A Dynamic Probabilistic Material Flow Modeling Method for Environmental Exposure Assessment of Engineered Nanomaterials

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Content

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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

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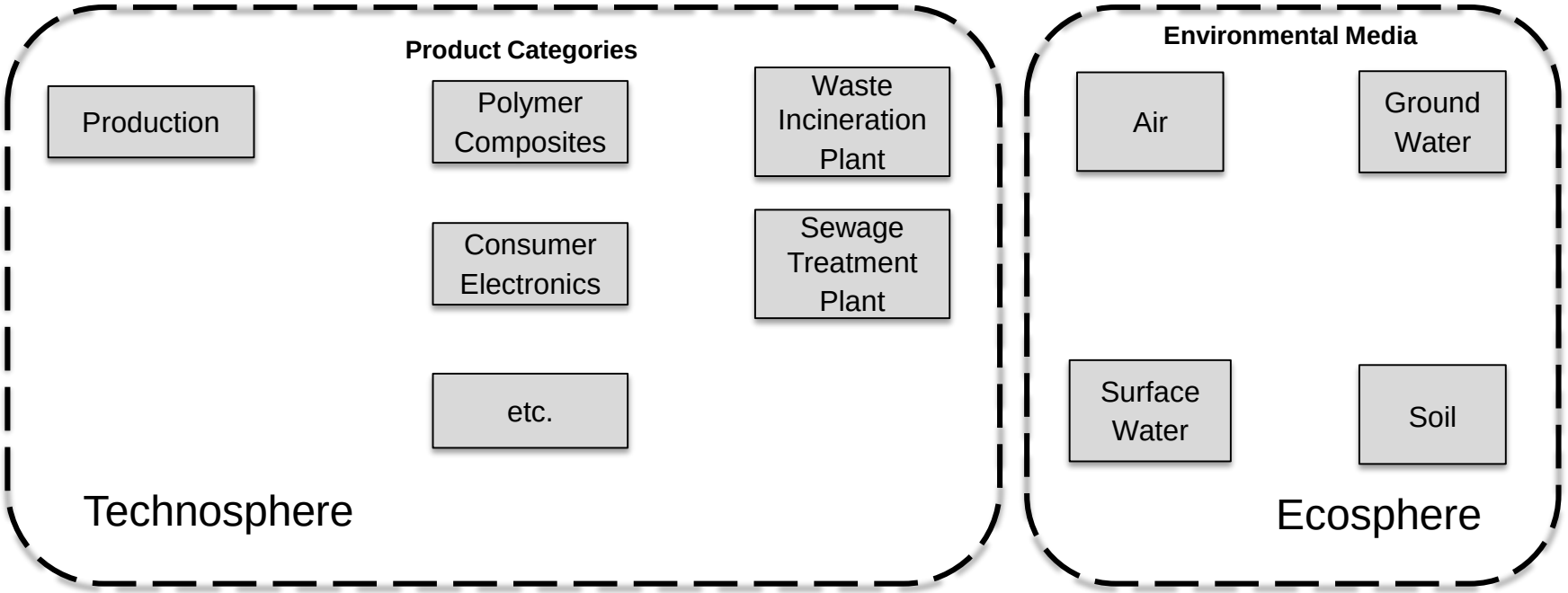
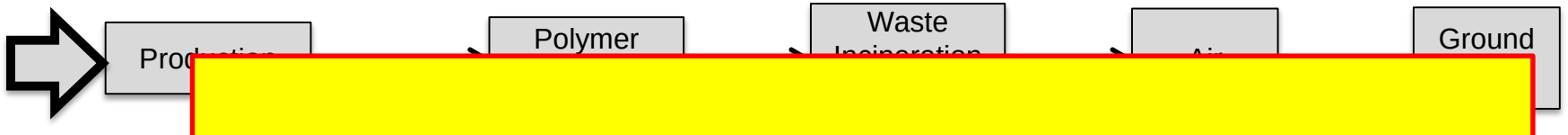
- Flow modeling anthropogenic pollutants in the environment
  - … enables to determine environmental stocks and concentrations
  - … and thus exposure and risk assessments,
  - … even where a direct measurement is not possible.

Identification of System Compartments



- Based on the investigated system and question

Mathematical Flow Representation



Challenges:

1. Time dynamic behavior

2. Fundamental uncertainties

$$Infl \qquad \text{oil}$$

$$+$$

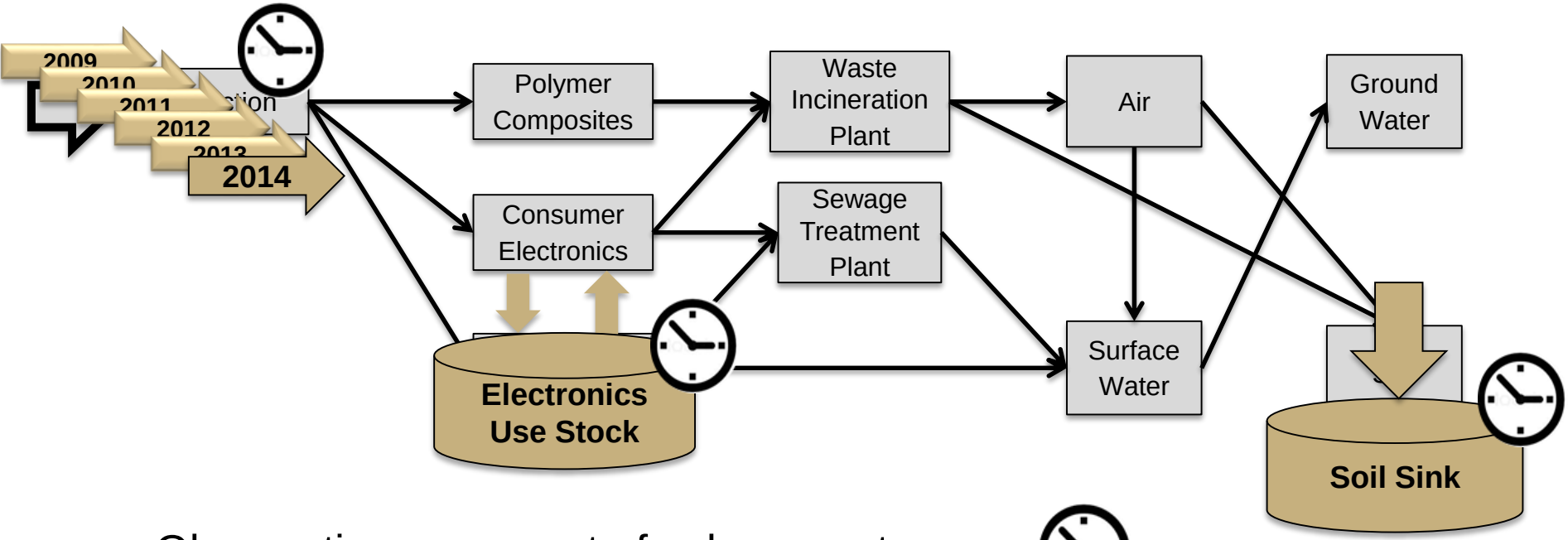
$$Inflow_{Prod.} * TC_{Prod.,\,Poly.} * TC_{Poly.,\,WIP} * TC_{WIP,\,Soil}$$

