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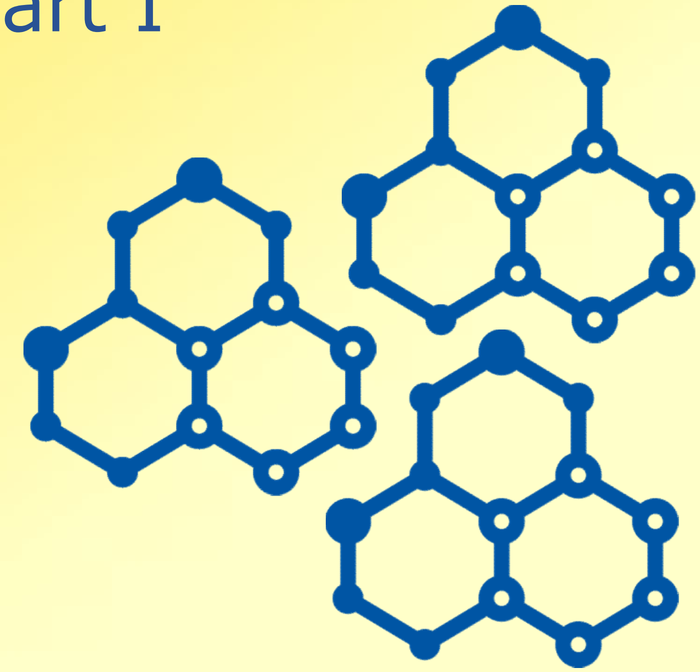
Current limitations and update needs identified by workshop organising committee – Part I

EUSES Update workshop
4 June 2018



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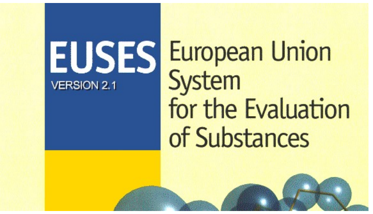
QSAR for Koc and BCF

Heike Schimmelpfennig, ECHA



QSARs in EUSES: current situation

- Two models considered, both of them require logkow as input
  - Koc – Sabljic et al. logkow range **1 - 7.5**
  - BCF – Veith et al. logkow range **1 – 10**

- However, EUSES does **not check** whether the predicted substance is **structurally related** to those used to create the model (structural domain)

Why to propose this change?

- Experience shows that the **error** of the calculation is **higher** for substances **outside of the structural domain.** This is not checked by EUSES for none of the two models
- The koc model requires manual selection of the chemical class to which the substance belongs.
    - Selecting the wrong chemical class for a substance can lead to considerable differences (up to **>3 log units**)
- Koc model performs **worse** for **ionic species**

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2) Change options

Option	Description	Pros	Cons
No update.	Same options as in current EUSES.	No cost.	No improvement.
Limit calculations.	Koc QSAR only for logkow<3 BCF QSAR only for logkow<> 4.5	Easy to implement. Lower risk of very erroneous predictions.	For some substances with logkow > 4.5, BCF may not be available.
Docking with QSAR platform.	Retrieve predictions from another software (e.g. CAESAR, ChemProp).	Automatic domain check of predictions.	Heavy IT implementation.

Option 2 + Implementation of new models

- From the proposed options, limiting the QSAR calculations seems the most cost-effective approach
- In addition, replacing the existing models by newer ones is possible:

- Koc model from Franco and Trapp.
    - Requires: **pka** and **logkow**
    - Aligned with **SimpleTreat**
    - Estimates better **ionisable molecules**
- Only for **logkow <3**

- BCF model?
    - Veith *et al.* (1979)(current)
    - Rorije *et al.* (2011)
    - Franco *et al.* (2011)
    - Others?
- Only for **logkow <4.5**

Priority level (for option 2)

- Ready for implementation and implementation in IT tools easy
- Increased reliability for regulatory purposes
- Lower risk of erroneous estimation for adsorptive or high BCF potential substances
- **High priority**

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Release scenarios: Proposal to revisit the current approach for designing the release module

Heike Schimmelpfennig, ECHA

Current situation (1)

- Release module (and part of subsequent fate and distribution) differentiated in EUSES between biocides and REACH:
  - Emission scenarios developed for biocides (specifically for consumption based approach) not available for REACH assessment although some may be relevant
  - SPERCs and emission scenarios are similar concepts although developed in different context. Likewise SPERCs could be useful for assessment of biocides (specifically for tonnage based approach)

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Current situation (2)

- Incremental implementation of biocide ESDs in current EUSES
    - ➢ Each scenario within each PT implemented individually although some scenarios are the same/similar (e.g. only volume of receiving compartment varies)
- Increased complexity due to incremental implementation
    - ➢ increased risk of bugs
- Not always a systematic approach in modelling releases/exposure across ESDs/EUSES
    - ➢ Some emission scenarios calculate local emissions as well as local concentrations/PECs (e.g. direct release) => reflection of exposure elements in release module of EUSES

FS4
TE3

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Proposal

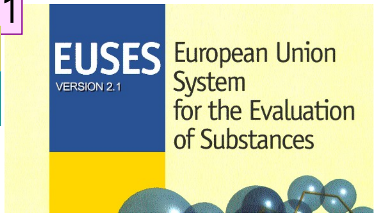
- Analyse various scenarios (release + local exposure) across ESDs to identify similarities/differences
- Develop a proposal for IT implementation for
  - improved consistency => local emissions in release module, local concentrations in fate & distribution module
  - consistent implementation for emission estimations
  - more robust implementation of new scenarios (e.g. harmonisation of parameters)

TE4

Slide 11

FS4	what is missing here is the fact that the proposal of "release scenario" harminization might help also REACH when there is a need to cover such case. Not only IT prospective. In general I found here to much emphasis on IT advantages. Would also mention business ones. FRATTINI Stefano, 29/05/2018
TE3	agree we need to indicate not only the IT advantages but also what this change would bring to the users of the tool (benefits from improved consistency and new scenarios) TSITSIOU Eleni, 30/05/2018
TE4	i dont understand this point TSITSIOU Eleni, 30/05/2018

