ECHA Workshop EUSES update, Brussels, 4-5 June 2018

Future developments in environmental risk assessment - SimpleBoxTreat4Solutions → SimplebBoxTreat4Reach?

Dik van de Meent[1,2], Jaap Struijs[1,2]

[1]Radboud University Nijmegen, NL
[2]Association of Retired Environmental Scientists ARES, Odijk, NL

Radboud University Nijmegen

Technical recommendations

by Jaap Struijs, Dik van de Meent

1. SimpleBox, SimpleTreat:
   a) SimpleTreat 4 (2016)
   b) SimpleBox 4 (2016)

   } the simpler, the better

2. Lessons learned from SOLUTIONS
   a) Integrate → SimpleBoxTreat
   b) Integrate Local and Regional → nested loc/reg Unit World; UBA's simple^{2}boxtreat?
   c) Substitute *PEC*/*PNEC*<*1* → Pr{C_W>*EC*} < 10^{-6}
   d) Consider mixtures
   e) 'safe use' = negligible contribution to ambient mixture toxic pressure

Recommended by Jaap:
EUSES 2 / SimpleTreat 3.1 → SimpleTreat 4.0

- Operation characteristics in SimpleTreat 3.1 reflect activated sludge technology in Europe 1980
  - Sludge loading rate = 0.15 kg/kg/d
  - Concentration suspended solids in effluent = 30 mg/L
- Partition coefficients based on:
  - QSARs for hydrophobic chemicals (Koc derived from Kow)
  - acid/base dissociation constants (pKa, pKb)

- In version 4.0 the operation characteristics represent the activated sludge technology in Europe 2010
  - Sludge loading rate = 0.10 kg/kg/d
  - Concentration suspended solids in effluent = 7.5 mg/L
- Partition coefficients based on:
  - New QSARs for Koc for organic chemicals computed from:
    - Chemical class (neutral or acid or base)
    - Acid dissociation constant (pKa)
    - Hydrophobicity (Kow)

Recommended by Dik:
EUSES 2 / SimpleBox 3.1 → SimpleBoxTreat4solutions

- separate STP simulation
- separate local calculation

- separate emission estimation
- Pr{*PEC*>*PNEC*}<5%
  - *PNEC* from IUCLID

- neutral hydrophobics only
- drizzle precipitation
- ….
- ….
- 40 compartments

- STP simulation integrated
- local nested inside regional
  - no overshoot local soil
- emission estimation integrated
- PR{*PEC*>*HC50*}<10^{-6}
  - Van Straalen-Aldenberg integrated

- partly ionized (organic acids and bases)
- rain episodes
- ….
- ….
- nested Unit World (simple^{2}boxtreat)?

Recommendation from the SOLUTIONS project:
Pr{*PEC*/*HC5* >1} < 5% → Pr{*PEC* > *HC50*} < 10^{-6}

- not different
- understandable, meaningful
- simple, robust
- scientifically sound
- ready to go
- demonstrates ‘safe use’

