

# Filling the gaps to better prioritize PMT/ vPvM substances under REACH

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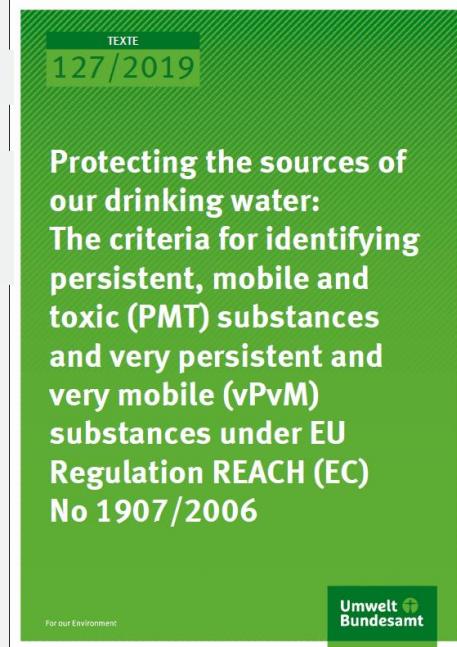
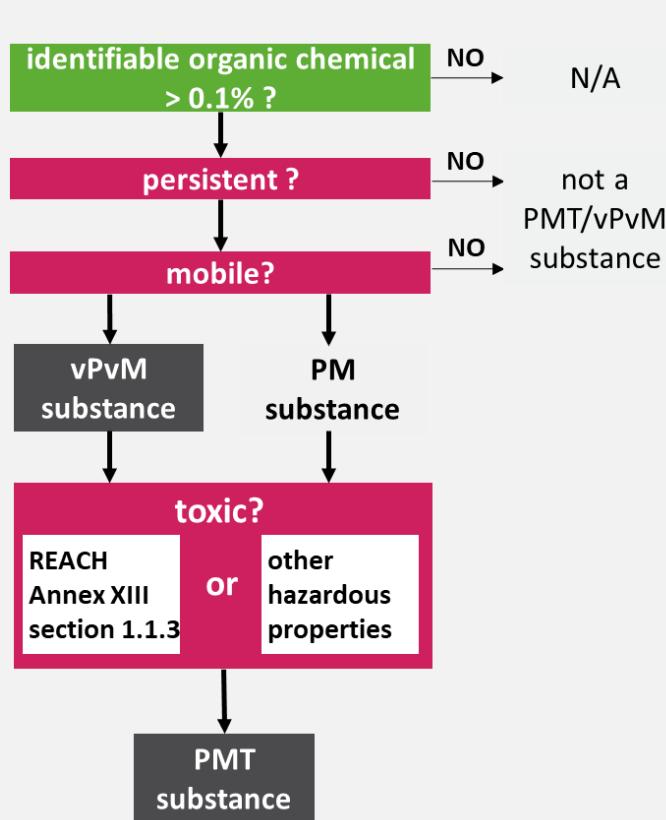
# Second #PMTWorkshop, Berlin 2018