MH1
FS5
TE5



Starting point for analysis

- Collecting the various fate and distribution models implemented for local exposure:

Release route	Local direct release to	Local exposure concentration based on the model for receiving compartment	Local exposure in subsequent compartment impacted
Air	Air (kg/day)	Local concentration in air: release from industrial site	• Local agricultural soil • MvE (man via environment)
		Local concentration in air: from application by spraying on a large surface (e.g. during spray application of mixtures on agricultural soil)	• MvE
Soil	Agricultural soil (kg/ha.day)	Local concentration in agricultural soil	• Local concentration in water: Small static water (ditch): • Local concentration in sediments: Sediment (of the ditch): • Concentration in groundwater • MvE • Secondary poisoning (terrestrial predators)
	Non agricultural soil (kg/day)	Local concentration in non agricultural soil	• Concentration in groundwater

Slide 12

MH1 is that useful?
MAGAUD Helene, 28/05/2018

FS5 I found it useful. Howver what is missing here a final slide with summary consideration. I would not end the presentation with tables
FRATTINI Stefano, 29/05/2018

TE5 agree as well
TSITSIOU Eleni, 30/05/2018

Release route	Local direct release to	Local exposure concentration based on the model for receiving compartment	Local exposure in subsequent compartment impacted
Water	Biological STP (kg/day)	STP concentration (Based on SimpleTreat)	• Local concentration in agricultural soil after 30 days (soil assessment) or 180 days (for MvE, sec pois.) • Air • Freshwater surface water/ sediments • Marine water/ sediments
	Surface water (kg/day)	Local concentration in water: flowing water	• Sediment • MvE • Secondary poisoning
		Local concentration in water: static water (Pond)	• Sediment • MvE • Secondary poisoning
		Local concentration in water: small static water surrounding agricultural field (ditch)	• Sediment • MvE • Secondary poisoning
	Marine water	Local concentration in marine water	• Marine Sediment • Secondary poisoning
		Local concentration in marine water (static: Oil platform)	• Marine Sediment • Secondary poisoning
		Local concentration in marine water (Harbour scenario, semi static)	• Marine Sediment • Secondary poisoning

Priority

- Approach for developing EUSES to be further analysed during pre-study expected to take place in early 2019
- Streamlining of implementation important from IT development perspective but increases also user friendliness
- Increase consistency and rationalisation within and between the regulatory areas

➢ **High priority**

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3. Releases estimation module update

Stefano Frattini, ECHA

Current situation in EUSES

- For biocides
    - Only release estimation modules from ESD before 2010 available (=> update of release module reflecting situation until end of 2017 under preparation)

- For REACH
    - Release estimation based on A (release factors) and B (amount, time of emission) tables

What and why to change

- Biocides[1]
  - Add new sub-scenarios prepared after 2017 per PT
  - Add new/revised ESD prepared after 2017
  - Adapt/change default values as agreed in WG

- REACH (based on R16 guidance):
  - Remove A-B tables (not further supported by R16)
  - Default ERC release factor (supported by use description)
  - Default site tonnage (=annual amount) and release days (R16 table) for industrial uses
  - Default site tonnage for widespread uses (R16 guidance)

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[1] Those scenarios and ESD available until end of 2017 implemented in EUSES 2.2.0 available, Q1 2019

Priority level

- High importance for both Biocides and REACH
    - Reflect current guidance, ESDs

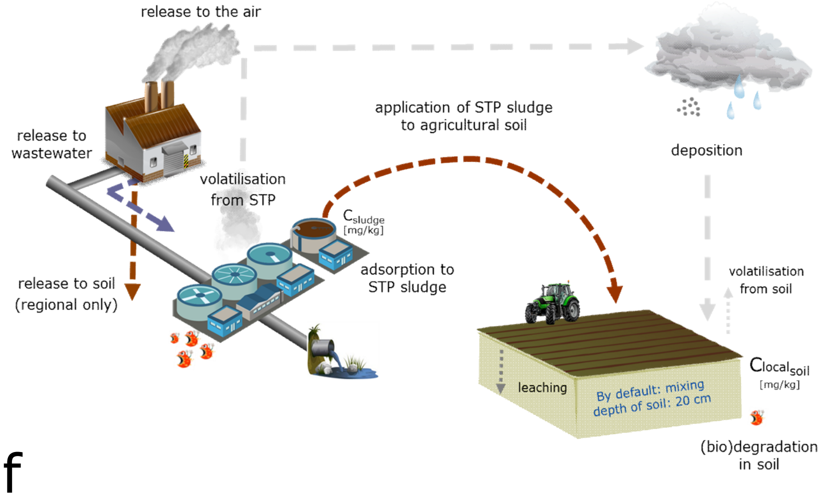
- Ready for implementation for both Biocides and REACH
    - ESD for biocide already implemented in EUSES 2.2.0 end 2018
    - Easy to implement R16 guidance provisions in EUSES (Chesar experience)

4. Direct releases to agricultural soil

Stefano Frattini, ECHA

Current situation in EUSES

- No direct releases of substances to agricultural soil at local scale
- Indirect release to soil at local scale only via
  - STP sludge application
  - Air deposition
- Soil Concentration calculated
  - After 10 years application of sewage sludge
  - Averaged over 30-180 days after last application



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What and why to change

- Implement direct release concept in EUSES as developed in LET/FEE tool
    - Initial proposal largely based on LET tool, need discussion with both tool developers
- Advantages of such change/new scenario in EUSES
    - Harmonisation
    - Easiness to take regional assessment into account
    - Connection of outcome of such scenario to Chesar

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What and why to change

- Proposal to implement only the default assessment
  - Simplified option (1 application only, no crops uptake, bare soil, etc.)
  - Relevant for generic assessment by registrant, Msafe calculation in absence of detailed info on uses
  - Not suitable for refined assessment (formulation / agricultural practice specific", like type of crops, number of application per year, etc.)
- Adaptation of the LET tool for 10 years of accumulation (like STP sludge scenario)
  - LET does not consider it while FEE does

