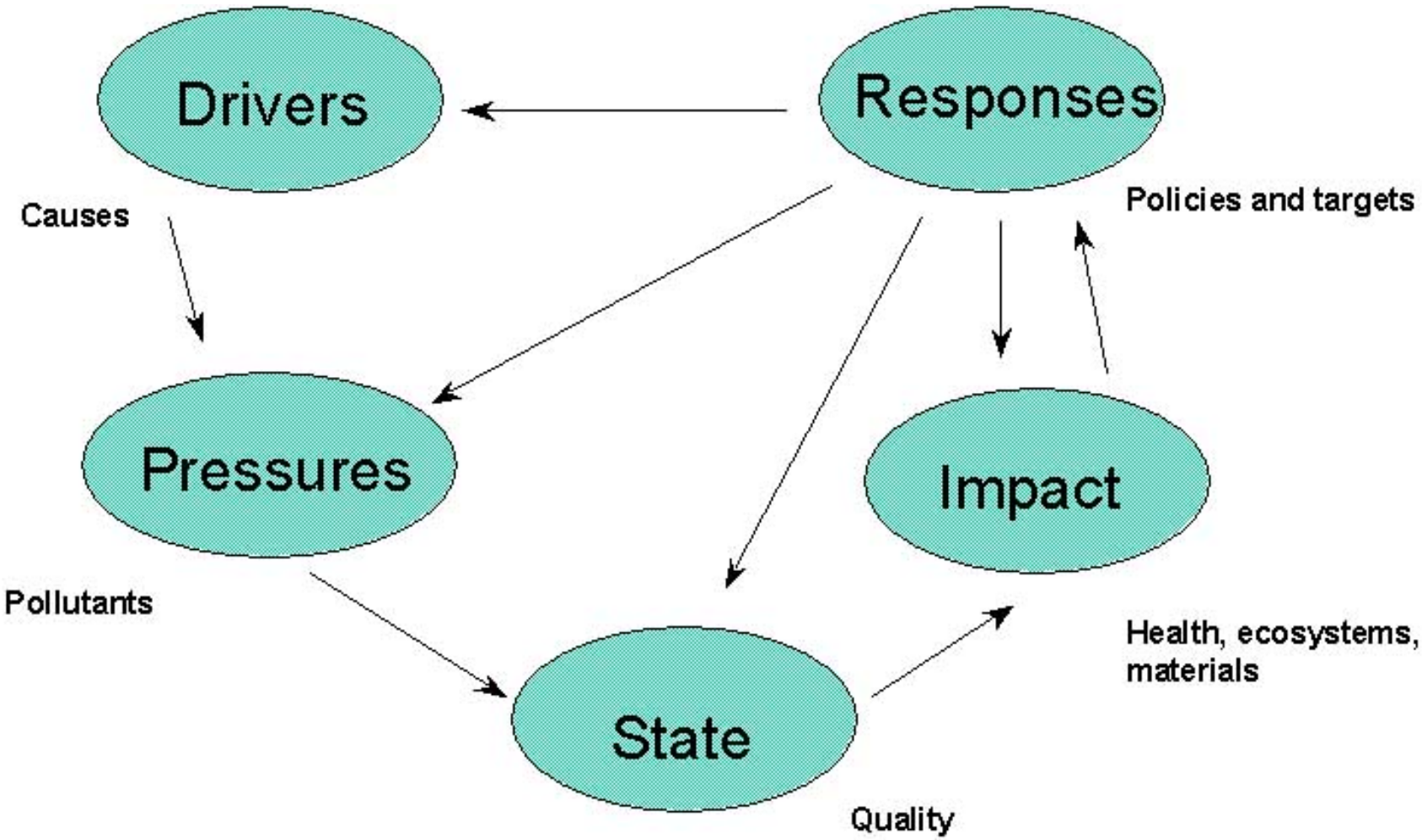


The EEA mandate

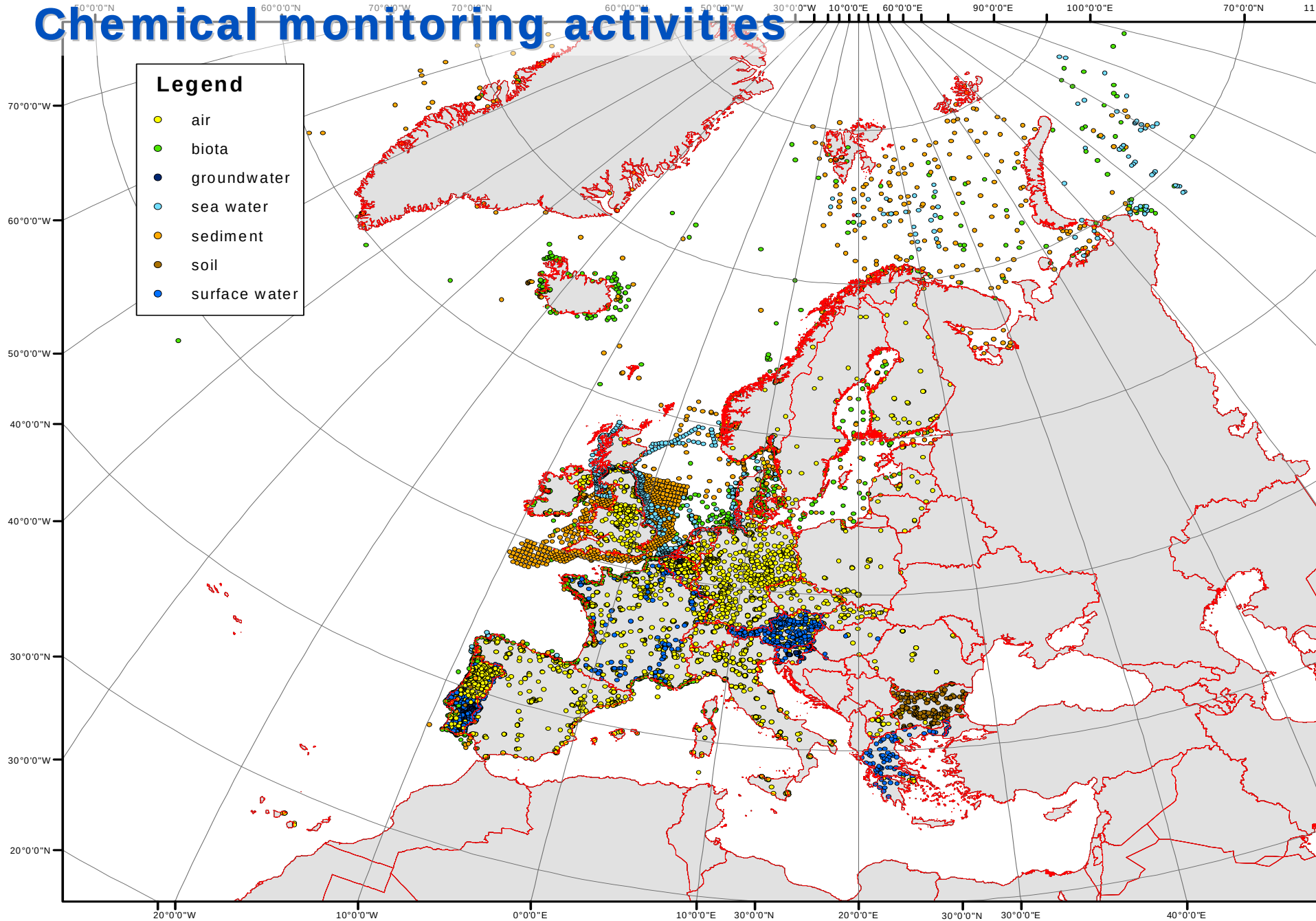
"To provide the Community and the Member States with objective, reliable and comparable information at European level enabling them to take the requisite measures to protect the environment,to assess the results of such measures and to ensure that the public is properly informed about the state of the environment,."

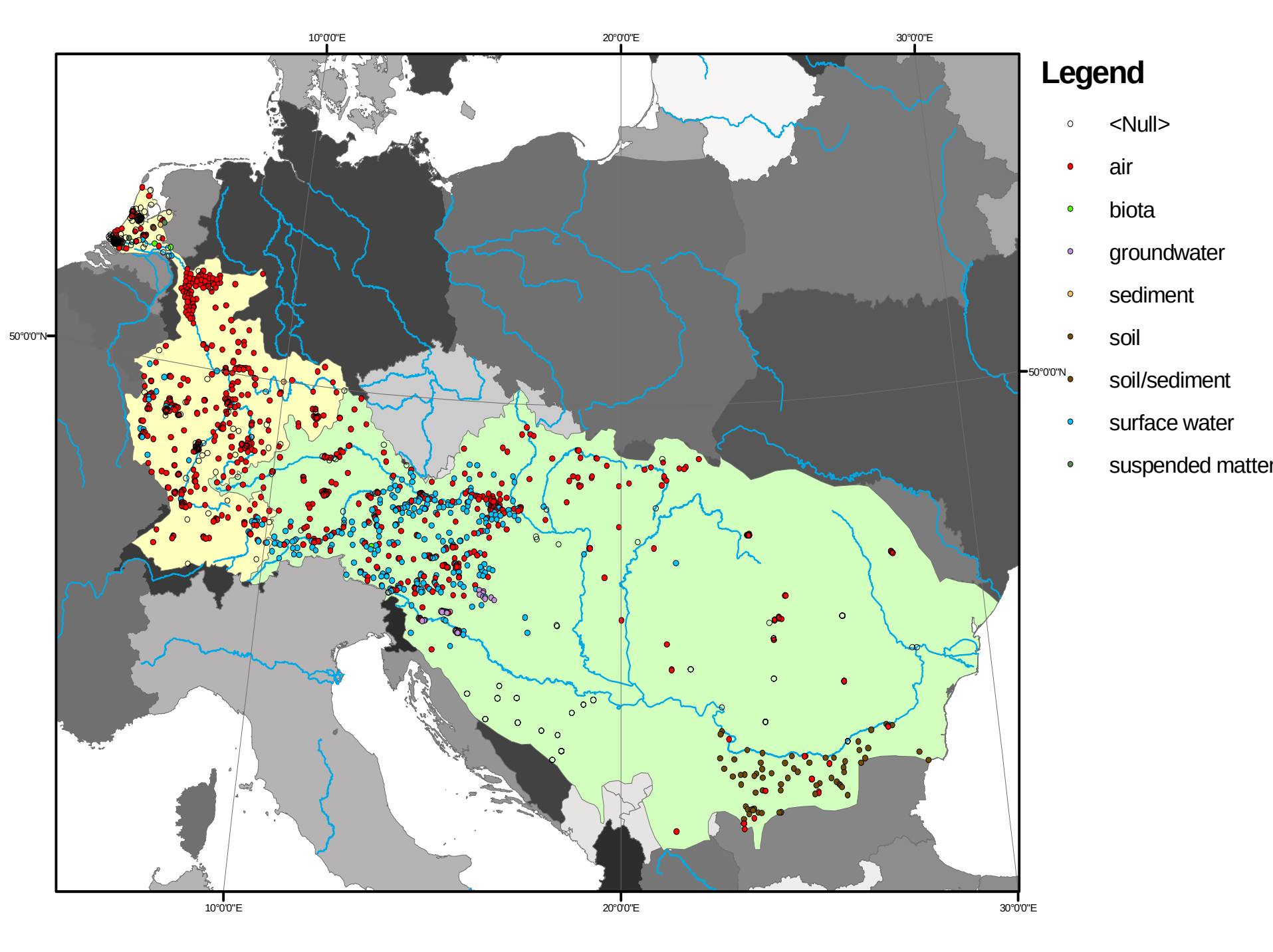
(Article 1 of EEA Regulation)

The DPSIR analysis framework



Chemical monitoring activities




10°0'0"E
20°0'0"E
30°0'0"E
50°0'0"N
Legend
<Null>
air
biota
groundwater
sediment
soil
soil/sediment
surface water
suspended matter

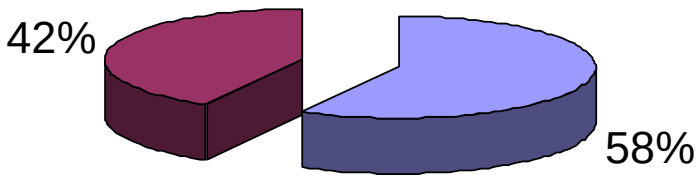
Data coverage*

N = number of substances

Available % of countries

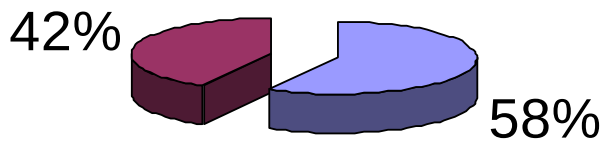
Not available % of countries

Sediment



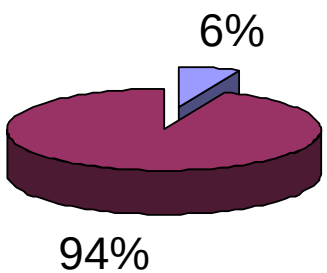
N= 3 - 99

Surface water



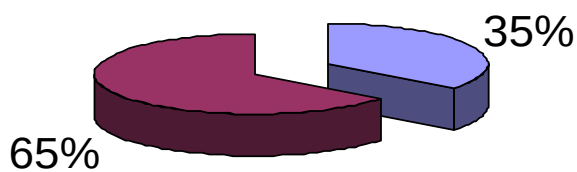
N= 1 - 168

Ground water



N= 64 - 65

Sea water



N= 1 - 157

* As of October 2004

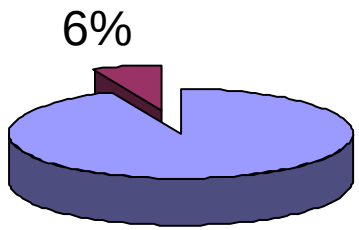
Data coverage cont.

N = number of substances

Available % of countries

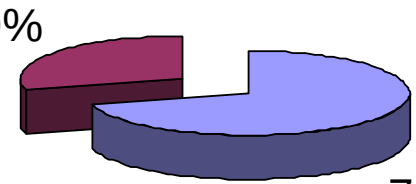
Not available % of countries

Air



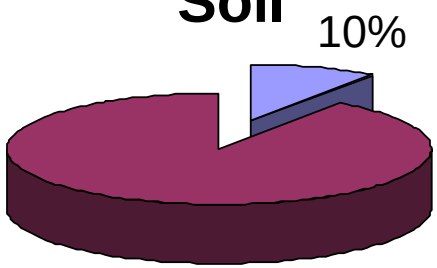
N= 5 - 46

Biota



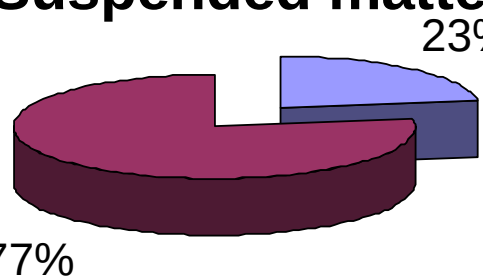
N= 1 - 126

Soil



N= 5 - 40

Suspended matter

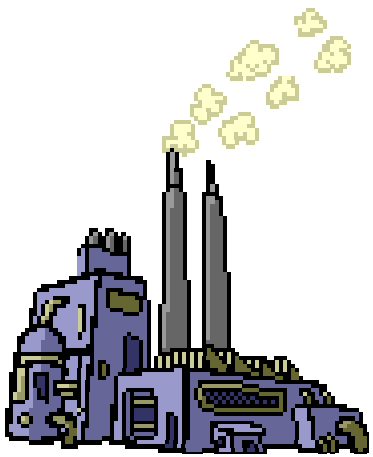


N= 3 - 95

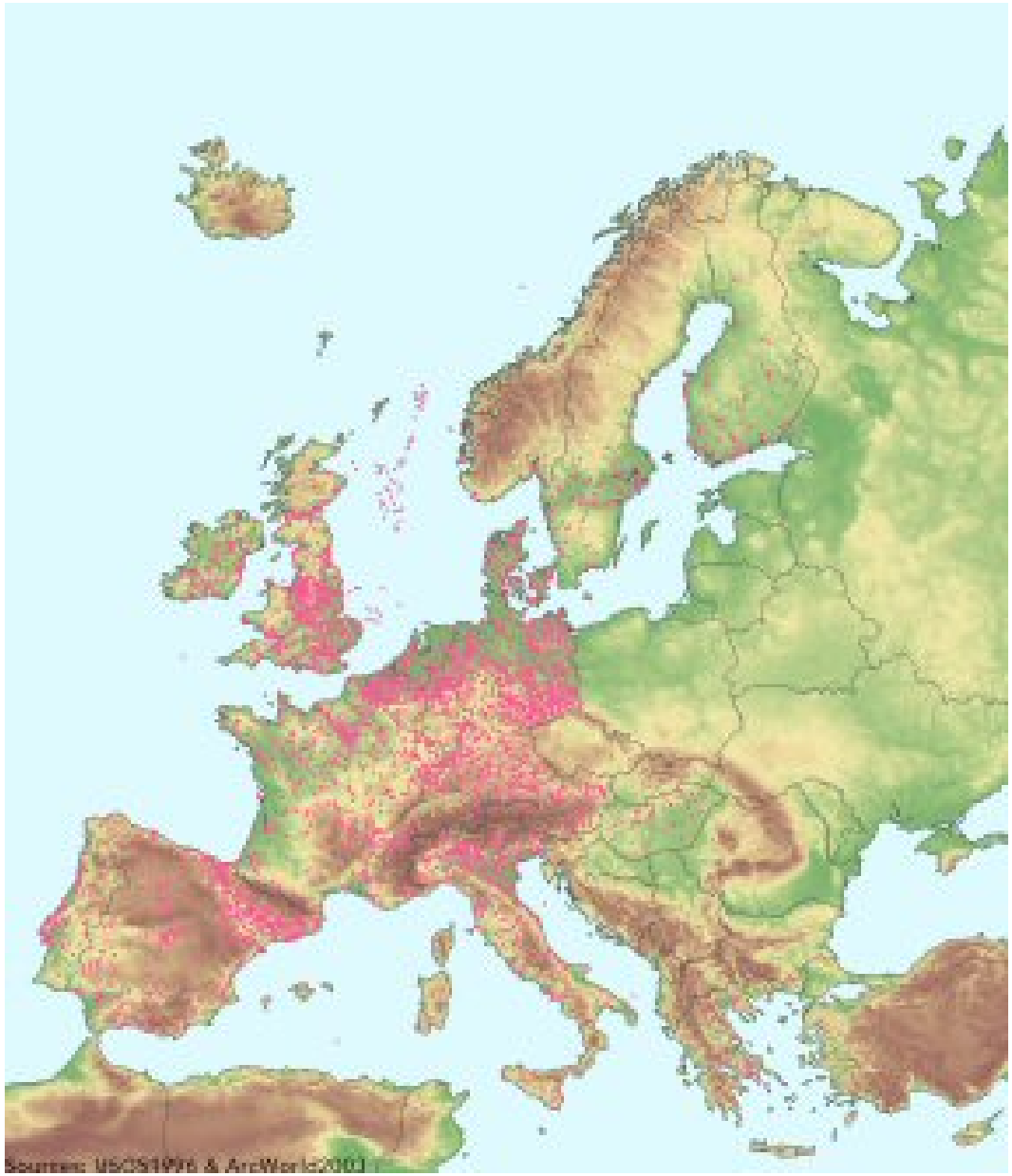
European Pollution Emission Registry

Launched 23 February 2004

Commission Decision to establish EPER (2000/479/EC):

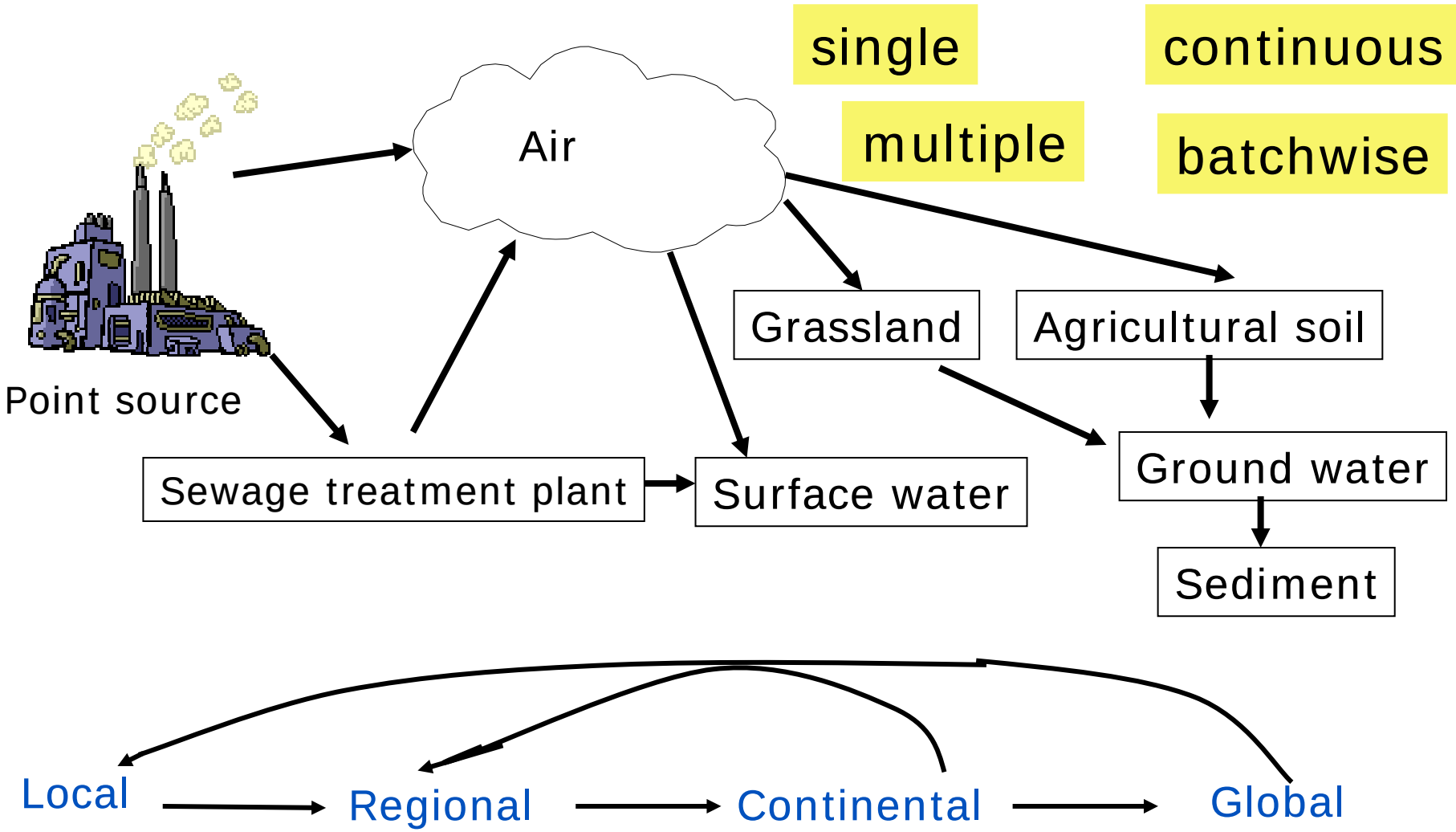


Europe-wide
(EU15, Hungary and Norway)
Industrial emissions into air and water.
50 Substances
10,000 large industrial facilities
Publicly accessible on the internet
http:// www.eper.cec.eu.int

