System Modeling

ESD.864
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The following hour-by-hour snowfall forecast is based on one computer model and is subject to change.

Updates arrive every three hours.

Plan for Today

- Reminders/Q&A
- System Modeling
- Last 15 minutes: Forum Discussion

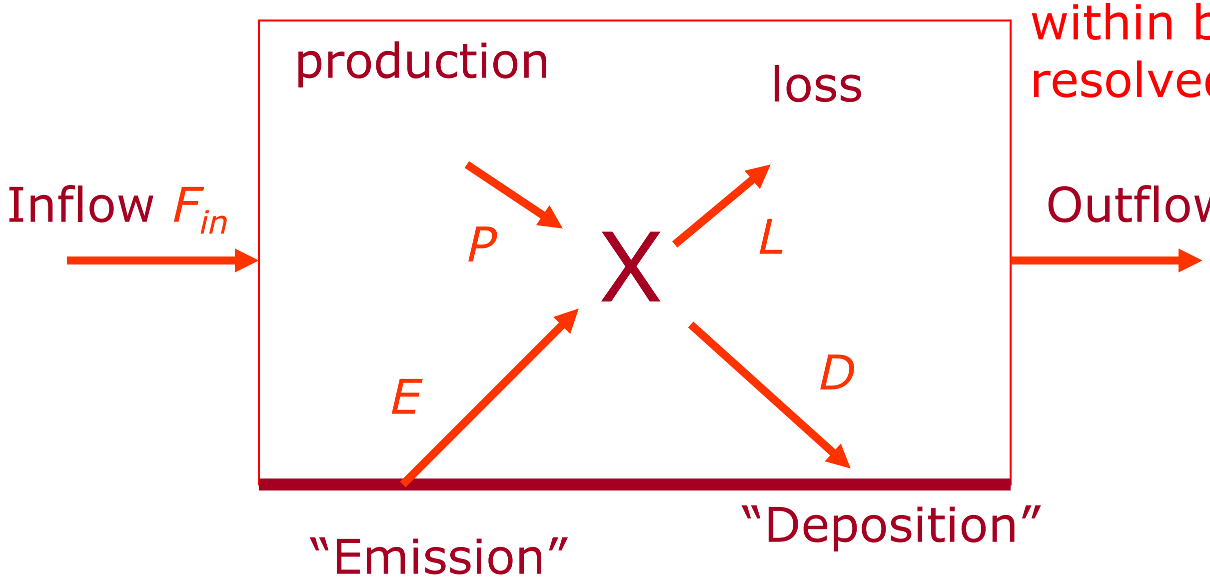
Outline

- System modeling: an introduction
- Box Modeling Principles
- Modeling in Engineering Systems
- Modeling in Context
- Analysis Techniques
- Application: Chemical box model (prep for PS 4)

Basic Modeling

- Many classes of models (e.g. system dynamics, stock-flow, complex climate models) are extensions of the "box model" concept
  - Including many we've seen in case studies
- Key concepts: mass balance and lifetime

One-Box Model



spatial distribution of X within box is not resolved

Mass balance equation: $\frac{dm}{dt} = \sum \text{sources} - \sum \text{sinks} = F_{in} + E + P - F_{out} - L - D$

Box model intuition quiz

- The lifetime of X in the box depends on which of the following:
  - A) inflow, production, and emission
  - B) outflow, deposition and loss
  - C) amount of X in the box
  - D) all of the above

Assume first-order loss rates.