$$+$$

$$Inflow_{Prod.} * TC_{Prod.,\,Elect.} * TC_{Elect.,\,WIP} * TC_{WIP,\,Air} * TC_{Air,\,Soil}$$

$$\ldots$$

Time Dynamic Behavior



- Observation over a set of subsequent years:

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

Uncertainty Handling

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- Existing (dynamic) material flow modeling methods
  - Often no uncertainty representation,
  - Value ranges,
  - Err
  - Var
  - => 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

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- Bayesian flow model[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

[a]static case in: Gottschalk (2010) in Environ. Modell. Softw. 25, 320-332

Simulation Framework

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

Model Structure - Components

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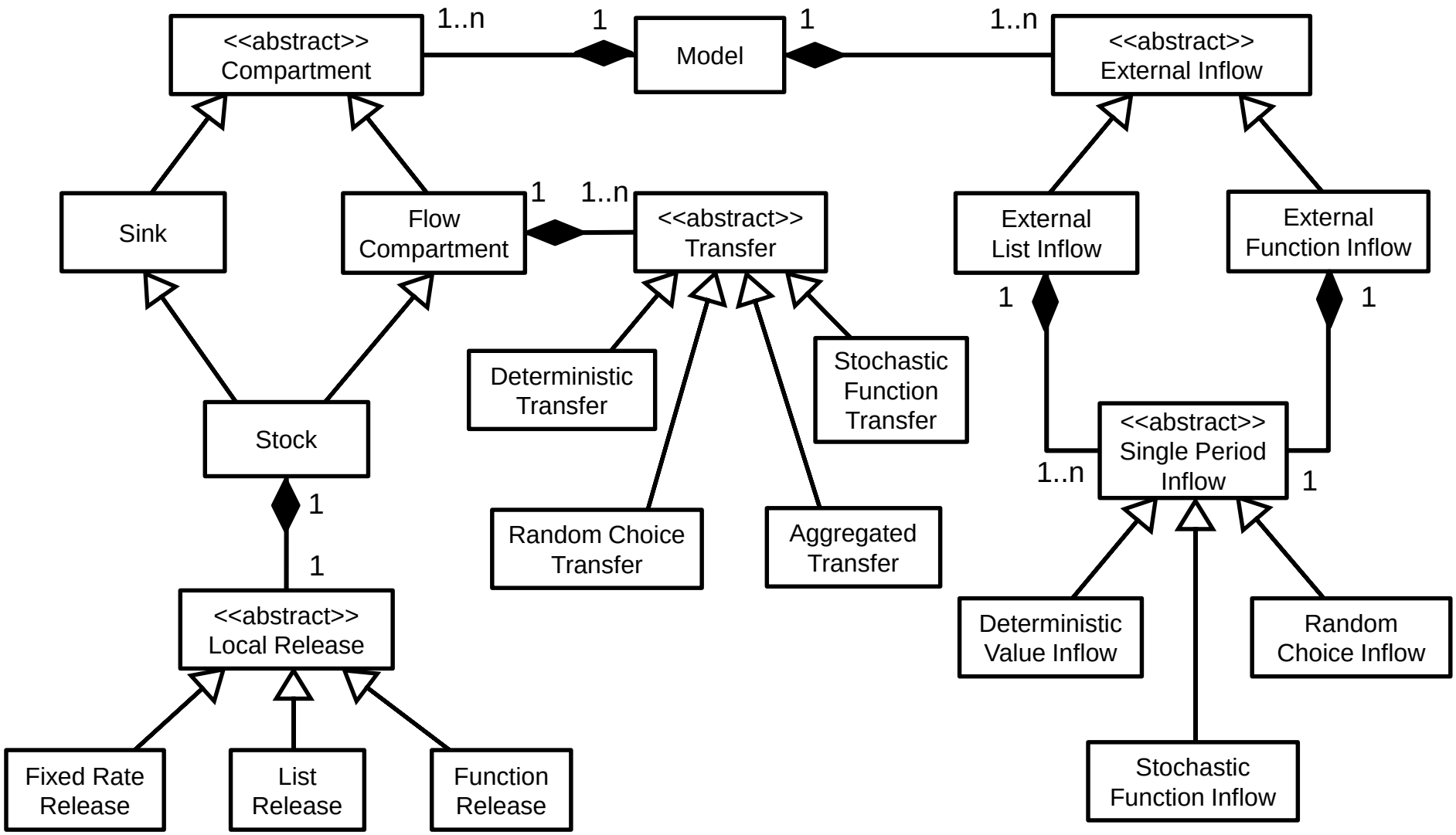
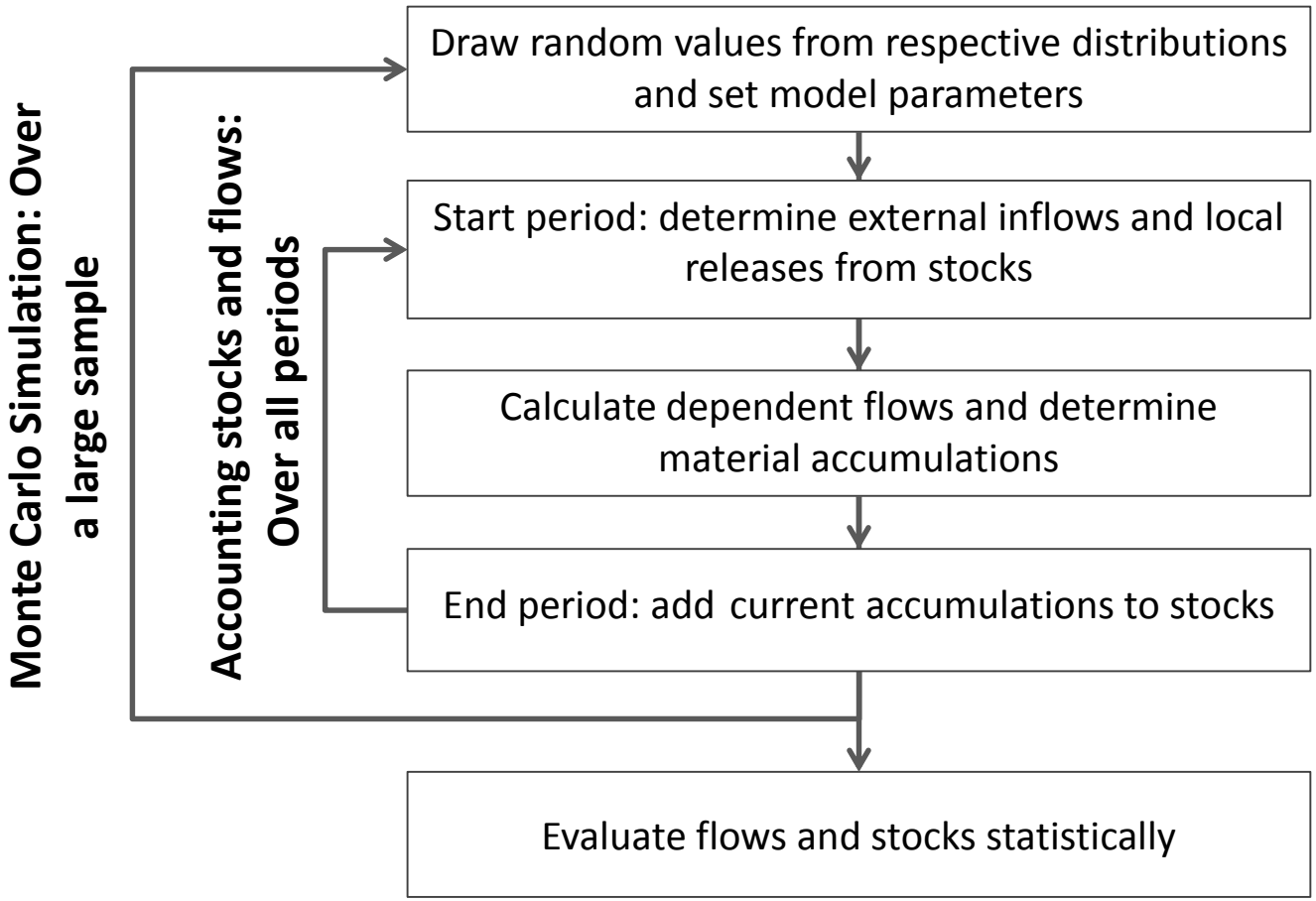


