Application of a multimedia activity model for evaluating the fate of persistent and mobile substances in soil

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ZeroPM Achieving Zero Pollution of Persistent and Mobile Substances: Prioritization through Substance Grouping and Risk Assessment; UBA Conference Center in Dessau-Roßlau, Germany, 19th -20th September 2024

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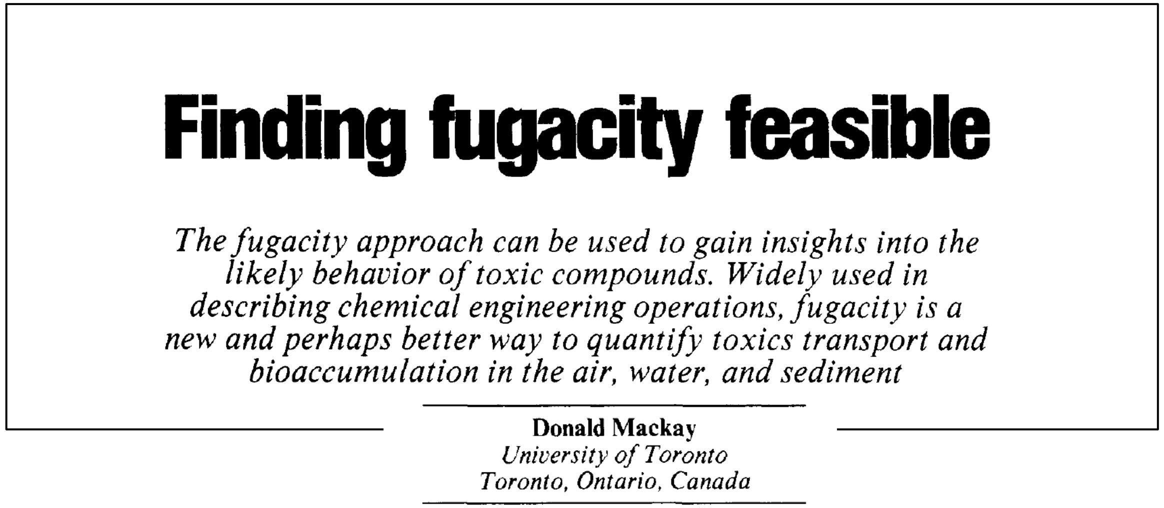
Brief model description

- Builds on the concept of fugacity
  - Concept of fugacity (f) introduced in 1901 by G.N. Lewis
    - Refers to the escaping tendency of a chemical
    - Units of pressure (Pa)
    - Convenient method for defining thermodynamic equilibrium criterion
  - Thermodynamic equilibrium occurs between two matrices when the fugacities in each matrix is equal

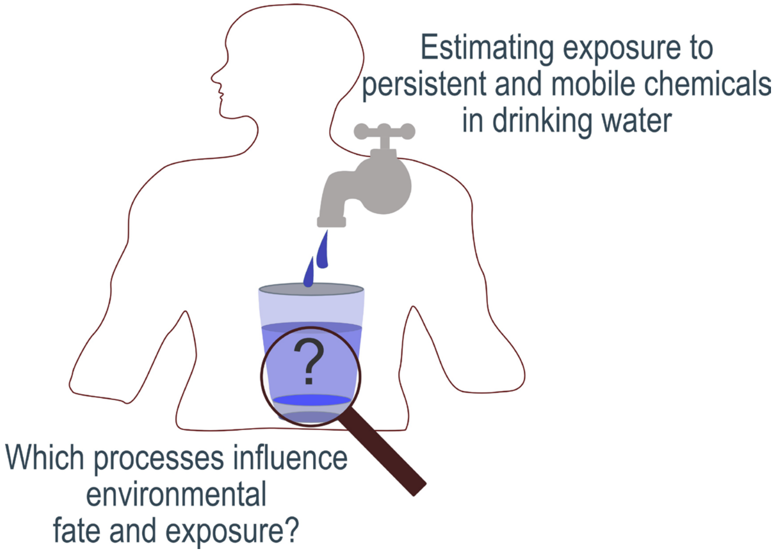


Finding fugacity feasible

The fugacity approach can be used to gain insights into the likely behavior of toxic compounds. Widely used in describing chemical engineering operations, fugacity is a new and perhaps better way to quantify toxics transport and bioaccumulation in the air, water, and sediment