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Main points for discussion

- Run off as source for surface water PEC
  - Worst case as suggested by LET?
- Sediment concentration not calculated as for EUSES standard scenario:
  - (Part of) releases to water are considered directly to sediment. Suitable even if deviating from R16 provisions?
- How to integrate MvE module in the tool?
  - Air emission for indirect exposure of humans
  - Food chain accumulation (crops, meat and milk) and uptake by humans

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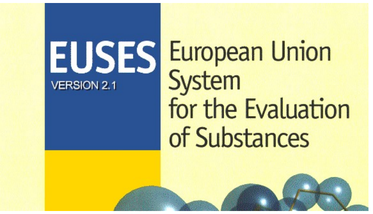
Priority level

- Medium importance
  - Fill a gap in the environmental assessment of chemicals under REACH
  - Limited number of substances affected (coformulants in pesticides and fertilizers)
- Nearly ready for implementation
  - Documented in other tools (LET/FEE)
  - Open points needs to be discussed before implementation
  - Harmonisation with R16 when reasonable/possible

5. Releases from reservoirs

Stefano Frattini, ECHA



Current situation in EUSES

- Time of emission (i.e. number of emission days per year) is a key parameter in EUSES to derive
  - Local concentration during episode (e.g. used for local concentrations in water, sediment, soil)
  - Annual averaged concentration (e.g. used for MvE, secondary poisoning)

- Only 1 Time of emission for both air and water emissions

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What and why to change

- Differentiate Time of emission to air and water to better support discontinuous releases to water
  - Wet scrubber (e.g. overspray collection)or bath (e.g. metal surface treatment) exchange
  - Releases from (not regular) cleaning operations
- Advantages of such “release scenario” in EUSES
  - No need to combine different EUSES runs to perform the assessment
  - Connection to Chesar

Priority level

- Low/Medium importance
  - Fill a gap in EUSES based assessment (workaround possible but cumbersome)
  - Only limited number of situations (e.g. SPERC covering discontinuous releases) are affected by this change so far
- Ready for implementation
  - Easy to implement in EUSES

6. Update of Simpletreat

Stefano Frattini, ECHA

Current situation in EUSES

- SimpleTreat 3.1 implemented, estimating chemical emission from sewage treatment plants

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What changes

- New SimpleTreat 4.0 will be implemented in EUSES with new default (compared to v 3.1) STP operational values
  - Higher BOD loading rate (from 54 to 60 g/p/d)
  - Lower Sludge Loading Rate (SLR from 0.15 to 0.1 kg BOD/kg MLSS/d)
  - These adaptations result in higher Hydraulic Retention Time (HRT from 7 to 11 h), meaning more time for degradation and/or adsorption
  - No new default for suspended solid concentration in the effluent (from 30 to 7.5 mg/l), since not yet supported EU wide
- Version 4.0 allows for ionizing organic partitioning (covered by Topic 1, QSARs)

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Points for discussion

- Allow for industrial site specific biological STP setting
  - Fraction settling in primary sedimentation phase
  - Fraction of BOD in raw sewage sludge solid/dissolved
  - Hydraulic Retention Time

- In general: possibility by the user to overwrite “agreed” default values

Priority level

- High importance
    - Affect exposure (via removal by STP) of all substances (degree of impact depending on substance properties)
- Ready for implementation
    - Simpletreat 4.0 already available as standalone estimation tool

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7. Sewer Removal Module

Diederik Schowanek, P&G

for ecetoc

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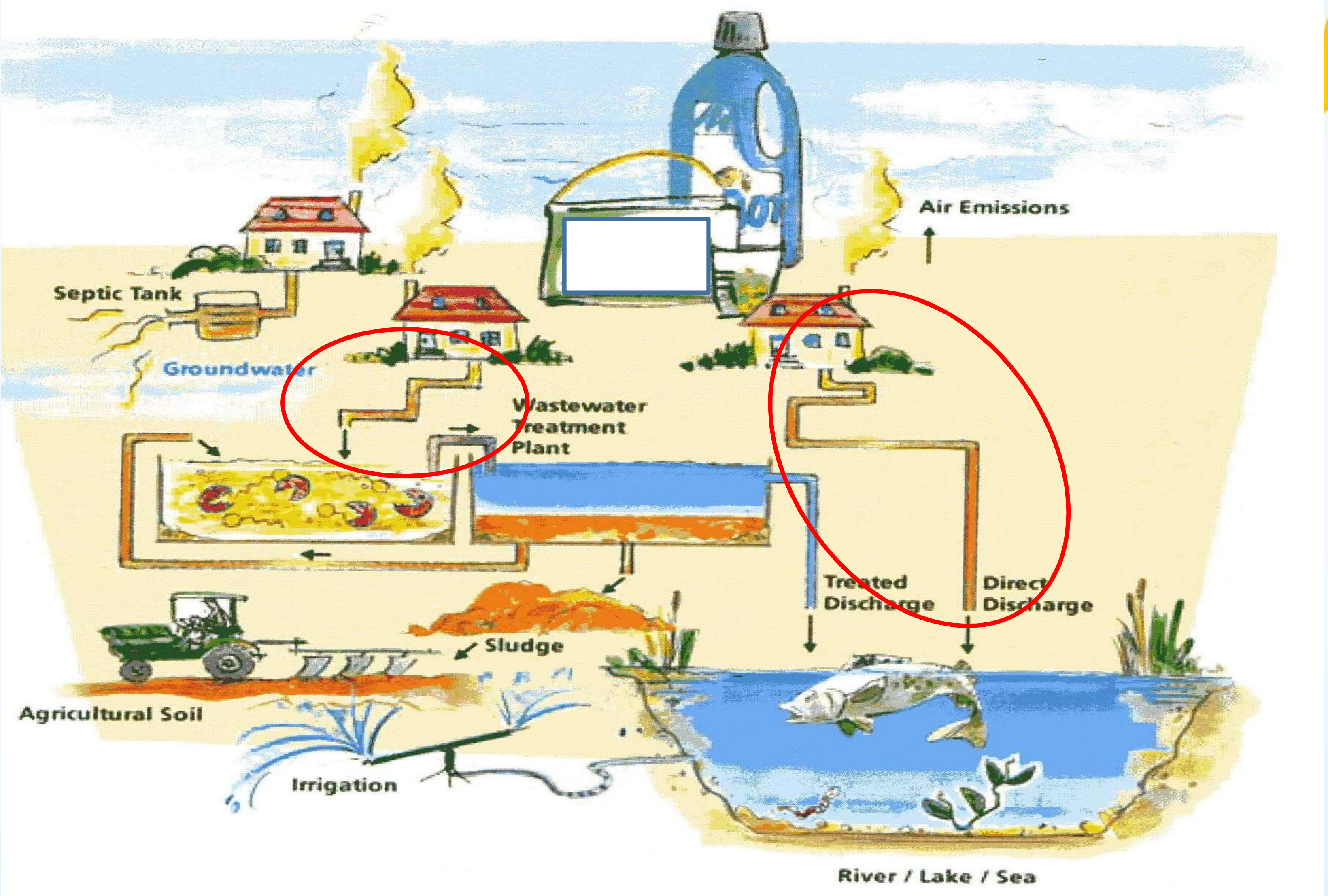
Sewer Removal / (Bio)Degradation Module