Differences  
of opinion

...but all in the  
same boat

# Outcome: Developed PMT Criteria and Guidelines



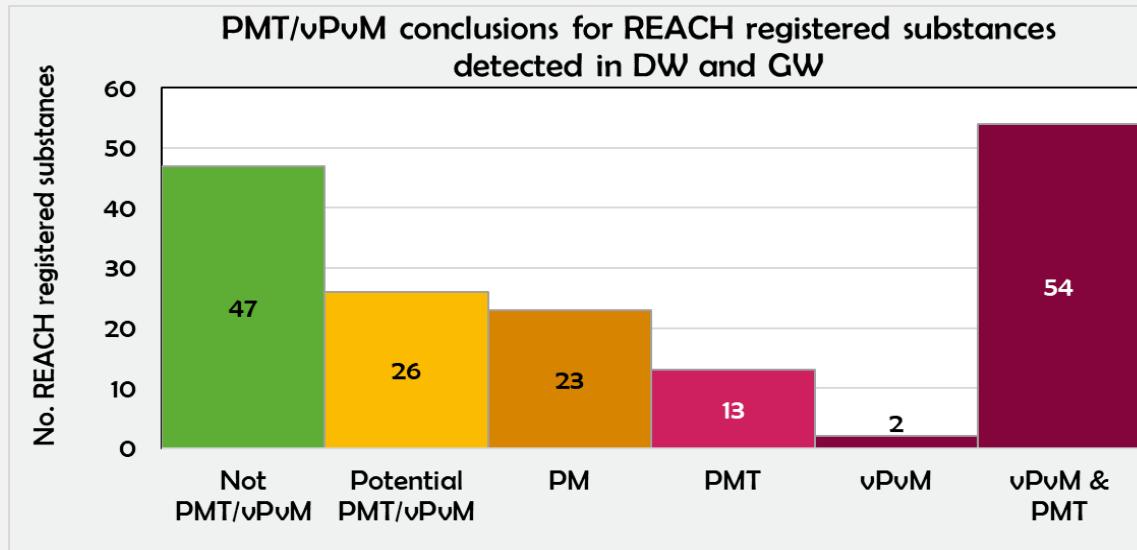
Scientific Background and Guidelines

# PMT/vPvM an Equivalent Level of Concern to PBT/vPvB



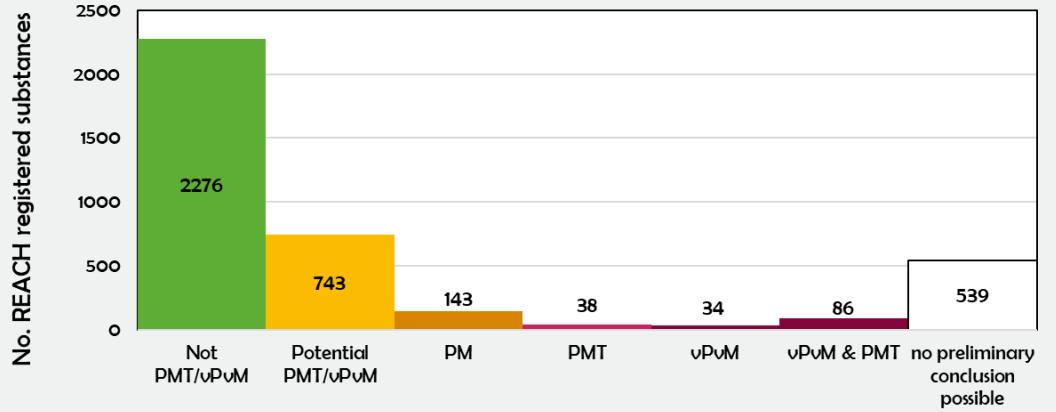
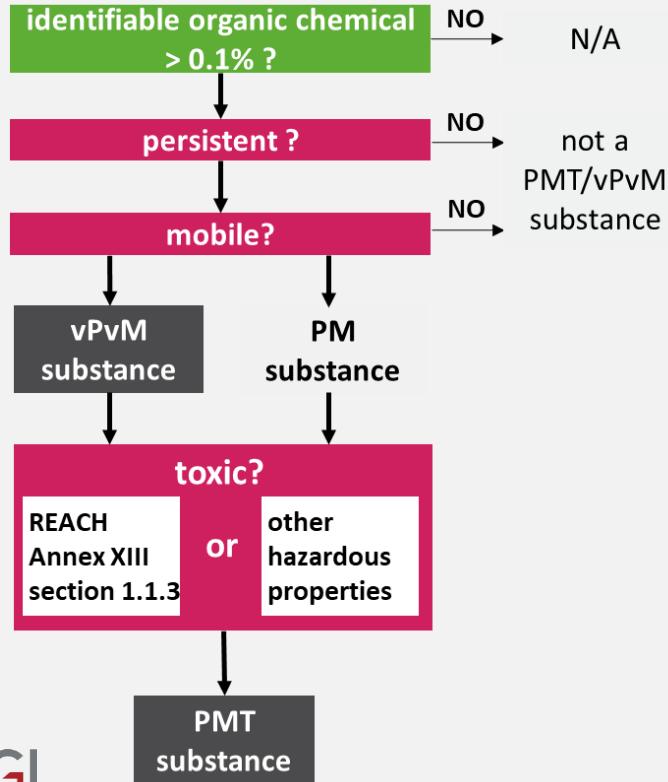
	REACH: PMT/vPvM Persistent, mobile, toxic	REACH: PBT/vPvB Persistent, bioaccumulative, toxic
<b>Persistency &amp; Toxicity</b>	Criteria for P/vP identical and T (nearly) identical	
<b>Exposure</b>	<i>Chronic, inter-generational presence</i> in fresh/drinking water sources; accumulates relative to dilution rates	<i>Chronic, inter-generational presence</i> in food chain; accumulates relative to depuration rates
<b>Criteria for Mobility (M) &amp; Bioaccumulation (B)</b>	<b>M:</b> Experimental log Koc < 4 ( <i>breakthrough WWTP, bank filtrate</i> ) <b>vM:</b> Experimental log Koc < 3 ( <i>groundwater transport</i> )	<b>B:</b> Bioconcentration factor > 2000 <b>vB:</b> Bioconcentration factor > 5000

Outcome: Not all chemicals in drinking water and ground water are PMT/vPvM  
*(false negatives expected)*



- 28% of «Not PMT/vPvM» in drinking water and groundwater are *not P*
- 6% of «Not PMT/vPvM» are *not M*
- Only 1 compound in DW that was *not P* and *not M* (butyl benzyl phthalate – drinking water contact material)
- Causes: Drinking water contact chemicals, local emissions, large emissions
- Non PMT/vPvM in drinking water short term concern: removed through risk mitigation/emission reduction....
- PMT/vPvM in drinking water long term concern: continuous exposure long after emissions stop

# Outcome: Initial list of PMT/vPvM substances



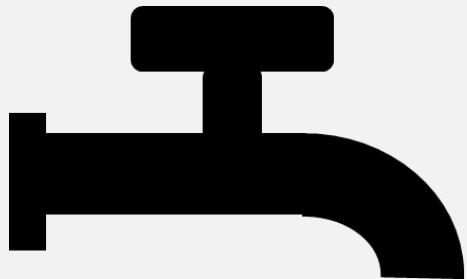
All REACH (2017)  
9742 substances with  
organic constituent