Donald Mackay
University of Toronto
Toronto, Ontario, Canada

D. Mackay, Finding fugacity feasible, Environmental Science & Technology, 1979, 13, 1218-1223.



Physicochemical Properties of Persistent and Mobile Organic Chemicals

Persistent (P) Criteria:

- Half-life >40 days in fresh or estuarine water at 9°C and pH 4-9 are considered to be persistent (P)
- Half-life >120d in either soil or fresh or estuarine sediment at 12°C and pH 4-9

Very Persistent (vP) Criteria:

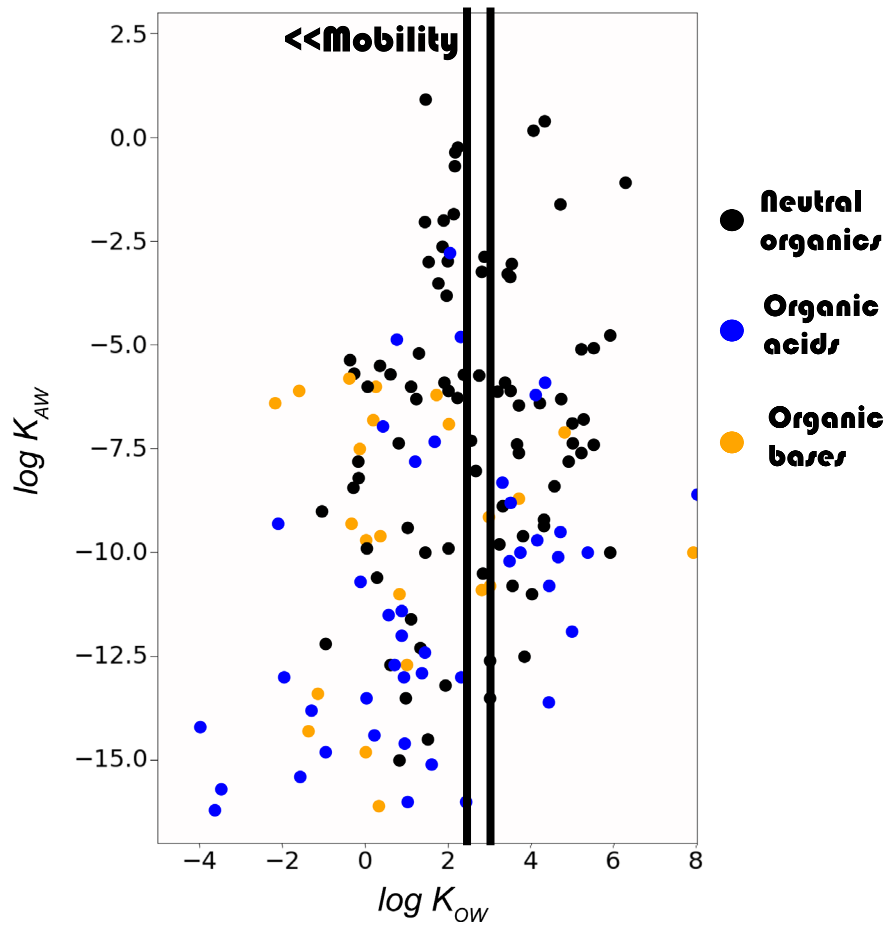
- Half-life >60 days in fresh or estuarine water at 9°C and pH 4-9 are considered to be very persistent (vP)
- Half-life >180 days in fresh or estuarine water at 9°C and pH 4-9 are considered to be very persistent (vP)