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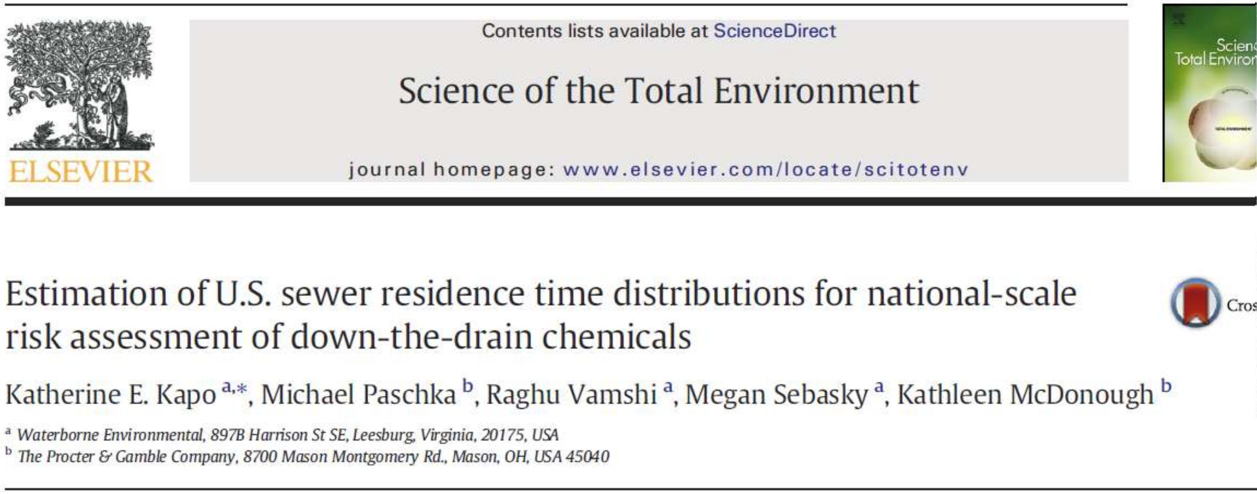
Why Needed? / Benefits

- Sewer system presently unmodelled in EUSES
- Evidence from environmental monitoring that for degradable, hydrolyzable and/or reactive chemicals the mass load of chemicals at emission point ≠ mass load at STP entry point
- Addition of a sewer model could refine Clocal estimation
- OECD method 314A allows to generate the kinetic degradation data needed for the model *('Evaluating the biodegradation of chemicals in sewage under simulated sewer conditions')*.
- Recent publications of average sewer residence times
- If no data: sewer removal = 0%

Concept ready for practical deployment

Literature References



Contents lists available at ScienceDirect

Science of the Total Environment

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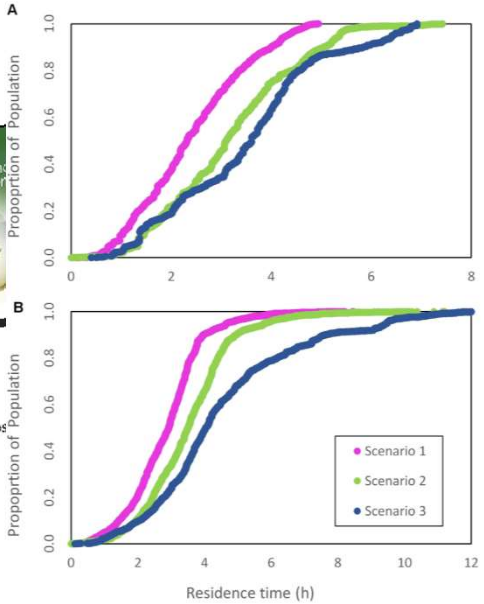
ELSEVIER

Estimation of U.S. sewer residence time distributions for national-scale risk assessment of down-the-drain chemicals

Katherine E. Kapo [a,*], Michael Paschka [b], Raghu Vamshi [a], Megan Sebasky [a], Kathleen McDonough [b]

[a] *Waterborne Environmental, 897B Harrison St SE, Leesburg, Virginia, 20175, USA*
[b] *The Procter & Gamble Company, 8700 Mason Montgomery Rd., Mason, OH, USA 45040*



Biodegradation
DOI 10.1007/s10532-016-9773-6

CrossMark

ORIGINAL PAPER

Biodegradation of nonionic and anionic surfactants in domestic wastewater under simulated sewer conditions

Jennifer Z. Menzies · Kathleen McDonough · Drew McAvoy · Thomas W. Federle

Technical Solution

- Model in its simplest form just a correction factor: % removed in sewer (R)

- Model should be simple and flexible such that it can model various decay processes in the same way
  - Chemical reaction (e.g. hypochlorite, peroxides, epoxides, …)
  - Hydrolysis
  - Aerobic and anaerobic biodegradation processes

- Settling and sorption not modelled

- First order decay model proposed:

$$y = A_o e^{-k_1 t} \qquad (1)$$

$$t_{\frac{1}{2}} = \ln(2)/k_1 \qquad (3)$$

$$R = 100 - \frac{100}{1 + k_1 HRT_{sew}} \qquad (4)$$

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What’s Needed & Next Steps?

