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Introduction: Flow modeling for environmental exposure assessment

Method: Development of dynamic probabilistic material flow modeling framework for exposure assessment

Results: Case study of CNT in Switzerland

Conclusions: Opportunities and limitations of the method based on the modeling and simulation process
Background

- Flow modeling anthropogenic pollutants in the environment

  - … enables to determine environmental stocks and concentrations
  - … and thus exposure and risk assessments,
  - … even where a direct measurement is not possible.
Identification of System Compartments

- Production
- Polymer Composites
- Consumer Electronics
- etc.

**Technosphere**

- Waste Incineration Plant
- Sewage Treatment Plant

**Product Categories**

- Environmental Media
  - Air
  - Ground Water
  - Surface Water
  - Soil

**Ecosphere**

- Based on the investigated system and question
Challenges:
1. Time dynamic behavior
2. Fundamental uncertainties

\[ \text{Inflow}_{\text{Prod.}} \times TC_{\text{Prod.}, \text{Poly.}} \times TC_{\text{Poly.}, \text{WIP}} \times TC_{\text{WIP}, \text{Soil}} + \]
\[ \text{Inflow}_{\text{Prod.}} \times TC_{\text{Prod.}, \text{Elect.}} \times TC_{\text{Elect.}, \text{WIP}} \times TC_{\text{WIP}, \text{Air}} \times TC_{\text{Air, Soil}} \]
...
Observation over a set of subsequent years:

- Varying annual inflows
- Delayed transfer in stocks
- Add up the inflows to model sinks
Uncertainty Handling

- Existing (dynamic) material flow modeling methods
  - Often no uncertainty representation,
  - Value ranges,
  - Error levels
  - Variance
  - $\Rightarrow$ Uncertainty as deviation from a (known) value

- Need for a new method!

- Exposure assessment modeling characteristics:
  - Fundamental uncertainties
  - Data from conflicting sources of varying reliability
Dynamic Probabilistic Material Flow Modeling

- Bayesian flow model\textsuperscript{a} with probability distributions for
  - Transfer Coefficients for dependent flows
  - For absolute volumes of external inflows for each year
- Deterministic time dependent release function of stocks

- Monte – Carlo simulation to propagate the assumptions (i.e. to stocks)

- Normalization of the material flows

\textsuperscript{a}static case in: Gottschalk (2010) in Environ. Modell. Softw. 25, 320-332
Simulation Framework

- Simulation package:
  - Ready to use infrastructure to facilitate simulation process
  - Components to implement and assemble the model
Model Structure - Components

- **Compartment**: 1..n
- **Model**: 1
- **External Inflow**: 1..n

**Sink**

**Flow Compartment**

**Stock**

**Local Release**

- **Fixed Rate Release**
- **List Release**
- **Function Release**

**Transfer**

- **Deterministic Transfer**
- **Stochastic Function Transfer**
- **Random Choice Transfer**
- **Aggregated Transfer**

**External Inflow**

- **External List Inflow**
- **External Function Inflow**

- **Deterministic Value Inflow**
- **Random Choice Inflow**
- **Stochastic Function Inflow**
**Simulation process**

- Monte Carlo Simulation: Over a large sample
- Accounting stocks and flows: Over all periods

1. **Draw random values from respective distributions and set model parameters**
2. **Start period: determine external inflows and local releases from stocks**
3. **Calculate dependent flows and determine material accumulations**
4. **End period: add current accumulations to stocks**
5. **Evaluate flows and stocks statistically**
Case Study - CNT in Soil in Switzerland
Model Parameter: CNT Production in 2012

The graph shows the probability density of CNT production volume (tons) for different studies:

- Hendren et al. 2011 (100%)
- Piccinno et al. 2012 (100%)
- Future Markets Report 2011 (100%)
- Ray et al. 2009 (25%)
- Healy et al. 2008 (25%)
- Schmid et al. 2008 (25%)
Model Parameter: CNT Production in 2012

Combined Sample
Model Parameter: CNT Production – Scaling

![Graph showing the production volume of CNTs over years with data points and regression function.](image)
Model parameters – Sewage treatment plant removal efficiency (TC)
Model parameters – Automotive product life time

- Normal distributed with $m = 11.9$ years
Model parameters - examples

Absolute Inflows for each period

Relative transfers (TCs)

Deterministic life-time distributions
Simulation Output: CNT stock in Soil
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![Graph showing the amount of CNT stock in soil over years with different quantiles represented.](image-url)
Simulation Output: CNT stock in Soil

- Mean value
- 15% quantile
- 85% quantile

- 2014
- Mean: 0.418 t
- Mode: 0.412 t
- 15% quant.: 0.351 t
- 85% quant.: 0.488 t
Simulation Output: CNT stock in Soil
Conclusions

- First time assessment of absolute ENM stocks and concentrations using a probabilistic model
- Time-dynamic system behavior
- Flow specific
- Explicit uncertainty representation and propagation

Limitations:
- At the moment no fate specific modeling
- Higher modeling effort
- Risk to pretend a too high certainty
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