Simulation process



Case Study - CNT in Soil in Switzerland

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Model Parameter: CNT Production in 2012

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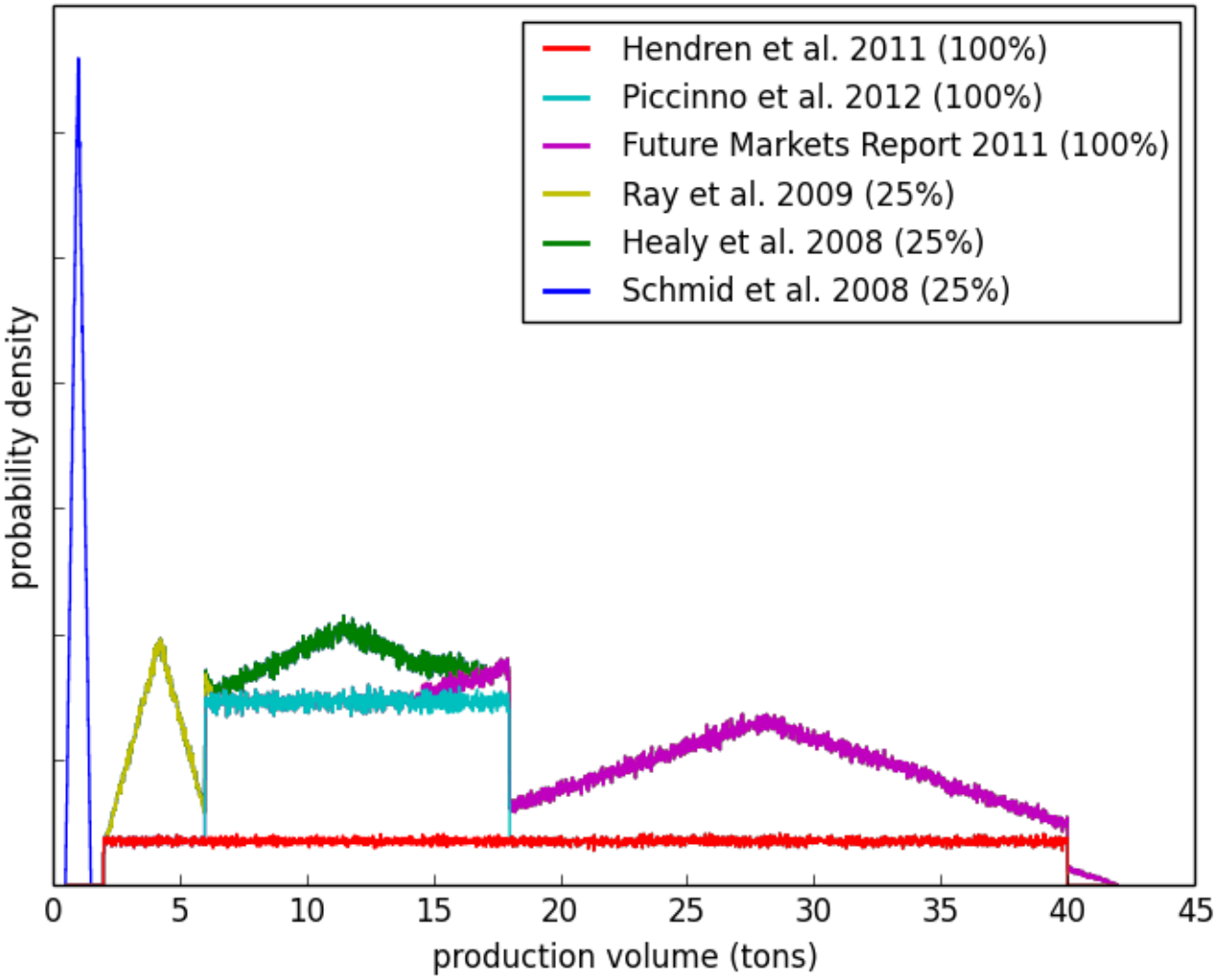