- Review and validation of proposed model concept with expert modellers (e.g. RIVM, ECHA)
- Confirm conceptual compatibility with SimpleTreat input (concentration of parent chemical)
- Develop a new section in REACH TGD R16 for sewer module on how to apply this in practice (ECETOC to lead?). Specify the conditions/data requirements under which the sewer module can be used. If not applicable or no data: removal = 0%
- Search for best data on EU sewer residence times to refine statistical distribution for EU. In meantime use conservative defaults

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8. Site specific local air and deposition

Joost Bakker, RIVM

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Current situation

- Local concentration in air is estimated from the standard air concentration at a source strength of 1 kg/d

- This standard factor is derived from the Gaussian plume model OPS assuming standard source characteristics and weather conditions

- Standard source characteristics cannot be changed in EUSES but have a large impact

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Current situation

- Although EUSES is designed as a first tier assessment tool it is also used in site-specific environmental exposure assessment for REACH-registrations or in applications for authorisation (AfA).

- Therefore desirable to implement a possibility for site specific environmental assessment

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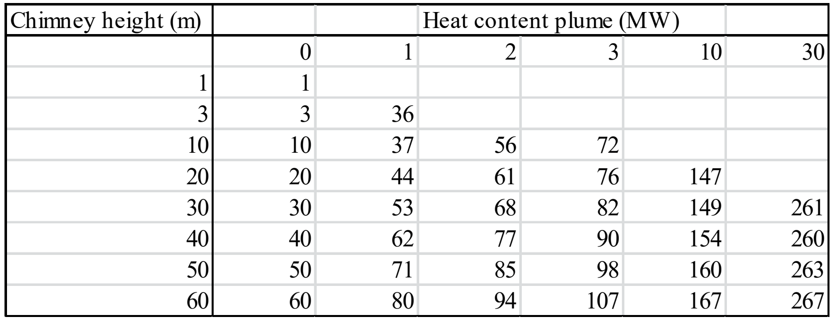
Solution

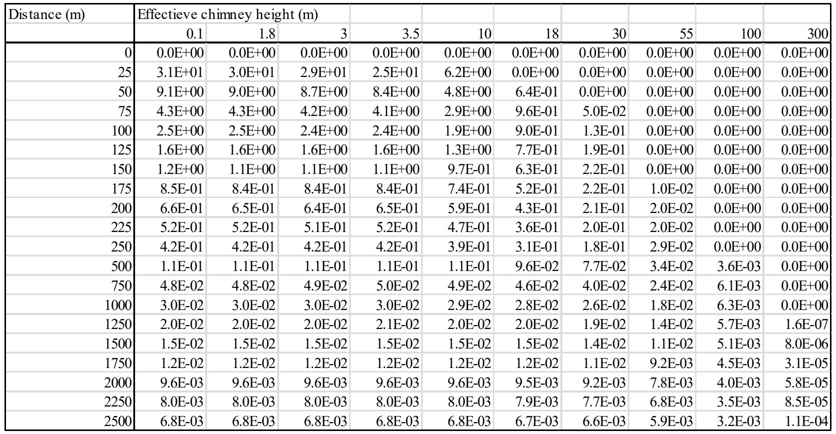
- Simple tool taking source characteristics into account calculating PECair
- Standard factors from effective chimney height and distance from source
- Effective height estimated from chimney height and heat content of plume

Chimney height & heat content



Chimney height (m)	Heat content plume (MW)					
	0	1	2	3	10	30
1	1					
3	3	36				
10	10	37	56	72		
20	20	44	61	76	147	
30	30	53	68	82	149	261
40	40	62	77	90	154	260
50	50	71	85	98	160	263
60	60	80	94	107	167	267

Effective height & distance



Distance (m)	Effectieve chimney height (m)								
	0.1	1.8	3	3.5	10	18	30	55	100	300
0	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
25	3.1E+01	3.0E+01	2.9E+01	2.5E+01	6.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
50	9.1E+00	9.0E+00	8.7E+00	8.4E+00	4.8E+00	6.4E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
75	4.3E+00	4.3E+00	4.2E+00	4.1E+00	2.9E+00	9.6E-01	5.0E-02	0.0E+00	0.0E+00	0.0E+00
100	2.5E+00	2.5E+00	2.4E+00	2.4E+00	1.9E+00	9.0E-01	1.3E-01	0.0E+00	0.0E+00	0.0E+00
125	1.6E+00	1.6E+00	1.6E+00	1.6E+00	1.3E+00	7.7E-01	1.9E-01	0.0E+00	0.0E+00	0.0E+00
150	1.2E+00	1.1E+00	1.1E+00	1.1E+00	9.7E-01	6.3E-01	2.2E-01	0.0E+00	0.0E+00	0.0E+00
175	8.5E-01	8.4E-01	8.4E-01	8.4E-01	7.4E-01	5.2E-01	2.2E-01	1.0E-02	0.0E+00	0.0E+00
200	6.6E-01	6.5E-01	6.4E-01	6.5E-01	5.9E-01	4.3E-01	2.1E-01	2.0E-02	0.0E+00	0.0E+00
225	5.2E-01	5.2E-01	5.1E-01	5.2E-01	4.7E-01	3.6E-01	2.0E-01	2.0E-02	0.0E+00	0.0E+00
250	4.2E-01	4.2E-01	4.2E-01	4.2E-01	3.9E-01	3.1E-01	1.8E-01	2.9E-02	0.0E+00	0.0E+00
500	1.1E-01	1.1E-01	1.1E-01	1.1E-01	1.1E-01	9.6E-02	7.7E-02	3.4E-02	3.6E-03	0.0E+00
750	4.8E-02	4.8E-02	4.9E-02	5.0E-02	4.9E-02	4.6E-02	4.0E-02	2.4E-02	6.1E-03	0.0E+00
1000	3.0E-02	3.0E-02	3.0E-02	3.0E-02	2.9E-02	2.8E-02	2.6E-02	1.8E-02	6.3E-03	0.0E+00
1250	2.0E-02	2.0E-02	2.0E-02	2.1E-02	2.0E-02	2.0E-02	1.9E-02	1.4E-02	5.7E-03	1.6E-07
1500	1.5E-02	1.5E-02	1.5E-02	1.5E-02	1.5E-02	1.5E-02	1.4E-02	1.1E-02	5.1E-03	8.0E-06
1750	1.2E-02	1.2E-02	1.2E-02	1.2E-02	1.2E-02	1.2E-02	1.1E-02	9.2E-03	4.5E-03	3.1E-05
2000	9.6E-03	9.6E-03	9.6E-03	9.6E-03	9.6E-03	9.5E-03	9.2E-03	7.8E-03	4.0E-03	5.8E-05
2250	8.0E-03	8.0E-03	8.0E-03	8.0E-03	8.0E-03	7.9E-03	7.7E-03	6.8E-03	3.5E-03	8.5E-05
2500	6.8E-03	6.8E-03	6.8E-03	6.8E-03	6.8E-03	6.7E-03	6.6E-03	5.9E-03	3.2E-03	1.1E-04