http://www.solutions-project.eu/

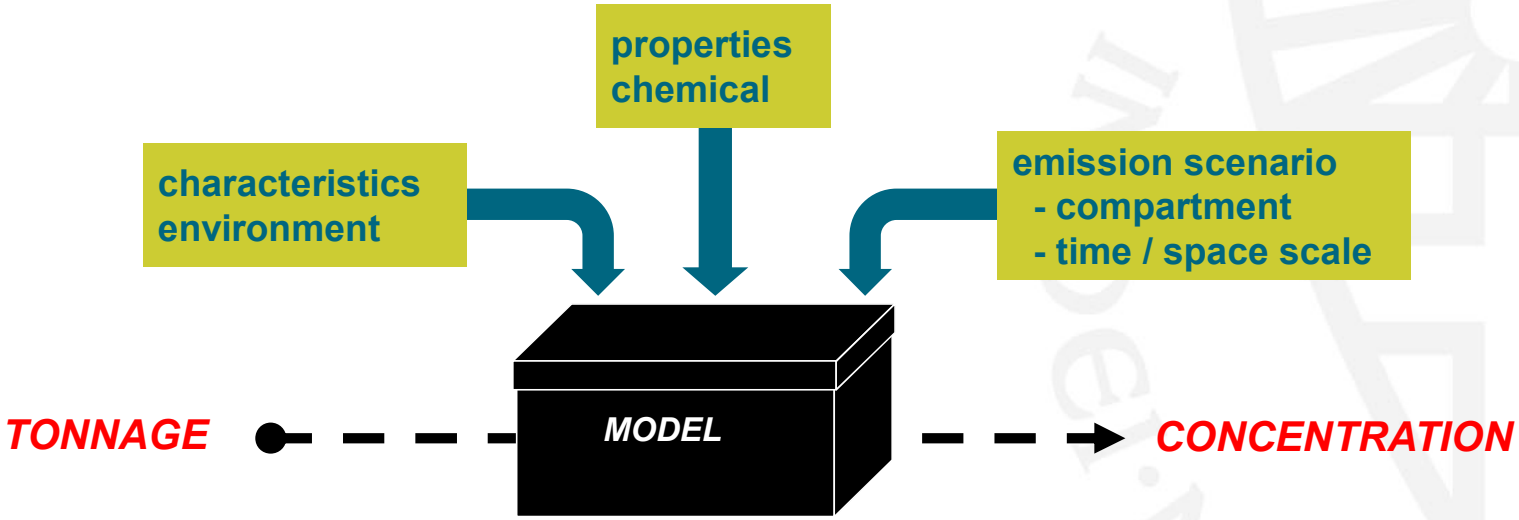
- EU FP7 project 10 M€
- UFZ Leipzig, RIVM, ARES
- ALL currently used substances
- Impacts aquatic ecosystems EU rivers

http://www.solutions-project.eu/

- EU FP7 project 10 M€
- UFZ Leipzig, RIVM, ARES
- ALL currently used substances
- Impacts aquatic ecosystems EU rivers