Mobile (M) Criteria

- Log organic-carbon water partition coefficient (K_{OC}) <3.0

Very Mobile (vM) Criteria

- Log organic-carbon water partition coefficient (K_{OC}) <2.0

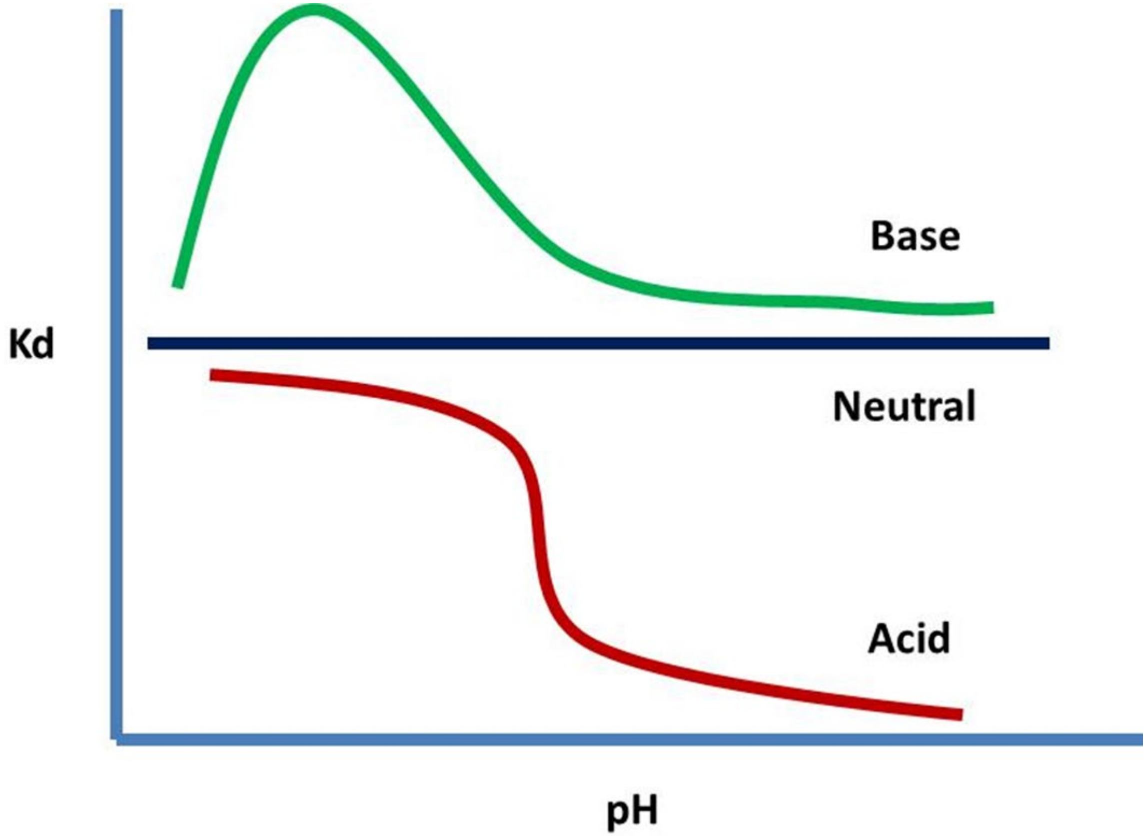


150/173 High-Priority Category

H. P. Arp, S. E. Hale, I. Schliebner and M. Neumann, Prioritised PMT/vPvM substances in the REACH registration database, Report (UBA-FB) FB001083/ENG, Umweltbundesamt, Dessau-Roßlau, Germany, 2023.

Properties of ionisable organic chemicals

- The potential to shift between the neutral and charged species as a function of shifting environmental pH, relative to the pKa of the chemical.



Activity-based Multimedia model

- Capability to simulate the environmental fate and transport of ionizable organics,
    - Activity-based approach is consistent with the concepts of fugacity
- Sorption of Organic acids and bases described by a suite of equations

For acids, neutral molecules:	$\log K_{OC} = 0.54 \times \log K_{OW,n} + 1.11$
For acids, anion:	$\log K_{OC} = 0.11 \times \log K_{OW,n} + 1.54$
For bases, neutral molecules:	$\log K_{OC} = 0.37 \times \log K_{OW,n} + 1.70$
For bases, cation (1):	$\log K_{OC} = 0.42 \times \log K_{OW} + 2.191.$
For bases, cation (2):	$\log K_{OC} = pK_a^{0.65} \times f^{\ 0.14}$