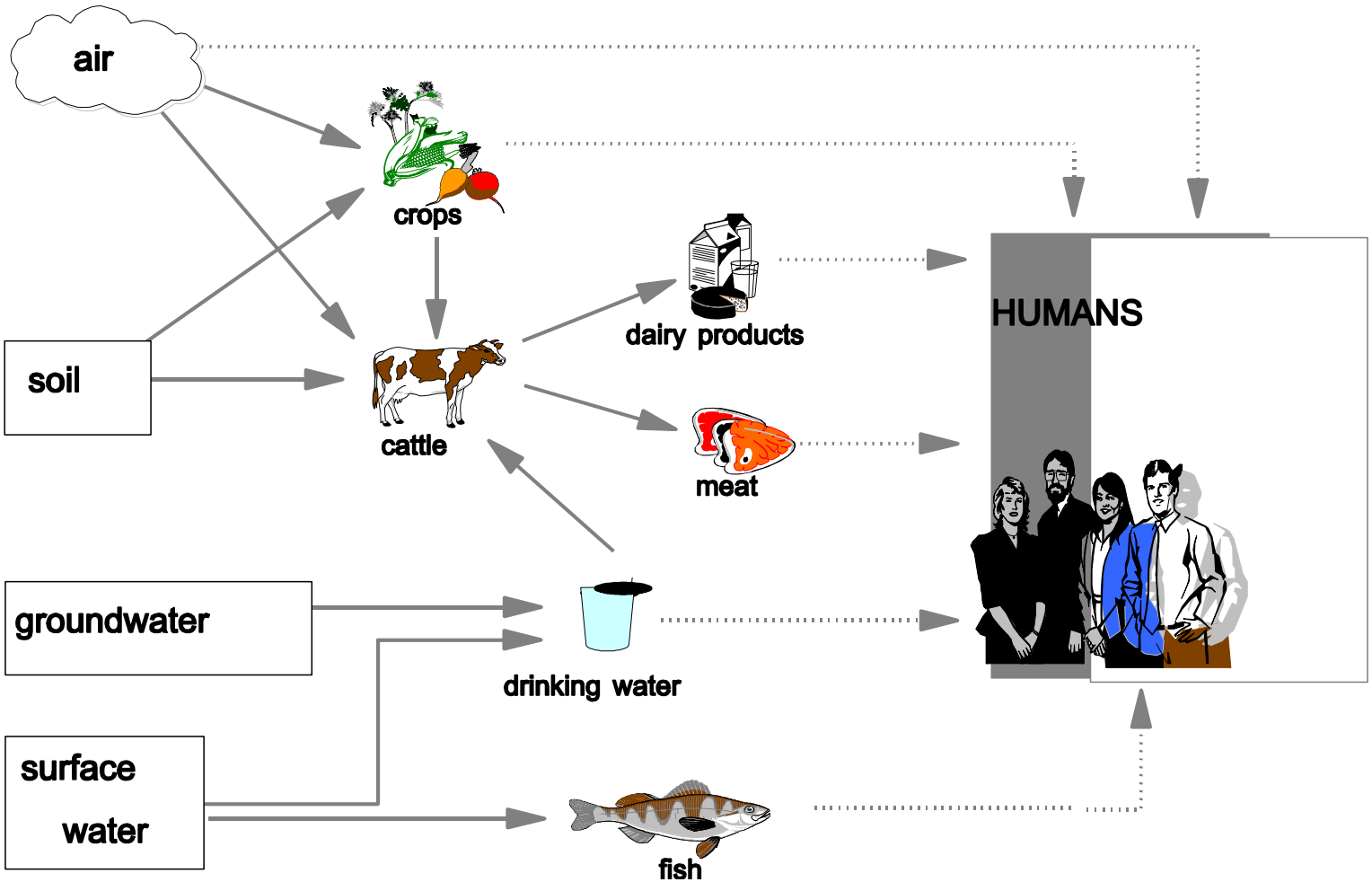


EPER facilities

Distribution routes of local emissions



Exposure of man via environment



Source: Technical Guidance Document for Risk Asessment

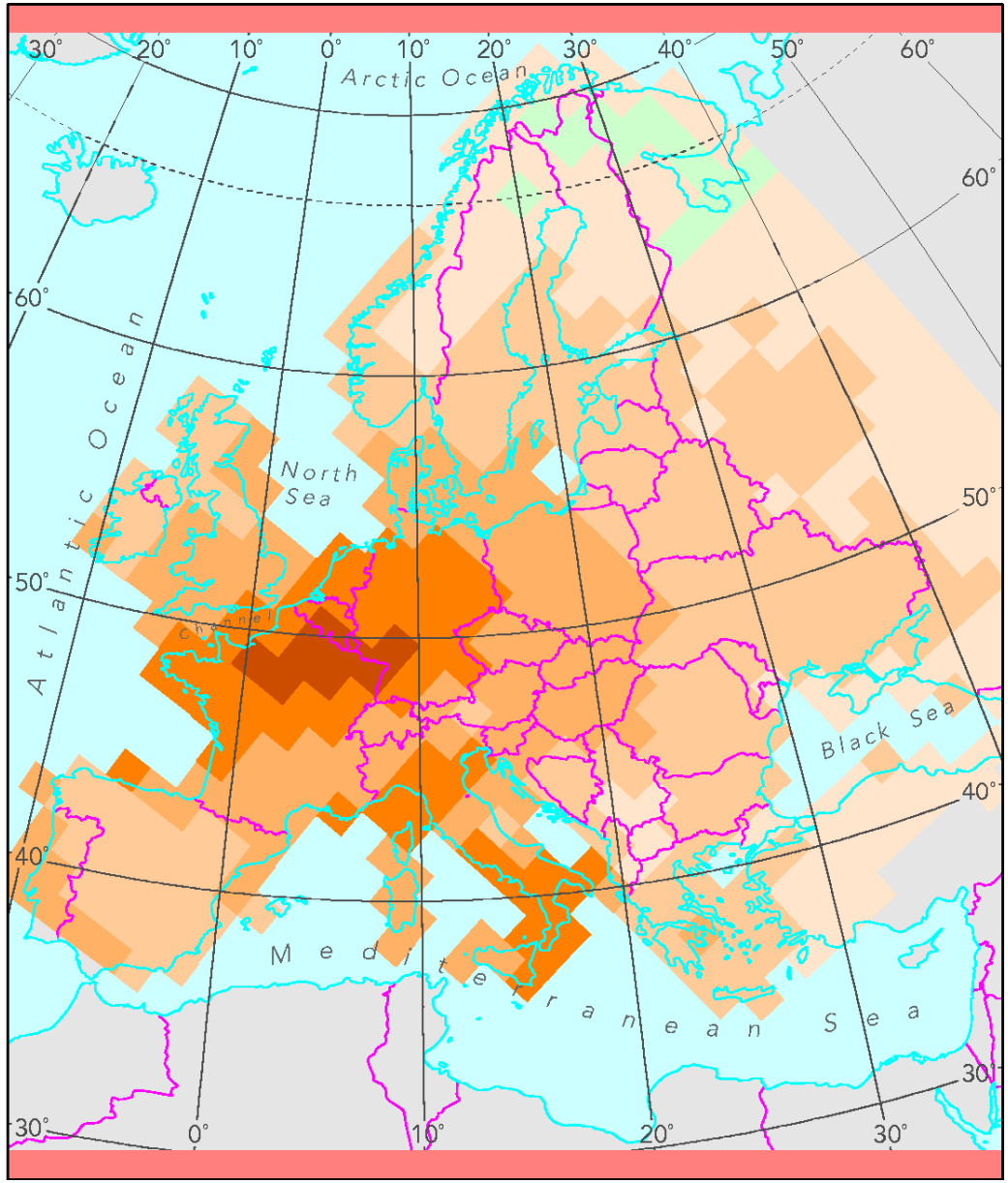
Accumulated excess of ozone concentration

0 1000 km

Concentration in µg/m³/h exceeding the threshold of 120 µg/m³/h in the EMEP 150–grid

- more than 12000
- 6000–12000
- 2000–6000
- 200–2000
- less than 200
- areas with no exceedance

Modelled from 1990 level emissions.
Meteorology from selected years.



Purpose of the feasibility study

- Develop a toolbox of available methodologies. Evaluate:
  - Availability
  - Validity and general acceptance
  - Ability to provide information on spatial distribution
  - Time and spation scale
  - Substance classes /EPER compounds
- Test run on selected modells and few compounds:
  - Map concentrations
  - Identify hot spots
  - Assess usefulness of EPER data format and added value compared to EMEP
- Draft a workplan how to extend to other modells and cover all EPER substances

Purpose of the feasibility study cont.

Develop a strategic proposal how

- based on European emission data - these models and derived data can be used to estimate and predict the concentrations, composition and distribution of chemicals in the European and wider environment to support EEAs integrated asessments.

Consider other potential users

EEA‘s clients:

Institution level:
European Commission, Parliament, Council, EEA member countries

General public:
NGOs, business, research community, media, advisory, groups/persons, debaters and the policy engaged public

Use of PRTR data

- By the Public: right to know, education, ‚pollution watch', influence industry and government
- By Industry: pollution prevention and reduction, cost reduction, public disclosure of environmental data, assistance to others, environmental management systems,
- By Government: Environmental improvements, development of policies and regulations, programme evaluation, compliance control, risk assessment tool, education, reporting:
- By Investment Community: assessing and tracking environmental performance of companies
- By Academic Research Institutions: basic and applied research, e.g. on socio-economic impacts, identify trends, *develop multimedia contaminant fate models that link releases to contaminant concentrations in air, water, and soil*

OECD ENV/JM/MONO(2005)3

Key use of models

applied by users of emission inventory data as identified in the brainstorming meeting

- Industry: demonstrate compliance, benchmarking environmental performance, driver for improvement
- Regulators: set emission levels in permits, assess consequences of excess emissions
- Policy makers: assess compliance with international obligations, assess cost of compliance
- Researchers: for many purposes that require understanding of spatial and temporal distribution of chemicals in the environment

Discussion points

- Is the „toolbox“ complete?
- Are the models adequately described?
- Which models do you use in your country/institution?
- Feedback on the proposed strategy:
  - Is the approach realistic
  - Do you see alternatives
- Further recommendations

Feasibility study: Modelling environmental concentrations of chemicals from emission data.

Keith Brown

John Abbott

AEA Technology

Harwell, UK

AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

Purpose of the work

'Develop a toolbox of available methodologies and a work plan for applying relevant models to substances reported under EPER in order to predict the concentrations, composition and distribution of these chemicals in the European environment'

AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

Main tasks

- Evaluate –
  - Which of the models are sufficiently validated for use in a policy context
  - Which of the models are suitable for EPER substances and other types of compound
- Make a test run
- Develop a strategic proposal to predict concentrations and distribution of chemicals based on emission data

Approach

- Phase 1 – Model evaluation
- Phase 2 – Test run and strategic plan

European Pollutant Emission Register (EPER)

- Established under Council Directive 96/61/EC (IPPC Directive)
- Emissions recorded for individual industrial facilities of specified types
- 50 substances listed
- Emissions in unit mass/year to air or water (direct and indirect)
- Updated every 3 years – current data is 2001.
- Due for replacement by EPRTR in 2009

EPER data

- Name of chemical (or mixture of chemicals)
- Facility identifiers – industry, site, operator etc
- Geographical coordinates
- Quantity emitted per year
- Measured, Calculated or Estimated data
- Receiving medium – air, water (direct & indirect)

Phase 1 - Model evaluation

- Evaluation criteria
- Information gathering

} Brainstorming meeting

- Types of models
  - **Atmospheric dispersion models** - Local and regional + scale, photochemistry, acid deposition
  - **Multimedia models** – screening and detailed
  - **Surface water models**
  - **Sewage treatment models**
- Suitability for modelling EPER substances
- Develop an outline strategy for phase 2

Model evaluation criteria

- Availability
- Peer review/quality status
- Adequacy of information
- History of usage and development
- Resource requirements
- Outputs
- Modelling principles
- Applications
- Input data requirements – (vs. data availability)

Input data requirements

- Models have a wide range of input data requirements
- Modelling scale determines the scale of input data – emission characteristics are important at the local scale
- Data for local modelling is often inaccessible
- Increasing model complexity demands greater detail in the input data
- Some of the input data required may be highly uncertain
- Increased model complexity does not always lead to increased accuracy

Conclusions from phase 1

- Detailed modelling for LOCAL concentrations is not feasible without detailed information on emissions characteristics
- Detailed modelling for REGIONAL + scale concentrations is feasible but:
  - Will be resource intensive to undertake
  - Will require specialist evaluation to ensure accuracy
- A staged approach to modelling, making use of available information, will offer a cost-effective solution.

The staged approach to modelling from emissions data

- Use a screening model to assess local and regional PECs from EPER emissions
- Make conservative assumptions for unknown input variables to predict reasonable ‘worst case’ output
- Compare PECs with background levels, EQS or other relevant criteria
- Undertake detailed modelling where regional criteria are exceeded
- Engage with industry to provide better information for local PECs

Demonstration of the staged approach

Our brief:

- Run one or more readily available models for one or more test substances using reported release data in the EPER database
- Map the concentrations
- Identify hot spots of predicted concentrations
- Assess usefulness of the EPER data format for this purpose
- Compare predicted levels with actual monitoring data on concentrations, if available

AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

Choice of EUSES for first stage screening

- Readily available: internet download
- Recognised : used for EU risk assessments
- EPER database provides sufficient input data to run the model
- EUSES predicts concentrations at the local, regional, continental and global (arctic, temperate and tropical regions) scales
- Has multi-media modelling capability: it predicts concentrations in air, water, soil, sediments, biota. For the feasibility study, we limited our interest to air, water and soil

Choice of substances

- Hexachlorobenzene: an example of a persistent organic pollutant
- Benzene: an example of a volatile organic substance
- Arsenic : an example of a heavy metal pollutant

Available monitoring data:

  - Air concentrations monitored under CLRTAP, reported by EMEP
  - EMEP summary reports on hexachlorobenzene and heavy metals
  - IUCLID database
  - Other national databases

Use of EPER data in modelling

The EPER database provides four pieces of information that can be used for modelling for each of the reported emissions:

- The pollutant
- The quantity emitted per year
- The medium into which the pollutant is released: air, direct to water or indirect to water
- The location of the emitting facility in latitude and longitude

Preparation of model inputs

Emission data was extracted from the EPER database using a simple Visual Basic in Excel ® script. The script:

- Summed local emissions of individual pollutants to the same media from each facility;
- Summed other EPER emissions to calculate a "regional EPER emission" over a 200 km x 200 km area centred on the source
- Summed continental EPER emissions outside the region to provide a "continental EPER emission"
- Also calculated a "regional background emission" on a pro-rata basis from national totals, where available
- Formatted emissions and physical property data for input
- Prepared batch files for EUSES operation

Physical property data

EUSES requires physical property data for each substance.

- For POPs and VOCs
  - Molecular weight, boiling point, melting point, vapour pressure, solubility, octanol-water partition coefficient, Henry's law coefficient, degradation rate in air, compound type for calculating other physical properties using QSARs
- For heavy metals
  - Vapour pressure (very low), solubility (very low), soil-water partition coefficient, sediment-water partition coefficient
- Data sources and input
  - EU Risk assessments, IUCLID, US EPA Human Health Risk Assessment Protocol, Data input to EUSES via input script.

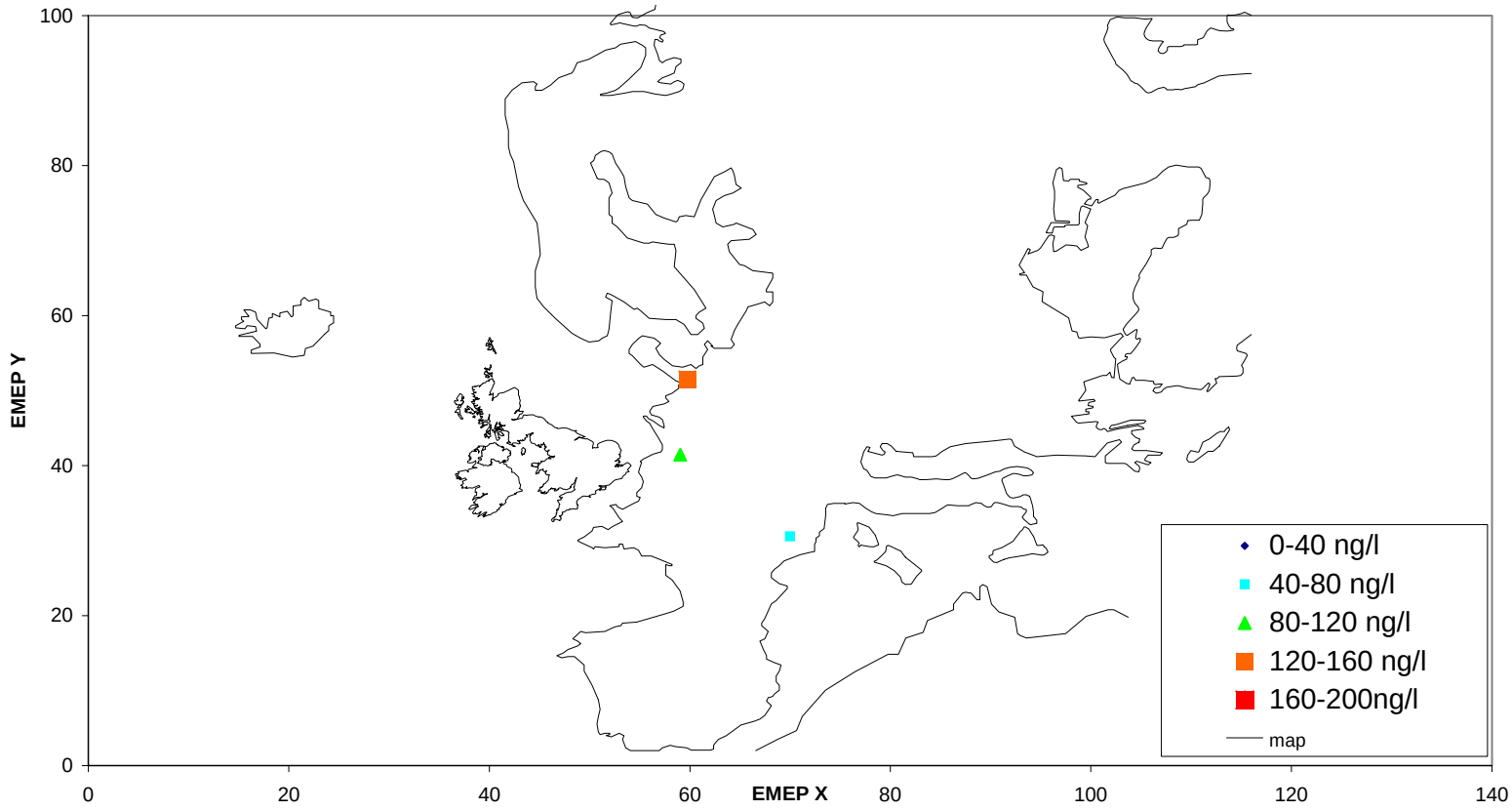
Other environmental data

- Other environmental data were not used for this feasibility study. EUSES defaults were used.
- The location (latitude, longitude, country) information provided by EPER could be used to extract other environmental data from databases.
- Examples include climatalogical data (temperature, precipitation), river catchment area data , land cover data (CORINE)
- Easily incorporated into input script

EUSES outputs

- EUSES provides numerical outputs
- For this feasibility study we used a simple Visual Basic in Excel® script to prepare simple European-scale maps showing the predicted concentrations in the vicinity of each emission source.

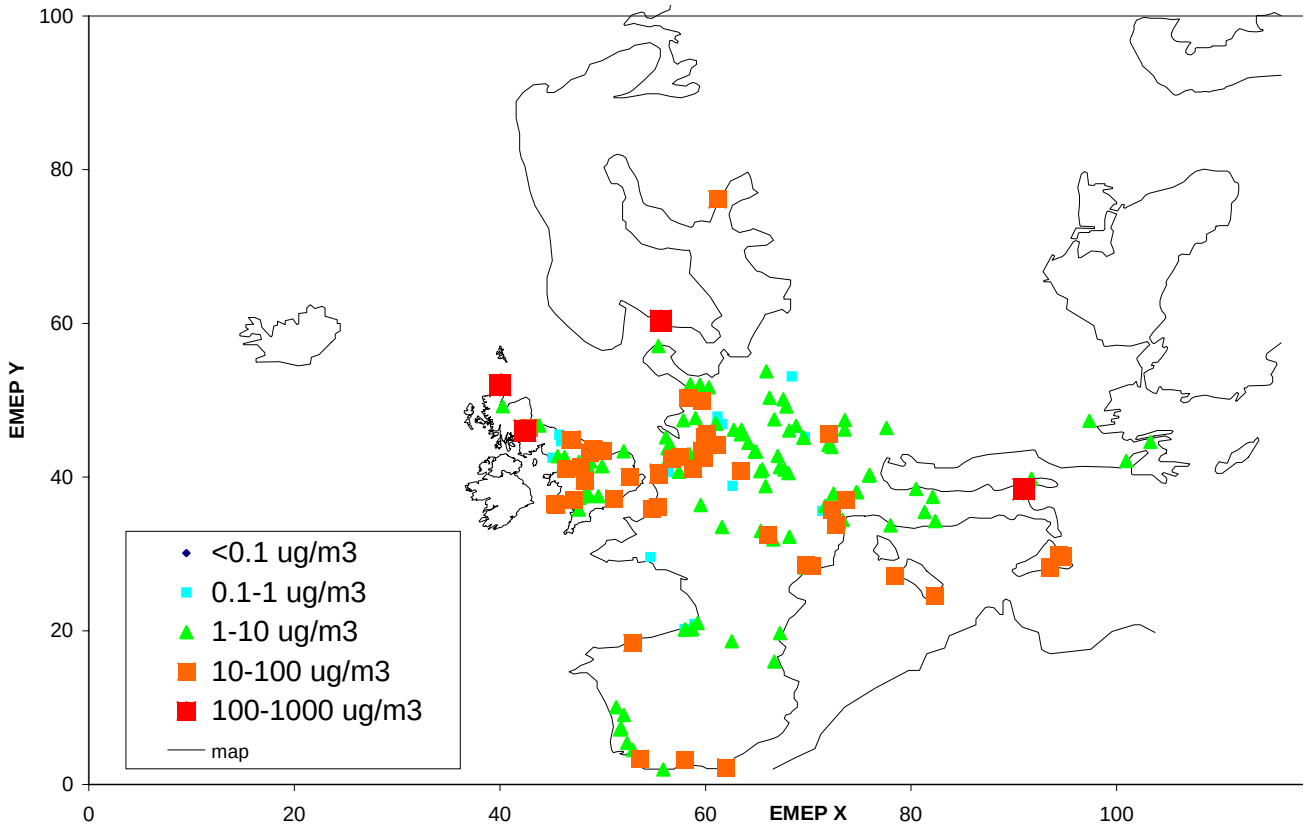
Predicted surface water concentrations of hexachlorobenzene



AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

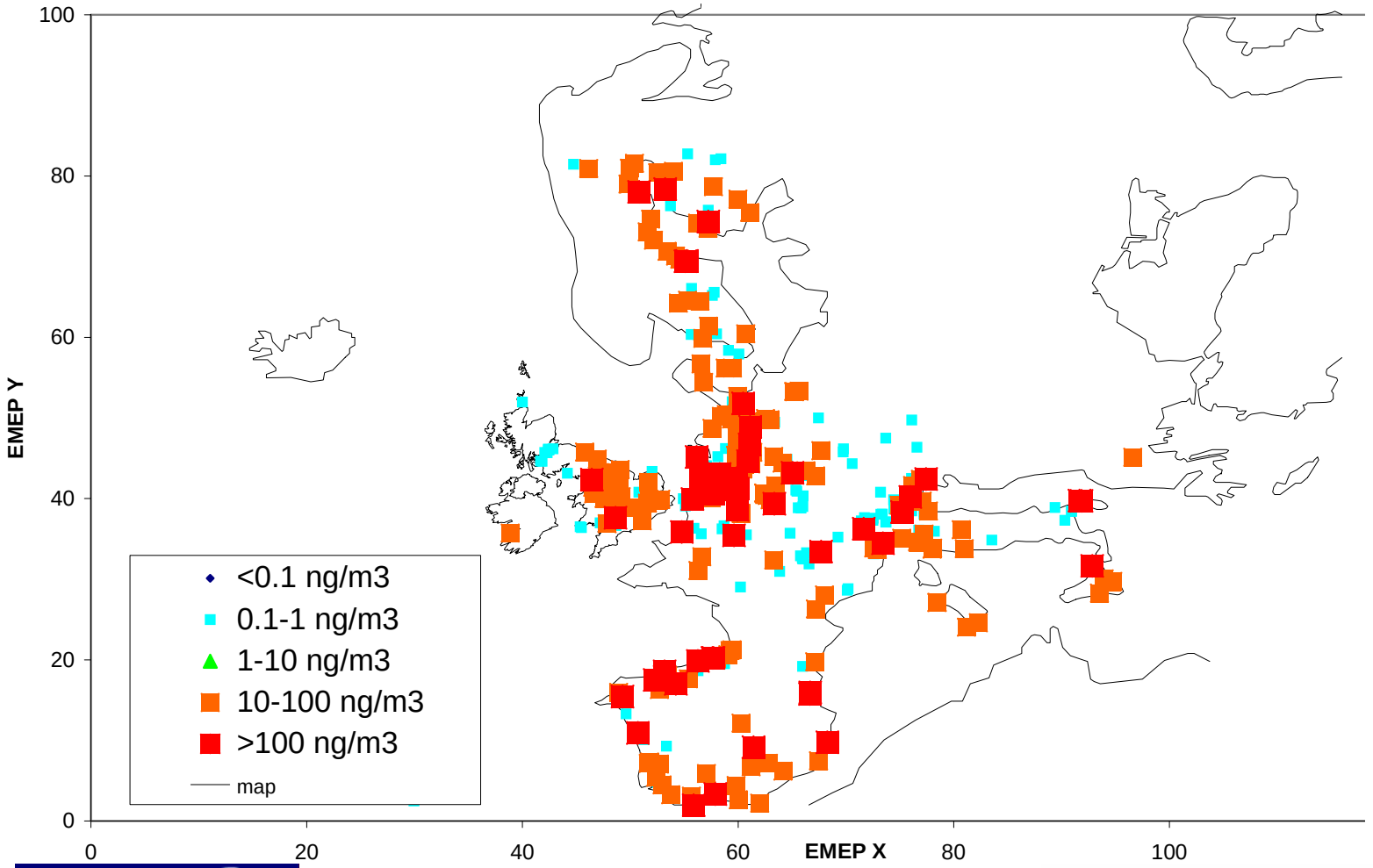
Predicted EPER contribution to local benzene concentrations in air



AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

Predicted contribution from EPER sources to arsenic concentrations in air



AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

EUSES model uncertainty

- EUSES model produces estimates of regional hexachlorobenzene concentrations in air and surface waters within an order of magnitude of measured values;
- EUSES model underestimated regional background benzene concentrations in air by typically an order of magnitude: emissions inventory incomplete
- The predicted regional background concentrations of arsenic in air are comparable with measured values. EUSES underestimates the arsenic concentrations in soils because the natural content of soils has not been taken into account

Scale of impacts: hexachlorobenzene

- Predicted environmental concentrations of hexachlorobenzene in surface waters may exceed 30 ng/l standards close to EPER data sources
- The predicted contribution from EPER sources to regional (or continental or global) is small (<0.02 ng/l) compared with the water quality standard

Scale of impacts: benzene

- The EUSES model predicts that the air quality limit value for benzene of 5 μg/m³ is currently exceeded close to many of the EPER source locations
- The predicted contribution from EPER sources to regional benzene concentrations is very small (0.02 μg/m³)

Scale of impacts: arsenic

- Local concentrations in air predicted by EUSES in the vicinity of several EPER sources exceed the 4th Daughter Directive target value of 6 ng/m^3.

- Local concentrations in surface waters predicted by EUSES in the vicinity of several EPER sources exceed national standards.

- The contribution from EPER sources to regional concentrations is very small.