Model Parameter: CNT Production in 2012

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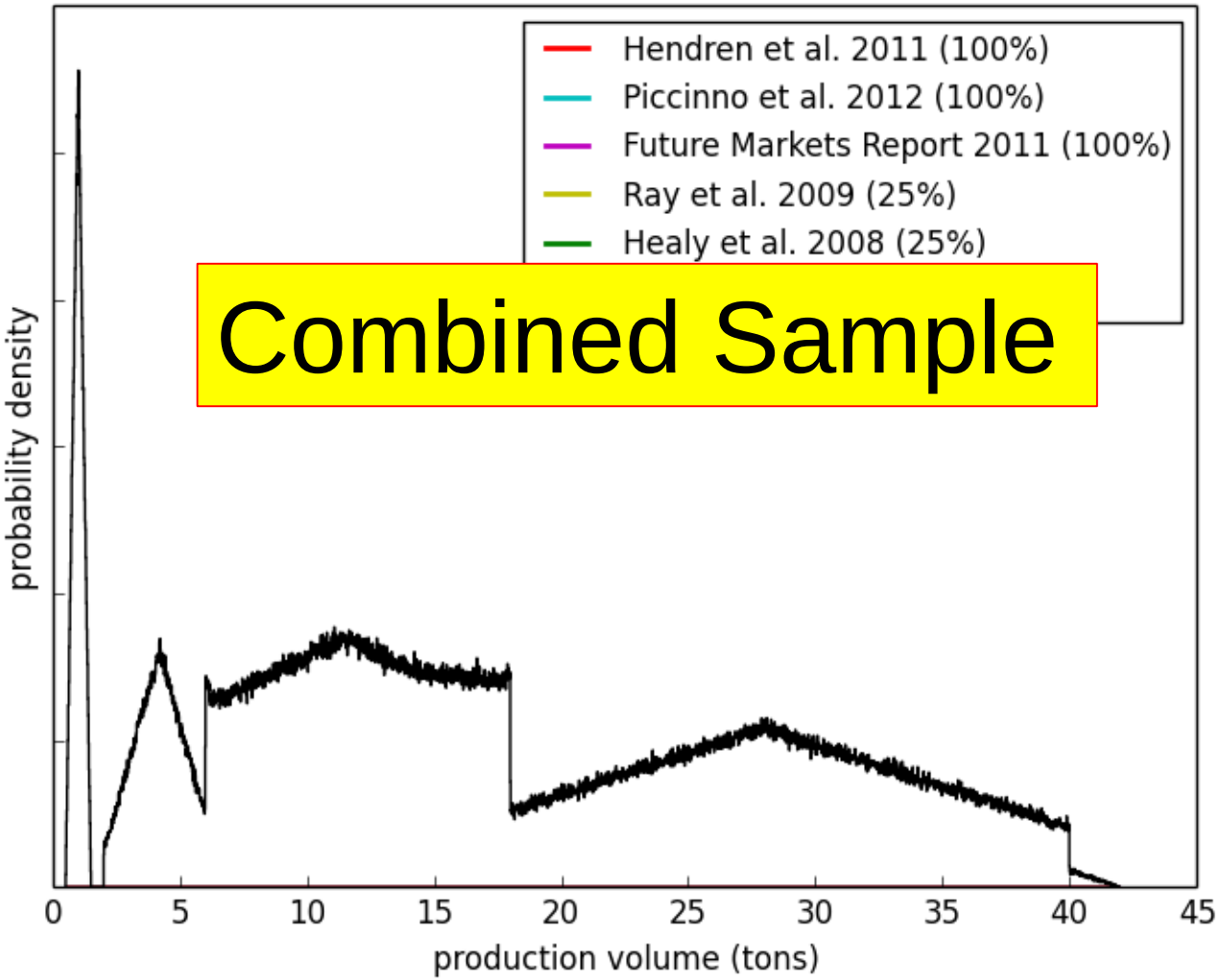