- Alternatively, measured K_d values can be used directly

Activity-Based Concept for Transport and Partitioning of Ionizing Organics

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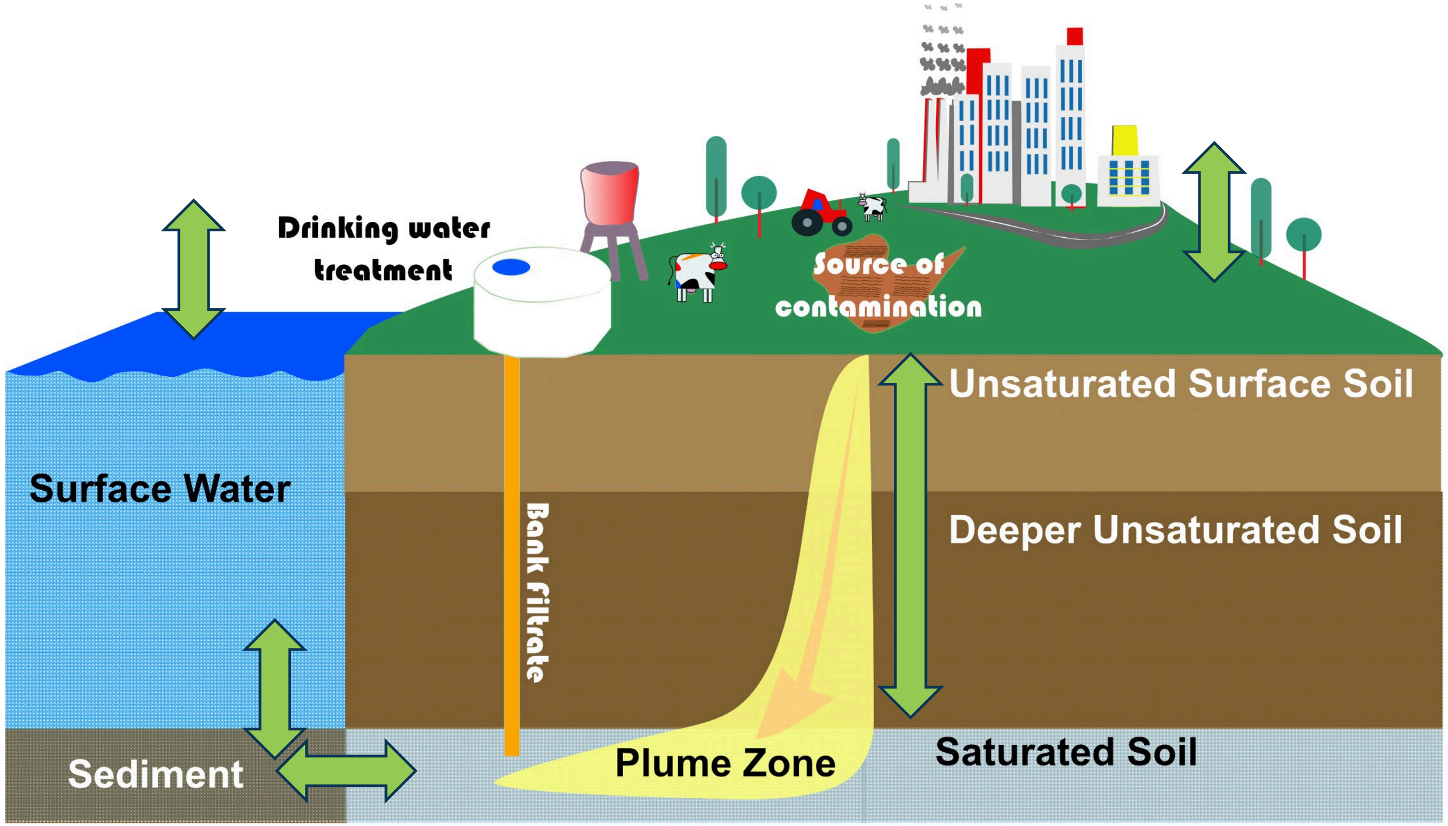
S. Trapp, A. Franco and D. Mackay, Activity-based concept for transport and partitioning of ionizing organics, Environ. Sci. Technol., 2010, 44, 6123-6129.