Scale of impacts

Common theme:

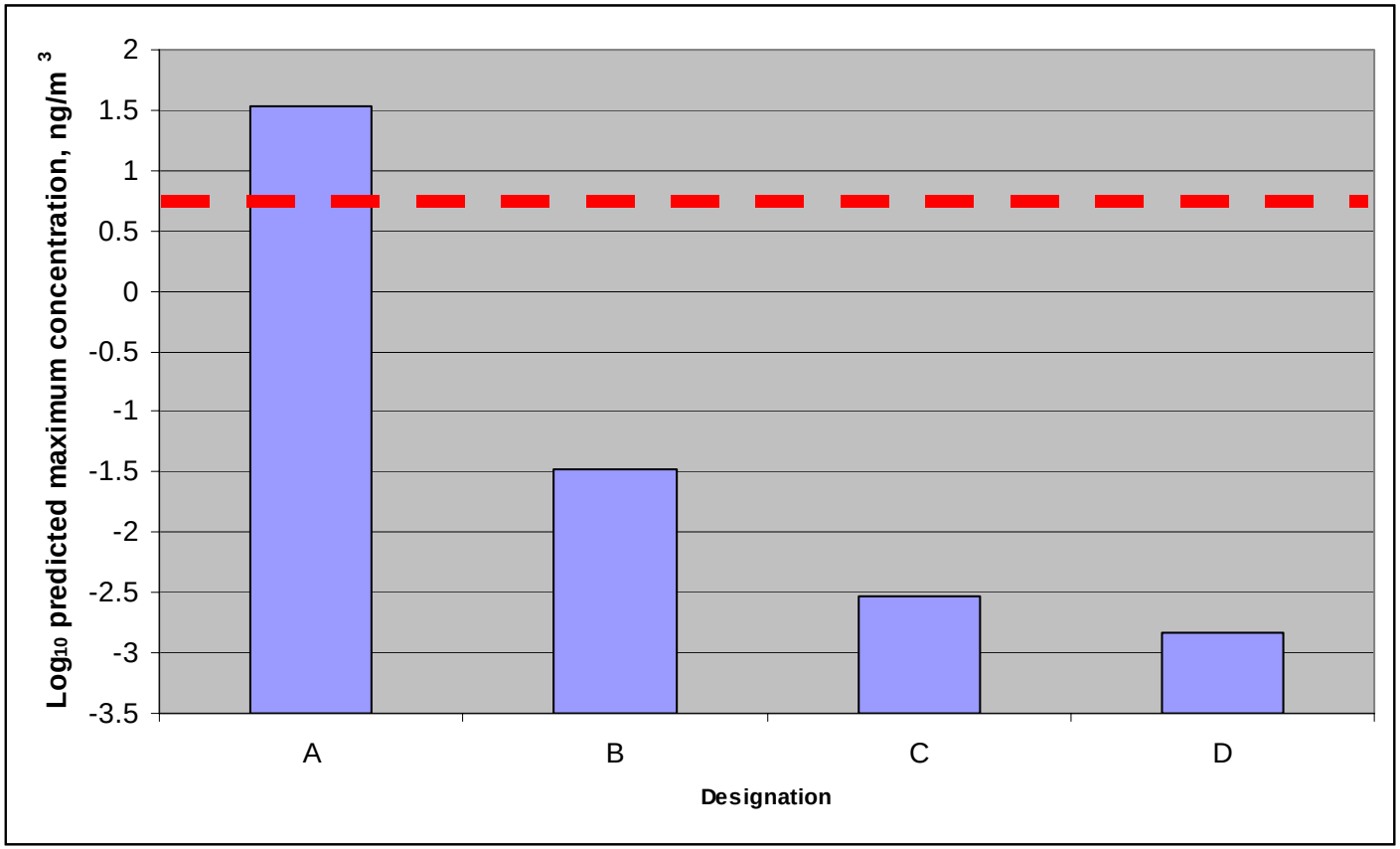
Largest predicted impacts are local to the source for hexachlorobenzene, benzene and arsenic

Effect of increased discharge information:

Arsenic discharge from coal burning power station

No	Additional Local Info	Model	Local PEC
A	None	EUSES	34.3
B	Stack height 198m	Worst case meteorological conditions & no plume rise (Environment Agency)	0.033
C	As above; Effective stack diameter = 12 m; Discharge temp= 130^{o}C, velocity= 27 m/s	Typical met conditions, includes plume buoyancy & momentum (Environment Agency)	0.003
D	As above; Hourly sequential meteorological data for region. Time varying emissions profile for UK coal-fired power stations	ADMS 3.2	0.0015

Increasing discharge information



AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

Usefulness of EPER data format

Strengths

- Provides information on geographical location
- Contains information on emissions to water and air
- Wider range of pollutants than EMEP/CLRTAP
- More frequently updated than EMEP
- Lower reporting thresholds than EMEP
- Data easily extracted for input to chemical fate models

Usefulness of EPER data format

Weaknesses

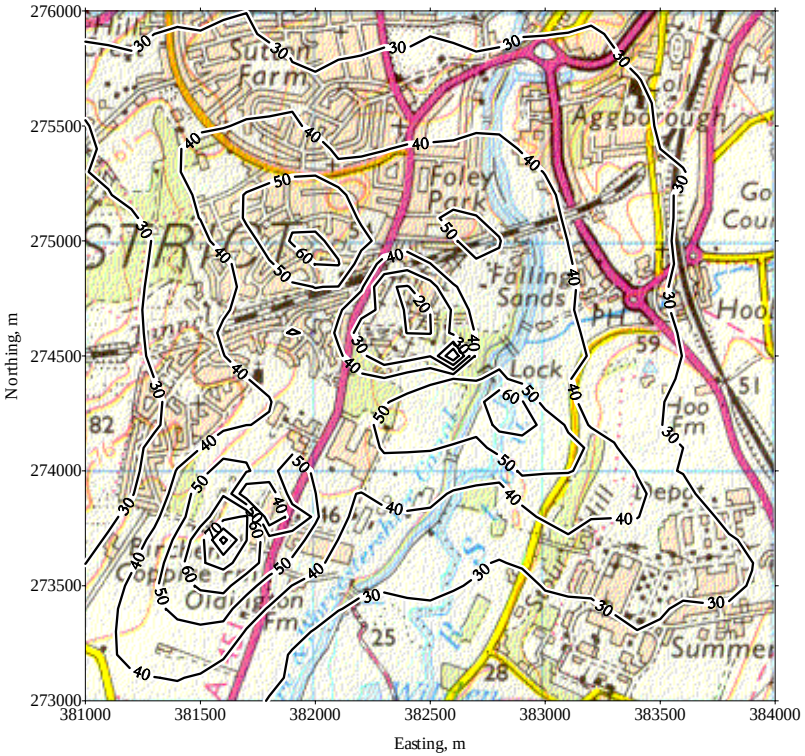
- No information on discharge characteristics
- Some emissions are combined e.g. BTEX: is it useful to model the impact of a mixture of chemicals with different properties and environmental impact?

Presentation of model outputs

- Our maps show the maximum process contribution or predicted environmental concentration close to each of the identified EPER sources
- These are the key outputs from the EUSES model
- Clearly shows the relative impact of each EPER source

Contour plots: short term SO_2 concentrations near an MSW incinerator

- Often suitable as output of detailed modelling. Example taken from Phase 1 of the work.
- Requires detailed information on discharge characteristics not available in EPER
- 1 km on a Europe scale map on an A4 page is approximately 0.04 mm



AEA TECHNOLOGY ENVIRONMENT

European Environment Agency

Detailed assessment: model selection

Two main factors determine the choice of model

- Scale of impact:
  - local, regional, continental, global
- Media affected:
  - air, water, soil, sediment or multi-media

Detailed assessment: model selection

Scale	Indicative model domain dimension	Indicative model resolution
Local	Up to ~50 km	Stack height (air dispersion) Water depth (hydrodynamic modelling)
Regional	~200 km	~2 km
Continental	EMEP grid	10-150 km
Global	Global	~2 degrees

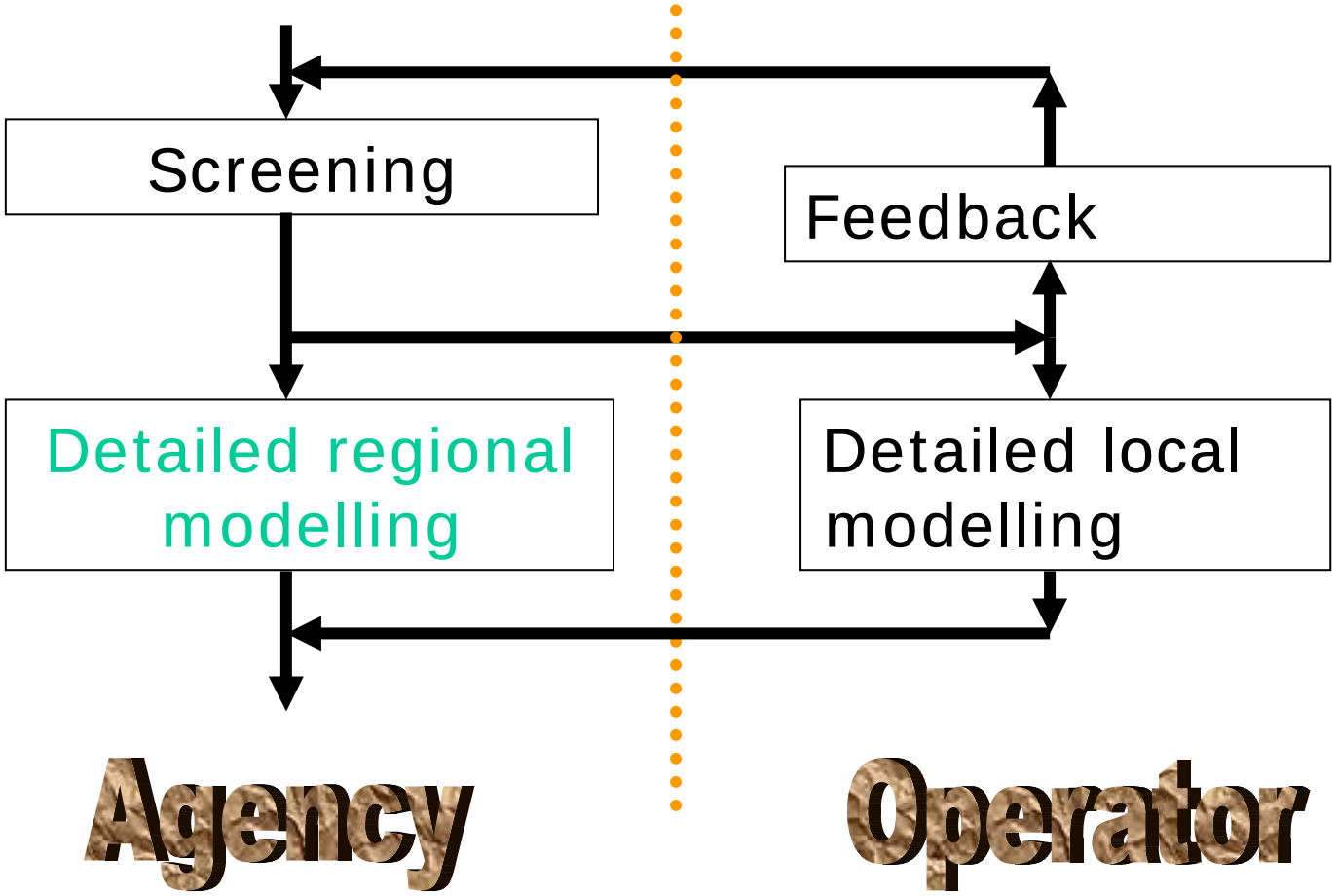
Additional information required from operators for local-scale modelling

Tier	AIR	Water (direct)	Water (indirect)
1 (EPER)	Emission Location	Emission Location	Emission Location
2	Stack height	Nature of receiving waters-river, coastal etc. Dilution factor	Effluent discharge rate of STP ⬅
3	Stack diameter Volume flowrate Discharge temperature Local surface roughness	Sediment concentrations, temperature of emission & receiving waters, Local solid-water partition coefficients	SimpleTreat input parameters ⬅
4	Temporal emissions & discharge rate profiles Details of buildings affecting dispersion, local terrain & exposure.	Local river/tidal flow patterns and turbulence patterns Temporal and spatial emissions and discharge rate profiles	

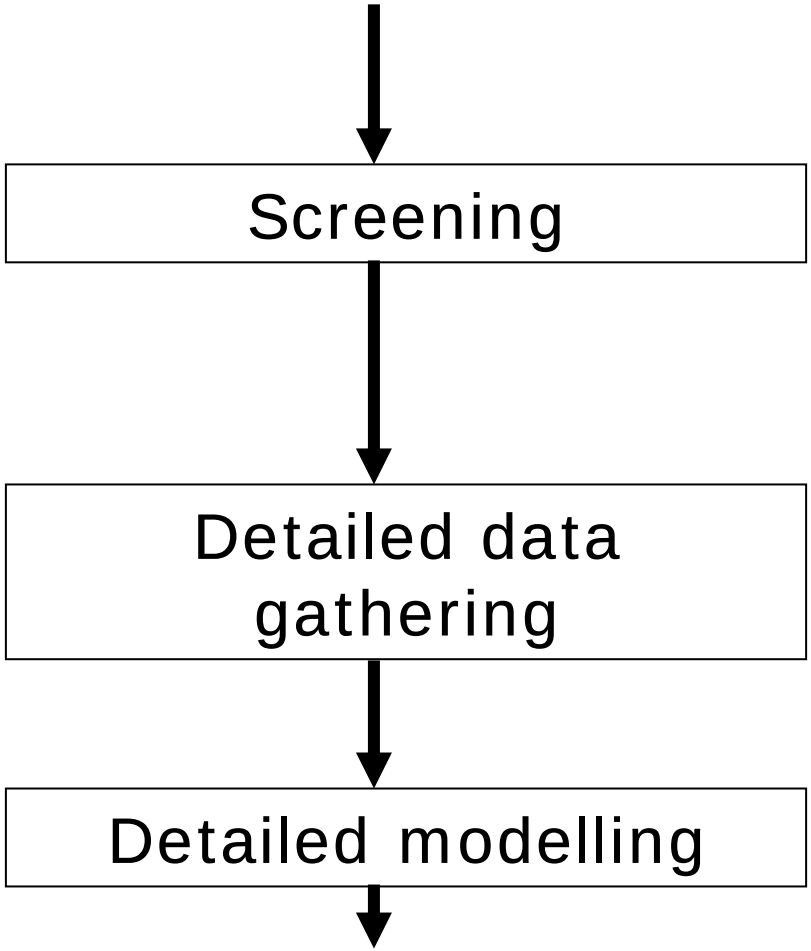
Problem with independent local scale modelling

- Requires detailed information about discharge characteristics
- Results may differ from operators own assessment used in the IPCC application
- Introduces potential conflict for the regulators
- Point made strongly at Harwell workshop
- Estimation of chemical concentrations throughout European environment requires input from operators and regulators
- Operators and regulators need “encouragement” to participate

Strategy: Feed-back / feed-forward model



Alternative strategy



How could the operators provide information?

We propose

- Additional optional fields on the EPER returns
- The fields would contain:
  - The EUSES parameter identifier e.g. PA CstdAir
  - The parameter value in SI units used in EUSES
  - A reference to the data source

Workplan: Phase 1

- Task A: Develop a prioritised list of EPER substances and run EUSES with default discharge characteristics and environmental data
- Task B: Run EUSES with sector-specific default discharge characteristics and regional environmental data
- Task C: Develop Internet website to show predicted concentrations and provide feedback
- Estimate resource requirements for detailed modelling in Phase 2

Workplan: Phase 2

- Task E: Assess feasibility of obtaining detailed information on discharge characteristics from IPPC applications
- Task F: Undertake detailed regional modelling where necessary
- Task G: Develop promotional plan

Conclusions from Phase 2

- Proposed a staged approach to assessing the chemical burden from point source emissions on Europe's environment
- Tested the feasibility of the staged approach using EUSES for an example POP, VOC and heavy metal
  - Mapped predicted concentrations
  - Compared predicted and measured environmental concentrations
- EUSES identifies whether there are significant impacts at the local, regional, continental or global scales

Conclusions from Phase 2 (2)

- EUSES identifies whether the pollutant remains in the emitting media and where cross-media transfer is important
- Greatest predicted impacts were at the local scale
- Local scale impacts depend on discharge conditions
  - Information not provided by EPER

Phase 2 conclusions (3)

- Independent local modelling will produce different results from IPPC applications-potential for conflict when reporting results
- Proposed a mechanism for operators to provide information
- Developed a workplan to achieve the aim of assessing the chemical burden from point source emissions on the European environment

Feasibility study: Modelling environmental concentrations of chemicals from emission data

European Environment Agency, Contract No. 3442/B02004.EEA.51980

AEA Technology, Harwell, UK
RECETOX - TOCOEN & Associates, Brno, CR

Expert Meeting on Modeling Chemical Concentrations in the Environment, EEA, Copenhagen, Denmark, 16 August, 2005

The purpose of the work is to develop a toolbox of available models, together with a work plan for enabling their use in conjunction with chemical emissions data, to predict the concentrations, composition, and distribution of chemicals controlled under Council Directive 96/61/EC concerning integrated pollution prevention and control.

Feedback on the report from the Brno Summer school

Summer School of Environmental Chemistry and Ecotoxicology

Approaches to the study of relationships between environmental levels of chemicals and their biological effects with special attention to the persistent, toxic substances

A. Environmental chemistry and exotoxicology of PTS

B. Modelling the environmental distribution of PTS

Brno, Czech Republic, 09-16/07/2005

Centre of Excellence

Feedback on the report from the Brno Summer school

Reviewers:

- Prof. Michael McLachlan, Stockholm University, Sweden
- Dr. Gerhard Lammel, Max Planck Institute, Hamburg, Germany
- Prof. Victor Shatalov, EMEP MSC-East, Moscow, Russia
- Dr. Johannes Ranke, University of Bremen, Germany
- Dr. Martin Scheringer, ETH, Zürich, Switzerland

General Comments

The report is well written and that the strategy adopted is in general good, collection of models is useful and interesting

Feedback on the report from the Brno Summer school

- **The review does not adequately address the key issue of steady state / non-steady state.**
- **However, these models will not be appropriate for higher tier assessment e.g. reconciling model predictions with measured concentrations.**
- **Furthermore, for persistent chemicals non-steady state models should have a key role in higher tier risk assessment, as monitoring will only give a snap shot.**
- **The future development of the environmental concentrations can only be evaluated with a non-steady state model.**

Feedback on the report from the Brno Summer school

- There may also be some limitations to using the standard **EUSES parameterization**.
- Emission data of organic chemicals, e.g. as reported by signatory states to the UNECE CLRTAP under the POPs Protocol or based on expert estimates, are considered to be very uncertain and vary between substances.
- The **mode of entry** (split among receptor compartments) is unknown for many relevant substances.
- The compartmental distribution as predicted by multimedia models (levels III and IV), however, is strongly influenced by the **mode of entry.**

Feedback on the report from the Brno Summer school

- **Region-specific models should be capable to account for the variety of significant mass transfer and partition coefficients in the region and for advection from the boundaries of the region.**
- **Application of EUSES - the fate model within the EUSES expert system is many years old nowadays; it is a good tool for doing risk analysis for a generic region, but it would be necessary to devise an alternative strategy based on a spatially resolved model with meteorological input data.**
- **EMEP model – will be presented by Sergey Dutchak**

Feedback on the report from the Brno Summer school

- **It is not sufficiently clear what the purpose of the intended modeling activity is**
- **Definition of chemical density**
- **Possible purposes of modeling studies, definition of modelling strategy – Martin Scheringer**

Role and requirements for detailed modelling

Sergey Dutchak
EMEP/MSC-E

Persistent Toxic Substances (PTS) modeling

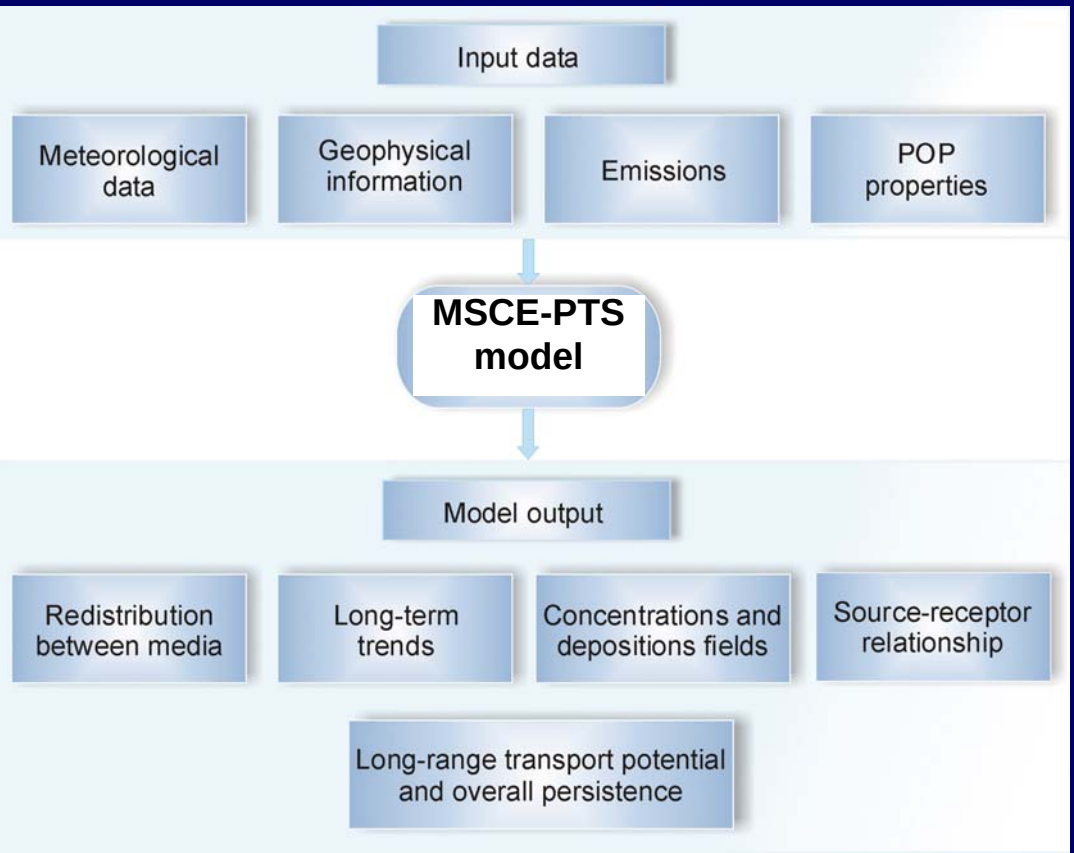
BOX MODELS

ChemRange	Switzerland
CliMoChem	Switzerland
GLOBO-POP	Canada
SimpleBox	Netherlands
EVN-BETR and UK-MODEL	UK
ELPOS	Germany
G-CIEMS	Japan

DETAILED TRANSPORT MODELS

CAM/POPs MEDIA	Canada
DEHM-POP	Denmark
MSCE-PTS	EMEP/MSC-E
ADOM-POP	Germany
HYSPLIT 4	USA
CMAQ	USA

Generic structure of EMEP / MSC-E model



List of PTS

POPs

PCBs, D&Fs, HCB, PAHs, γ-HCH

New substances

HCBD, PeCB, PCP, PCN-47, dicofol, α- and β- endosulfans and BDE-28, BDE-47 and BDE-99. . .

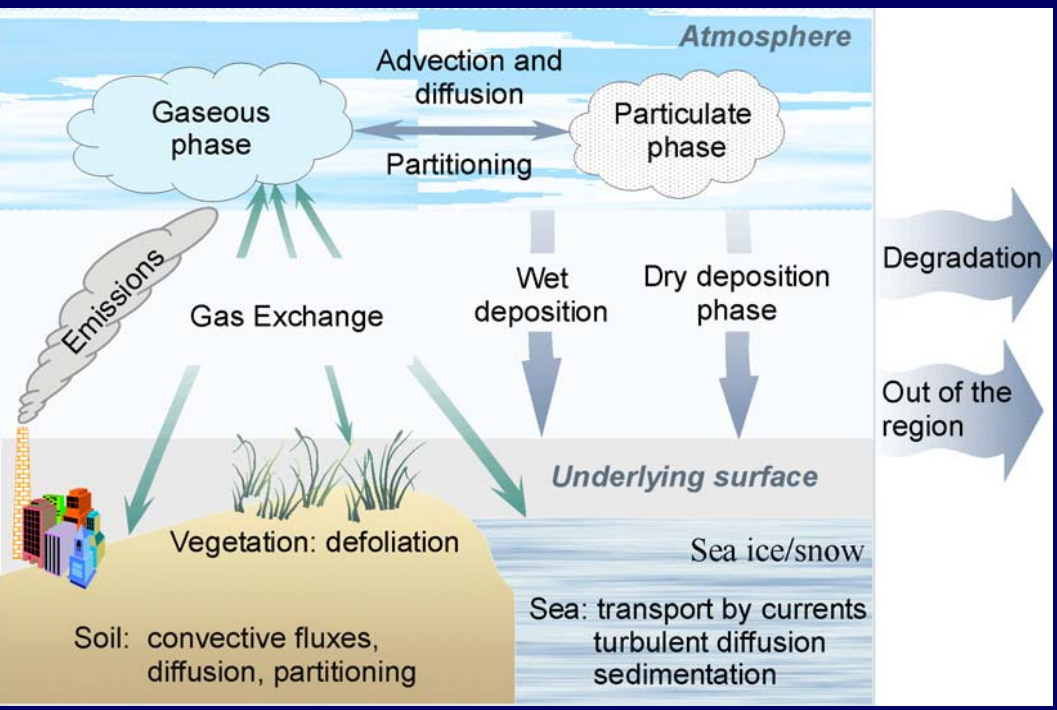
HMs

Pb, Cd, Hg

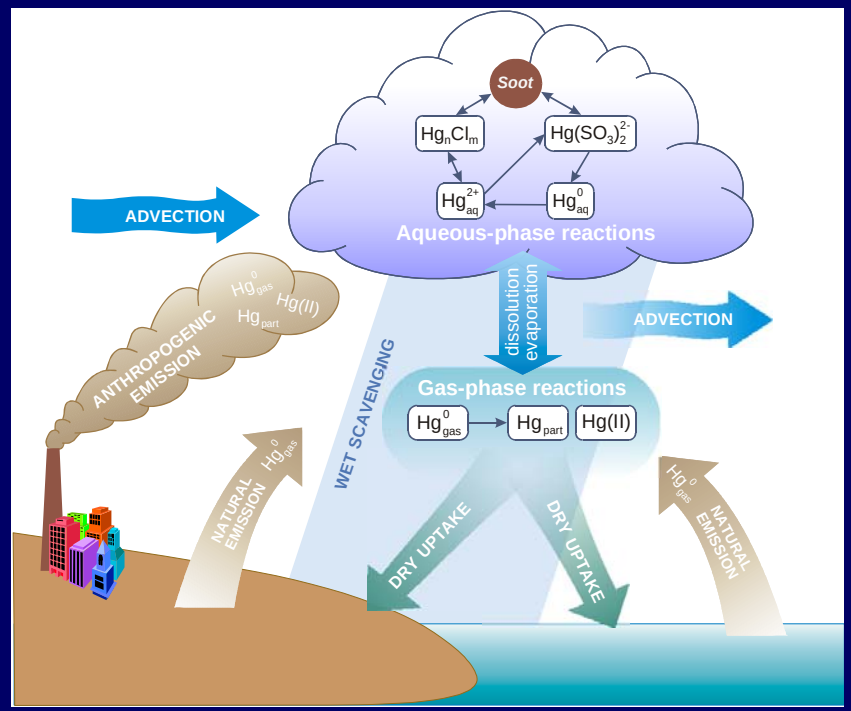
New substances

Ni, Cu, As, Cr, Zn, Se . . .