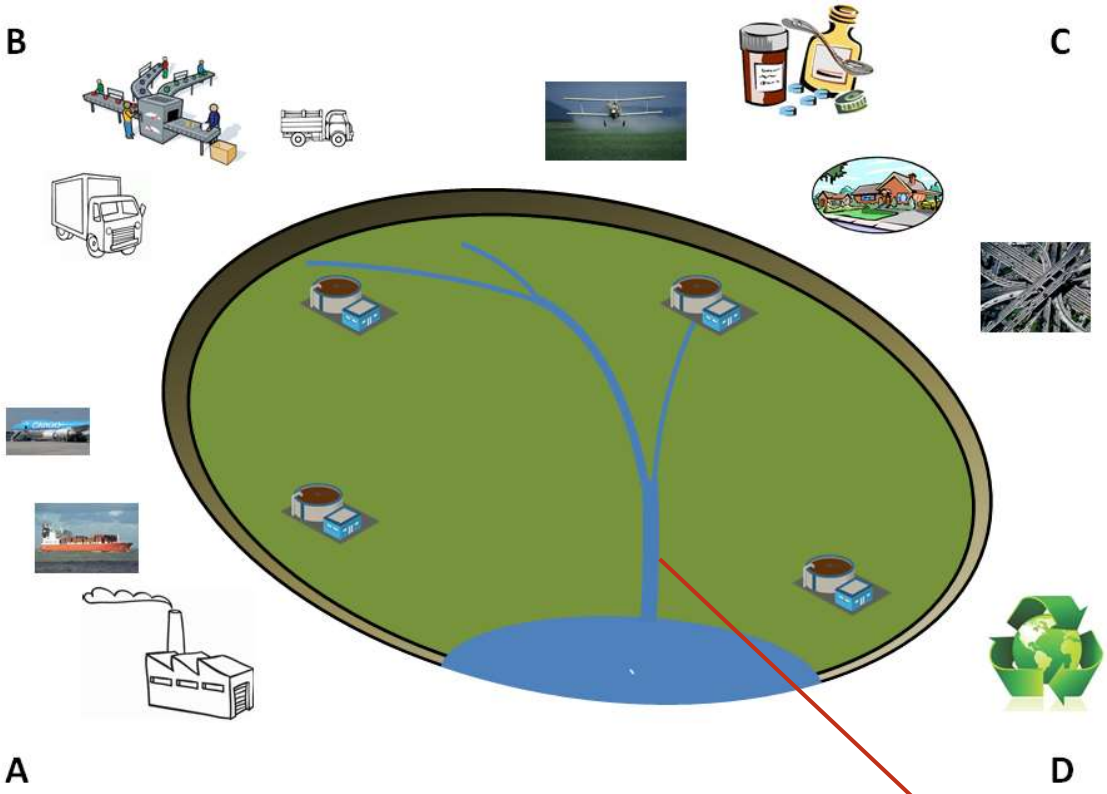
SOLUTIONS exposure modeling

- Concentrations proportional to emission rates
- Exposure function of EU tonnage



