Modelling the fate of POPs on European scale using a gridded multi-media box model.

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International regulation POPs

UNEP – Stockholm Convention on POPs

UNECE Long Range Atmospheric Transport Protocol

Intended to restrict or ban chemicals that are: persistent, bioaccumulative, subject to long-range atmospheric transport

Strategic Approach to International Chemicals Management (SAICM)

Adopted in 2006, SAICM is an international policy framework to foster the sound management of chemicals

Also REACH... PBTs, and vBvP
What information/tools are required? How can we link sources, measurements and modelling to ensure effectiveness of regulation?

**Key areas**
1. Reliable source inventories
2. Ability to understand environmental fate and behaviour
3. Effective use of measurements to quantify effectiveness

Source inventories

Scale-up emission estimates using surrogates such as population density

Distribute emissions using regional scale multi-media models

Compare air/soil PECs with spatial datasets - not usually internally consistent
Development of modelling tools: European scale multi-media model (European Variant of BeTr North American model)

Distribution of B(a)P with NE UK grid cell
(1000 kg h\(^{-1}\) lower atmosphere)

Key inventory information

- **Air (lower)**: 2.7%
- **Air (upper)**: 0.25%
- **Soil**: 59%
- **Vegetation**: 1.5%
- **Coastal water**: 36%

**Air-Soil**: 16 kg h\(^{-1}\)
**Air-Veg.**: 53 kg h\(^{-1}\)
**Air-coastal water**: 265 kg h\(^{-1}\)

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**Legend**
- Regional Persistence
  - Total: 34,038.65 days
  - Reaction: 118.3949 days
  - Advection: 47.7336 days

- Total Inputs: 1021.548 kg/y
- Total Inventory: 95.266 kg

**Fluxes in kg/year**
- Air (lower) - Soil: 16 kg h\(^{-1}\)
- Air (upper) - Vegetation: 53 kg h\(^{-1}\)
- Air - Coastal water: 265 kg h\(^{-1}\)
Simple what-if scenarios: 10000 kg emitted in region 24
Air concentration as percentage of concentration in region 24
Emission/source inventories are usually provided on a country by country basis.

Legend

BaP emissions (g/km$^2$/yr)

- Light blue: 0 - 5
- Teal: 6 - 20
- Green: 21 - 50
- Yellow: 51 - 100
- Orange: 101 - 200
- Red: 201 - 300
- Maroon: 301 - 1000
- Dark grey: 1001 - 5000
- Black: 5001 - 10200

TNO 2000 per country

EMEP 2004 per country

EMEP 2004 50x50 grid
Steady state gridded output

PEC in air (pg m⁻³)

- 24.70 - 50.00
- 50.01 - 100.00
- 100.01 - 150.00
- 150.01 - 200.00
- 200.01 - 360.10
PEC in air (ng m\(^{-3}\))

- 0 - 0.005
- 0.005 - 0.1
- 0.1 - 0.25
- 0.25 - 1
- 1 - 2.5
- 2.5 - 10

UK air quality standard

EU limit
Case study: Penta-BDE life cycle

- Br production ➔ Brominated Flame retardant industry ➔ Penta-BDEs
- European market ➔ PBDEs ➔ Penta-BDEs

- Vapour pressure based EF
- Log Koa based EF
- Other approaches
EVn BeTr - example of temporal and spatially variable emissions - PeBDE

Emission scenarios - population density, regional hotspots, PCB surrogate
Predicted time trends in three model regions.

(a) BDE-47 in air

(b) BDE-47 in soil
Comparison of predicted and measured air concentrations for BDE-47.
Time trend for measured BDE-47 concentrations in archived pasture versus the modelled trend of European atmospheric emissions.
Spatial Distribution of BDE-47 in ambient air

Range 0.8 to 107 ng per sample

Sampling rate 3 m$^3$ per day (42 days) = 130 m$^3$ = 6 to 820 pg m$^{-3}$
ALARM Climate Scenarios

- **BAMBU (Business As Might Be Usual) Scenario**: continue economic growth; biggest warming, biggest rain difference
- **GRAS (Growth Applied Strategy) Scenario**: some controls
- **SEDG (Sustainable European Development Goal) Scenario**: shock scenarios, GRASCUT - gulf stream cut off

Predicted landcover changes
Predicted climate changes

GRAS scenario

Temp Max 1991-2020

Temp Max 2071-2100
Looking to the future: climate change and pollutant behaviour
Modelling POPs - future challenges

• Use of scientific evidence in public policy making contains varying levels uncertainty that must be assessed, communicated and managed.

• Weighing of scientific evidence balanced against the beneficial use.

• Important that emission databases, environmental fate and behaviour models and measurement studies are developed in conjunction with each other.

• Models can used to clearly demonstrate uncertainty and identify key research areas.