The structure of multicompartment model

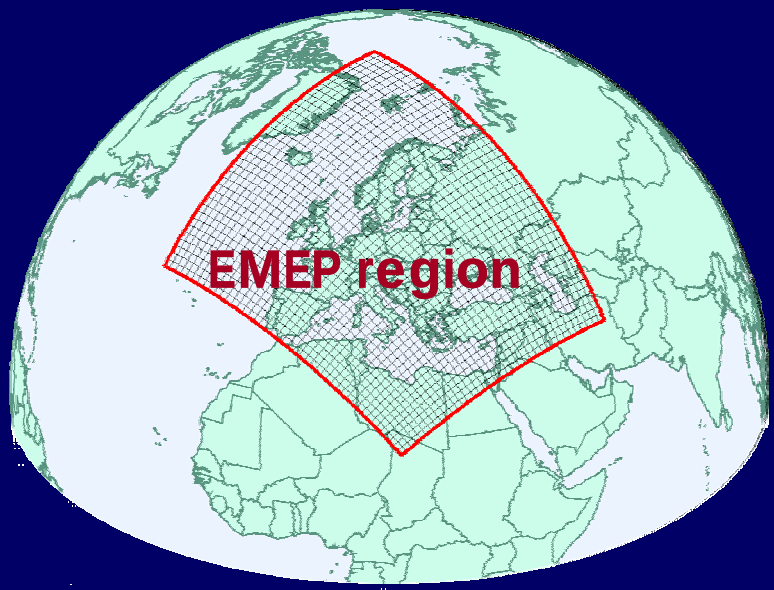


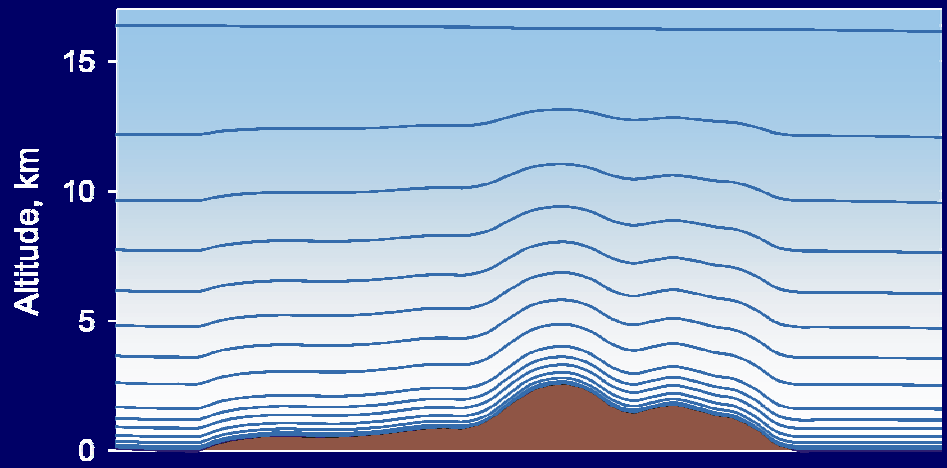
Model compartments and processes



Atmospheric chemistry module

Computation domain





Regional model – 3d Eulerian type

- Coverage – EMEP region
- Resolution – 50×50 km^2

Hemispheric model – 3d Eulerian type

- Coverage – Northern Hemisphere
- Resolution – 2.5°×2.5°

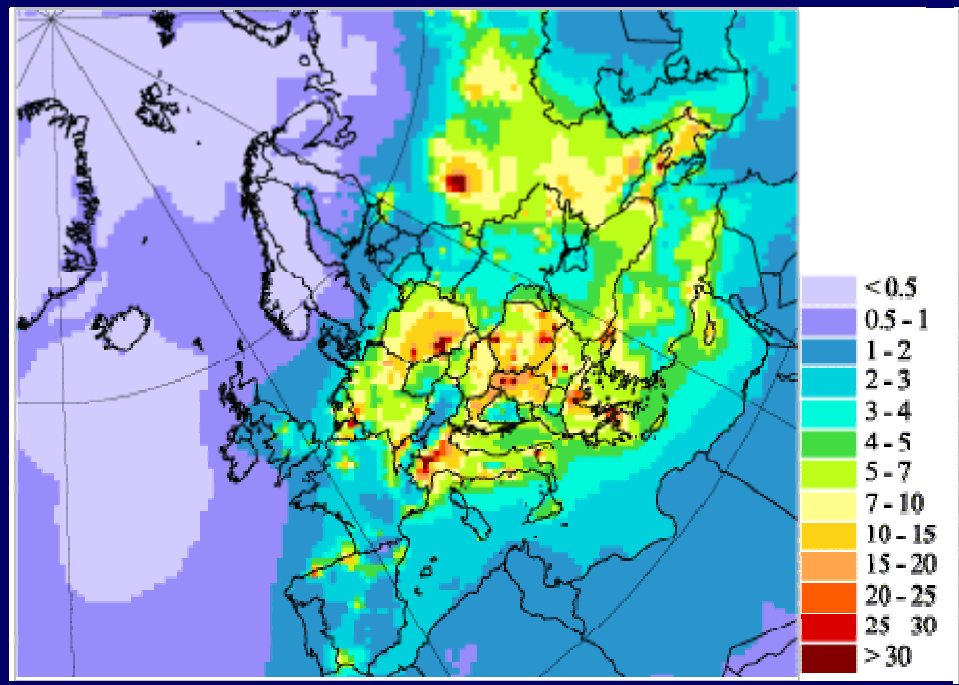
Vertical structure:

- (σ-p) coordinate system
- 15 layers up to 15 km
- First layer height ~ 70 m

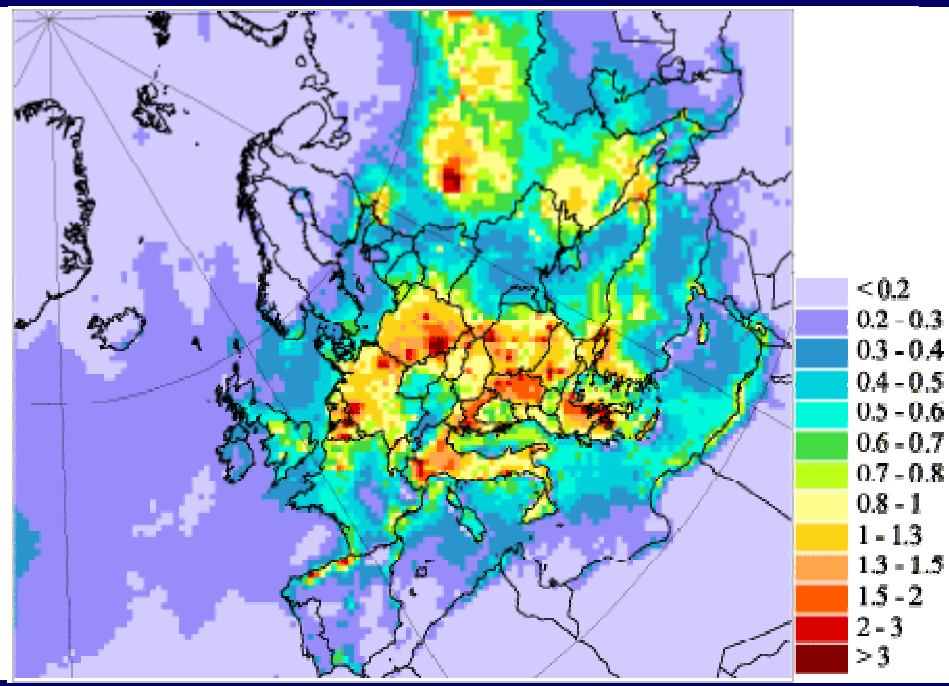
Model application

- Annual concentration and deposition level in Europe
- Background pollution level for countries or specific locations
- Concentrations and depositions from source categories
- Deposition to different underlying surface (grass, forest …)
- Mass balance
- Concentrations in different environmental media (soil, seawater, vegetation)
- Source-receptor relationship and transboundary transport
- Long-term trends
- Seasonal (monthly) variations
- Short-term episodes (days)
- Projections and scenario
- Evaluation of new substances

Annual pollution levels in Europe, 2002



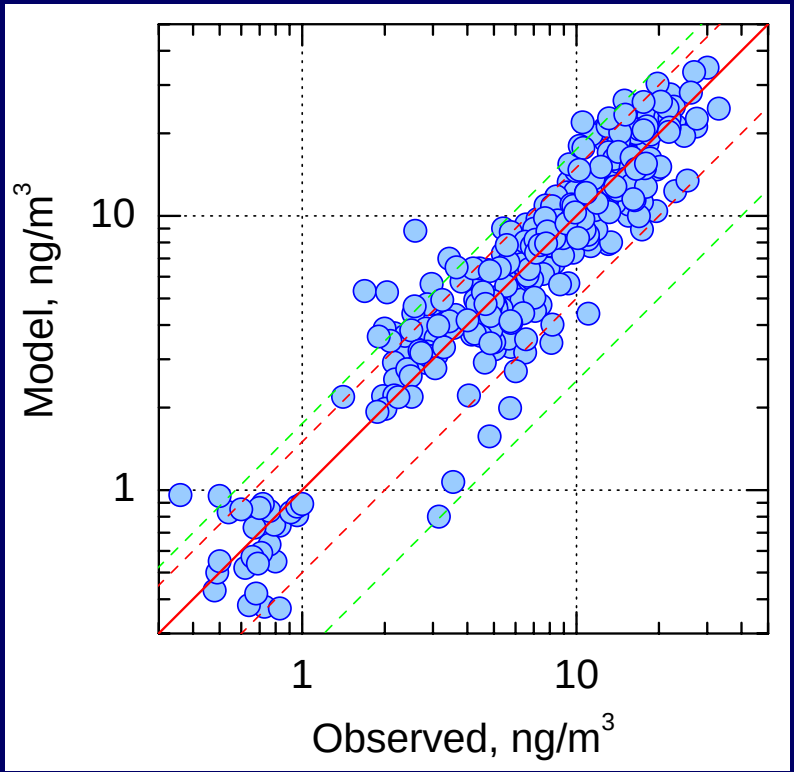
Annual mean air concentrations of lead in 2002, ng/m^3



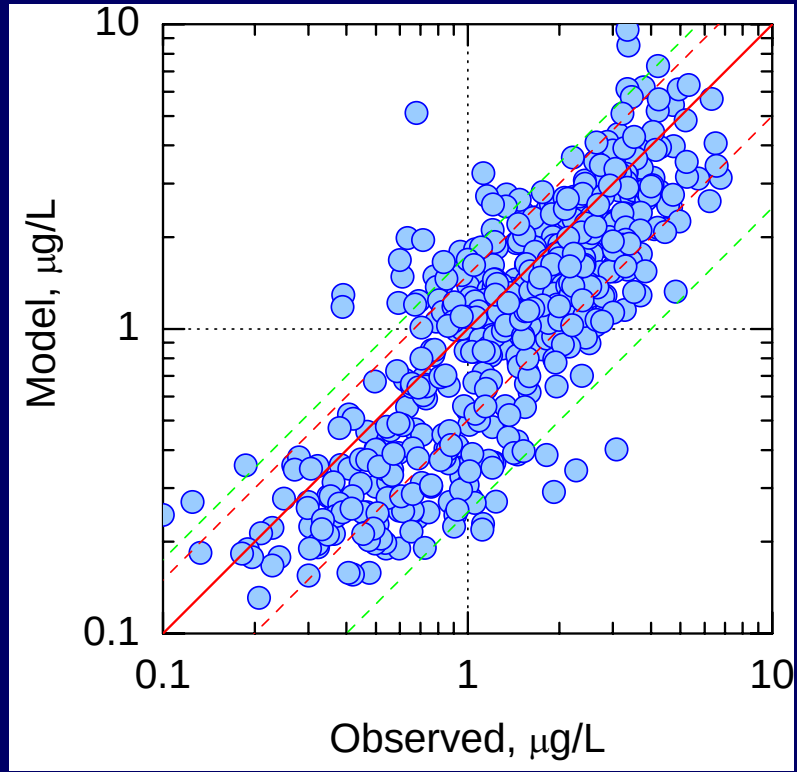
Total (dry and wet) deposition of lead in 2002, kg/km^2/y

Model validation

in air

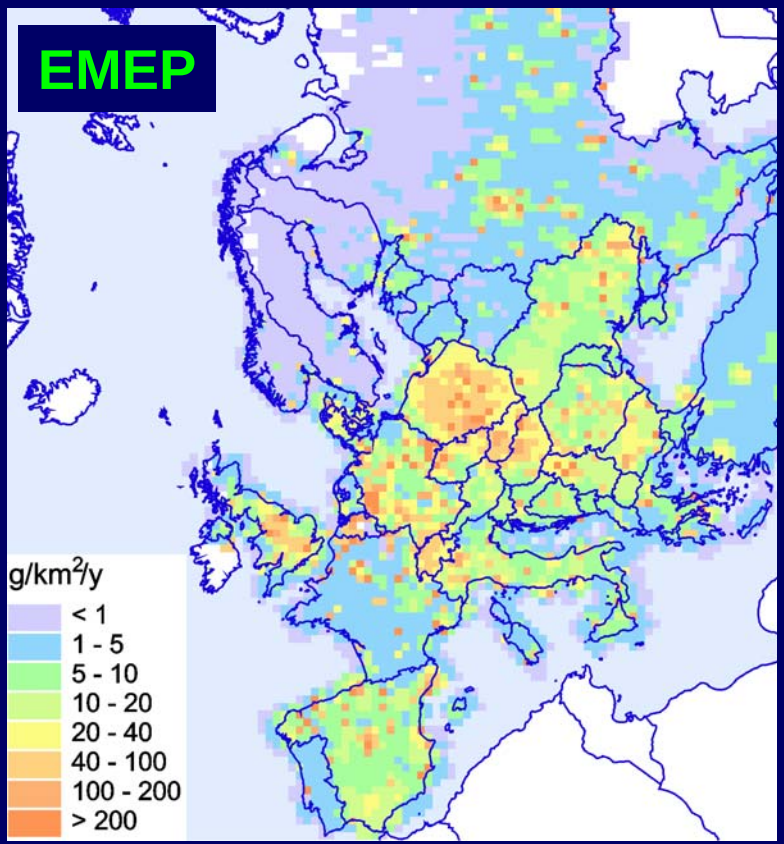


in precipitation

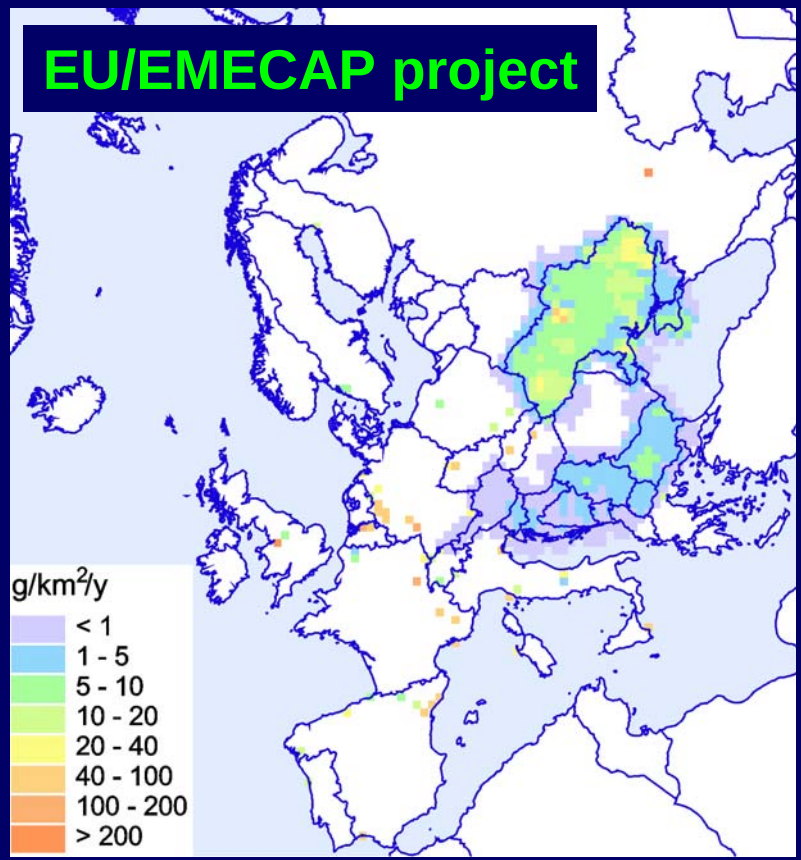


Comparison of annual mean modelled and measured concentrations of lead for 1990–2003

Contribution of source-categories (chlor-alkali plants)

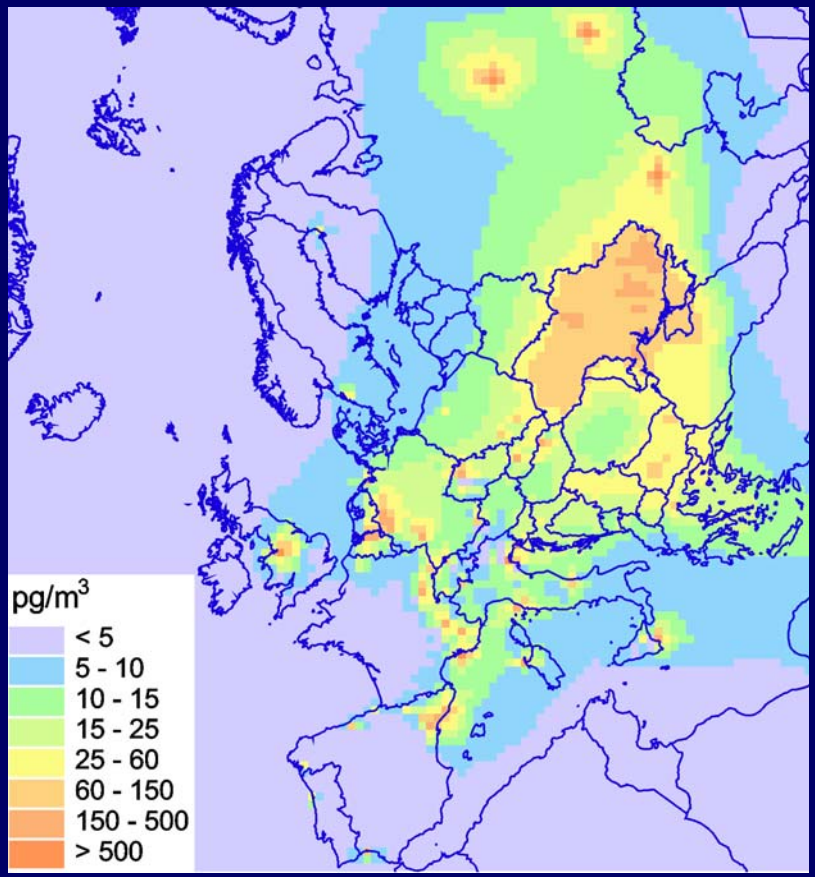


Spatial distribution of mercury anthropogenic emissions in Europe in 2000 with resolution 50x50 km^2

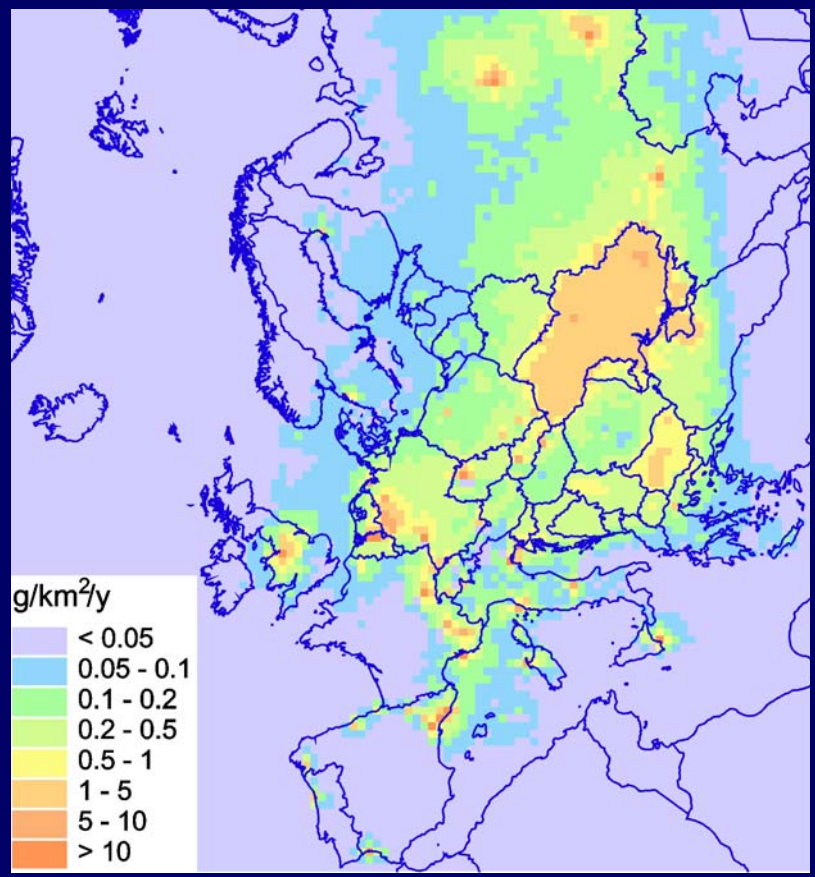


Mercury emissions from chlor-alkali production in Europe in 2000 (point sources with exception for some south-east European countries)

EU/EMECAP project

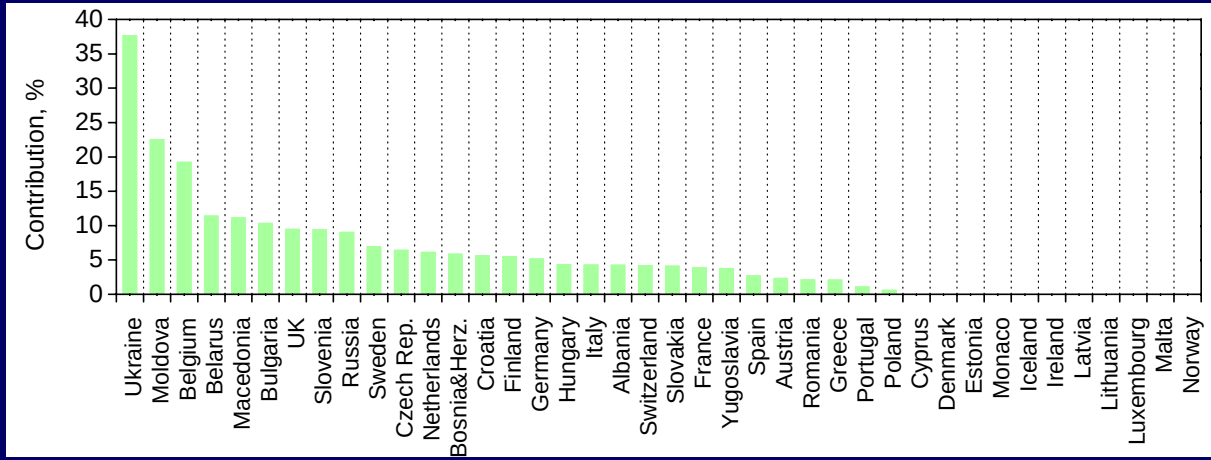


Mean annual concentration of total gaseous mercury in the ambient air from emissions of chlor-alkali plants in Europe, 2000

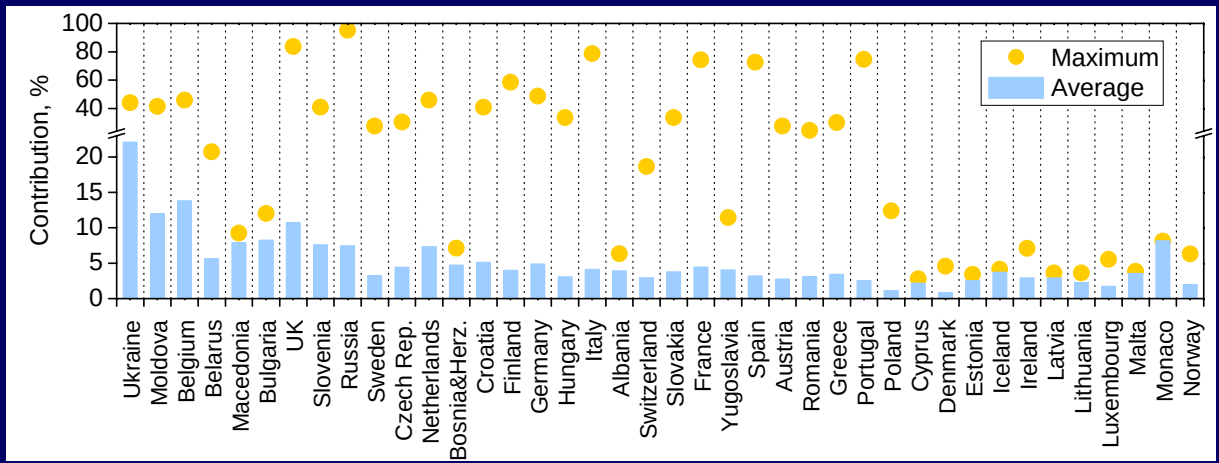


Annual mercury deposition from emissions of chlor-alkali plants in Europe, 2000

EU/EMECAP project



Relative contribution of chlor-alkali plants to total anthropogenic emissions of mercury in European countries in 2000