Constant source, 1st order sink

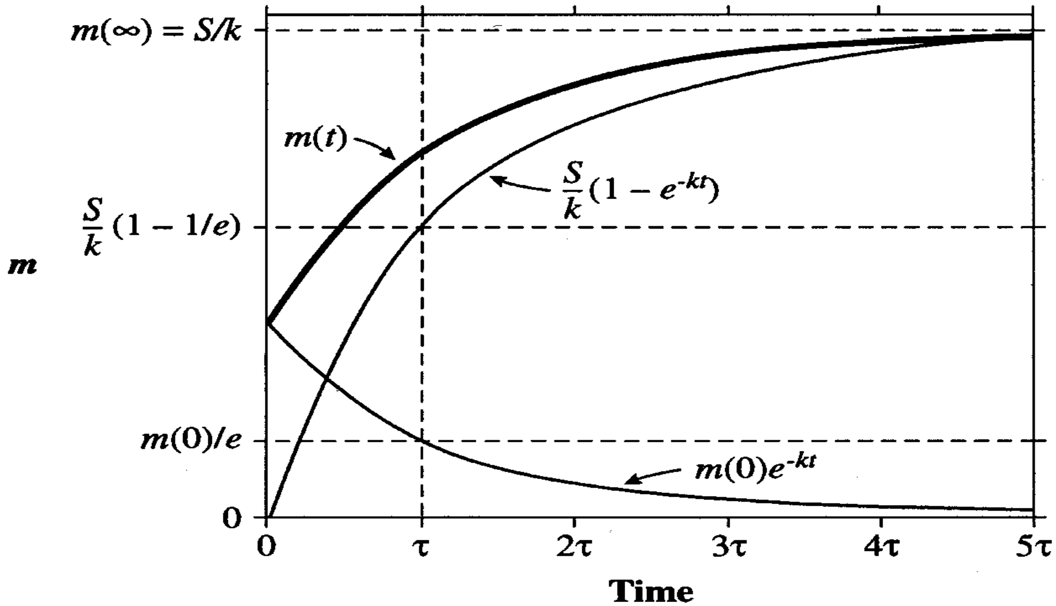
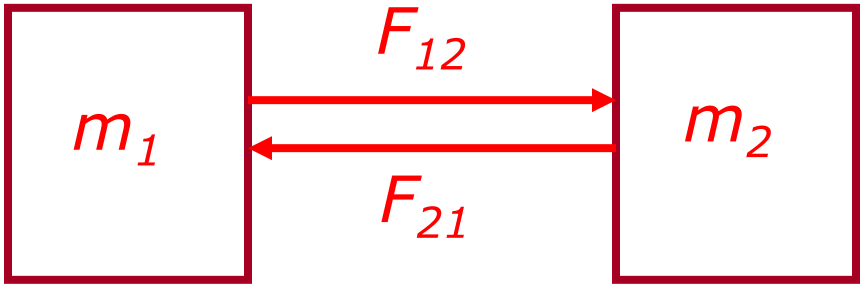


Fig. 3-2 Evolution of species mass with time in a box model with first-order

Source: Figure 3-2 in Jacob, Daniel. Introduction to Atmospheric Chemistry. Princeton University Press, 1999.

$$\frac{dm}{dt} = S - km \quad \Rightarrow \quad m(t) = m(0)e^{-kt} + \frac{S}{k}(1 - e^{-kt})$$

Two-box model



Mass balance equations: $$\frac{dm_1}{dt} = E_1 + P_1 - L_1 - D_1 - F_{12} + F_{21}$$

(similar equation for dm_2/dt)

If mass exchange between boxes is first-order:

$$\frac{dm_1}{dt} = E_1 + P_1 - L_1 - D_1 - k_{12}m_1 + k_{21}m_2$$

⇨ system of two coupled ODEs (or algebraic equations if system is assumed to be at steady state)