Concentration air at 1 kg per day emission

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Way forward

- Not available yet but also needed for calculating deposition flux to soil in EUSES
- More recent version of OPS is used to derived standard factors
- Recalculation of the default EUSES factor needed

Priority level

- Medium importance
  - No standard requirement, only useful in limited number of cases such as for site-specific assessments in applications for authorisation.
- Not ready
  - Can be implemented for calculating $\mathrm{Clocal}_{\mathrm{air}}$
  - Additional calculations needed to derive standard deposition factors for the gaseous and particulate phase
  - Guidance needed on procedure for site specific assessment

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9.Local deposition volatile substances

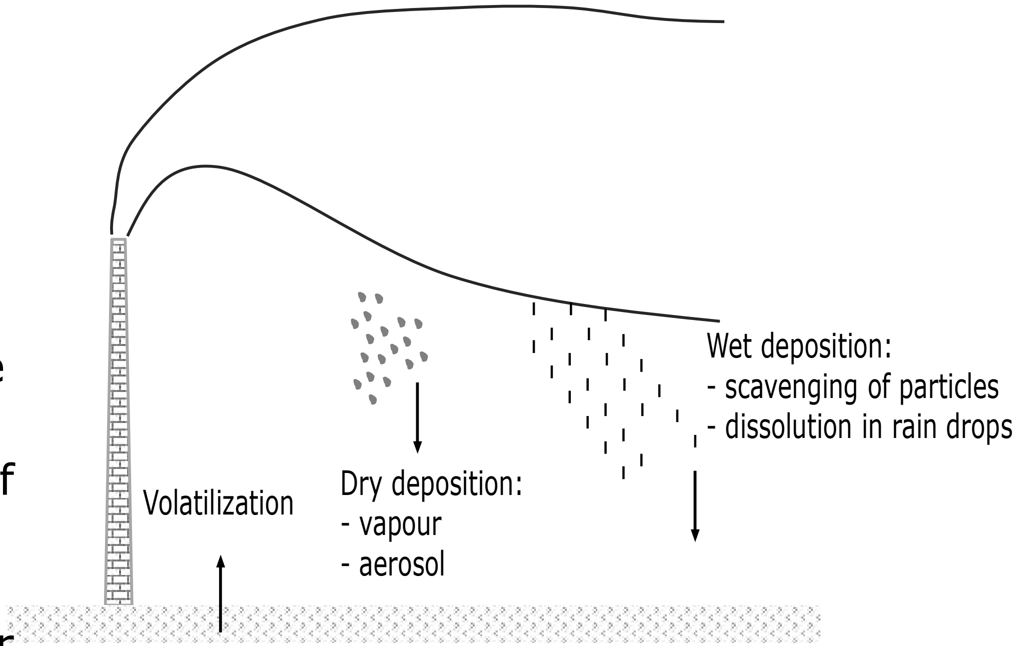
Joost Bakker, RIVM

Issue

- Industry communicated that an unexpectedly high concentration in the local soil is calculated in EUSES for very volatile substances emitted to air.

Current situation local atmospheric fate

- Aerosol bound deposition: not relevant
- Deposition of gaseous fraction through gas absorption and wet deposition
- Wet deposition based on Henry’s law coefficient. Usually negligible for very volatile chemicals
- Gas absorption/ dry deposition of gaseous fraction to soil has a fixed value (0.01 cm.s^{-1}).
- This value is possibly too high for volatile chemicals, or
- Volatilization from soil is too low



Solution

- Gas absorption and volatilization are now independent parameters for the local scale
- The algorithm for gas absorption for the regional scale could be used to make the dry deposition velocity at local scale substance dependent.
- It should be further analyzed how the regional algorithm and fixed value relate in order to facilitate a proposal for the correction of the default dry deposition velocity in EUSES.

Priority level

- Important
  - The impact may be large, the proposed change would lead to considerably lower concentrations in soil at the local scale
- Not ready
  - It should be further analyzed how to properly calculate the dry deposition velocity at the local scale.
  - The standard deposition flux for gaseous compounds should be corrected accordingly.

10. Modelling episodic rain

Joost Bakker, RIVM

Current situation

- EUSES regional distribution part (according to Simplebox 3.0) assumes constant drizzle which is unrealistic.
- Consequently the atmospheric fate of highly soluble chemicals is predicted incorrectly.

Solution

- Modelling episodic rain improves the precision between steady-state and complex dynamic models

- The proposed change will affect predicted concentrations in air, water and soil at the larger spatial scales, the local concentrations would not be affected.