Excluding Article 14  
Exemptions, <10 ton/y &  
intermediates: 3859 substances

vPvMT (155 substances)  
vPvM (47 substances)  
PMT (152 substances)

vPvMT (86 substances)  
vPvM (34 substances)  
PMT (38 substances)

# Impact Assessment



- ↗ 119 substances prioritized for follow up.
- ↗ Upgrading AC and ozonolysis in Germany to partially treat some PMT/vPvM nationwide will cost 0.8-1.5 billion € year .
- ↗ Costs to Europe could get up to the hundreds of billions € year just for drinking water and groundwater remediation actions.
- ↗ Public health costs would only add on top of this.

# Follow-up: PMT/vPvM Substances: Identification and Regulation under REACH

## (2019-2021) FKZ 3719 65 408 0

- ☛ Identify PMT on REACH list from Sept 2019 (**22400 Substances**) and compare to May 2017 (**15469 Substances**)
- ☛ Expand monitoring literature review
- ☛ monitor German bank filtrate and raw water for PMT/vPvM substances
- ☛ Identify the state of «**Gaps**» in addressing PMT/vPvM substances
- ☛ RMOA for 10 substances
- ☛ Disseminate the PMT/vPvM criteria and concern



Hans Peter Arp (NGI), Sarah Hale (NGI), Ivo Schliebner (UBA), Vassil Valkov (IWW), Michael Neuman (UBA), Ulrich Borchers (IWW), Karsten Nödler (TZW), Daniel Zahn (HSF), Isabelle Neuwald (HSF)

# Yesterday's Poll: what are the most important gaps? (Pick 3)

## Substance Assessment

- ✓ Availability of Persistency data?
- ✓ Availability of Mobility data?
- ✓ Availability for Toxicity data?
- ✓ Availability of Analytical methods?
- ✓ Availability of Monitoring data?
- ✓ Availability of transformation products and mixture composition?

## Risk Governance

- ✓ Missing risk assessment tools/models?
- ✓ Missing water remediation infrastructure?
- ✓ Missing chemical legislation?
- ✓ Missing safe and sustainable substitutes?



# Yesterdays Poll: what are the most important gaps? Results

## Substance Assessment

- Availability of Persistency data? (rank 9/13%)
- Availability of Mobility data? (rank 8/14%)
- Availability for Toxicity data? (rank 7/15%)
- Availability of Analytical methods? (rank 2/28%)
- Availability of Monitoring data? (rank 3/24%)
- Availability of transformation products and mixture composition? (rank 1/30%)

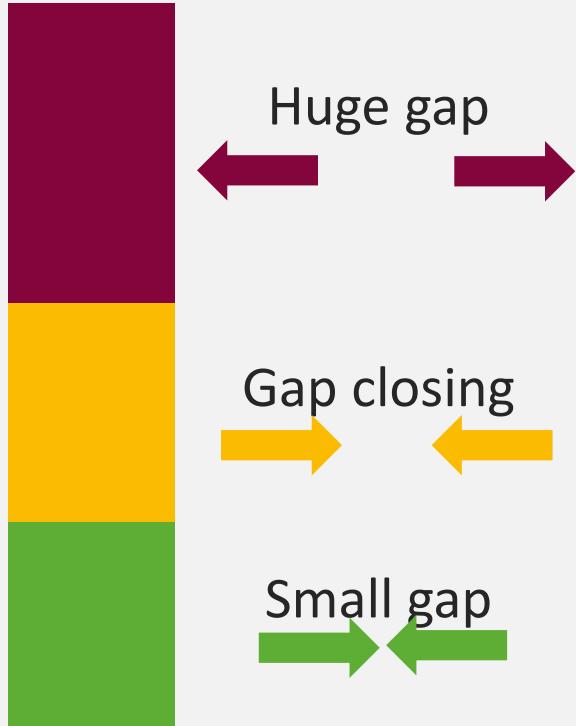
## Risk Governance

- Missing risk assessment tools/models? (rank 4/18%)
- Missing water remediation infrastructure? (rank 10/10%)
- Missing chemical legislation? (rank 6/17%)
- Missing safe and sustainable substitutes? (rank 5/18%)

■ N=371



# Towards closing the gaps: Opinion and New Poll!



- Will present first glimpse at new project results in relation to each “gap”
- End of presentation we will poll if you think each gap is huge, closing or small*
- I will present a case for each and **make a prediction of audience response**
- Results will be shared after workshop