Modeling in engineering systems

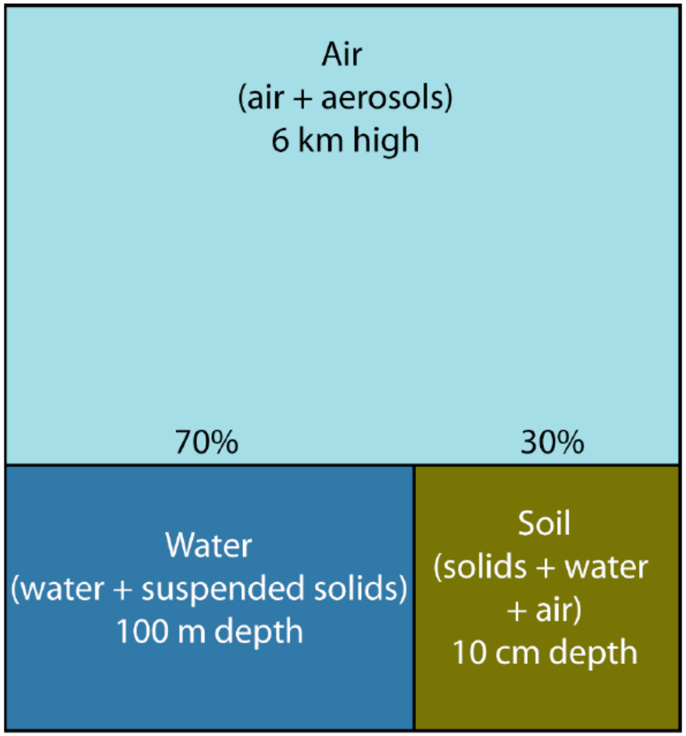
Modeling and user understanding

Analysis Techniques

- Sensitivity analysis
- Uncertainty analysis (Monte Carlo)

Chemical Box Model: The OECD Screening Tool (PS 3)

- Single region
- Global dimensions
- Air, water, soil



POPs: Specific category of particularly hazardous chemicals

- "Persistent organic pollutants"
- Characteristics: persistence in environment (air, soil, water); bioaccumulate (fish, marine mammals); toxic
- Category of "POPs" is a science-policy hybrid
- Subject to international agreements (global Stockholm Convention)

What are POPs and why are they a problem?

- Pesticides, e.g. DDT, Chlordane: carcinogenic, ecotoxic
- Subject to international regulation because of long-range transport
- Accumulation in the Arctic, in traditional foods, far from location of use/release

How to determine whether a chemical is a POP?

- Data requirements for persistence, bioaccumulation
- "Environmental fate properties and/or **model results** that demonstrate that the chemical has a potential for long-range environmental transport…" [Stockholm Convention]

Stockholm Convention and additional POPs

- The 2001 Stockholm Convention initially dealt with only 12 persistent organic pollutants (POPs)
- It included a procedure for adding future substances to the agreement, based on scientific criteria of persistence, bioaccumulation, toxicity
- 10 additional substances have so far gone through the process

Adding POPs to the Stockholm Convention: 5-step review process

- Party submits a proposal to regulate a new chemical based on information requirement in Annex D (Persistence, bioaccumulation, toxicity info)
- POPs Review Committee (POPRC): 31 government-designated experts decides whether criteria met
- Soliciting of technical comments, development of risk profile by POPRC
- Soliciting of comments, POPRC develops risk management evaluation and submits to the Conference of Parties (COP)
- Conference of Parties takes final decision on whether to list chemical and where

Review Committee Issues

- Composition: regional, disciplinary
- Language
- Procedure and timing (meeting frequency)
- Capacity (for proposing, and analyzing)

INTERNATIONAL CRITERIA FOR POPs

Bioaccumulation:
- Bio-accumulation factor (aquatic) > 5000 or log Kow > 5, OR
- Evidence of high bioaccumulation in other species, high (eco)toxicity, OR
- Monitoring data in biota

Persistence:
- Half-life of 2 months in water, or 6 months in soil, or 6 months in sediment, OR
- Evidence of sufficient persistence to justify consideration

Long-range transport potential:
- Measured levels in locations far from releases, OR
- Monitoring showing long-range environmental transport may have occurred, OR
- Environmental fate properties or model results showing potential for transport
- Air half-life > 2 days for chemicals transporting through air