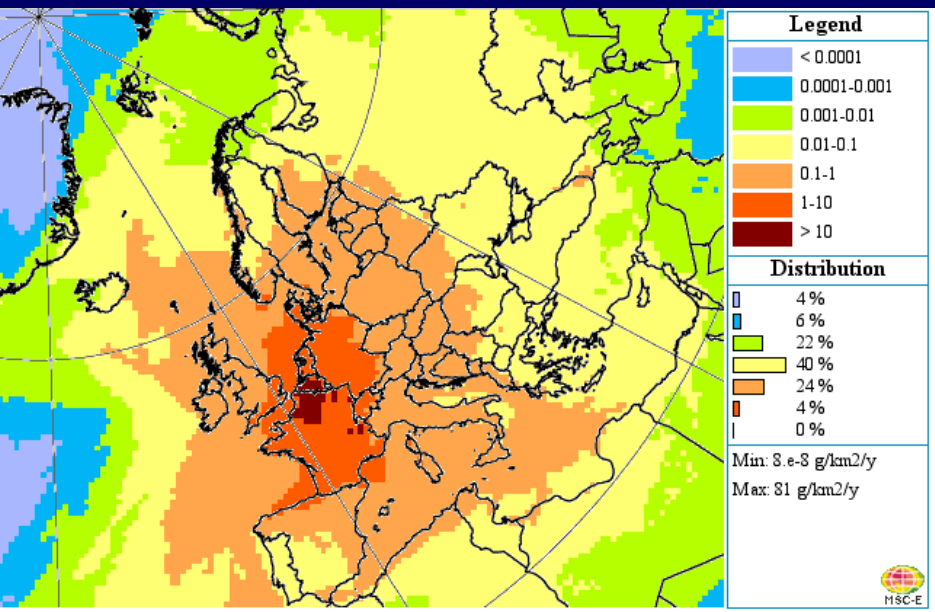


Relative contribution of chlor-alkali plants to deposition of anthropogenic mercury to European countries in 2000

EMEP/MSC-E

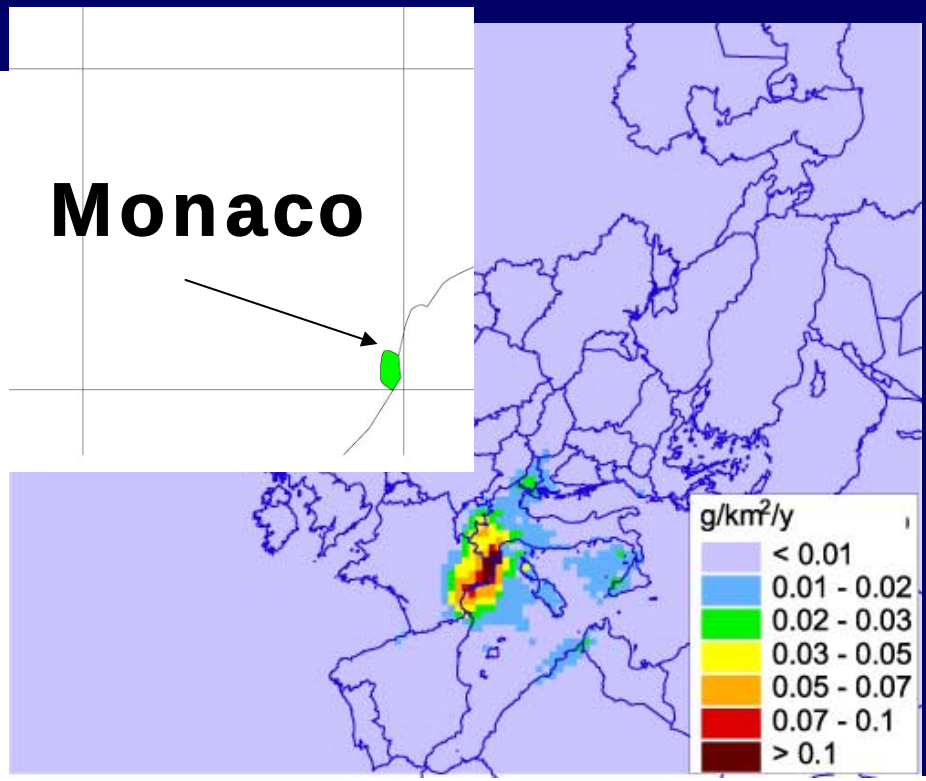
Source –receptor relationship

Cadmium



From national sources of **France** in 2002, g/km²/y

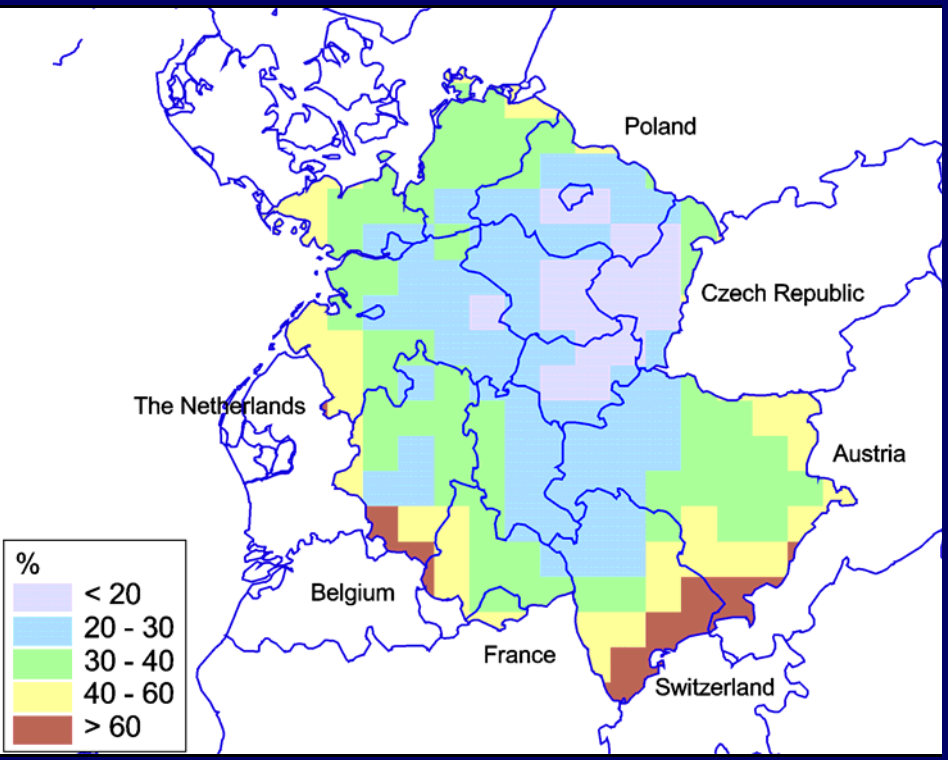
Lead



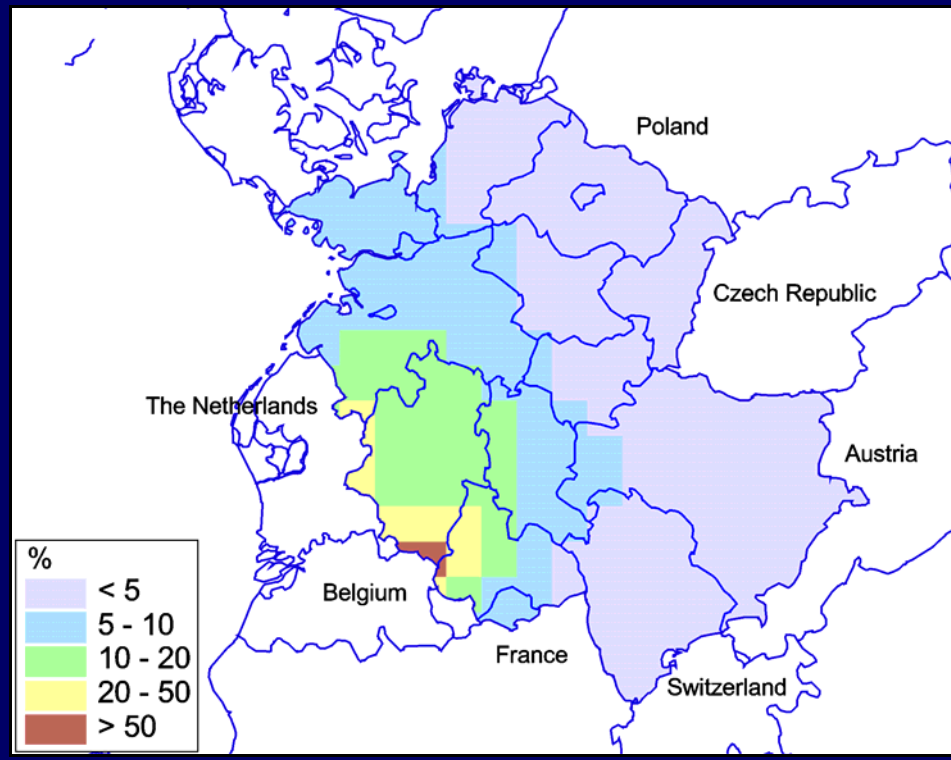
From national sources of **Monaco** in 2002, g/km²/y

Atmospheric transport from different sources

Background levels

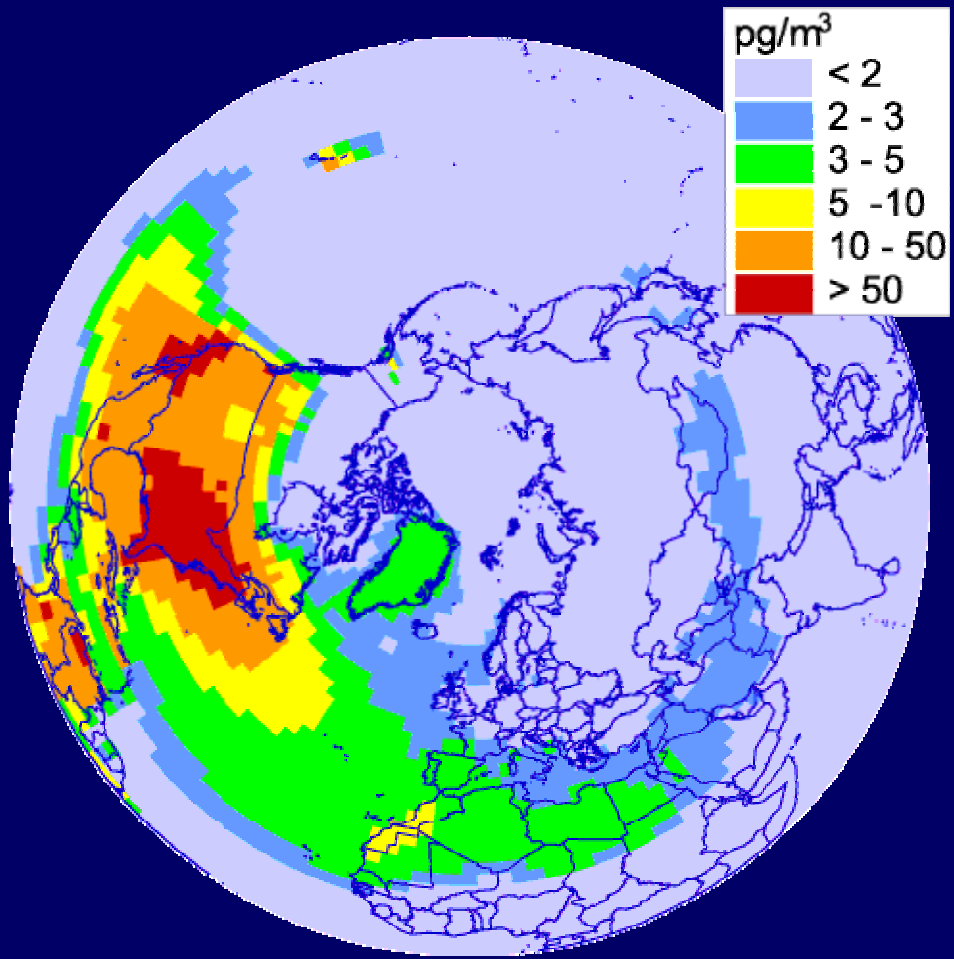


Contribution of external European anthropogenic sources to depositions of lead in Germany in 2002



Contribution of external anthropogenic sources from Belgium to depositions of lead in Germany in 2002

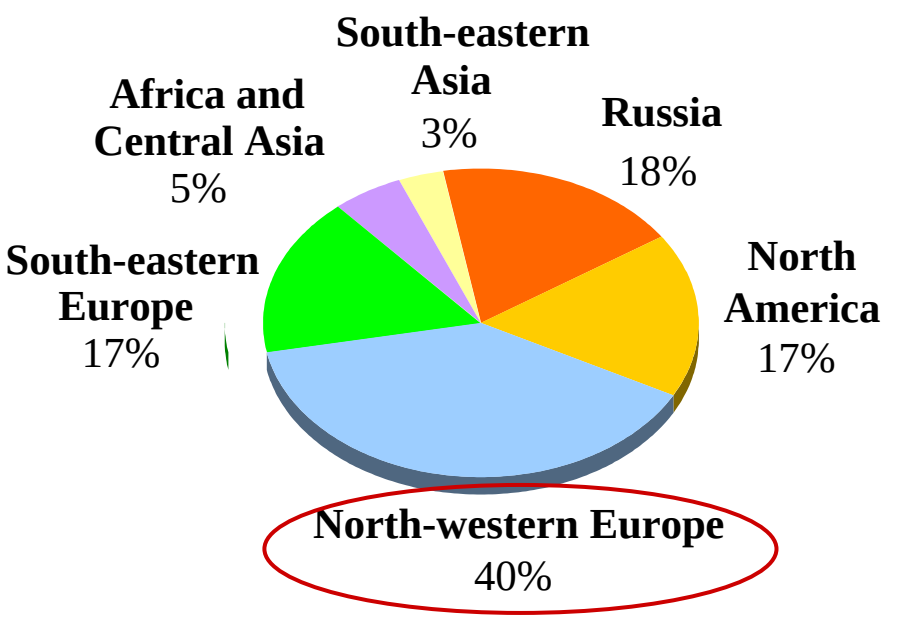
Background levels



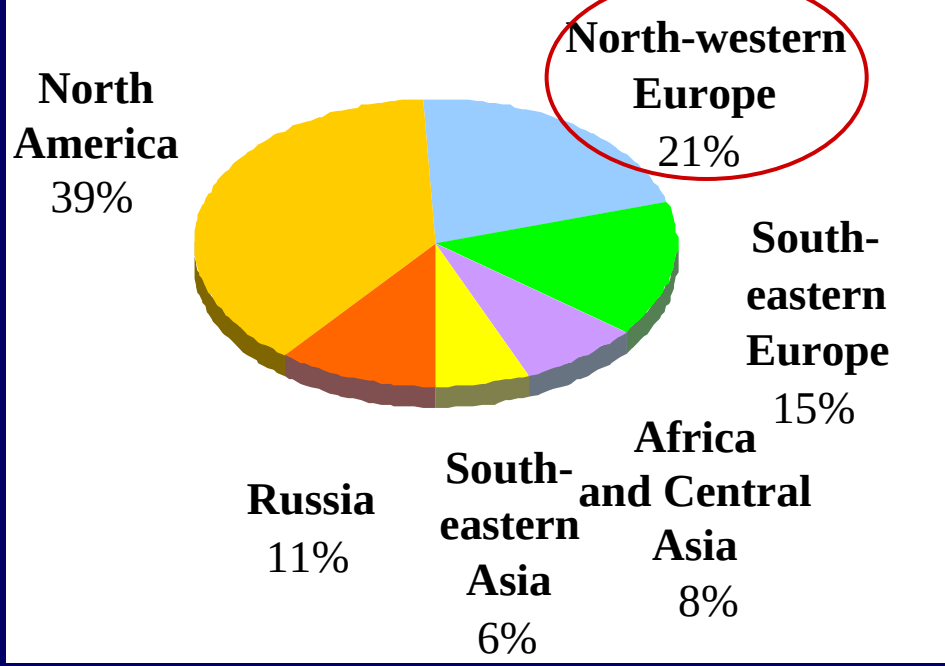
Intercontinental transport of PCB-153 from North America

Source-receptor relationships at the hemispherical scale

Deposition to the Arctic



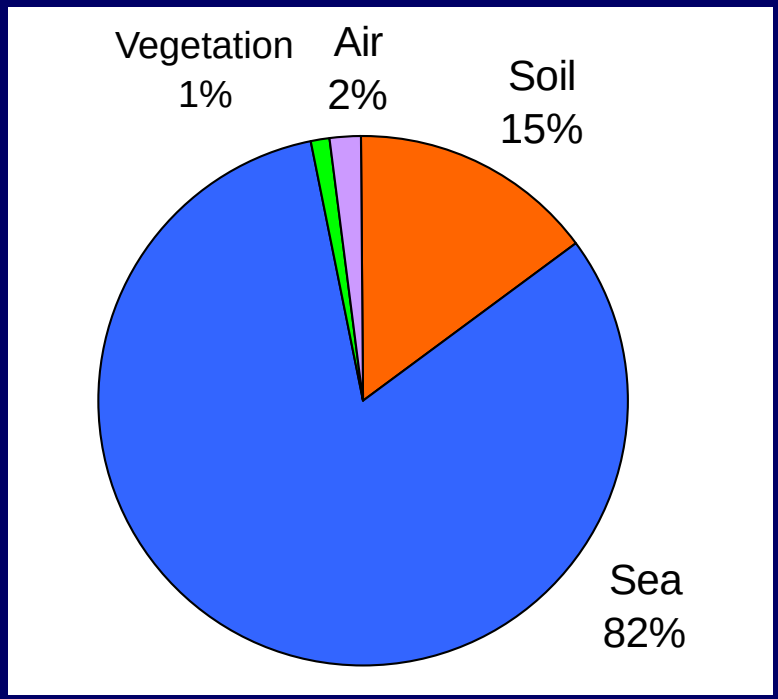
Canadian Arctic



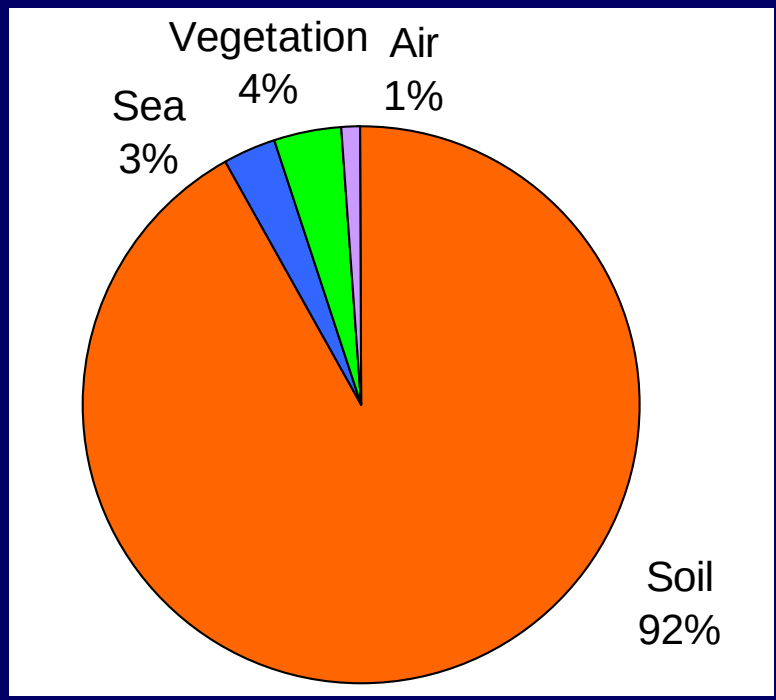
Contributions of main source groups to PCBs deposition to the Arctic

Mass balance

γ-HCH

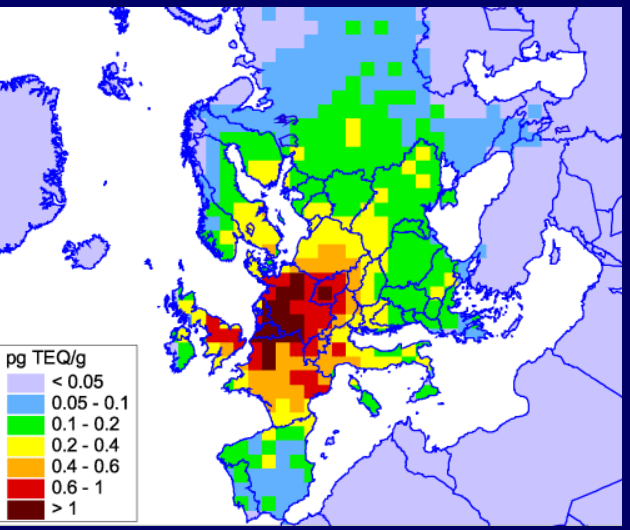


PCB-153

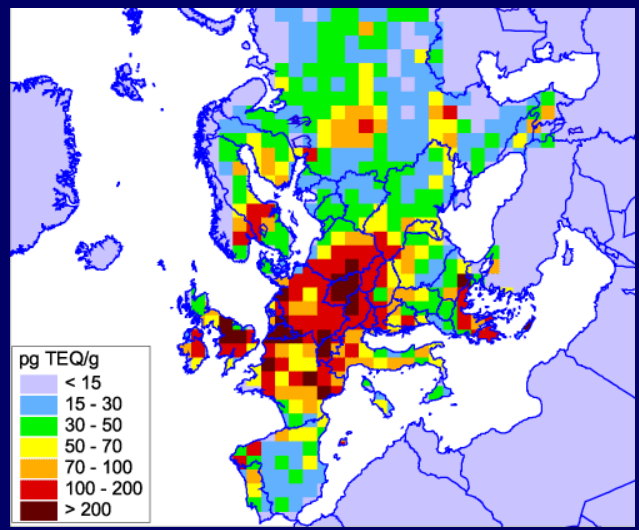


Distribution of pollutants between media depending physical-chemical properties (11 years calculation period)

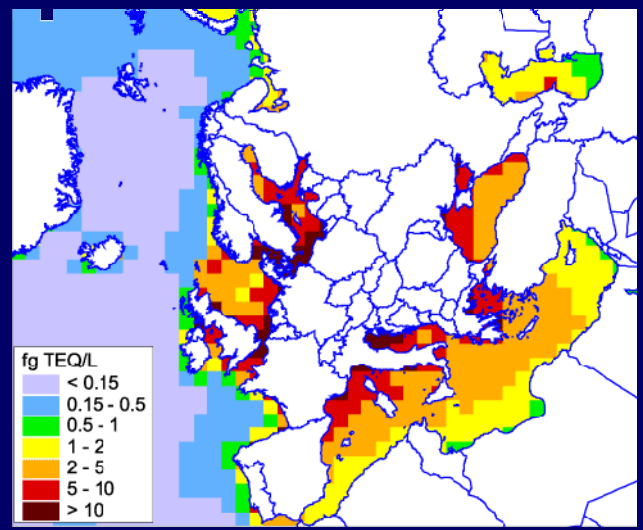
Spatial distribution of PCDD/Fs concentrations in different compartments in 2001



Soil

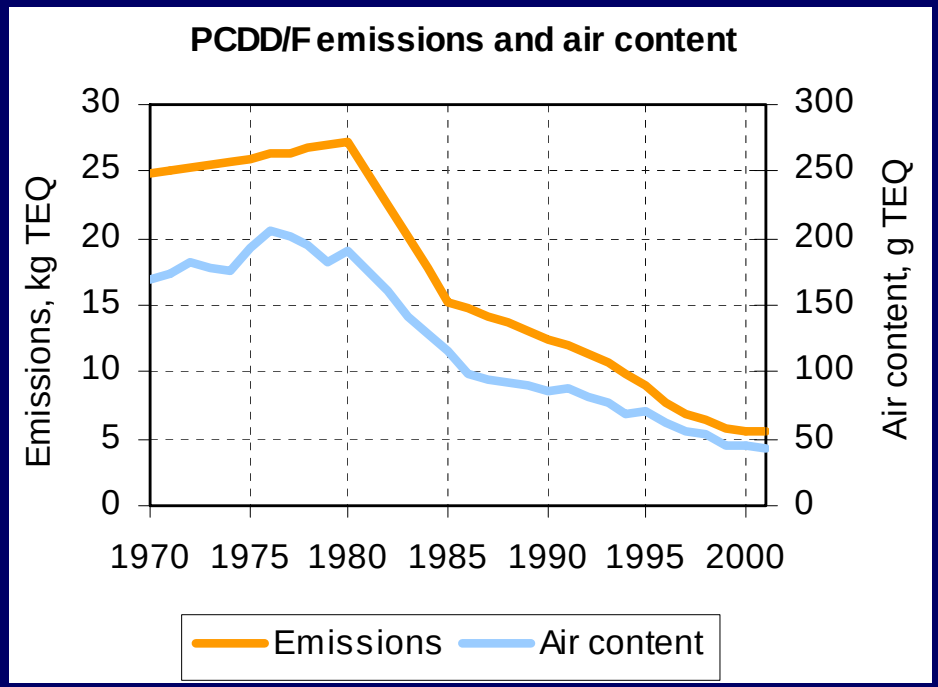


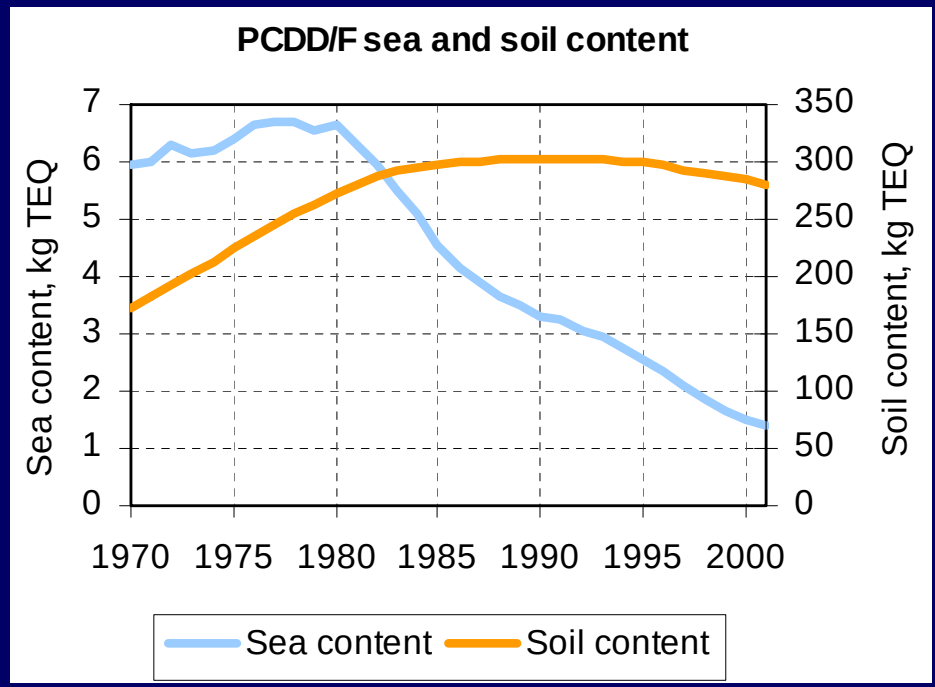
Vegetation



Seawater

Long-term trends of contamination

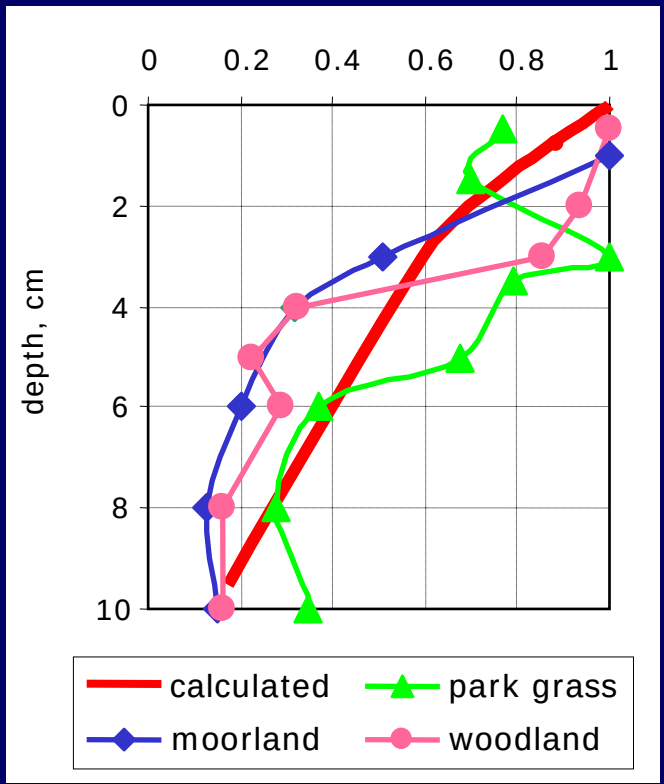




Trend of PCDD/Fs content in the main environmental compartments as compared with that of emissions in Europe for a period from 1970 to 2001