# Gap 1: Availability of Persistency data? (ranked 9)

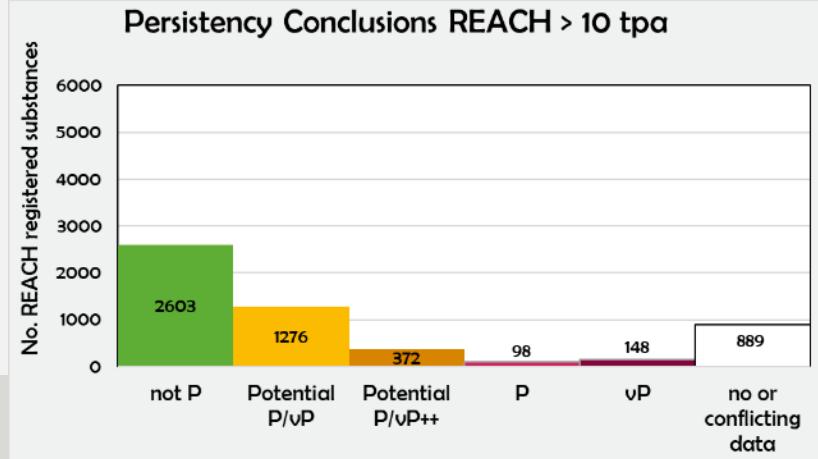
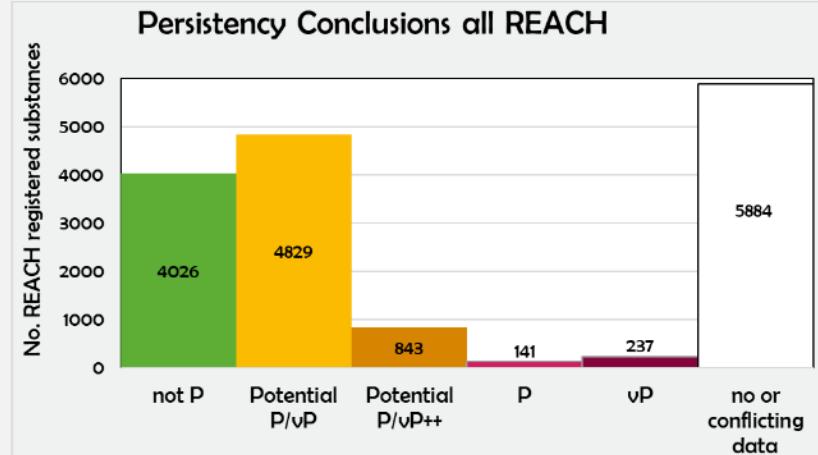
40%

- Little/no information for low volume/intermediate REACH substances
- Mandatory PBT assessment for substances > 10 tpa contributes to more testing: Effect of PBT/vPvB regulation
- Screening tests for ready/inherent biodegradability useful for demonstrating «Not P»

20%

Relevant talks:

Roberta Hofman-Caris (KWR), Martin de Jonge (Vitens)



# Gap 2: Availability of Mobility data? (rank 8)

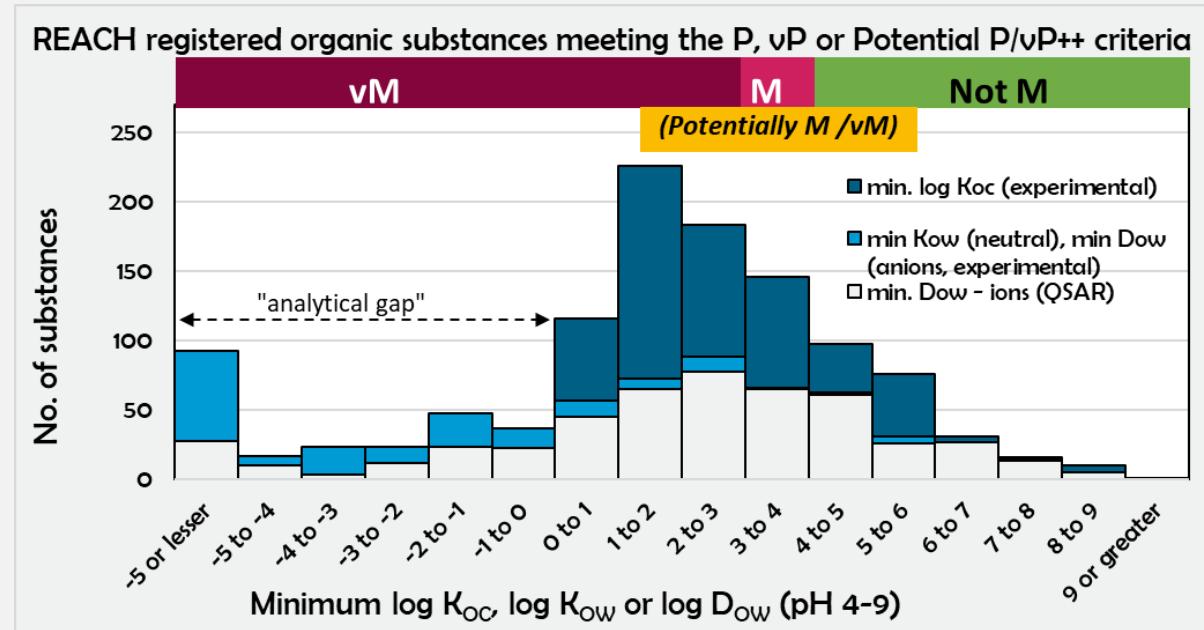
20%

20%

60%

→  $K_{oc}$  data for ionic substances rare and scattered,  $D_{ow}$  does not account for ion-exchange