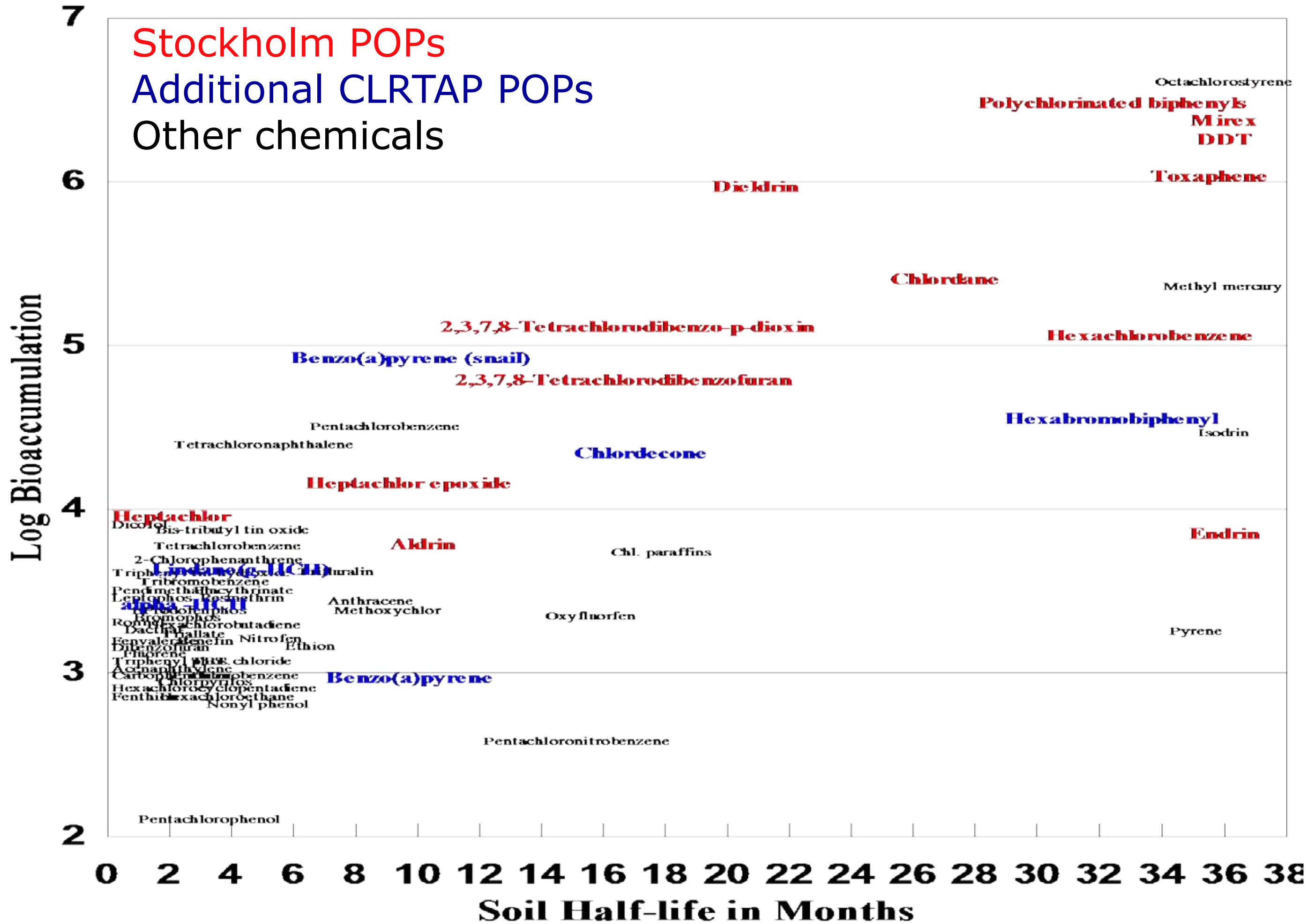
Adverse effects

Criterion		Stockholm	CLRTAP
Bioaccumulation	Log Kow	5	5
	Bioaccumulation Factor	5000	5000
Persistence	Water	2 months	2 months
	Soil	6 months	6 months
	Sediment	6 months	6 months
Transport	Air	2 days	2 days

Log Kow=octanol-water partition coefficient, measure of lipophilicity
Bioaccumulation factor: takes into account environmental and dietary sources