Model Parameter: CNT Production – Scaling

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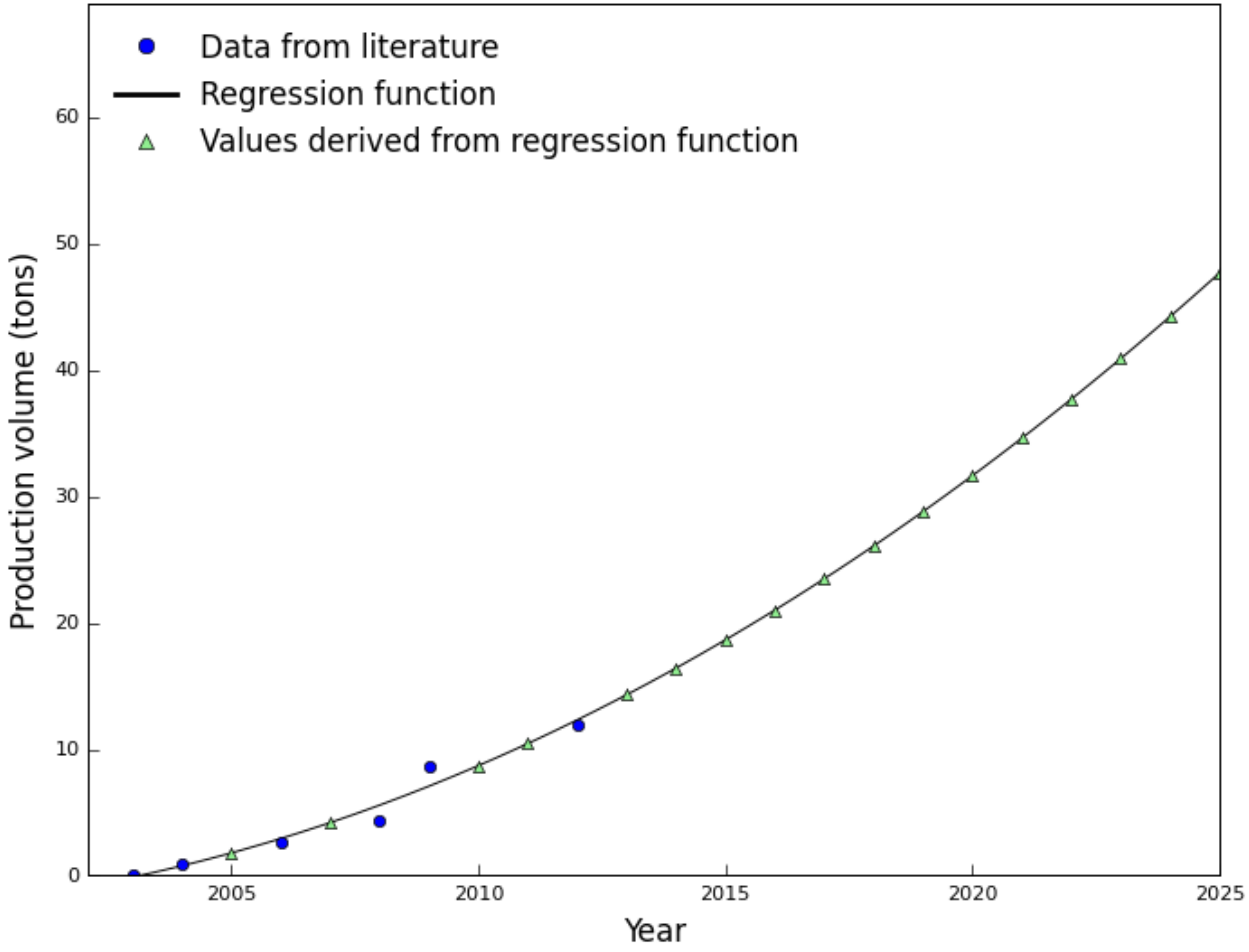
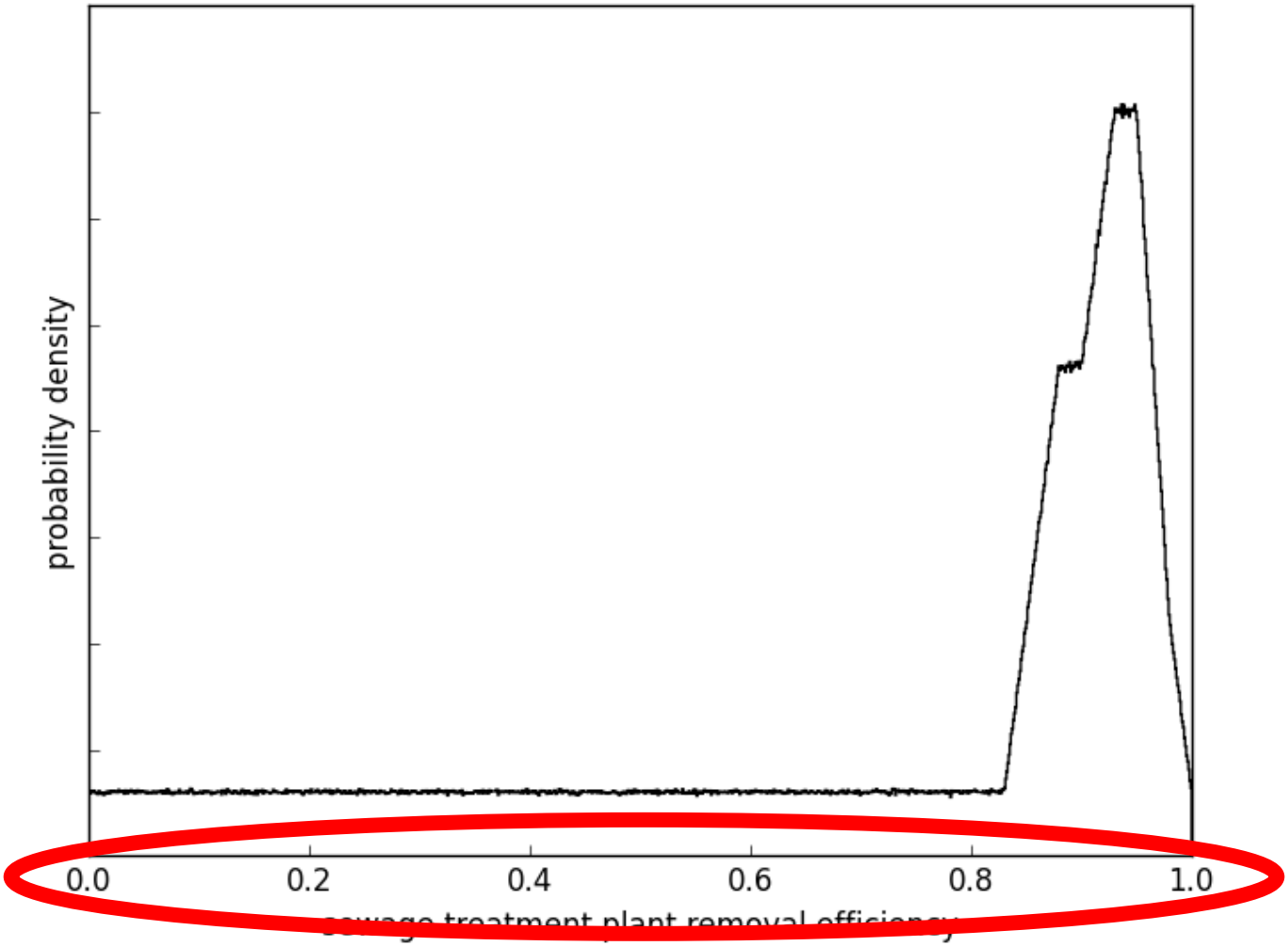