$$C^{ss}{}_W = m(P^s, S^s, K_{OW}, k^{deg}, env) \cdot e$$

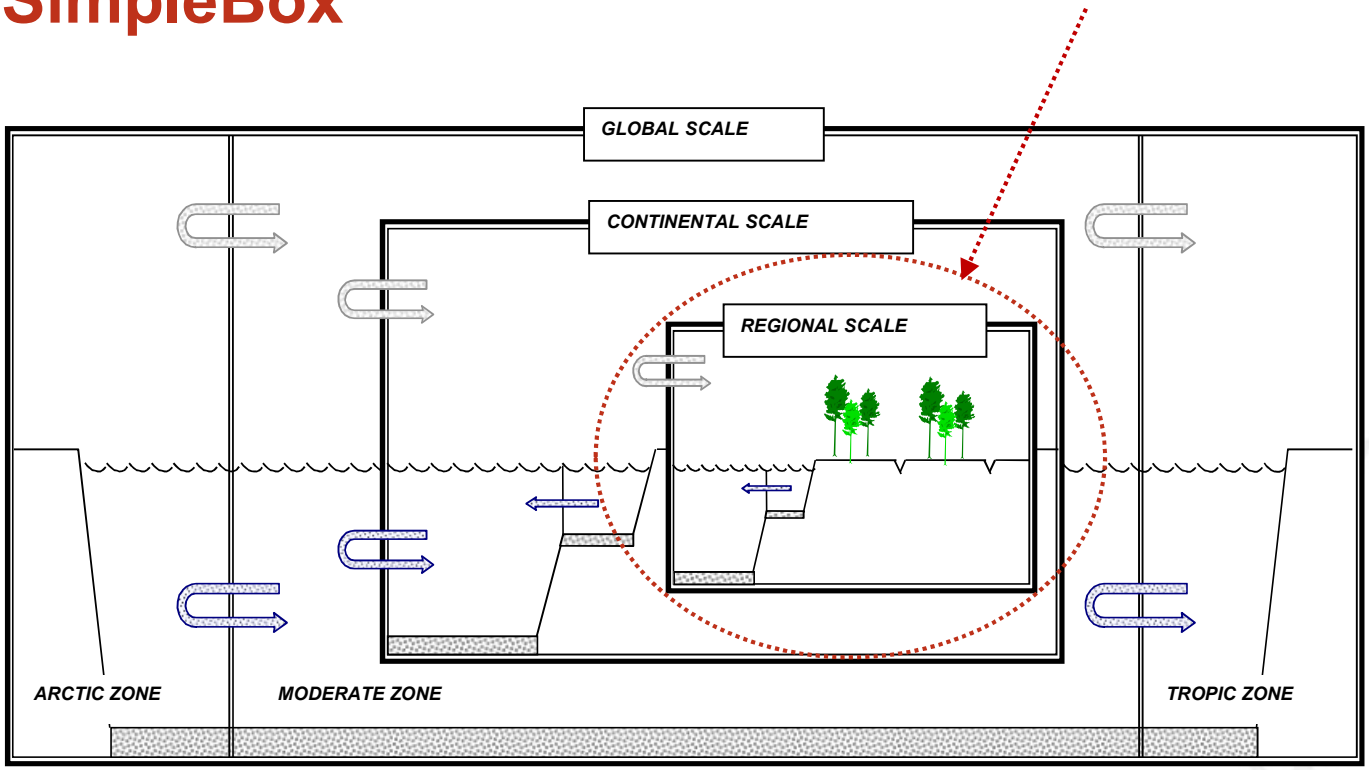
SOLUTIONS emission estimation



- EUSES 2.1.2: ***A/B tables***
  - REACH: ***ERC***
  - SOLUTIONS project: ***spERC***

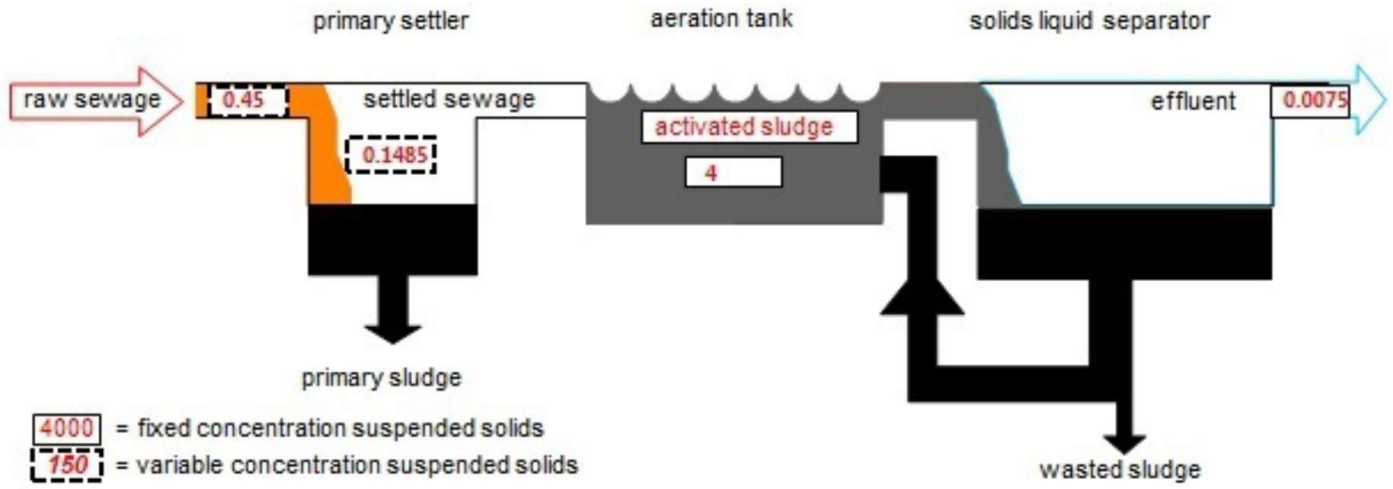
$$\text{Release}_i = \sum_i USE_i \cdot RF_i \cdot F_{STP}$$