Vertical profile of soil concentrations

Calculated PCB-153 vertical soil concentration profiles in comparison with measurements at three locations in the UK; relative units

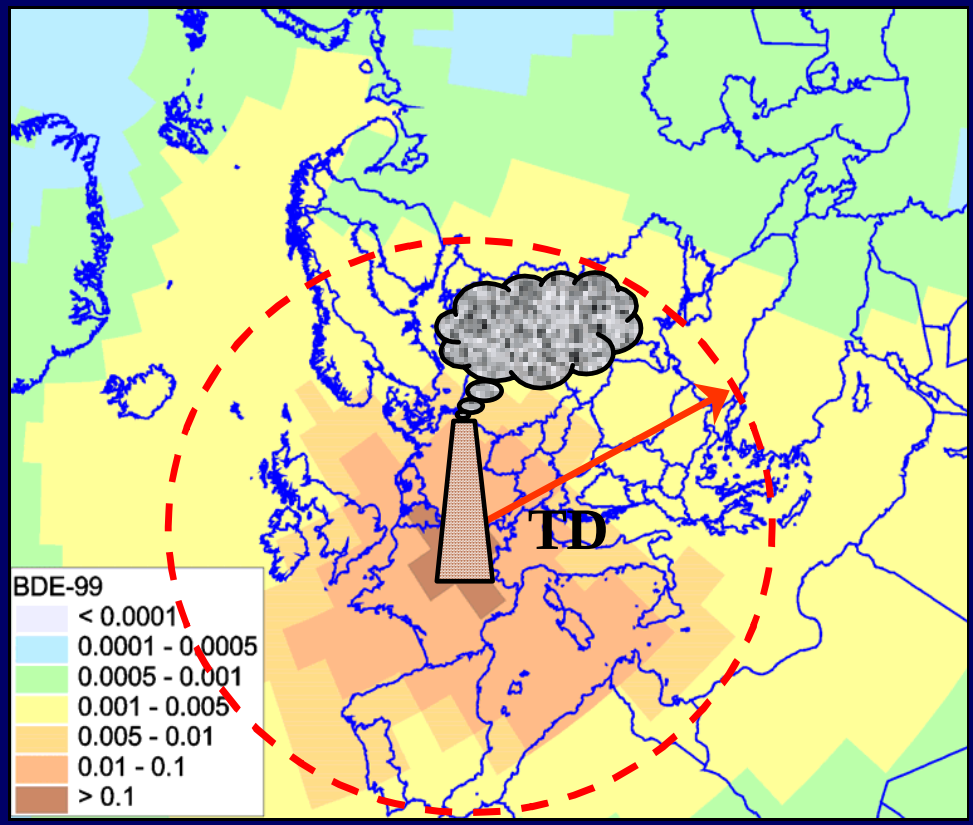


Measurements taken from: Cousins I.T., B.Gevao and K.C.Jones, *Chemosphere*, v.39, No.14, 1999

Model assessment of new substances

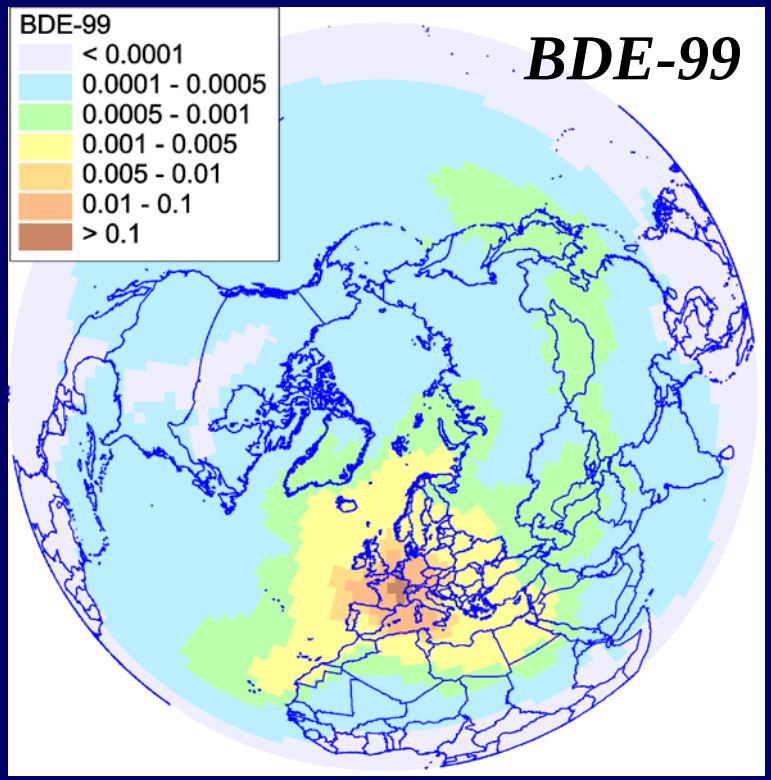
hexachlorobutadiene (HCBD), pentachlorobenzene (PeCB), pentachlorophenol (PCP), polychlorinated naphthalenes (PCN-47 congener), dicofol, α- and β- endosulfans and polybrominated diphenyl ethers (BDE-28, BDE-47 and BDE-99) . . .

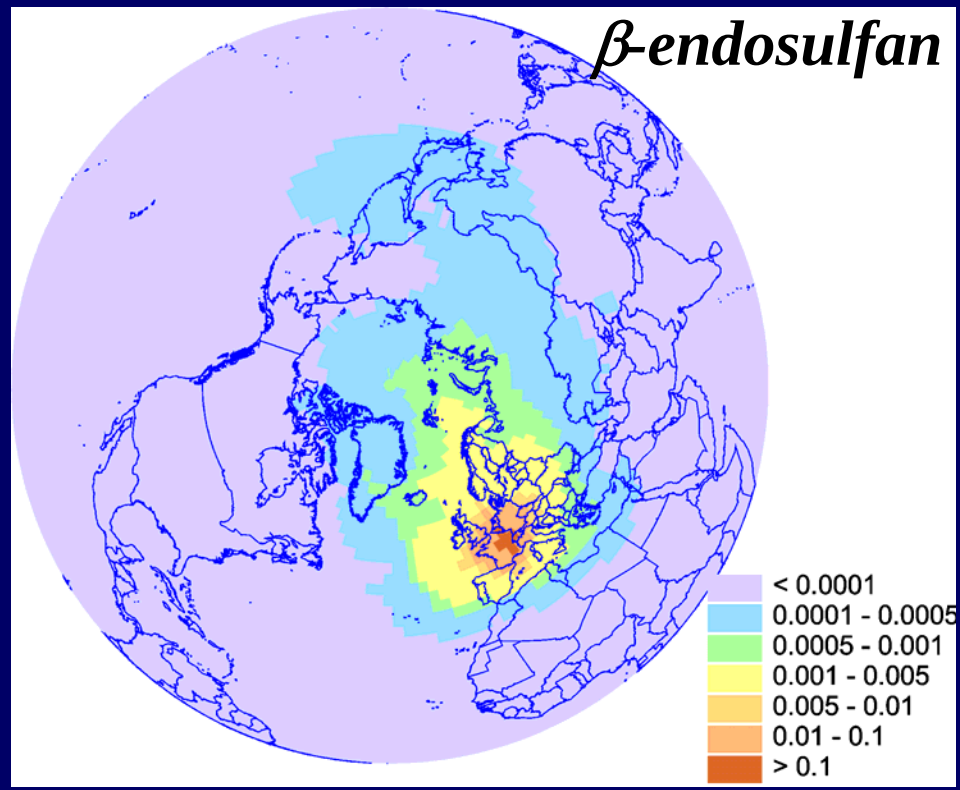
Transport and spatial distribution of pollutants from point source



TD - distance from the source at which annual mean atmospheric concentration of a chemical in question drops 1000 times compared with the concentration near the point source

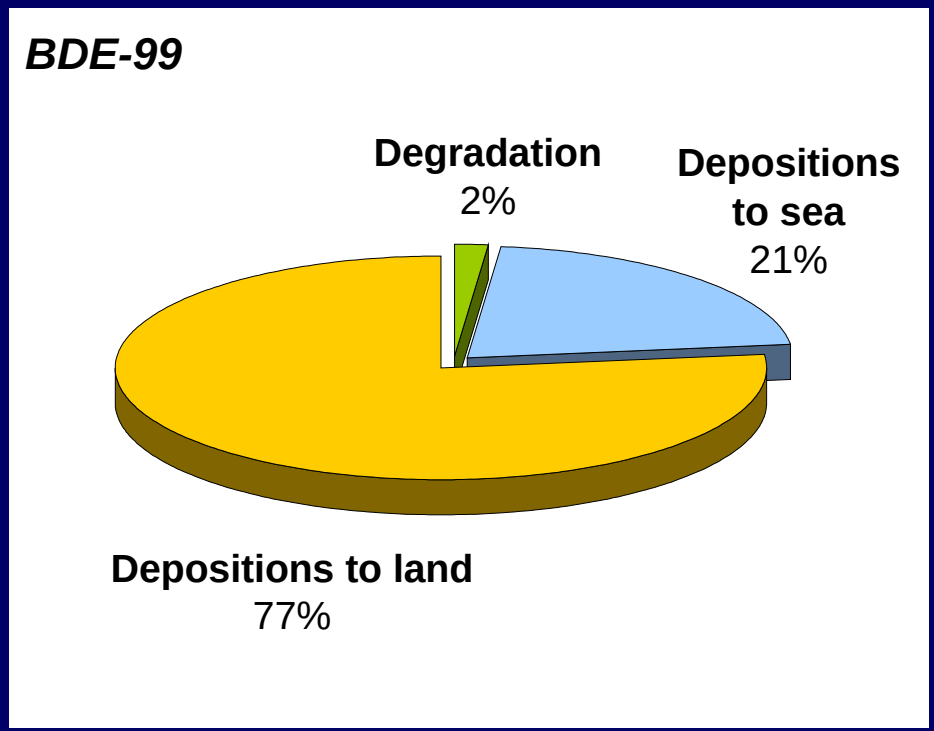
Evaluation of new substances

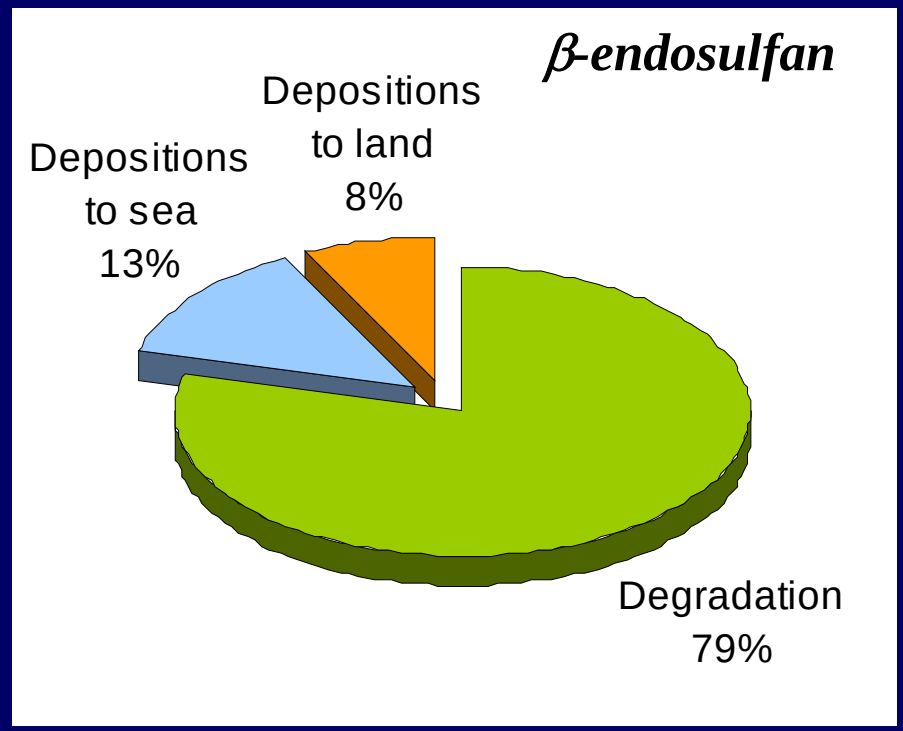




Spatial distribution of air concentrations in the Northern Hemisphere from point source 1 t per year located in France, Paris

Evaluation of new substances

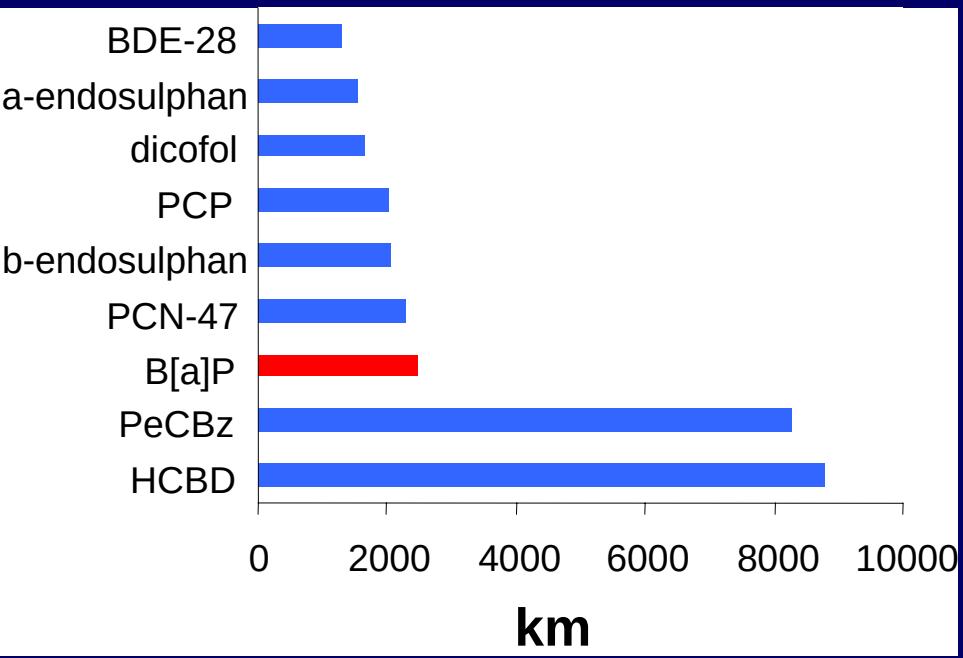




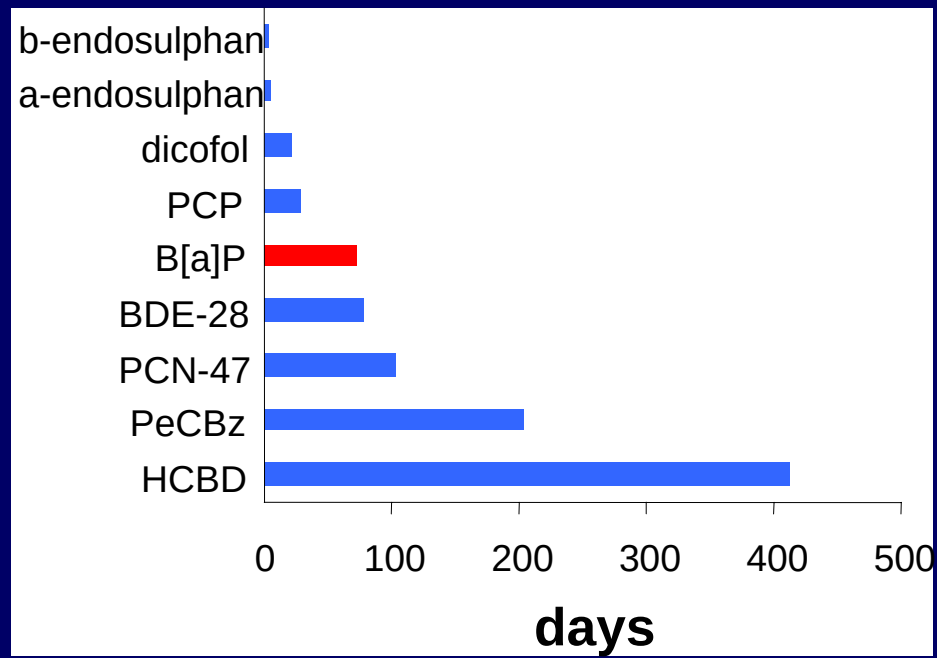
Calculated annual balance of BDE-99 and β-endosulfan removal from the atmosphere

Evaluation of new substances

Transport distance



Overall persistence



Scientific validity

Annual consideration of technical and scientific work on modelling at meetings of EMEP Task Force on Modelling and Measurement

- Workshops and conferences
- Scientific publications
- Model intercomparison
- Comparison of modelling results against measurements
- Model sensitivity studies
- Detailed model description

EMEP / MSC-E Scientific and Technical publications

Model description and sensitivity study

- Regional Multicompartment Model MSCE-POP - 5/2005
- Regional Model MSCE-HM of Heavy Metal Transboundary Air Pollution in Europe - 6/2005

Model intercomparison

- Methodology and Results for Pb in 1990 2/96
- Model intercomparison study for cadmium. 2/2000
- Intercomparison Study of Numerical Models for Mercury. Stage I–III – 2000-2005

New Substances

- Model Assessment of PentaBDE – 10/2004
- Model Assessment of Endosulfan – 11/2005

Articles

- *Environmental Science and Pollution Research, 2002* "Regional background monitoring of PBT compounds. The comparison of the results from measurements and modelling."
- *Atmospheric Environment, 2003* "Comparison of mercury chemistry models"
- *Environmental pollution, 2004*
  "Numerical evaluation of the PCBs transport over the Northern Hemisphere"

Transparence of information

- Emissions
- Measurements
- Model output
- Model description

Model requirements

Emission data	Gridded emission data 50x50 km^2 (EMEP), low and high sources, point-sources
Meteorological data	MM5, NSEP/DOE and ECMWF re-analysis data
Land use/Land cover	Based on CORINE and SEI database, EUNIS classification, LAI/NASA
Physical-chemical properties of pollutants	Literature sources
Environmental properties	Air – OH-radical and aerosol concentrations Soil – Organic content, volumetric water content Sea – currents, ice cover, organic matter, thickness of upper of mixed layer

Computer resources

Personal computer based on PC AMD Atlon 64 3800+ (2.4. GHz)

Softwhere: Windows, Excel, ArcView, Winword, Dreamveawer

Computer time for calculations of deposition and concentrations fields for 1 year from point source or group of sources:

for Northern Hemisphere:

POPs/HMs ~ 3 h (resolution 2.5^o x 2.5^o)

for Europe:

HMs ~ 7 h
POPs and Hg ~ 24 h (resolution 50 x 50 km^2)

EMEP emission database (model requirements)

Minimum reporting / yearly

National totals and NFR sector emissions

Minimum reporting / five yearly

Energy consumption data

Electricity and heat production and consumption

Energy consumption data for transport sector

Agricultural activity data

Gridded national totals

Gridded sector data for each of the relevant aggregated NFR sector

Large point sources

LPS data for each relevant aggregated NFR

Additional reporting

Height distribution

Land-use data

Mercury breakdown

% of toxic congeners of PCDD/F

Other HMs and POPs

Natural emissions

Pre- 1990 emissions of PAHs, HCB, PCDD/Fs and PCB (historical emissions)

Meteorological data

PSU/NCAR mesoscale model MM5

There are several useful features of this system:

- This system can work with different sets of initial meteorological data (NCEP/DOE and ECMWF re-analyses etc.)
- Various parameterisations of physical processes (atmospheric boundary layer, precipitation, radiation transfer etc.) are available.
- This system allows operations in different map projections. In particular, the polar stereographic projection is supported.
- Nesting is available in this system. A user can perform calculations both on regional and local scales on the base of the same data assimilation system.
- The MM5 community model is spread worldwide and tested for various geographical and climatic regions. Besides, the model improvement and development are going on.
- This system can be deployed on a personal computer and can provide simulations of meteorological data for reasonable time.

Research Perspectives on Modeling Strategies

Martin Scheringer
Swiss Federal Institute of Technology, Zürich
European Environment Agency, August 16, 2005

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Safety and
Environmental
Technology Group

What is a Model?

- All models are simplifications of reality.
  Here: environmental fate models
- Selection of processes
  - Considered **relevant** for the problem investigated;
    here: phase partitioning, degradation, transport, bioaccumulation
  - **Quantitatively** described within a consistent mathematical framework;
    here: mass balance equations for a chemical in different media
- Solution of the model:
  - Calculate masses of a chemical in all compartments of the model as function of time

Model Choices

- Type of model:
  - Models with high temporal and spatial resolution
    - ➔ Higher computational effort
    - ➔ More environmental and chemical-specific parameters to be known
  - Box models (lower resolution)
- Model purpose:
  - „realistic“ description of the environment: **simulation models**
    - ➔ Prediction of concentrations
  - Sketch of the environment: **evaluative models**.
    - ➔ Understanding of processes and their interplay;
    - ➔ Compare environmental fate of different compounds,
    - ➔ „Screening“, „Ranking“ of chemicals.
- Scope, geometry
  - Local, regional, global models

Recent Developments in Modeling

- Many new models available
- Computer hardware improved
- Modeling software improved
- Setting up a new model easy to do
- Running a model easy to do
- But ...

Recent Developments in Modeling

- Many new models available
- Computer hardware improved
- Modeling software improved
- Setting up a new model easy to do
- Running a model easy to do
- But ...
- ... what are fruitful modeling strategies?

Five Elements of a Modeling Strategy

- Define model **purpose**
  - Model quality determined by fit of model and purpose
- Make model **transparent**
  - Sensitivity and uncertainty analyses
- Include findings from **recent environmental research**
  - Evaluate influence of improved process descriptions
- Relate model to **other models**
  - Model comparison methods
- Relate model to **field data**
  - Select appropriate data

Model Purpose

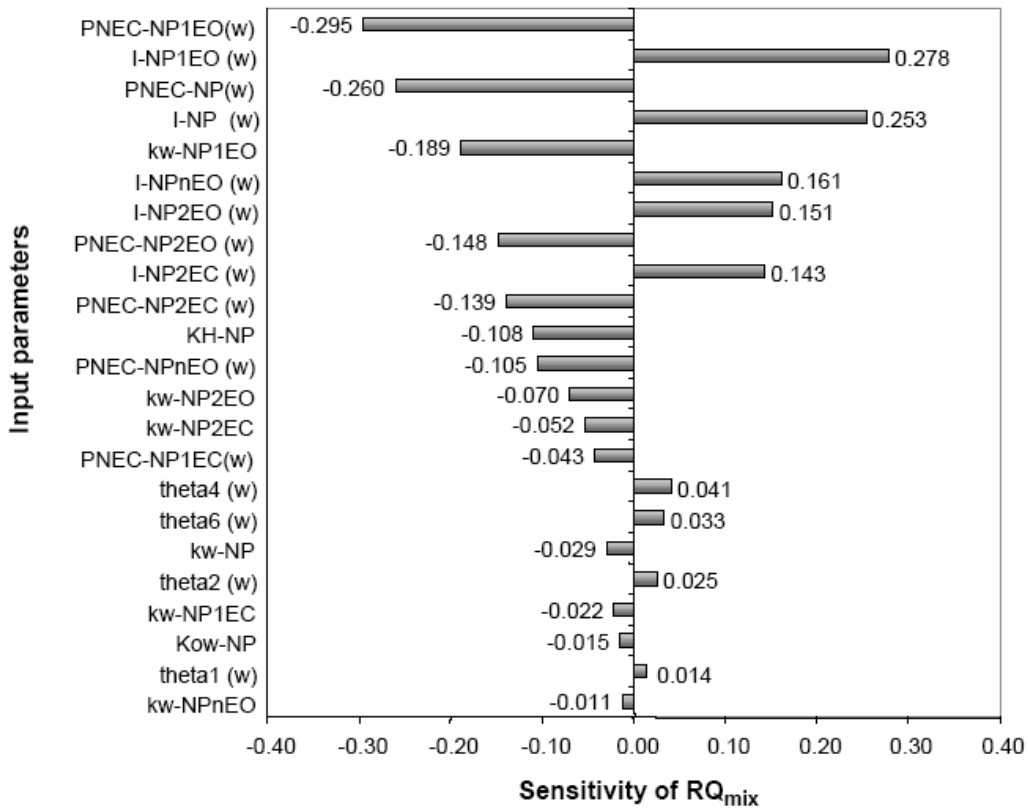
- Guiding Questions:
  - Which „**endpoint**“? – concentrations, mass fluxes, persistence, human exposure, ...
  - Which **chemicals**? How many? – organic compounds; heavy metals, ...
  - Which region or „**system**“? – regional/open vs. global/closed, different types of soil; freshwater vs. seawater; vegetation; ice/snow?
  - Which **processes**? – formation of metabolites; ...
  - What is the temporal and spatial **resolution**? – steady state vs. dynamic, temperature constant or variable; rain constant or variable; ...
  - Which **data** are available?
  - What is the **computational effort**? – PC vs. main frame; Excel, Matlab, Mathematica, C++, ...