[Eckley, *Environment*, 2001; Rodan et al., *ES&T*, 1999]

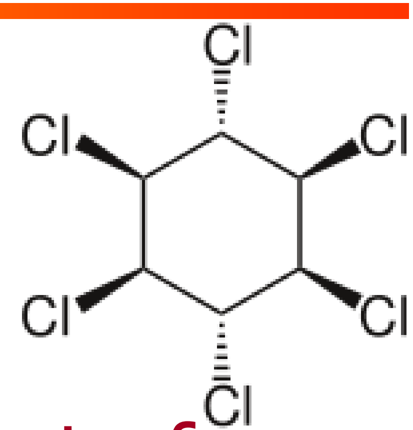
SETTING CRITERIA: WHERE ARE THE DIRTY DOZEN?



Source: Figure 2 in Rodan, Bruce D., David W. Pennington, et al. "Screening for Persistent Organic Pollutants: Techniques to Provide a Scientific Basis for POPs Criteria in International Negotiations." *Environmental Science & Technology* 33, no. 20 (1999): 3482-8.

[Rodan et al., *ES&T*, 1999]

Example review process: Lindane



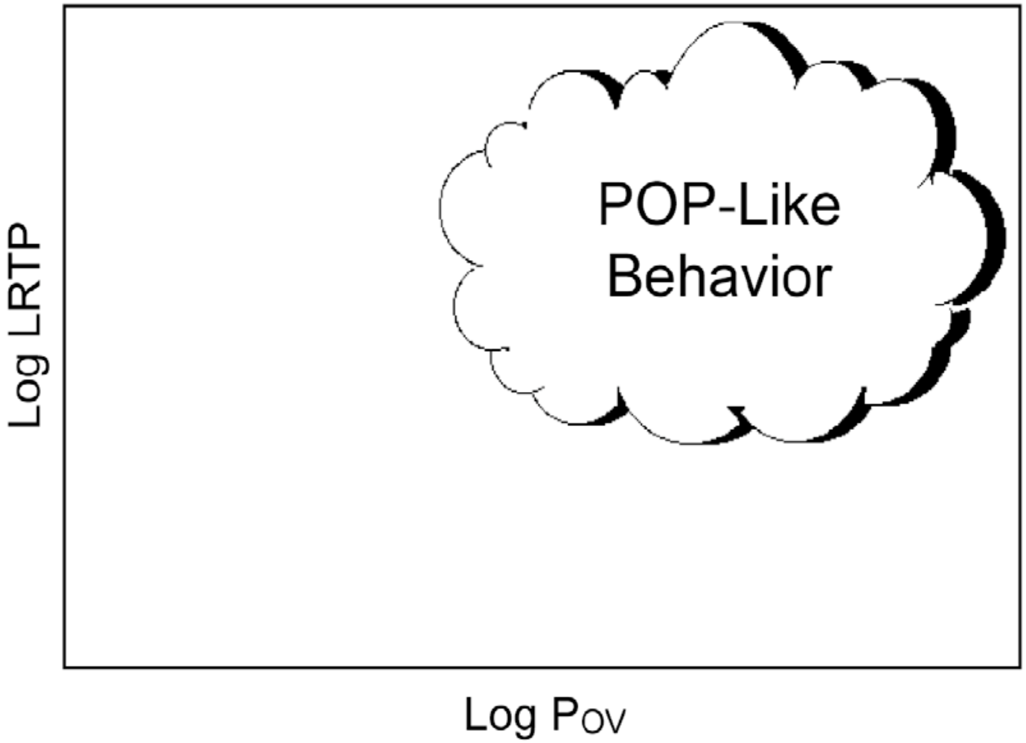
- Proposed by Mexico, June 2005
- Lindane=gamma-hexachlorocyclohexane
- Agricultural insecticide, treatment of head lice
- Measured in the Arctic; toxic to rats; carcinogenic in mice; accumulates in humans

Procedure (Lindane example)