SimpleBox



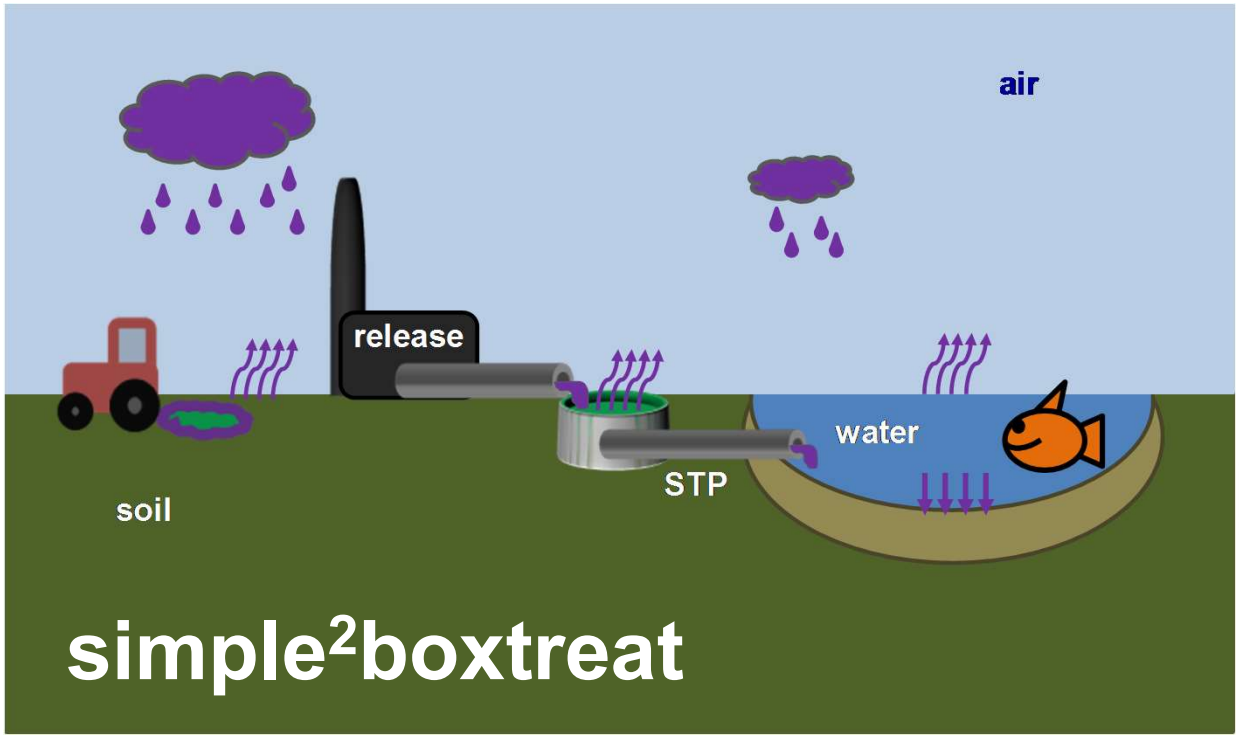
- SimpleBox 4.0 (2016); most RIVM-recommended improvements included
- simulates hypothetical ‘evaluative’ environment
  - Regional scale: Rhine/Meuse/Scheldt catchment
  - Local spatial: 15x15 km, nested in regional (not shown in this Figure)
  - Integrated with SimpleTreat → SimpleBoxTreat

SimpleTreat



- SimpleTreat 4.0 (2016); most RIVM-recommended improvements included
- Simulates 'Classical Activated Sludge' water treatment system
  - SimpleTreat 4.0 (2016)
  - Integrated with SimpleBox → SimpleBoxTreat