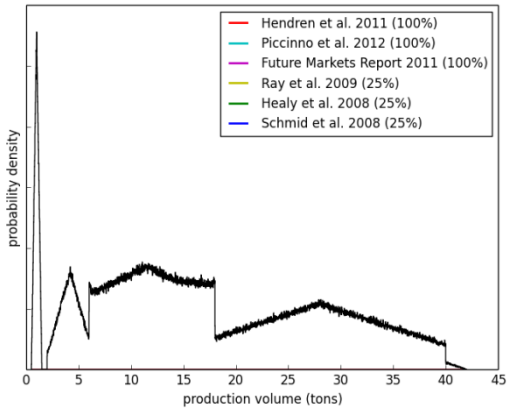
Model parameters – Sewage treatment plant removal efficiency (TC)

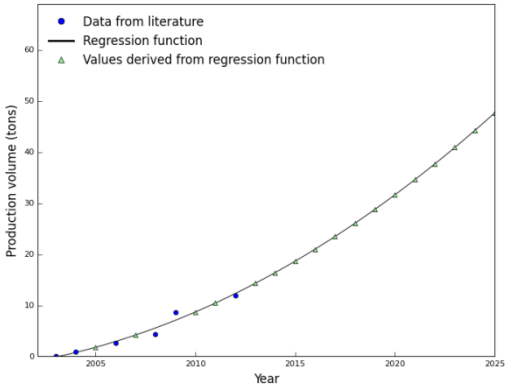


Model parameters – Automotive product life time

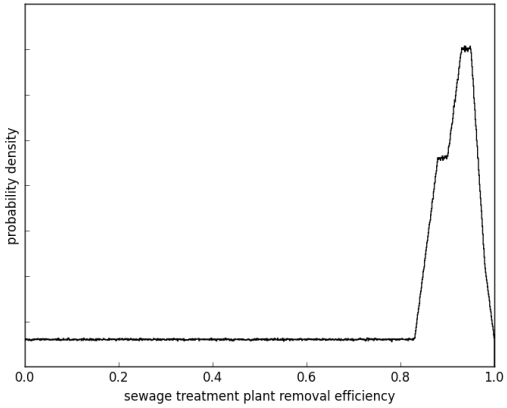
- Normal distributed with $m = 11{,}9\ years$

Model parameters - examples

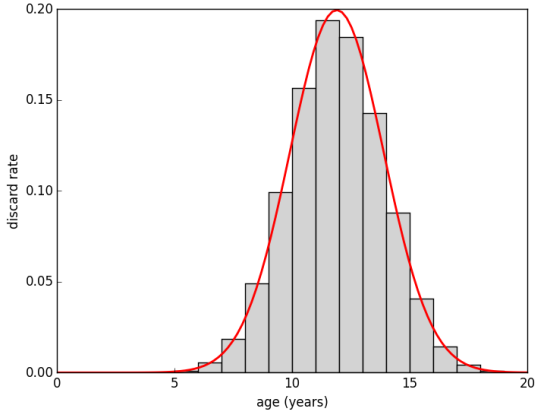




Absolute Inflows for each period



Relative transfers (TCs)



Deterministic life-time distributions

Simulation Output: CNT stock in Soil

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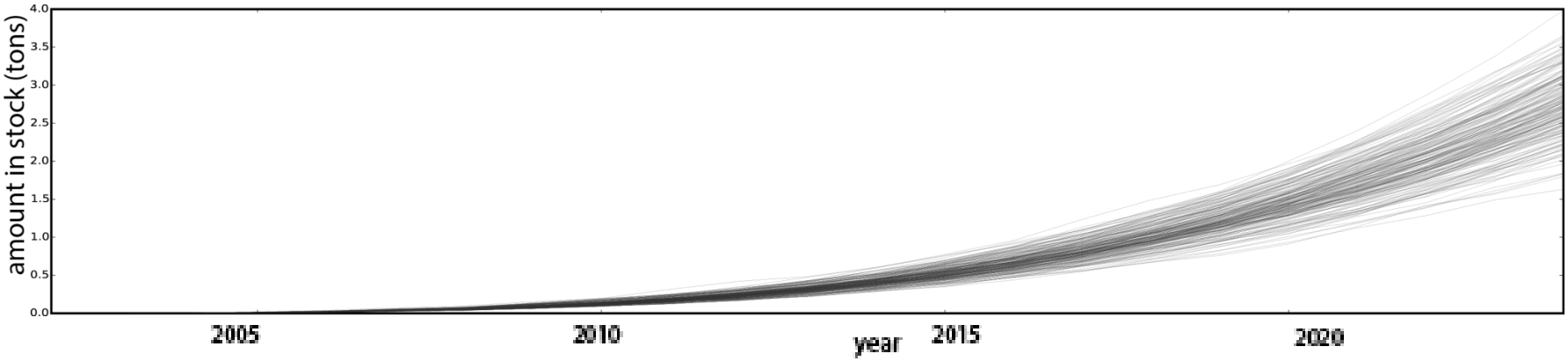