Way forward

- Implementation of model formulation worked out and published by Jolliet and Hauschild (2006)
- Their approximation is designed to be implemented in multimedia models
- Model formulation is implemented in SimpleBox 4.0

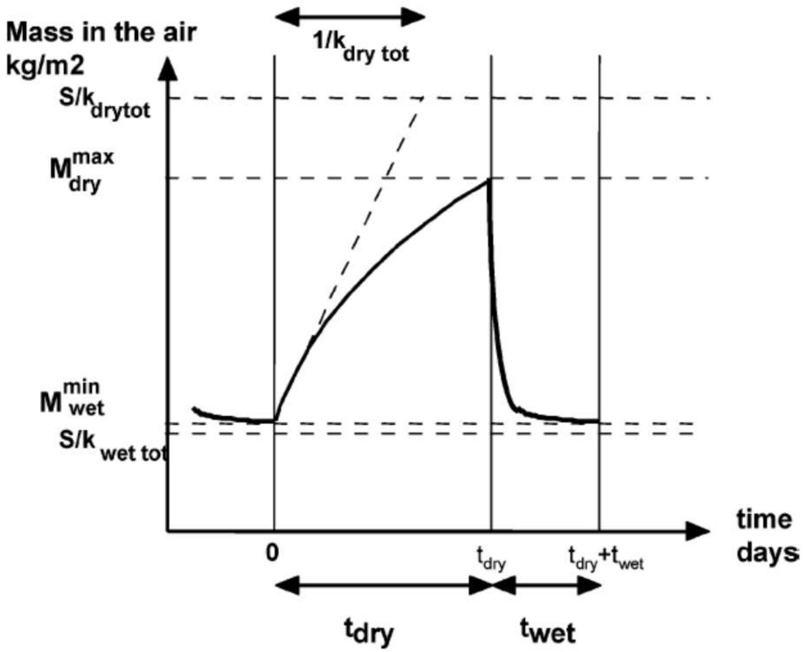


FIGURE 2. Mass of substance present in the air compartment as a function of dry and wet deposition under a regime of intermittent precipitation.

Priority level

- Low importance
  - Would affect fate at larger spatial scales not at the local
  - Would mainly affect highly soluble chemicals
  - For these kind of chemicals, considerably lower concentrations in air and higher concentrations in soil and water would be predicted
- Ready to implement
  - proposed method is fit for multi-media mass balance models and is already implemented in SimpleBox 4.0

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11. Assessment of photolytic degradation

Joost Bakker, RIVM

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Current situation

- Environmental half-life for photolysis can be entered in EUSES
- Often only information based on the OECD Technical Guideline 216 for phototransformation of Chemicals in Water is available
- Photolysis half-life under real environmental conditions is often hard to find
- EUSES provides no assistance to derive half lives under real environmental conditions

Solution

- Environmentally relevant half-lives in water can be derived from standard photolysis test using the calculation procedure proposed by Castro Jimenez and van de Meent (2011).

Priority level

- Low importance
  - Impact on exposure is expected to be relatively low as photodegradation is often not very relevant under field conditions
  - Photodegradation is not included in the local exposure calculations (local environment and STP). It will only affect concentrations at larger spatial scales
  - may be relevant for chemicals that are persistent to biodegradation but readily degradable by photolysis
- Technically ready
- Implemented in a SimpleBox vs. 3 test version, which can be integrally copied into the EUSES fate model.

12 Initial Local PEC soil

Joost Bakker, RIVM

Current situation

- The local PEC in soil (e.g. following sewage sludge application) is calculated as an averaged value over 30 days and 180 days after the last of yearly applications for 10 consecutive years.

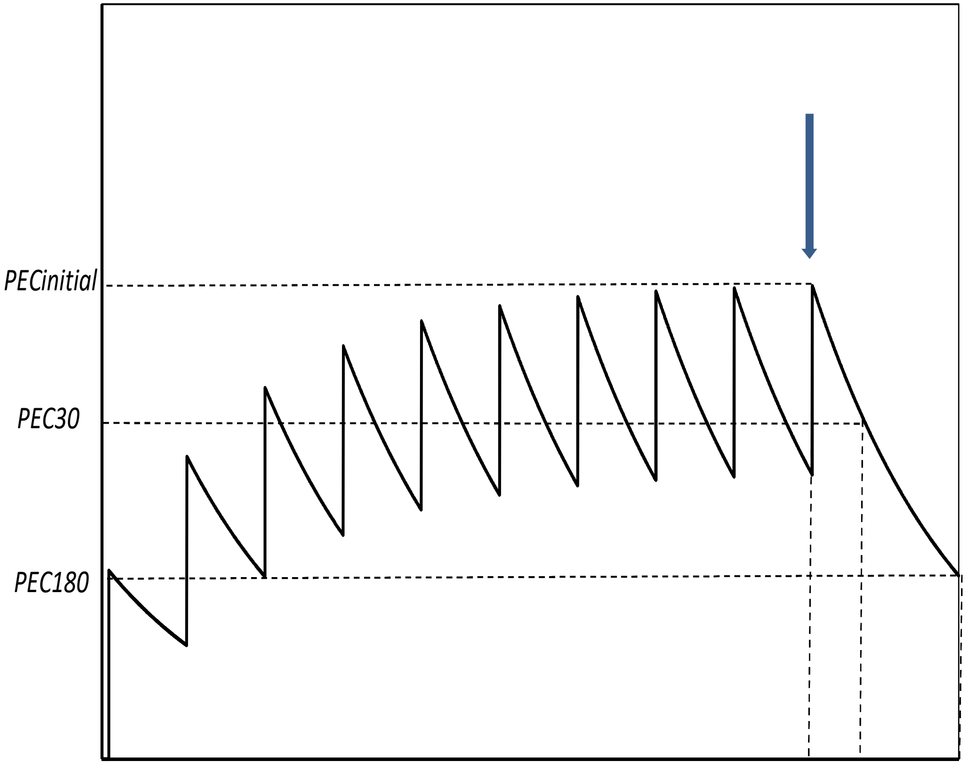
- The results of currently available standardised terrestrial ecotoxicity tests are generally expressed on the basis of initial, nominal concentrations.

Current situation

- This means that degradation of the substance in the soil is not consistently taken into account in both the exposure (PEC) and effect (PNEC) parameters.