SOLUTIONS exposure modeling: SimpleBoxTreat

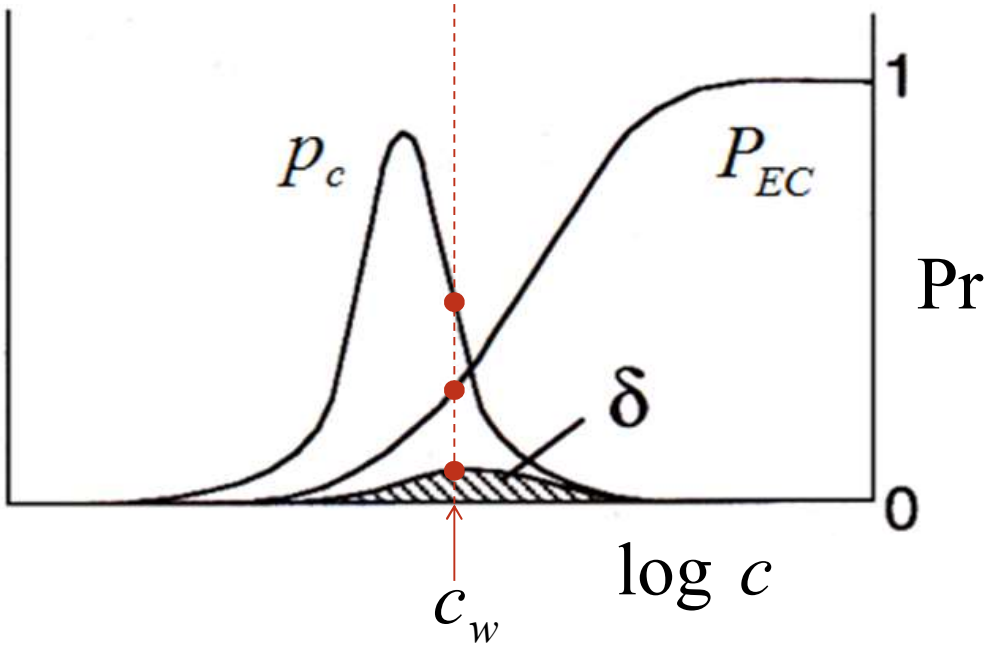


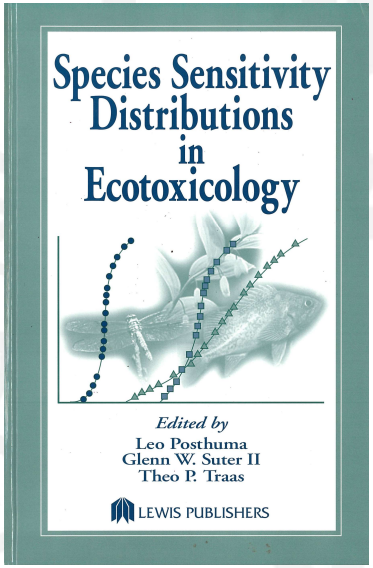
by Joris Meesters
Radboud University / RIVM

- UBA - KnowSEC
- SimpleTreat vs 4 + local SimpleBox vs 4
- Calculate REACH ‘Characterization Factors’