Sensitivity and Uncertainty Analyses

- Sensitivity analysis
  - shows most influential model parameters
  - vary parameter x, calculate change in result y and determine elasticity $\alpha = (\Delta y/y)/(\Delta x/x)$

Sensitivity and Uncertainty Analyses

- Sensitivity analysis
  - shows most influential model parameters
  - vary parameter *x*, calculate change in result *y* and determine elasticity $\alpha = (\Delta y/y)/(\Delta x/x)$



Fenner et al.
Environ. Sci. Technol.
36 (2002), 1147–1154

Sensitivity and Uncertainty Analyses

- Sensitivity analysis
  - shows most influential model parameters
  - vary parameter *x*, calculate change in result *y* and determine elasticity $\alpha = (\Delta y/y)/(\Delta x/x)$
- Uncertainty analysis
  - determines contribution of variable/uncertain parameters to variability of model results
  - Methods:
    - ➔ Monte Carlo: much knowledge about parameter distributions required (!)
    - ➔ Estimation based on assumption of log-normally distributed input parameters (MacLeod et al. 2002).

Contributions to Output Variability

- Assume log-normal distributions for input parameters:
  - $\Delta x/x = \Delta \ln x$ represents standard deviation of parameter x, σ_x
  - Result from sensitivity analysis: $(\Delta x/x) \cdot \alpha = (\Delta y/y)$
  - Therefore: $\sigma_{output} = \alpha \cdot \sigma_{input}$

Contributions to Output Variability

- Assume log-normal distributions for input parameters:
  - $\Delta x/x = \Delta \ln x$ represents standard deviation of parameter x, σ_x
  - Result from sensitivity analysis: $(\Delta x/x) \cdot \alpha = (\Delta y/y)$
  - Therefore: $\sigma_{output} = \alpha \cdot \sigma_{input}$
- Method described by MacLeod et al., Environ. Toxicol. Chem. **21** (2002), 700–709.

SETAC PRESS

Environmental Toxicology and Chemistry, Vol. 21, No. 4, pp. 700–709, 2002

Printed in the USA
0730-7268/02 $9.00 + .00

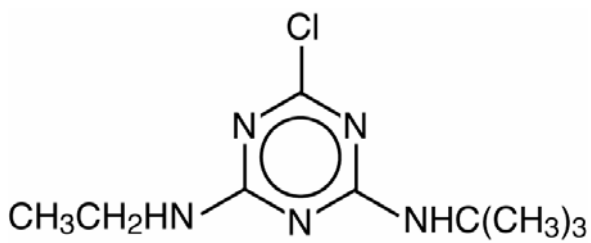
EVALUATING AND EXPRESSING THE PROPAGATION OF UNCERTAINTY IN CHEMICAL FATE AND BIOACCUMULATION MODELS

MATTHEW MACLEOD, ALISON J. FRASER, and DON MACKAY*
Canadian Environmental Modelling Centre, Environmental and Resource Studies, Trent University, Peterborough, Ontario K9J 7B8, Canada

(*Received* 9 *March* 2001; *Accepted* 25 *September* 2001)

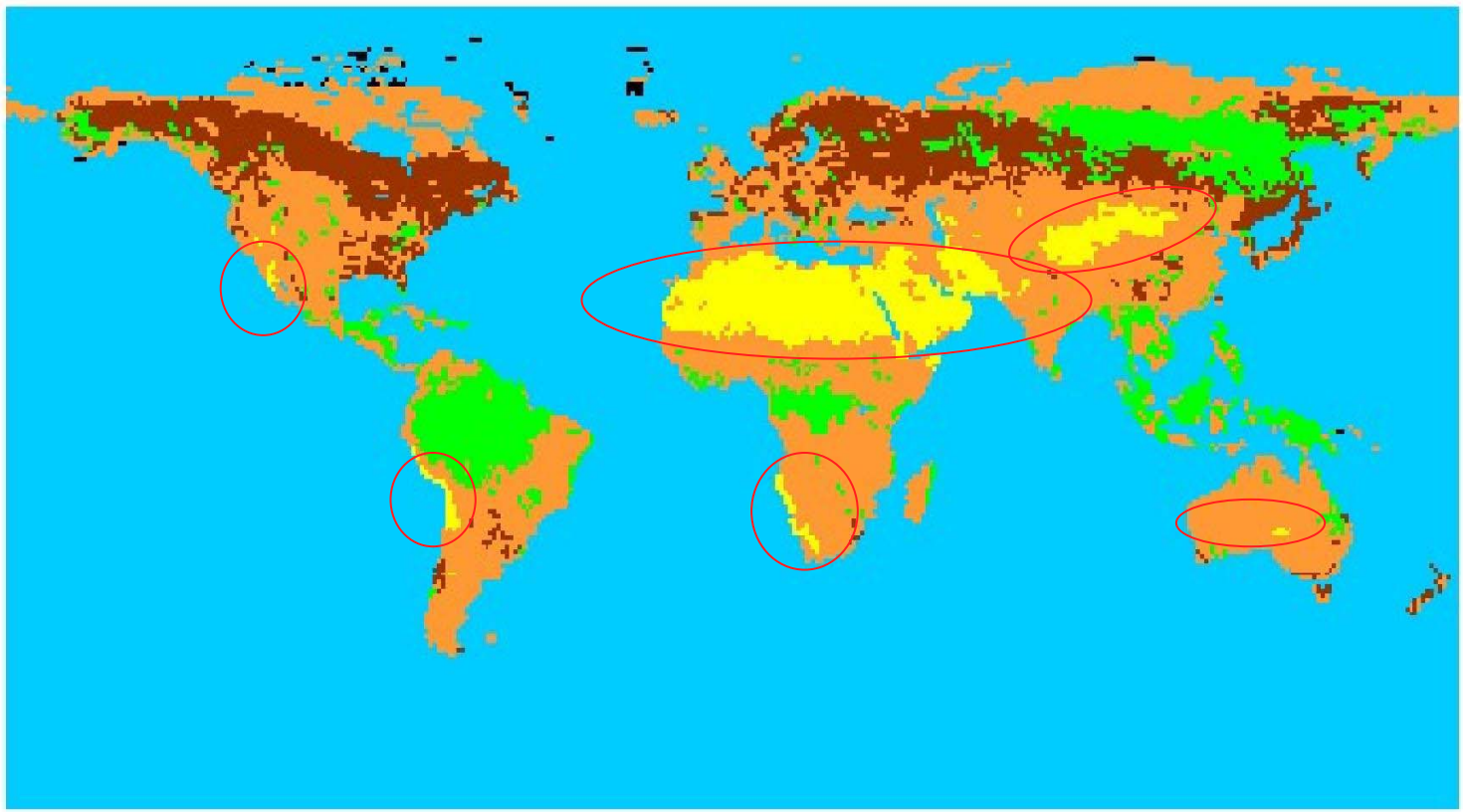
Include New Findings from Environmental Research

- Develop two versions of a model
  - With the process/compartment of interest
  - Without the process/compartment of interest
- Compare results from the two versions
  - **Example:** influence of dry soils (deserts) on long-range transport of terbuthylazine (TBA)



Influence of Dry Soils on LRTP

- Types of soil cover from DeFries and Townsend, *Int. J. Remote Sensing* **15** (1994), 3567–3586



yellow: **bare soil,** 3.4% of global surface
orange: grassland
brown: coniferous forests
green: deciduous forests

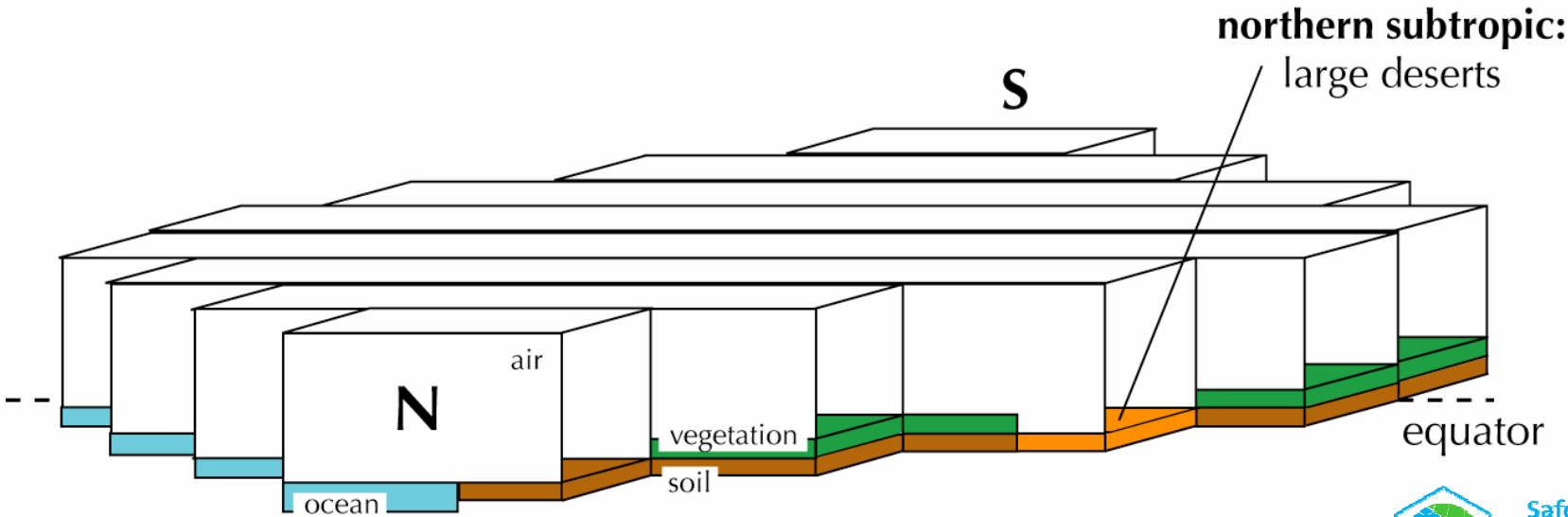
Element 3

«CliMoChem» Model with Dry Soils

- Two model versions in comparison:
  - version 1:

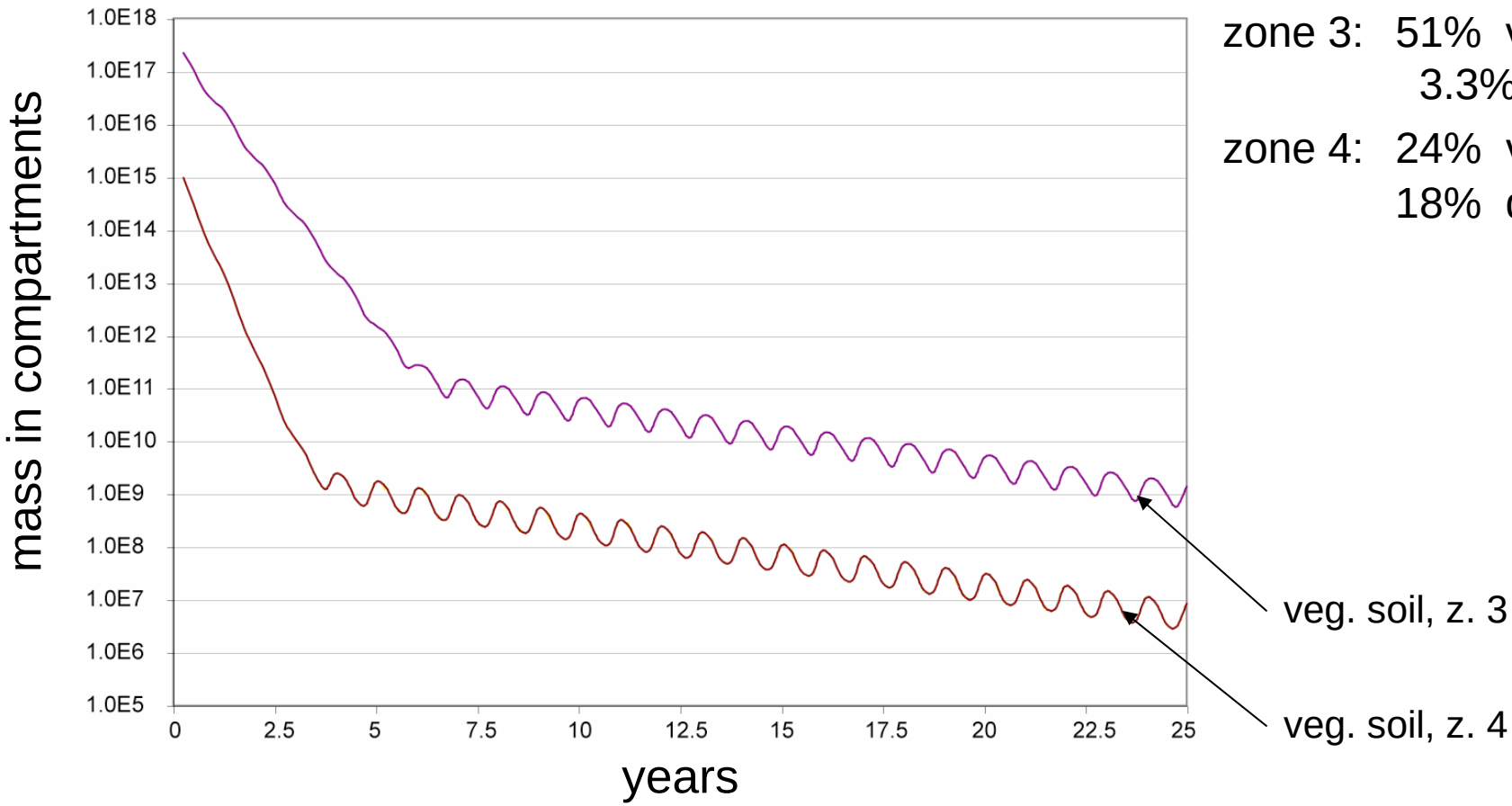
    $K^{\text{total}}_{\text{dry soil-air}} = K^{\text{aBs}}_{\text{dry soil-air}}$ (only absorptive capacity)
  - version 2:

    $K^{\text{total}}_{\text{dry soil-air}} = K^{\text{aBs}}_{\text{dry soil-air}} + K^{\text{aDs}}_{\text{dry soil-air}}$ (absorptive and adsorptive capacity)
  - Masses in compartments as functions of time



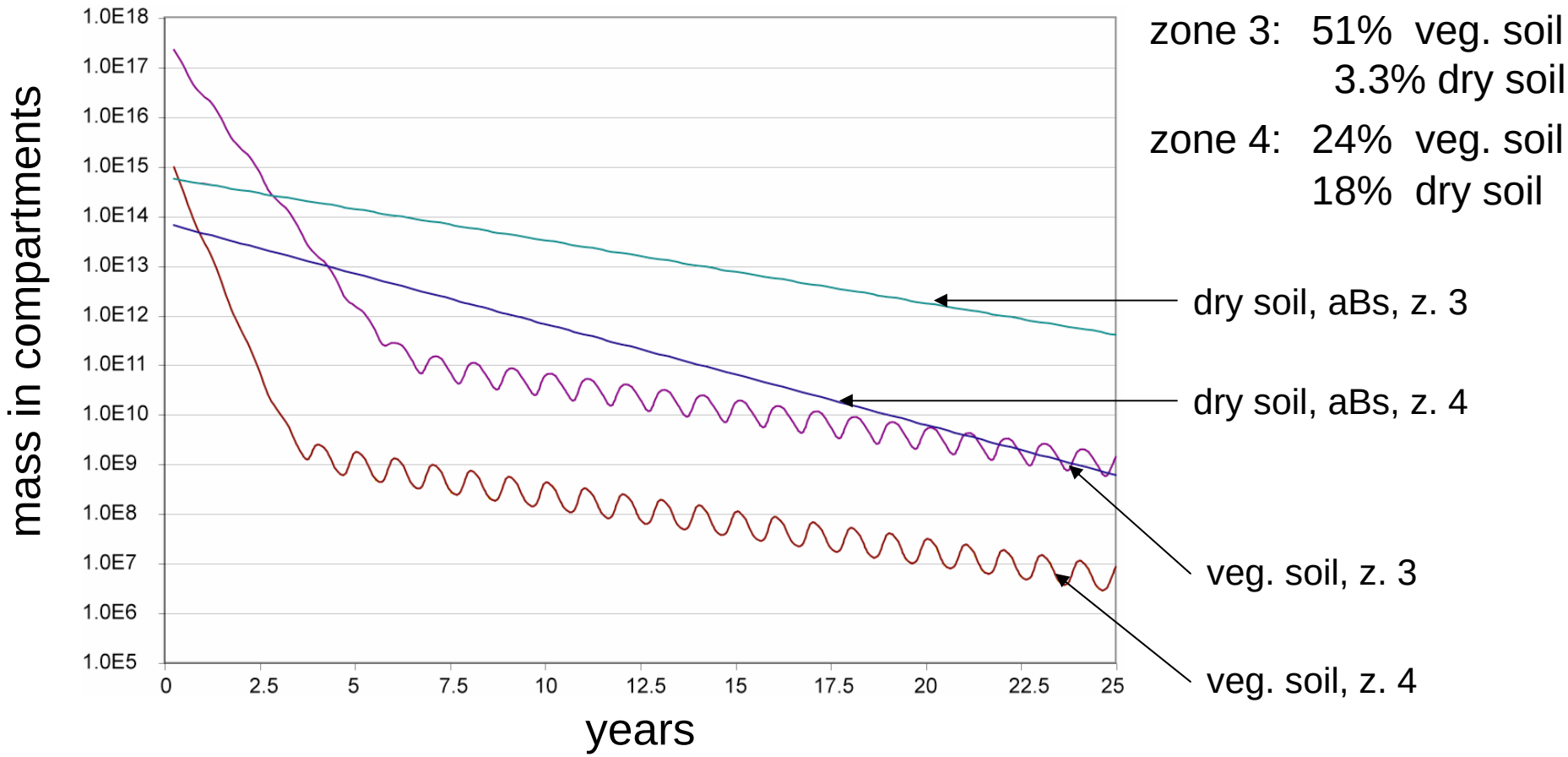
CliMoChem Results for TBA (I)

- Emission of TBA to air of zone 3 of 10 (northern temperate)



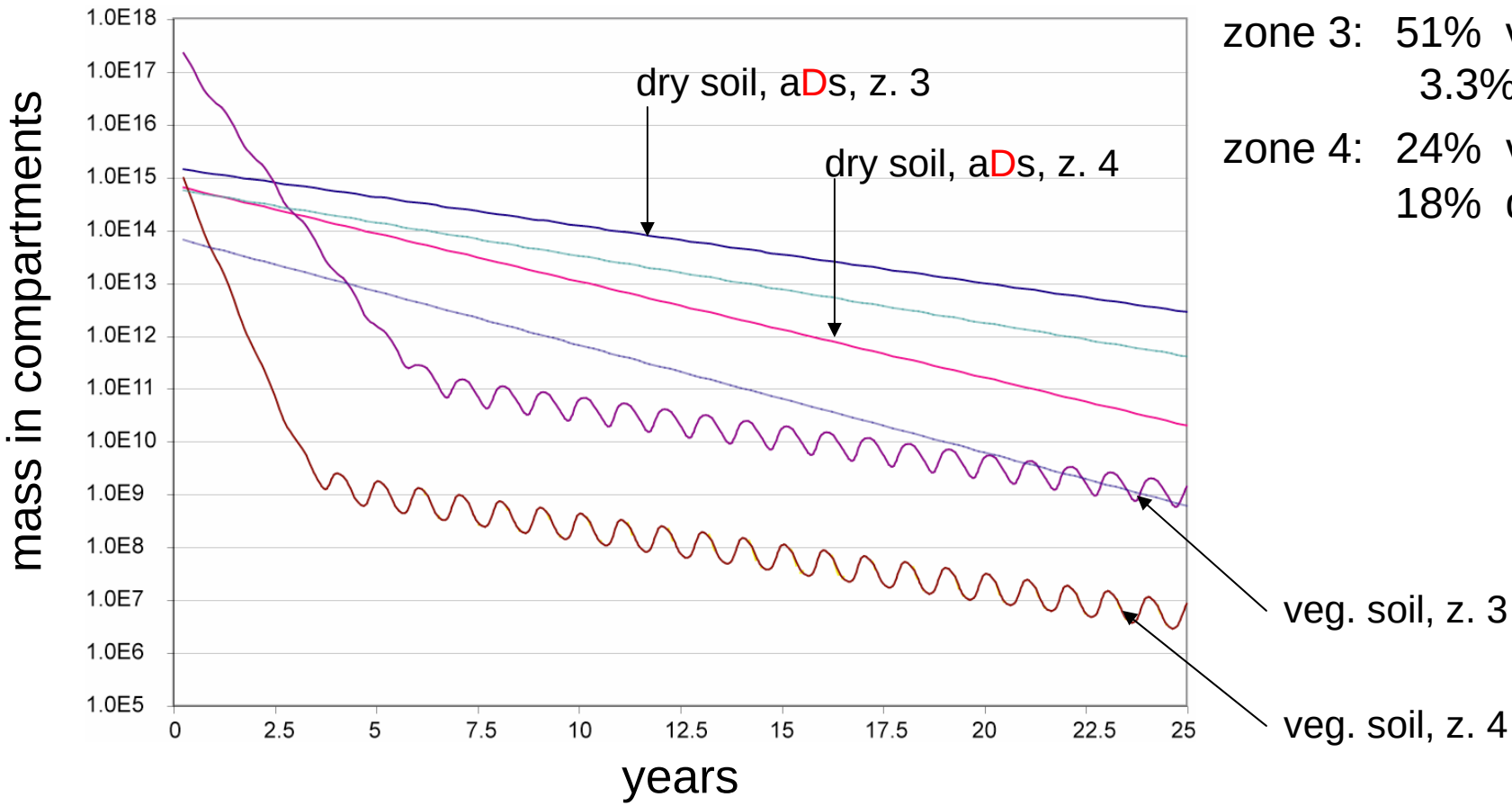
CliMoChem Results for TBA (II)

- Emission of TBA to air of zone 3 of 10 (northern temperate)



CliMoChem Results for TBA (III)

- Emission of TBA to air of zone 3 of 10 (northern temperate)



zone 3: 51% veg. soil
3.3% dry soil

zone 4: 24% veg. soil
18% dry soil

Model Comparison Studies

- **OECD** model comparison: nine relatively similar multimedia box models
- **EMEP** POP model intercomparison: 10 different models for the environmental fate of persistent organic compounds (box models and highly resolved models)
- Method for **mechanistic analysis** of differences between two models

Model Comparison Studies

- **OECD** model comparison: nine relatively similar multimedia box models
- **EMEP** POP model intercomparison: 10 different models for the environmental fate of persistent organic compounds (box models and highly resolved models)
- Method for **mechanistic analysis** of differences between two models

SETAC PRESS

Environmental Toxicology and Chemistry, Vol. 23, No. 10, pp. 2433–2440, 2004

Printed in the USA
0730-7268/04 $12.00 + .00

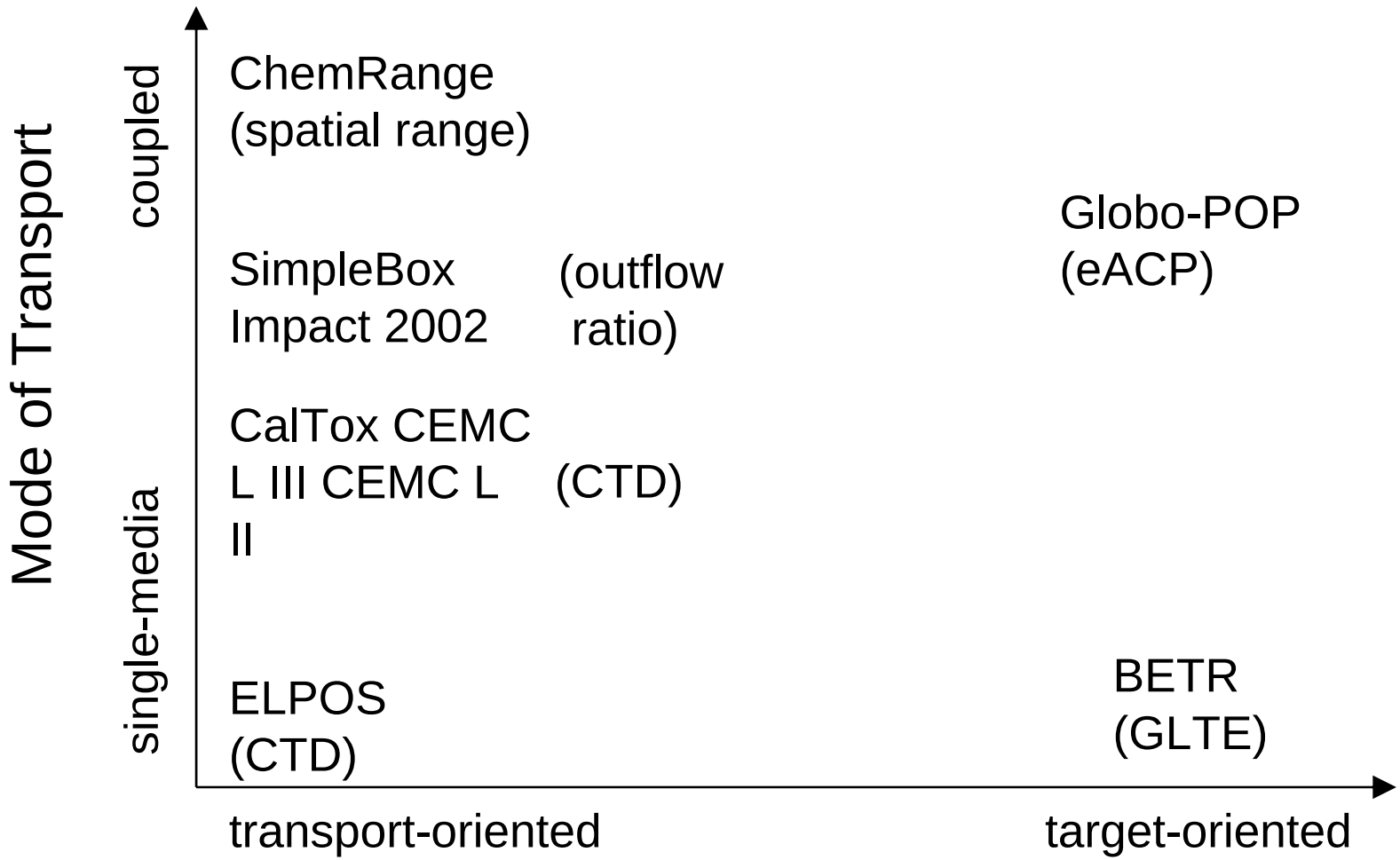
Special Issue Honoring Don Mackay

INVESTIGATING THE MECHANICS OF MULTIMEDIA BOX MODELS: HOW TO EXPLAIN DIFFERENCES BETWEEN MODELS IN TERMS OF MASS FLUXES?