Solution

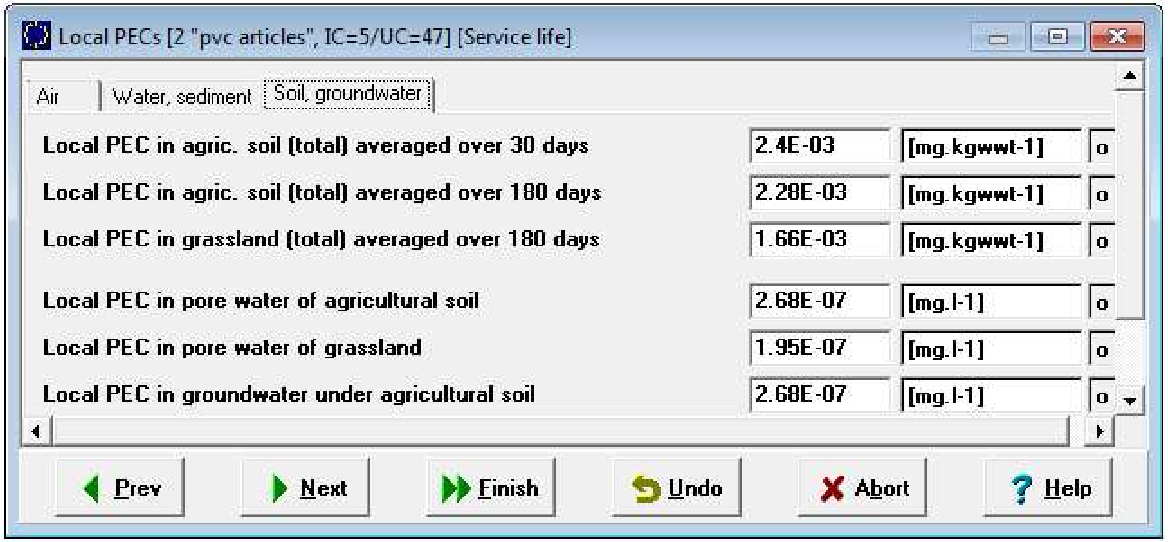
- The PNECsoil based on nominal concentrations should therefore be compared with the initial PECsoil, which is the PECsoil directly after the last sludge application (before degradation takes place).
- This has been agreed for the biocides assessment
- Therefore it is suggested that EUSES should additionally provide initial PEC in soil.



Way forward

- The initial concentration in soil is already calculated by EUSES as an intermediate result only not presented as such

- Initial PEC should be presented in the Local PECs screen



Local PECs [2 "pvc articles", IC=5/UC=47] [Service life]

Local PEC in agric. soil (total) averaged over 30 days	2.4E-03	[mg.kgwwt-1]	o
Local PEC in agric. soil (total) averaged over 180 days	2.28E-03	[mg.kgwwt-1]	o
Local PEC in grassland (total) averaged over 180 days	1.66E-03	[mg.kgwwt-1]	o
Local PEC in pore water of agricultural soil	2.68E-07	[mg.l-1]	o
Local PEC in pore water of grassland	1.95E-07	[mg.l-1]	o
Local PEC in groundwater under agricultural soil	2.68E-07	[mg.l-1]	o

Priority level

- Important
  - Required for biocides assessment
  - This issue is not discussed for REACH but could be used for all chemicals if wished
- Ready to be implemented
  - No extra calculations required
  - Can easily be implemented: only output screens have to be adapted

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13 Depth dependent soil concentration

Joost Bakker, RIVM

Current situation

- Multimedia mass balance models typically assume that compartments are well mixed over a certain depth
- This is not true for real soils
- According to theory concentrations in soil decline exponentially with depth (e.g. McKone and Bennett (2003)

Solution

- Transport processes from soil take place at a certain depth (z) rather than over the average depth <c>

- Therefore transport coefficients need to be corrected

- The correction factor is c(z) / <c>:

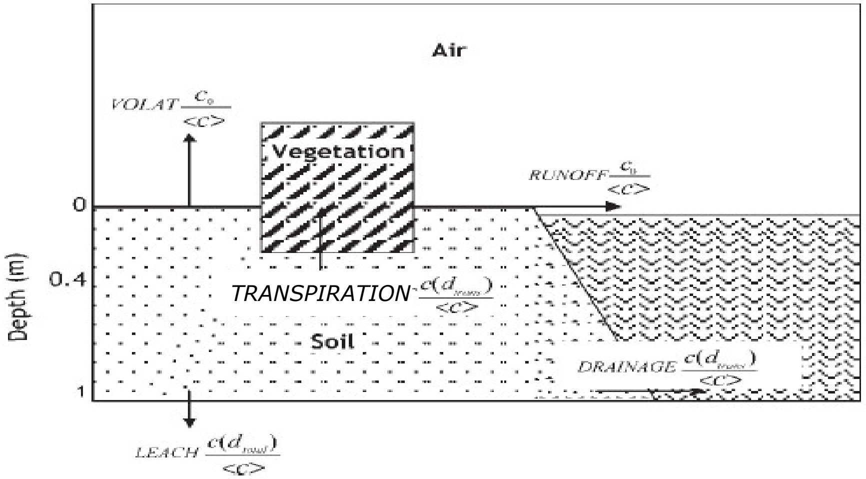
$$\frac{d_t/d_p}{1-e^{(-d_t/d_p)}}e^{(-z/d_p)}$$

Where:

- dt the total depth, or the fixed soil depth in EUSES
- d_p the chemical dependent characteristic soil (penetration) depth

Way forward

- Relevant depth have to be set for relevant processes
- In Simplebox 4.0 a fixed value is used for dp valid for compounds with log Kow > 3
- dp is substance dependent and already implemented in EUSES for the regional scale



Transport process	*Relevant depth z*
Volatilization	$z = 0$ (air/soil interface)
Leaching	$z = d_t$ (lower boundary)
Surface run-off/erosion	$z = 0$ (air/soil interface)
Drainage	$z = 1$ m (tube depth)
Transpiration	$z = 0.4$ m (rooting depth)

Priority level

- Important
  - The impact on the exposure calculation may be high
  - Proposed changed will affect the soil compartment at the local scale (including vegetation) and at the regional scale all compartments directly connected to soil.
- Ready to be implemented
  - The proposed method is documented, verified (Hollander et al., 2004) and implemented in SimpleBox 4.0 (Schoorl et al., 2014).

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Thank you!