SOLUTIONS effects modeling: Van Straalen-Aldenberg

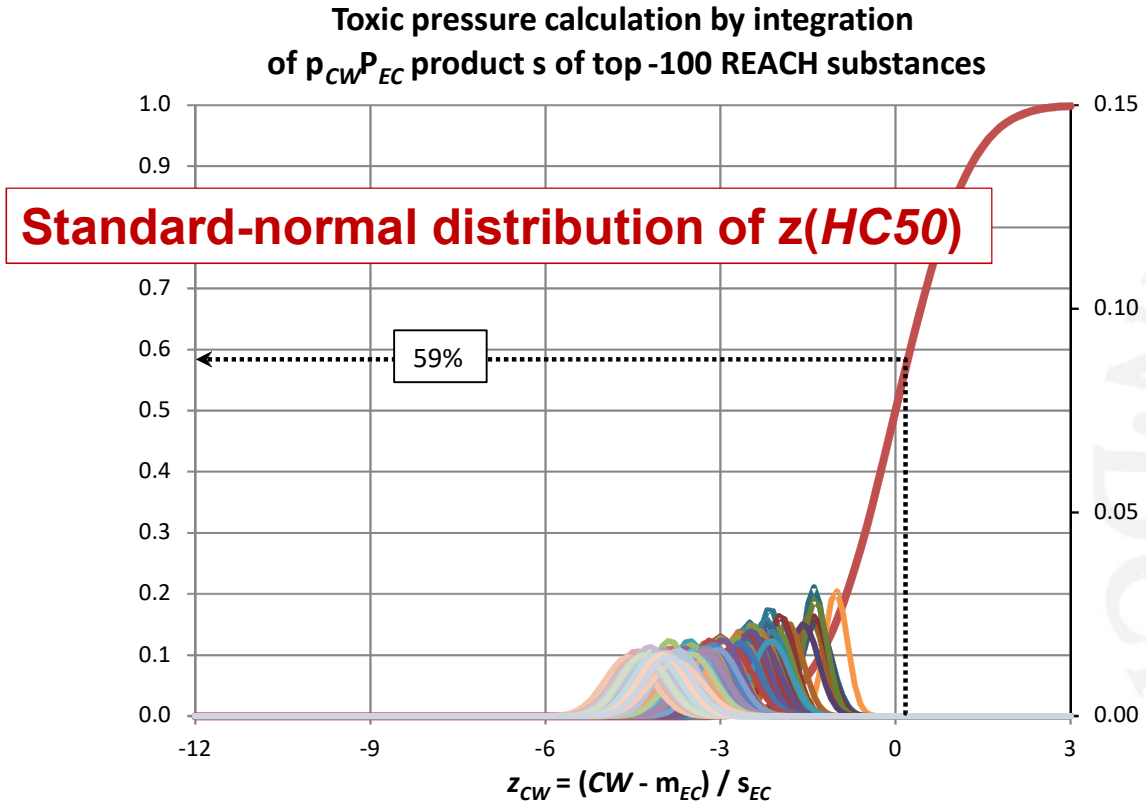
- Van Straalen and Aldenberg et al. (2002). In SSD-book, pp 37-102





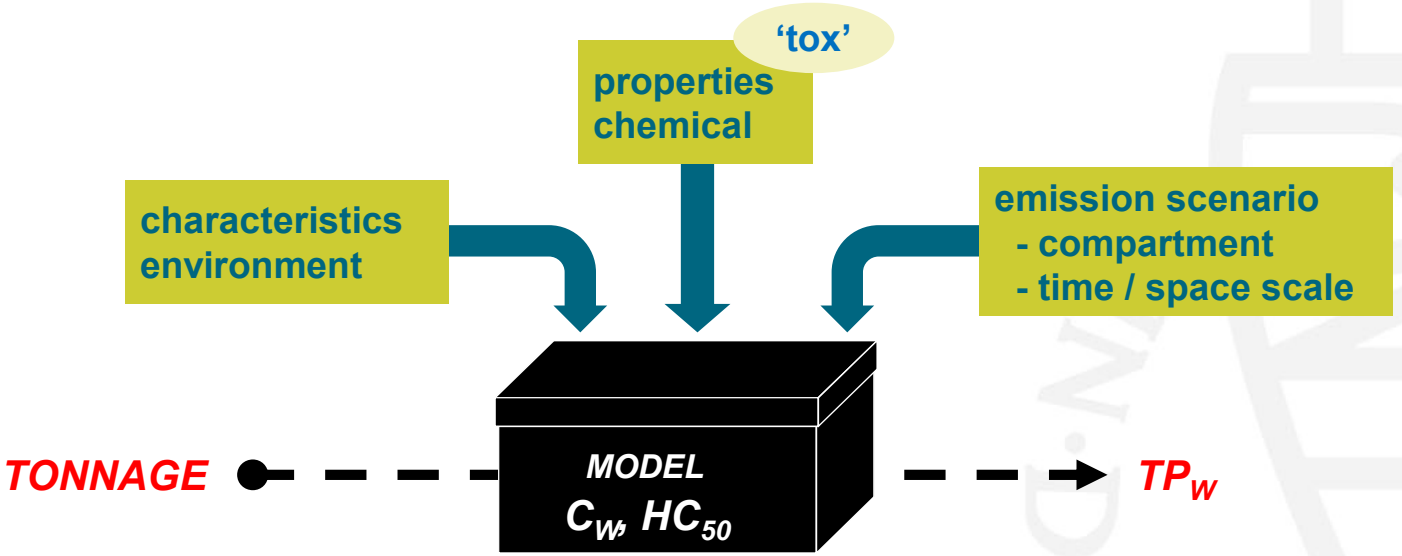
$$\textbf{Toxic Pressure} = \textbf{PAF} = \Pr\{\text{EC} < c_W\} = \Pr\{c_W > EC\} = \int_{-\infty}^{\infty} pdf(C_W) \cdot CDF(EC)dc = \delta$$