Illustrative schematic of model structure



Multimedia, Multilayer soil model with a maximum of 20 different soil layers

- Simulate leaching of chemical contaminants through soil horizon

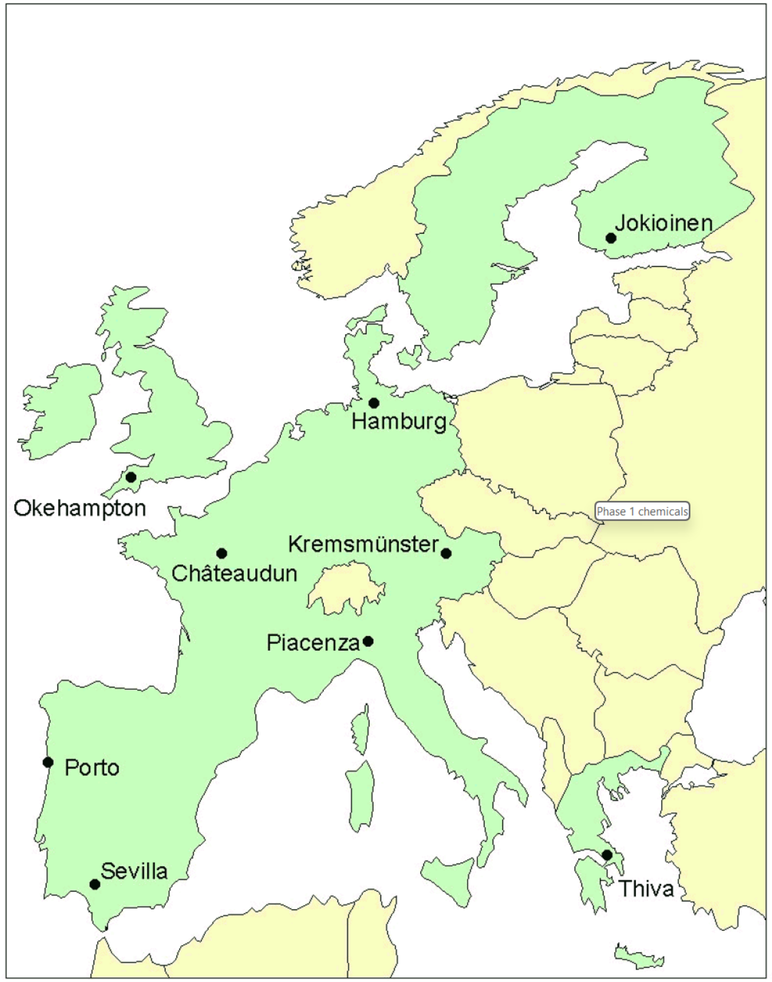
Sediment compartment coupled to saturated soil/groundwater compartment

- Darcy's Law

Parameterizing the soil compartment

- Significant heterogeneity with respect to soil and geologic properties, which can influence the interactions between chemical contaminants and their leaching
- FOCUS ground wate scenarios represent an opportunity to evaluate leaching potential across different soil types typical of the EU

Location	Mean Annual Temp. (°C)	Annual Rainfall (mm)	Topsoil Texture†	Topsoil Organic Matter (%)
Châteaudun	11.3	648 + I*	silty clay loam	2.4
Hamburg	9.0	786	sandy loam	2.6
Jokioinen	4.1	650	loamy sand	7.0
Kremsmünster	8.6	899	loam/silt loam	3.6
Okehampton	10.2	1038	loam	3.8
Piacenza	13.2	857 + I*	loam	2.2
Porto	14.8	1150 + I*	loam	2.5
Sevilla	17.9	493 + I*	silt loam	1.6
Thiva	16.2	500 + I*	loam	1.3



Phase 1 chemicals

PFAS

- Dominated by strong acids, i.e. pKa <2

- Triazines
  - Five neutral organics
  - Six organic bases (pKa values range between about 2 to 5, depending on environmental pH a mixture of charged and neutral species can occur)
  - Two organic acids (pKa values estimated between 7-8)
- Triazoles
  - Split between neutral organics and organic acids, pKa values for acids >7)