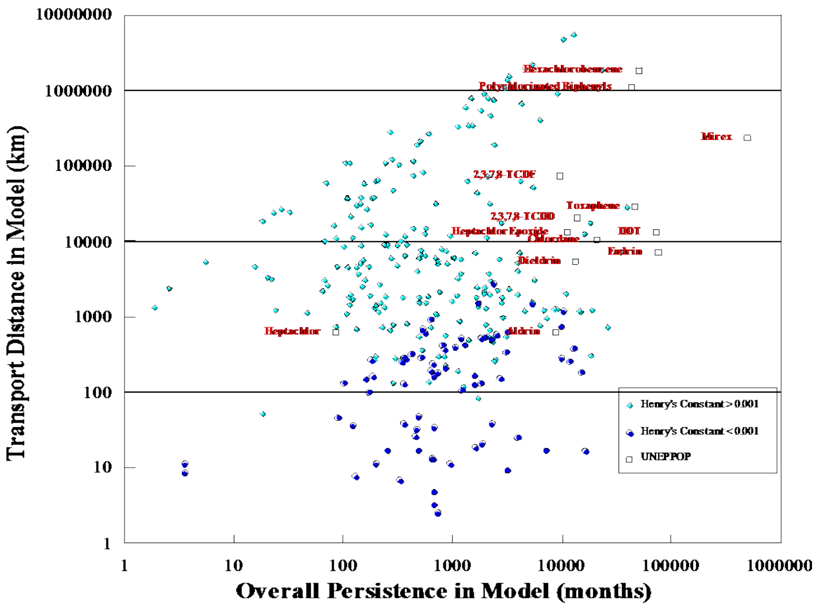
- 6/05: proposal by Mexico
- 11/05: POPRC says satisfies screening criteria
- 11/06: POPRC adopts risk profile
- 11/07: POPRC adopts risk management evaluation
- 5/09: COP includes Lindane on Annex A (Elimination), with specific time-limited exemptions for some head lice use

LRTP vs Pov

- LRTP=long-range transport potential
- Pov=overall persistence



Transport distance v. overall model persistence



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[Rodan et al., *ES&T*, 1999]

- Other approaches to identify POPs:
  - Model overall environmental persistence (sometimes, different results from half-life approach, see *Klasmeier et al. 2006)*
  - Screening based on quantitative structure-property relationships (*Muir and Howard*, 2006 identified 30 with bioconcentration potential and 28 with transport potential)
- *But, challenges in monitoring and measurement exist.*

Long-range transport potential

- Characteristic travel distance (unit:km): the distance at which concentration has decreased to 37% assuming constant flow of air
- Air speed: 4 m/s, Water speed: 0.02 m/s
- Calculated for release to water and air
- Decrease in concentration from degradation, transfer

Figure of characteristic travel distance (CTD) removed due to copyright restrictions. Please see figure 2 in Scheringer et al. (2006) at http://www.sust-chem.ethz.ch/downloads.

Scheringer et al., http://www.sust-chem.ethz.ch/docs/POP_Candidates_OECD_Tool.pdf

Figure of transfer efficiency (TE) removed due to copyright restrictions. Please see figure 2 in Scheringer et al. (2006) at http://www.sust-chem.ethz.ch/downloads.

Scheringer et al., http://www.sust-chem.ethz.ch/docs/POP_Candidates_OECD_Tool.pdf

Chemical property inputs

- Kaw=air water partition coefficient; related to Henry's Law (which deals with pressures not concentration). [air]=[water]*Kaw
- Kow=octanol-water partition coefficient. Measure of lipid solubility.

Screening Tool Results

Figure of "Results from the Tool for the four POP candidates and 10 generic PCB homologues in comparison" removed due to copyright restrictions. Please see figure 4 in Scheringer et al. (2006) at http://www.sust-chem.ethz.ch/downloads.

Uncertainty

Figure of "Results from a Monte Carlo calculation for gamma-HCH." removed due to copyright restrictions.
Please see figure 6 in Scheringer et al. (2006) at http://www.sust-chem.ethz.ch/downloads.

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