→ Neutral substances – lots of data and good models. Many ionic substances have  $K_{oc}$  values orders of magnitude from threshold



# Gap 3: Availability of Toxicity data? (rank 7)

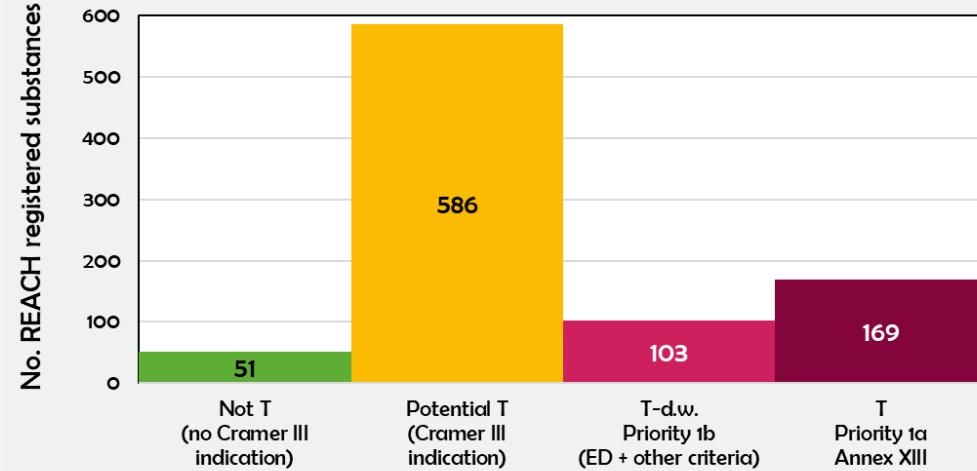
40%

20%

40%

- Lack of data on PM/vPvM chemicals, despite chronic exposure. Few long-term physiologically based pharmokinetic (PBPK) models.
- Attention on PFAS is inspiring increasing research on effects from chronic water exposure
- Lots of required testing due to CLP

Toxicity Conc. for PM/vPvM substances registered under REACH



# Gap 4: Availability of Analytical methods? (rank 2)

30%

- Target analysis still needed for extremely mobile substances (e.g.  $\log D < -2/3$ ); standards HARD to come by

40%

- VAST improvements in the past 5 years in relation to target and non-target analysis (e.g. HILIC columns, Super critical fluid chromatography, suspect screening databases such as the Norman Network SLE)

30%

NCI

Relevant talk: Thomas Letzel, TUM; Juliane Hollander, EAWAG. Chat – Coordination of NORMAN and DG Sante for non-target data

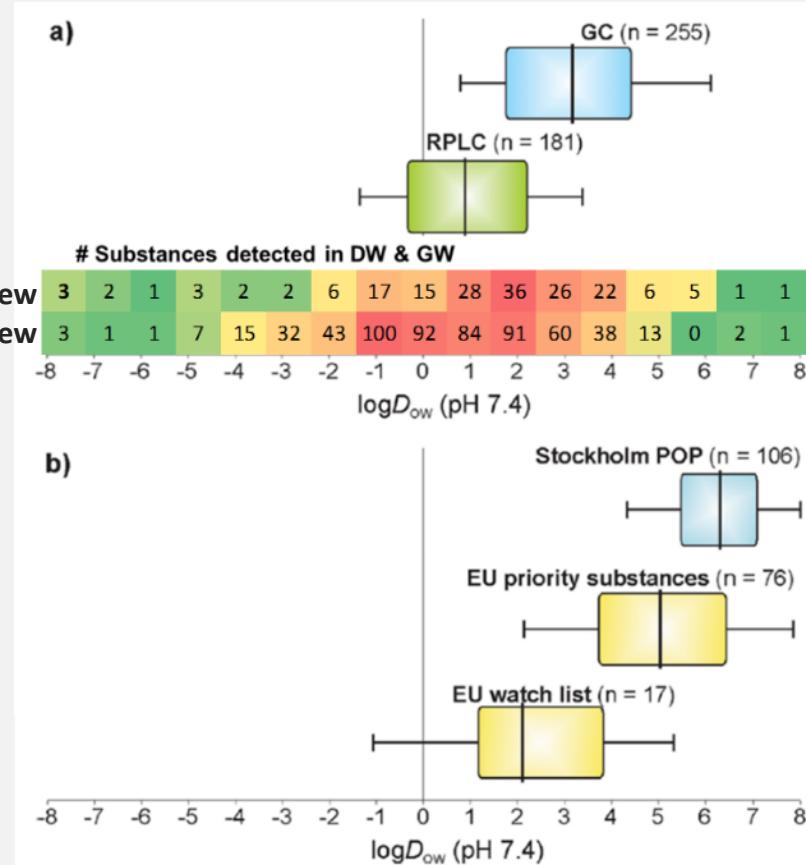


Figure adapted from Reemtsma et al. ES&T 2016

# Gap 5: Availability of Monitoring Data? (rank 3)

70%

- An **incentive gap**: why monitor unless requested/share data unless requested. Only seeing tip of the «chemical iceberg» via research community