Level 3 model

- Environmental system parameterization
  - FOCUS Models
    - The Hamburg scenario selected as representing the worst-case leaching soil, exceeding the target of the 80th percentile soil

Horizon	Depth (cm)	Classification	pH-H_2O^*	pH-KCl†	Texture (µm)			om (%)	oc (%)	Bulk Density (g cm^{-3})	Depth Factor@
					<2	2-50	>50				
Ap	0-30	sandy loam	6.4	5.7	7.2	24.5	68.3	2.6	1.5	1.5	1.0
BvI	30-60	sandy loam	5.6	4.9	6.7	26.3	67	1.7	1	1.6	0.5
BvII	60-75	sand	5.6	4.9	0.9	2.9	96.2	0.34	0.2	1.56	0.3
Bv/Cv	75-90	sand	5.7	5	0	0.2	99.8	0	0	1.62	0.3
Cv	90-100	sand	5.5	4.8	0	0	100	0	0	1.6	0.3
Cv	100-200	sand	5.5	4.8	0	0	100	0	0	1.6	0.0

† These values are estimated from the measured KCl values by assuming a standard difference of 0.7 pH units (Barrere et al, 1988)

* Measured at a soil solution ratio of 1:2.5

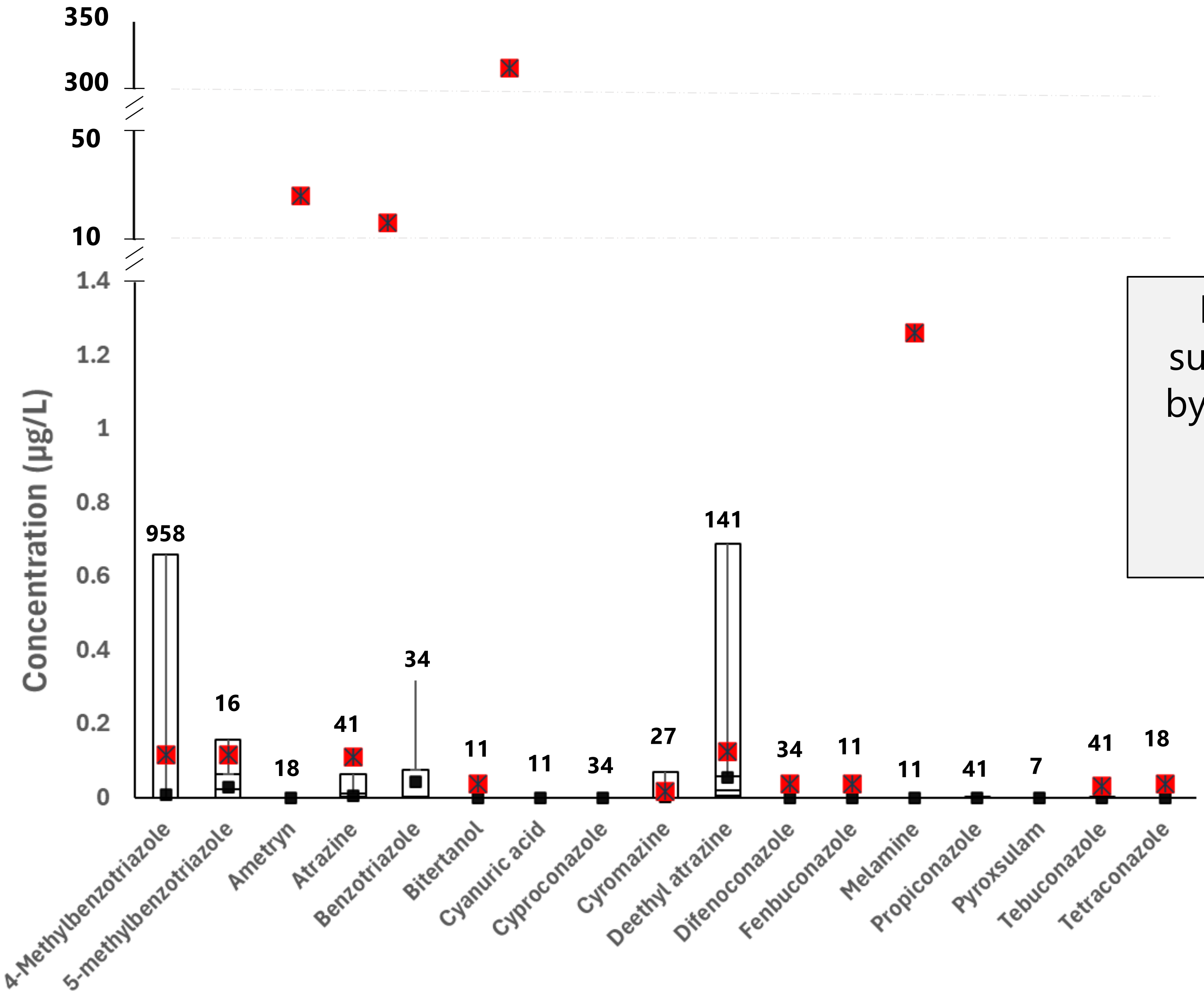
@ The depth factor indicates the relative transformation rate in the soil layer.