Van Straalen-Aldenberg applied to 6409 substances under uncertainty



- Concentration distributions of top-100 REACH substances overlap EC-distribution
  - means and standard deviations of exposure concentrations modeled by SimpleBoxTreat
  - mean and standard deviations of substance-specific HC50-acute from registration data

SOLUTIONS impact modeling



$$TP_W = f(\mu_{c_W}, \sigma_{c_W}, \mu_{EC_{50}}, \sigma_{EC_{50}})$$

- Toxic Pressure = Pr{C_W>EC} simple (model) function of EU tonnage
- Robust, useful

SOLUTIONS impact assessment: findings/conclusions

1. Estimated emission rates greatly uncertain

   'right on average, but wrong most of the time' (V Forbes, 2010)

   but good enough to serve the purpose

2. Estimated emission rates + simple unit world model

   good enough to rank substances

3. Pareto distributions (*'80-20 rule'*)
   a) of C_W
   b) of Pr{C_W>EC}
   c) Pareto ratio 95-5

4. Most Pr{C_W>EC} small (below 10^{-6})

5. >95% 'negligible risk'

SOLUTIONS impact assessment: recommendations to EUSES updating

1. Parsimony principle confirmed in SOLUTIONS
   a) Exposure modeling
   b) Impact modeling
   c) SimpleBoxTreat4solutions recommend to EUSES/REACH
2. Recommended for exposure modeling
   a) Emission estimation integrated
   b) STP simulation integrated
   c) Nested local/regional Unit World
3. Recommended for impact assessment
   a) Van Straalen-Aldenberg integral for calculating Pr{C_W>EC}
      mean + standard deviation C_W + mean and standard deviation *EC50*
4. Recommended for demonstrating possibility of 'safe use'
   a) with $EC = EC50$, Pr{C_W>EC} < 10^{-6}

Acknowledgement

- Colleagues in Academia, Government, Industry 1984-2018
  - Don Mackay, Frank Wania, Ian Cousins, Todd Gouin, ….. (Univ of Toronto, Trent Univ, Canada)
  - Tom McKone, Randy Maddelena, Matt Mcleod, ….. (Lawerence Berkeley Lab, UC Berkeley, CA)
  - Lee Wolfe, Sam Karickhoff, Richard Zepp, Larry Burns, ….. (USEPA Athens, GA)
  - Michael Matthies, Stephan Trapp, Andreas Beyer, Jörg Klasmeier, ….. (Univ of Osnabück)
  - Tjalling Jager, Theo Traas, Joost Bakker, Leo Posthuma, Tom Aldenberg, ….. (RIVM, Bilhoven)
  - Nico van Straalen (Free University Amsterdam, ARES)
  - Michael Hausschild, Mark Huijbrechts, Ralph Rosembaum, ….. (USEtox)
  - Johannes Tolls, Frank Schnoeder, Volker Koch, ….. (Ecetoc TRA)
  - Albrecht Striffler (denkbares), Nannett Aust (UBA KnowSEC)