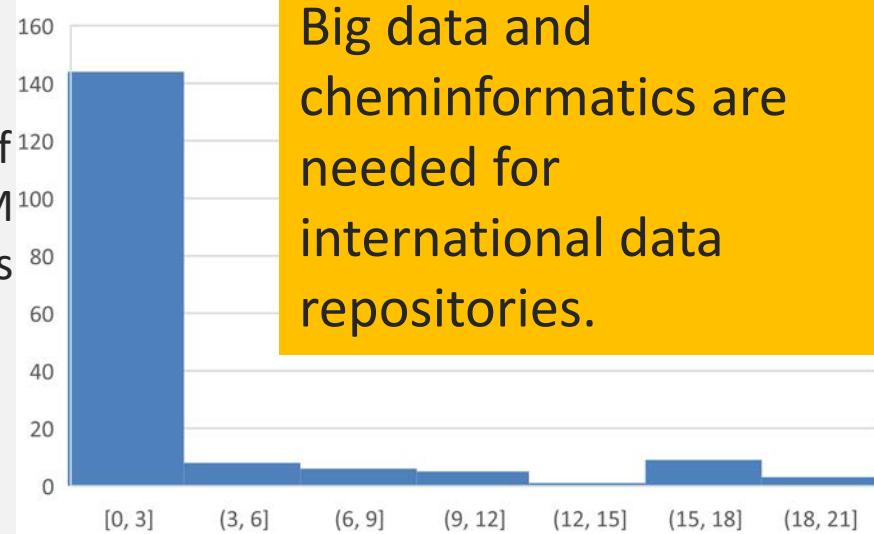
20%

- State-of-the-art research labs paving the way!

10%

NGI

Number of PMT/vPvM substances



Big data and cheminformatics are needed for international data repositories.

Number of water analysis labs in Germany that routinely analyze for them

# Sneak preview of new German monitoring data



- 81 PMT/vPvM substances plus additional PFAS
- 13 sources of German drinking water
- Detected 57 substances, including 8 for the first time
- e.g. 1,1,1,3,3-hexafluoropropan-2-ol at 0.4 µg/L in bank filtrate
- Confirms **again\*** that PMT/vPvM criteria and emission/use information can be used to predict chemicals in drinking water sources

\* JPI Promote - Schulze et al. Water Research 2019

<https://www.sciencedirect.com/science/article/pii/S0043135419300363>

# Gap 6: Transformation products and mixture composition? (rank 1)

80%

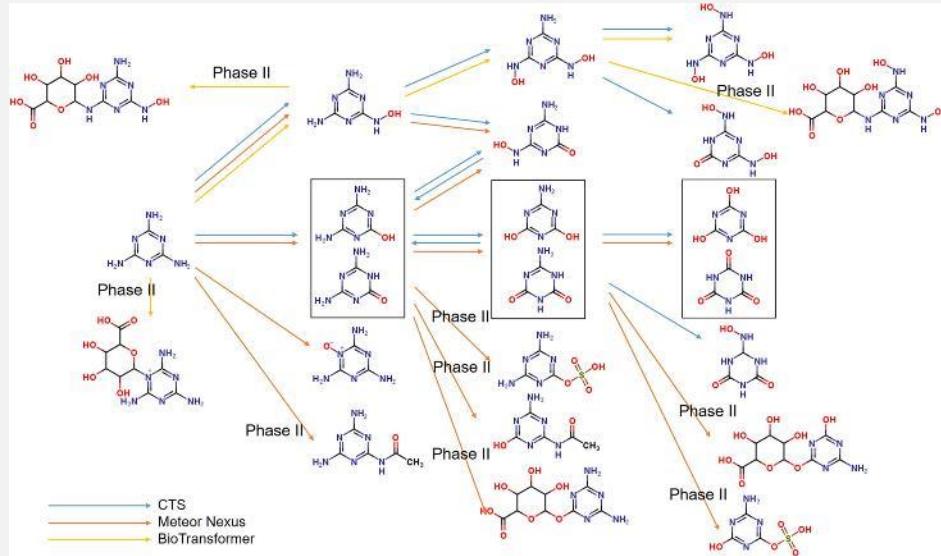
10%

10%

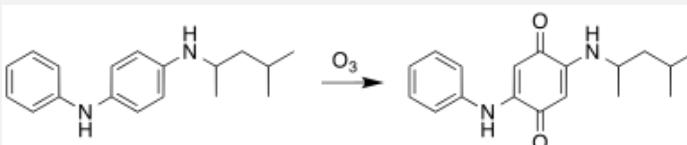
NGI

Relevant talks: Karsten Nödler  
TZW, Frauke Averbeck BauA

- For all REACH:
  - ONLY 451 transformation products identified through **experimental** databases (EAWAG BBD, Norman SLE)
  - QSARs give multiple predictions (see Zheng et al.)
  - Ca 30% of organic substances in REACH are complex mixtures (UVCBs)



- Melamine transforming to even more vPvM chemicals (Zheng et al. ES&T 2020, 10.1021/acs.est.0c02593)