Ground water depth of 2 m (estimated by IUCT).

Phase 1 chemicals

- No emission data readily available
  - Preliminary estimates based on tonnage bans
  - Emission to soil only
- Environmental monitoring data summarized from Norman database

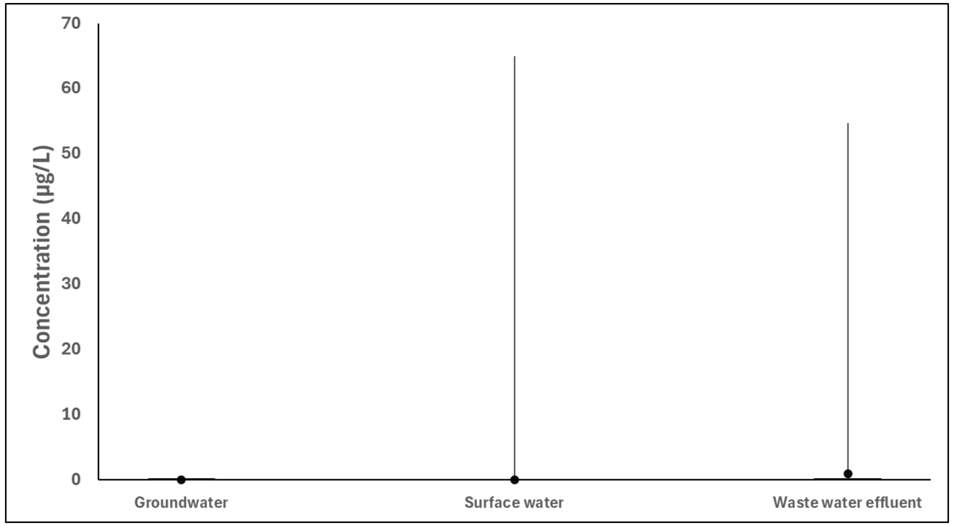
Preliminary Results



Box and whisker plots summarize data reported by the NORMAN network and which reflect concentrations in groundwater.

Challenges and limitations / next steps

- Emissions data represent the fundamental input parameter!!
- Environment-specific variability – How important is it?
  - E.g. Emission uncertainty versus environment-specific parameters
  - Sensitivity be evaluated using the different scenarios described in the different FOCUS models
- Removal via Drinking Water Treatment
  - Not currently considered, but….
- Monitoring data
  - Presentations from Abishek and Sylvia rely on applying these data (Surface and Groundwater) within the context of the risk matrix after the coffee break…



Tebuconazole

Norman data		Concentration (µg/L)			
	Groundwater	Surface water		Waste water effluent	
min	0		0	0	
25th quartil	0		0	0	
Median	0		0	0.00125	
75th quartil	0		0	0.006239	
Max	0.000665		65	54.8	
Mean	1.89E-05		0.010042	0.935275	
Std dev	0.000105		0.203992	5.962775	
Number	41		216417	244	