Simulation Output: CNT stock in Soil

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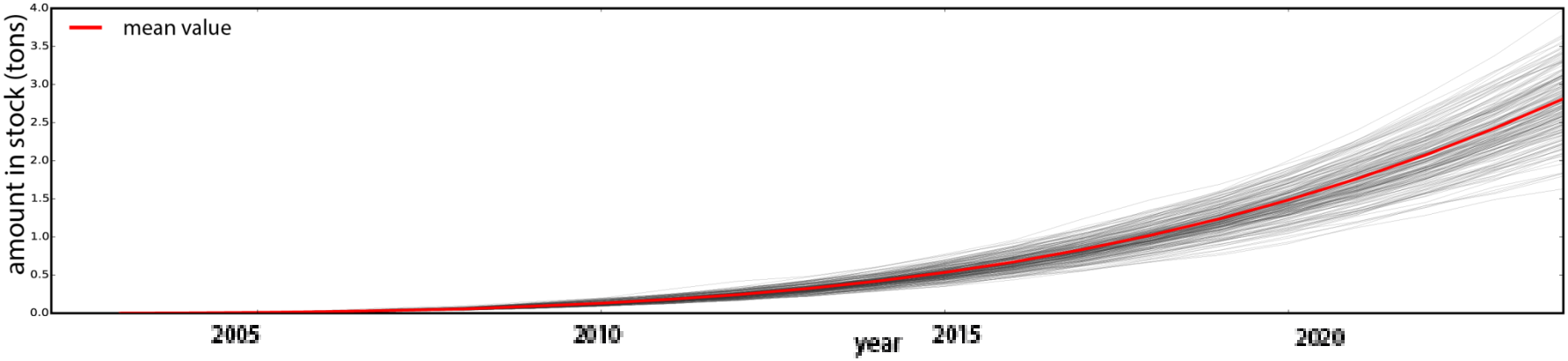

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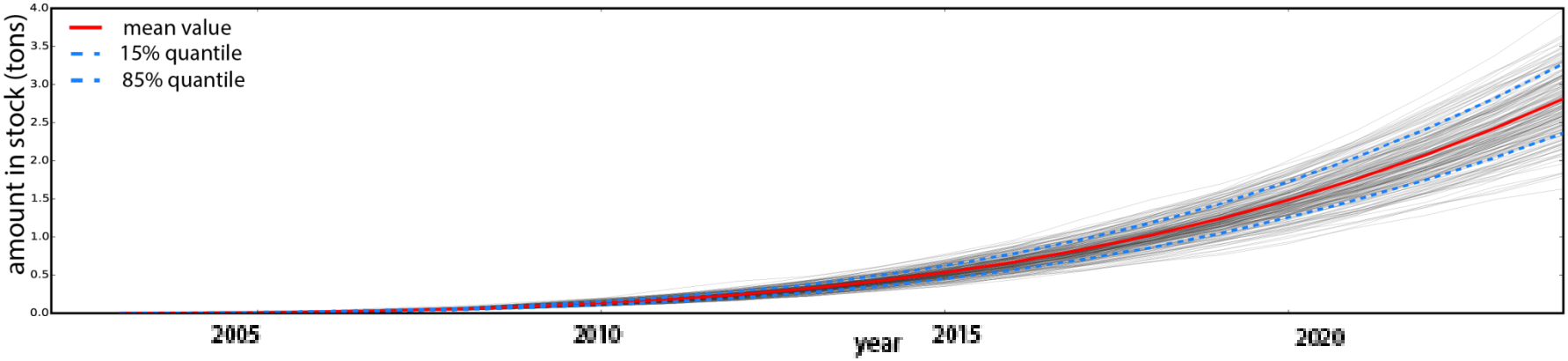

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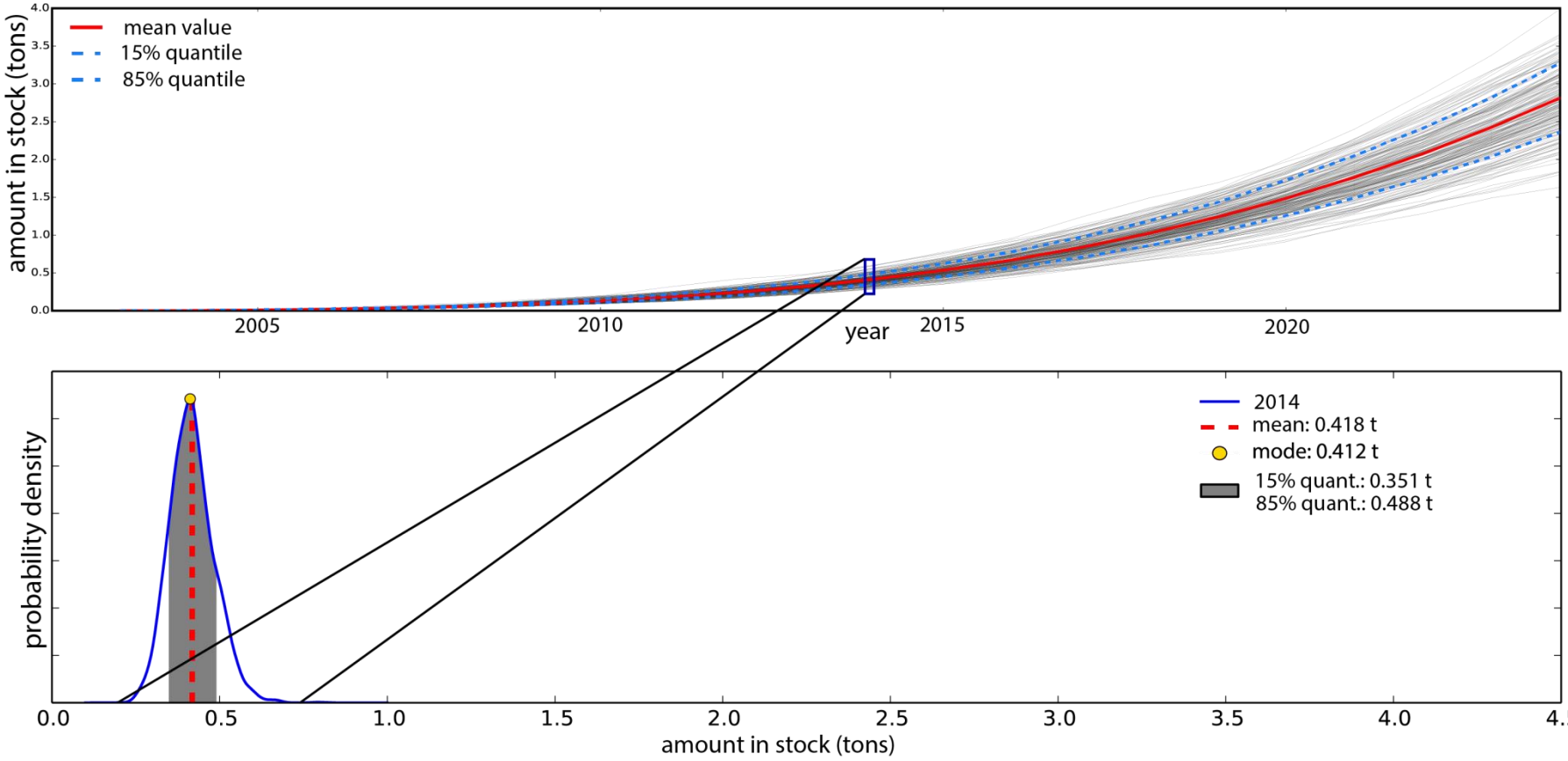