- 6PPD (REACH vPvM & PMT) -> killer of Coho Salmon (Tian et al. Science 2020 <https://science.sciencemag.org/content/371/6525/185>)

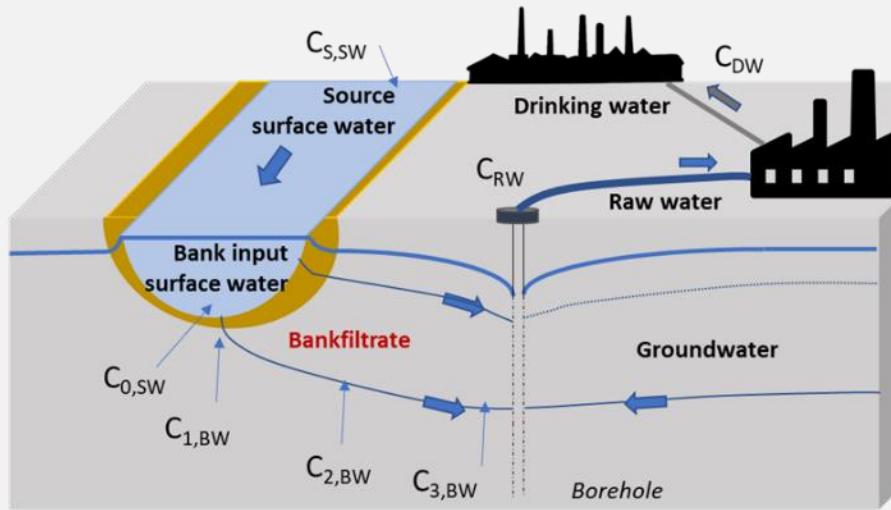
# Gap 7: Missing risk assessment tools/models? (rank 4)

60%

10%

30%

- Mobility gap – ionic substances have complex behaviour
- Toxicity gap – unknown long term exposure effects
- Diffuse emissions, bank filtrate/ground water are inherently complex and not covered by generic models



- Well established agriculture plant protection product (PPP) and waste water treatment plant (WWTP models for specific scenarios (EUSES, SimpleTreat)

# Gap 8: Missing water remediation infrastructure? (rank 10)

70%

20%

10%

- ↗ **A gap that cannot be fully closed.** Many “pristine”, or developing countries have limited drinking water production infrastructure – rely on chemical regulation to ensure protection.
- ↗ **Regrettable remediation:** Most PMT/vPvM only removable with RO / super expensive, resource intensive treatment: Economic, Efficiency and Sustainability concerns.
- ↗ **Advance treatment methods work best at emission source**



Relevant talks: Claudia Castell-Exner (Eureau), Ivo Schliebner (UBA), Karsten Nödler (TZW), Luisa Rabe & Pia Schumann (UBA), Gabriel Sigmund (University of Vienna)

Screening of 158 PMT/vPvM substances Arp and Hale 2019. Suitable water treatments:

Technique	%
Neither O <sub>3</sub> nor AC	52,5
Only O <sub>3</sub>	15,8
Only AC	20,9
Both	10,8

K.Nödler, preliminary results

Setting the agenda in research

**Comment**



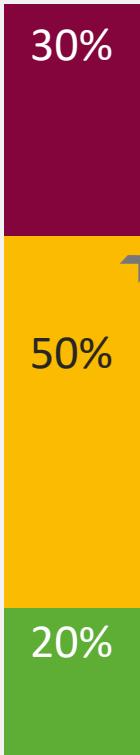
One of five water-reuse plants in Singapore, which together supply about 40% of the nation's water for drinking and other uses.

Drink more recycled wastewater

Cecilia Tortajada and Pierre van Rensburg

Tortajada and van Rensburg, Nature, 2019

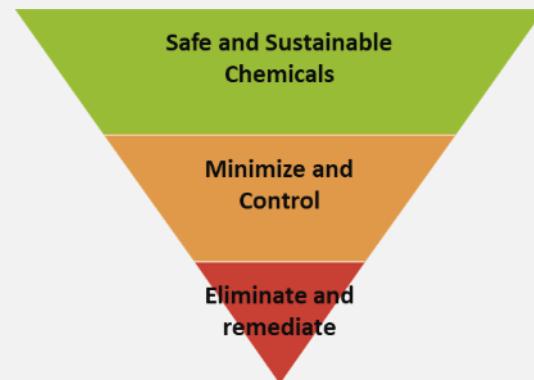
# Gap 9: Missing chemical legislation? (rank 6)



- Harmonization to be explored across risk and hazard based legislation and regulation (CLP, REACH, PPPR, WHO GV, DWD, E-PRTR)
- The Chemicals Strategy for Sustainability and Zero Pollution Ambition
  - Inclusion of PMT/vPvM in for REACH / CLP
  - PFAS restriction
  - Safe and Sustainable by Design
- Existing tools
  - Article 57f
  - PPPR