MARTIN SCHERINGER,* FABIO WEGMANN, and KONRAD HUNGERBÜHLER
Institute for Chemical and Bioengineering, Swiss Federal Institute of Technology Zürich, CH-8093 Zürich

(*Received* 14 *July* 2003; *Accepted* 20 *November* 2003)

OECD Model Comparison: Nine Multimedia Box Models



Models and Indicators for P_{ov} and LRTP

- Overall persistence
  - $P_{ov} = \tau_{ov} = M_{tot}/N_{r,tot}$ with
  - M_{tot} = total mass in the system (mol),
  - $N_{r,tot}$ = sum of all reactive fluxes (mol/d)

- Long-range transport potential (LRTP)
  - transport-oriented LRTP (open scale): ELPOS, CalTOX, CEMC Level II and III
  - transport-oriented LRTP (limited scale): ChemRange, SimpleBox, Impact
  - target-oriented LRTP: BETR, Globo-POP

3175 Hypothetical Chemicals

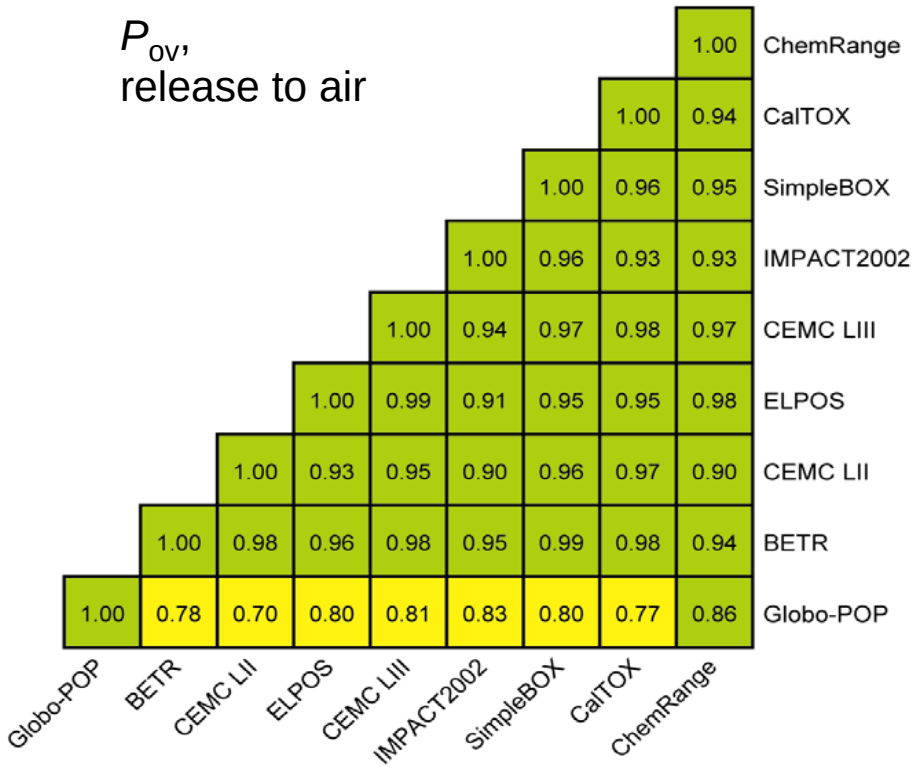
- Variation of
  - **half-life in air:** 5 steps from 4 h to 8760 h (1 year)
  - **half-life in water:** 5 steps from 1 day to 10 years

    –> half-life in soil: $t_{1/2,s} = 2 \cdot t_{1/2,w}$

    –> half-life in sediment: $t_{1/2,sed} = 10 \cdot t_{1/2,w}$
  - **log K_{aw}** from –11 to 2 in units of 1
  - **log K_{ow}** from –1 to 8 in units of 1
  - additional restriction: log K_{oa} between – 1 and 15
- Result: 3175 combinations, called hypothetical chemicals

Rank Correlation Coefficients

P_{ov},
release to air



green: > 0.85

yellow: 0.65–0.85

red: < 0.65

Rank Correlation Coefficients

P_{ov},
release to air

	Globo-POP	BETR	CEMC LII	ELPOS	CEMC LIII	IMPACT2002	SimpleBOX	CalTOX	ChemRange
ChemRange	0.86	0.94	0.90	0.98	0.97	0.93	0.95	0.94	1.00
CalTOX	0.77	0.98	0.97	0.95	0.98	0.93	0.96	1.00	
SimpleBOX	0.80	0.99	0.96	0.95	0.97	0.96	1.00		
IMPACT2002	0.83	0.95	0.90	0.95	0.94	1.00			
CEMC LIII	0.81	0.98	0.95	0.99	1.00				
ELPOS	0.80	0.96	0.93	1.00					
CEMC LII	0.70	0.98	1.00						
BETR	0.78	1.00							
Globo-POP	1.00								

LRTP,
release to air

	Globo-POP	BETR	CEMC LII	ELPOS	CEMC LIII	IMPACT2002	SimpleBOX	CalTOX	ChemRange
ChemRange	0.52	0.62	0.64	0.76	0.69	0.75	0.88	0.74	1.00
CalTOX	0.31	0.70	0.82	0.96	0.97	0.98	0.89	1.00	
SimpleBOX	0.39	0.69	0.73	0.90	0.86	0.89	1.00		
IMPACT2002	0.31	0.71	0.78	0.95	0.96	1.00			
CEMC LIII	0.28	0.69	0.81	0.96	1.00				
ELPOS	0.40	0.79	0.72	1.00					
CEMC LII	0.20	0.33	1.00						
BETR	0.60	1.00							
Globo-POP	1.00								

green: > 0.85

yellow: 0.65–0.85

red: < 0.65

Results Model Comparison

- Chemicals with strongly different results in two models:
  - What model environment is most appropriate for what context/purpose?
  - **Land:** freshwater and sediment;
    water shallow;
    no transport in water;
    high net deposition of SOCs to soils
  - **Ocean water:** water much deeper;
    transport in water relevant;
    export to deep ocean relevant,
    net deposition of SOCs with intermediate K_{ow} lower

OECD Model Comparison Study

Comparing Estimates of Persistence and Long-Range Transport Potential among Multimedia Models

KATHRIN FENNER,[†]
MARTIN SCHERINGER,[*,‡]
MATTHEW MACLEOD,[§]
MICHAEL MATTHIES,[∥]
THOMAS MCKONE,[§]
MAXIMILIAN STROEBE,[‡]
ANDREAS BEYER,[⊥] MARK BONNELL,[#]
ANNE CHRISTINE LE GALL,[®]
JÖRG KLASMEIER,[∥] DONALD MACKAY,[○]
DIK VAN DE MEENT,[×]
DAVID PENNINGTON,[+]
BERND SCHARENBERG,[◇]
NORIYUKI SUZUKI,[◆] AND FRANK WANIA[▽]
Swiss Federal Institute for Environmental Science and

process descriptions) affect the results for P_{ov} and LRTP. Using a set of 3175 hypothetical chemicals covering a broad range of partition coefficients and degradation half–lives, we systematically analyze the P_{ov} and LRTP results obtained with nine multimedia models. We have developed several methods that make it possible to visualize the model results efficiently and to relate differences in model results to mechanistic differences between models. Rankings of the hypothetical chemicals according to P_{ov} and LRTP are highly correlated among models and are largely determined by the chemical properties. Domains of chemical properties in which model differences lead to different results are identified, and guidance on model selection is provided for model users.

Introduction

High persistence and long-range transport potential are

Environ. Sci. Technol. **39**, 2005, 1932–1942

- OECD/UNEP workshop with a consensus model for P_{ov} and LRTP, August 30/31 2005, ETH Zürich

Field Data

- Key question: Do the field data represent the assumptions of the model?
  - Sources: within the model domain vs. background
  - Spatial, temporal resolution
  - Compartments, processes included
- Scatter in field data
  - Noise (values close to limit of detection) vs. environmental variability
  - Which factors determine environmental variability?

Outlook for EEA Project

- Discuss/refine purpose
  - Define criteria for concentration evaluation (legal standards, toxicity thresholds, measured concentrations?
- Review and update – if necessary – the model
  - Steady-state assumption justified? If not, no match between field data and model results
- Identify major uncertainties
  - Are they in the emission data?
  - Are they in the model?
- Compile suitable field data

REGULATORY PERSPECTIVE ON MODELLING STRATEGIES

A PERSONAL VIEWPOINT

Dr Jose V. Tarazona

Director

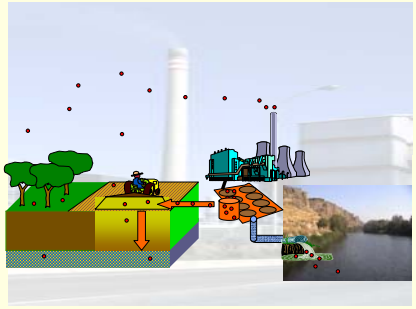
Department of the Environment, INIA, Spain

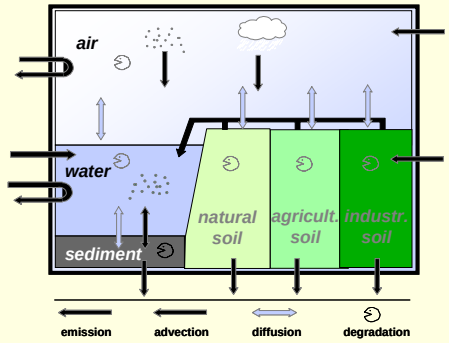
Major needs for the regulatory use of models

- Assessing current status
  - Cost/effective tool for assessing exposure
  - Setting priorities for monitoring efforts
  - Covering spatial and temporal variability
- Predictive tool
  - Assessing the risk of new activities
  - Assessing the benefits from risk management options
  - Setting priorities for control efforts

Assessing current status

- Cost/effective tool for assessing exposure
  - EUSES
    - Assessing the risk of existing chemicals where monitoring data are not available
    - LOCAL PEC
      - Based on SPECIFIC emission scenarios
    - REGIONAL AND CONTINENTAL PEC
      - Based on GENERIC emission scenarios





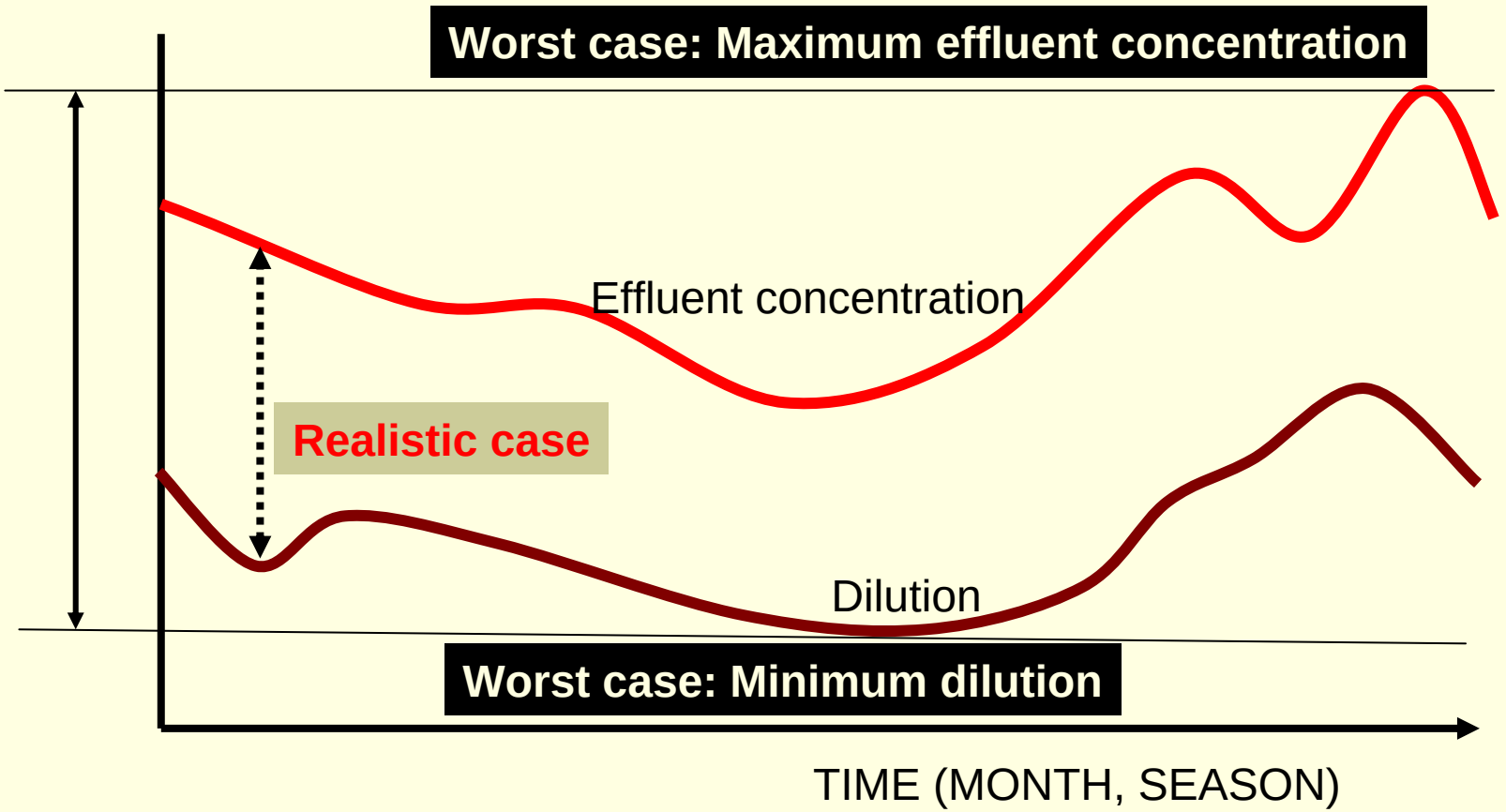
IF A POTENTIAL RISK IS IDENTIFIED, MONITORING CONFIRMATIONS CAN BE SUGGESTED BEFORE SETTING RISK MANAGEMENT REQUIREMENTS

Assessing current status

- Setting priorities for monitoring efforts
  - LIST OF PRIORITY CHEMICALS UNDER THE WATER FRAMEWORK DIRECTIVE
    - Selecting chemicals requiring a continuous control at the pan European level

Assessing current status

- Covering spatial and temporal variability



Predictive tool

- Assessing the risk of new activities
  - FOCUS GROUND WATER
    - PREDICTING THE EXPECTED CONCENTRATION OF A PESTICIDE IN GROUND WATER IF A NEW MOLECULE IS AUTHORIZED BASED ON
      - THE GOOD AGRICULTURAL PRACTICES PROPOSED BY THE INDUSTRY
      - THREE MODEL OPTIONS
      - TEN EUROPEAN SCENARIOS

Predictive tool

- Assessing the benefits from risk management options
  - Comparative risk assessment of Cadmium/Nickel batteries management:
    - Incineration
    - Land-filling
    - Combination of both

Predictive tool

- Setting priorities for control efforts
  - Selecting chemicals to be monitored in an industrial facility
    - 30 industrial companies
    - >300 hazardous chemicals used at different quantities and under different conditions

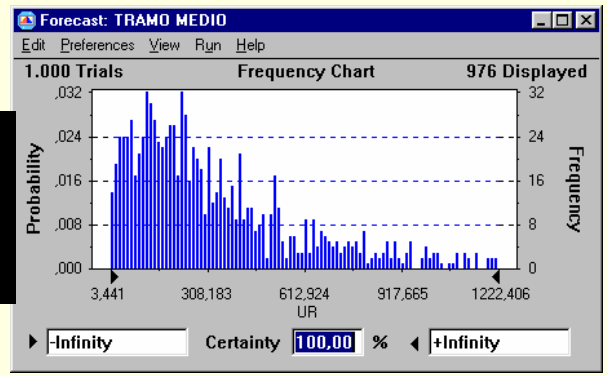
Modelling versus Monitoring

- In general, monitoring data are expected to prevail on model estimations if:
  - Monitoring compilations and modelling estimations cover similar scenarios:
    - E,g, downstream concentration of industrial chemicals after the mixing zone
  - Monitoring efforts and raw data supporting model estimations have equivalent statistical power.

Modelling versus Monitoring

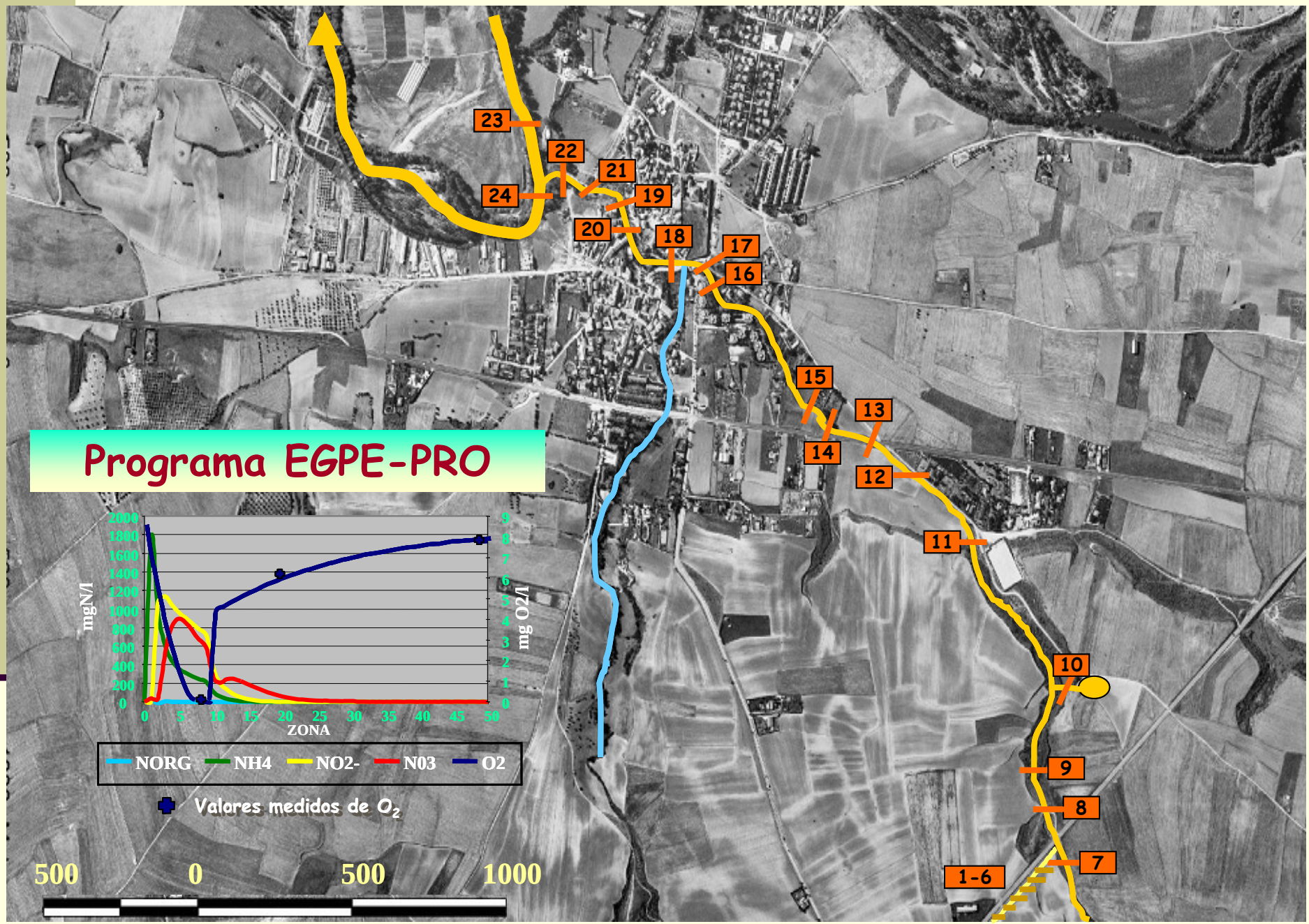
- But, well **calibrated** and **validated** models may offer more powerful estimations than poor monitoring programmes, e.g.:
  - Annual maximum and average concentrations based on seasonal measurements on single upstream and downstream sampling stations, *versus*,
  - GIS modelling estimations, based on calibrated emissions, >500 estimations of WWTP dissipation and 50 years of daily dilution factor estimations.

ERCHITOX model estimations at downstream Zaragoza based on 20 years daily flow and emission data



Modelling versus Monitoring

- The best option:
  - A proper monitoring programme covering measurements at critical time and space levels
  - Allowing the calibration, validation and confirmation of models covering the expected temporal and spatial variability.

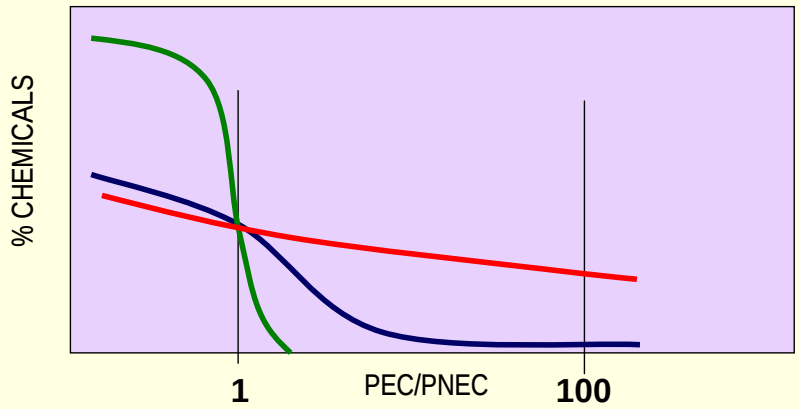

Programa EGPE-PRO
23
22
21
24
19
20
18
17
16
15
13
14
12
11
10
9
8
7
1-6
mgN/l
mg O2/l
ZONA
NORG
NH4
NO2-
N03
O2
Valores medidos de O2
500
0
500
1000

Uncertainty in model extrapolation

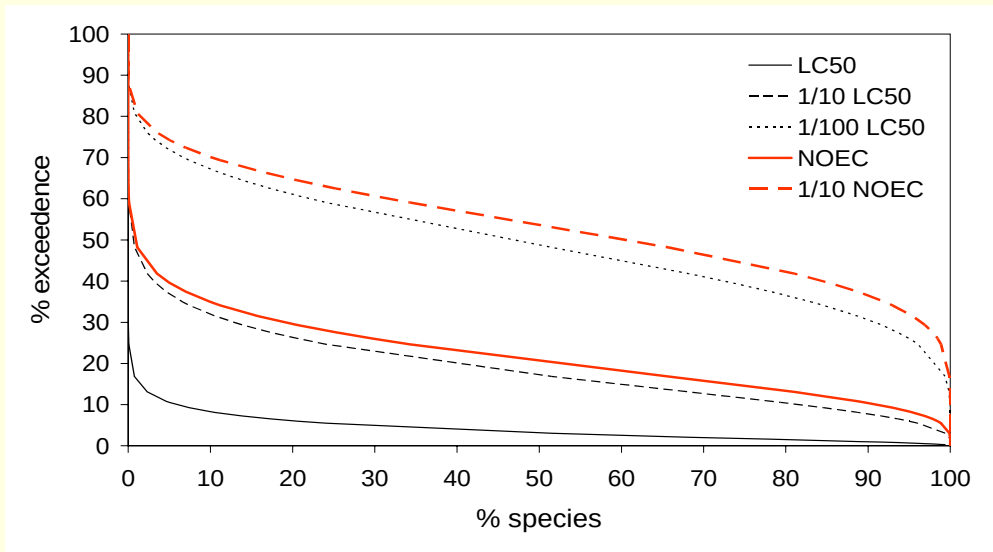
- Uncertainty in model assumptions
  - Bioaccumulation based on Kow does not predict the bioaccumulation potential (e.g. perfluorinated surfactants)
- Uncertainty in model methods
  - Soil partition and leaching based on Koc where clay absorption plays a main role (e.g. tetracyclines)
- Uncertainty in (default) model data.
  - E.g. dilution factor of 10

Proposals for covering variability and uncertainty

- Realistic versus simplified assessments



- Moving probabilistic



Additional uses

- Landscape based risk assessment/risk management, combining:
  - GIS based modelling tools
  - Level of protection for different ecosystems, communities, populations or individuals: combining Chemicals` risk assessment and Nature 2000 biodiversity protection goals

Draft conclusions….
…. for further discussion

- Modelling approaches are essential tools in the regulatory context for
  - Covering estimations not (well) covered by monitoring programmes
  - Estimating the expected benefices from management options
  - Addressing temporal and spatial variability
- Models must be validated and calibrated.
- Modelling approaches require a proper estimation of their predicting power, as well as conceptual, methodological and technical uncertainty
- Suitable models may cover local/temporal risk estimations in a better way than lower tier monitoring efforts.,., but monitoring is essential for calibrating and validating the models.

Thank you

MINISTERIO
DE EDUCACIÓN
Y CIENCIA

INIA
Instituto Nacional de Investigación
y Tecnología Agraria y Alimentaria