Simulation Output: CNT stock in Soil

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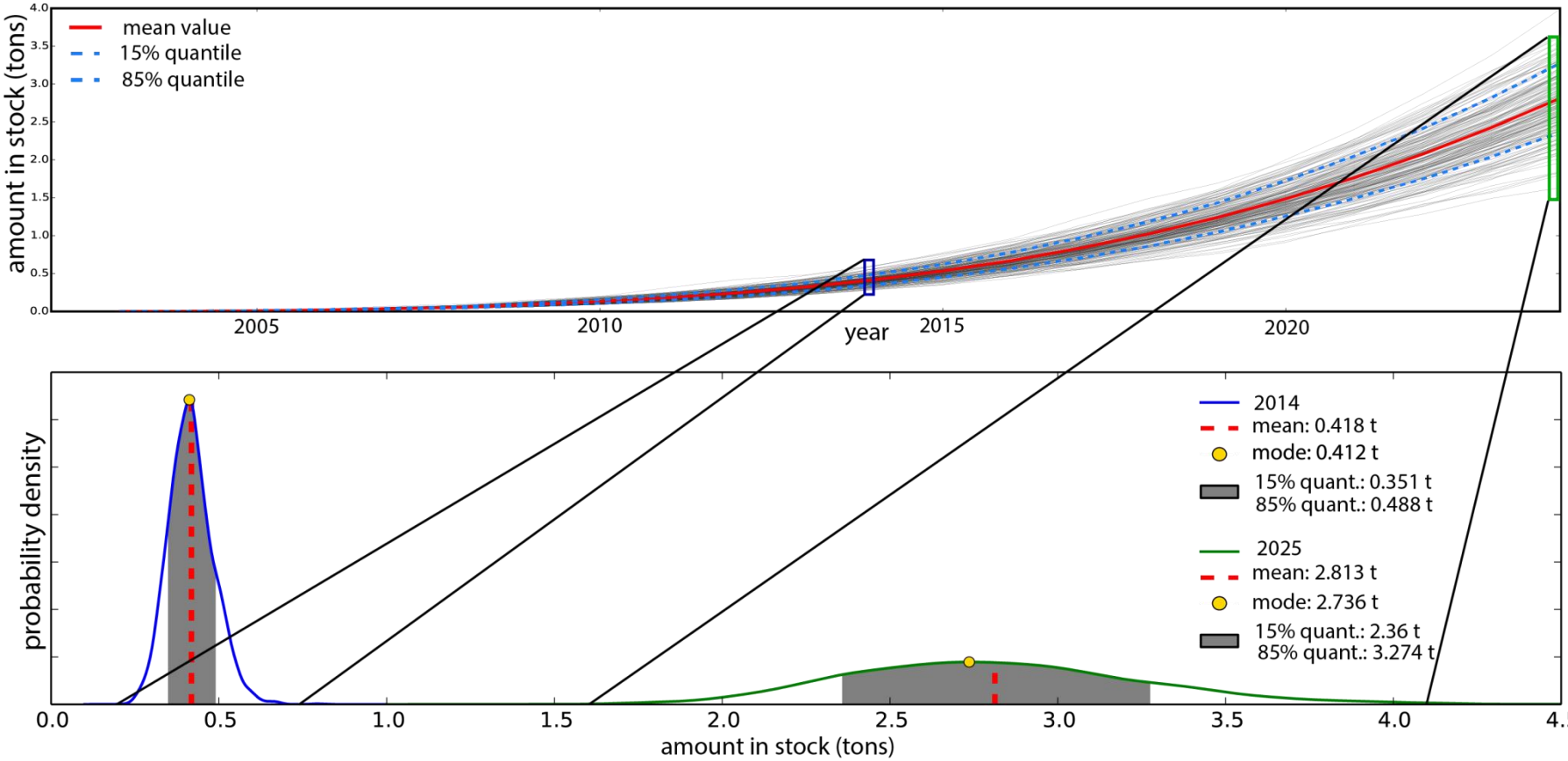

Conclusions

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- 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

Acknowledgements

Thank you for your attention!

Contact: Nikolaus.Bornhoeft@empa.ch

Nikolaus A. Bornhöft, Tian Yin Sun, Lorenz M. Hilty, Bernd Nowack: A Dynamic Probabilistic Material Flow Modeling Method; submitted to Environmental Modeling & Software (2015)