Jin et al. <https://pubs.acs.org/doi/10.1021/acs.est.0c04281>



# Gap 10: Missing safe and sustainable substitutes (rank 5)

40%

- Technical / economic challenges
- Definition of «essential use»
- Safe and sustainable by design / green chemistry techniques concept and techniques rapidly developing
- Sustainable material and process engineering
- Majority of high production chemicals are NOT PMT/vPvM
- Strong societal/industry support
- Humans are innovators

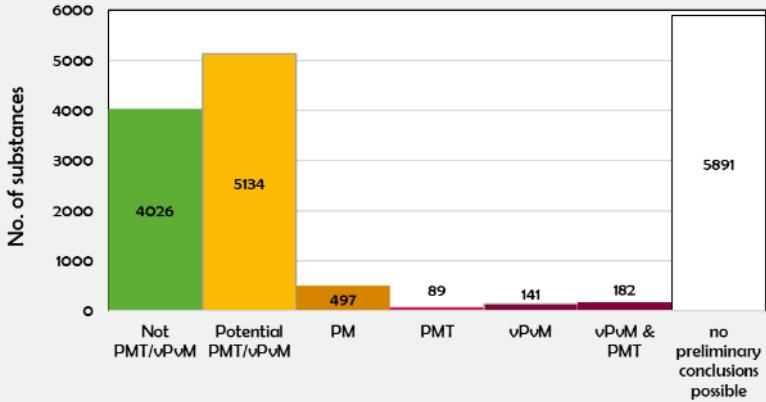
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30%

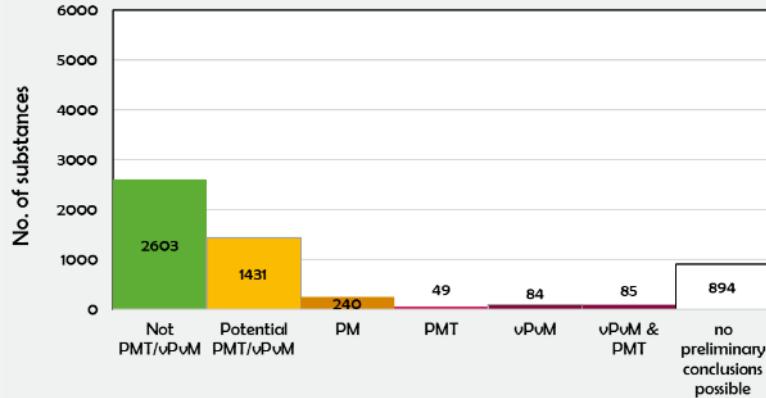
NGI

Relevant talk: Xenia Trier (EEA), Ninja Reineke (ChemTrust)

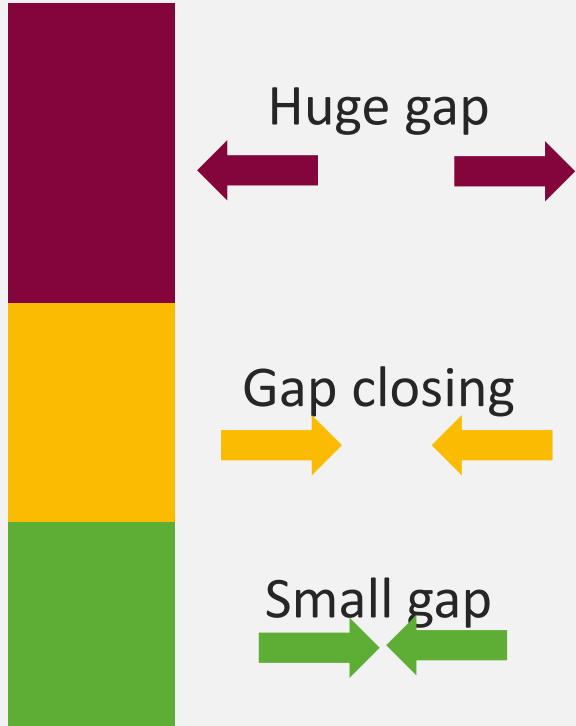
A) PMT/vPvM Conclusions for all REACH Registered Substances with identified organic constituent (as of September 2019)



B) For REACH Registered Substances with Organic Constituent > 10 tonnes per annum



# Please open the poll!



## Substance Assessment

- ↗ Availability of Persistency data?
- ↗ Availability of Mobility data?
- ↗ Availability for Toxicity data?
- ↗ Availability of Analytical methods?
- ↗ Availability of Monitoring data?
- ↗ Availability of transformation products and mixture composition?

## Risk Governance

- ↗ Missing risk assessment tools/models?
- ↗ Missing water remediation infrastructure?
- ↗ Missing chemical legislation?
- ↗ Missing safe and sustainable substitutes?



# We have the tools, let us close the gaps to get control!

## Stewardship + Risk Governance + Science



- PMT/vPvM In CLP & REACH
- Harmonization of PMT/vPvM definitions within risk assessment models and regulations
- Big data monitoring data and suspect list harmonization (e.g. non-target in E-PRTR)
- Remediation at emission sources rather than downstream
- Safe and sustainable chemistry

Non-toxic hierarchy of the Chemical Strategy for Sustainability

Safe and Sustainable Chemicals

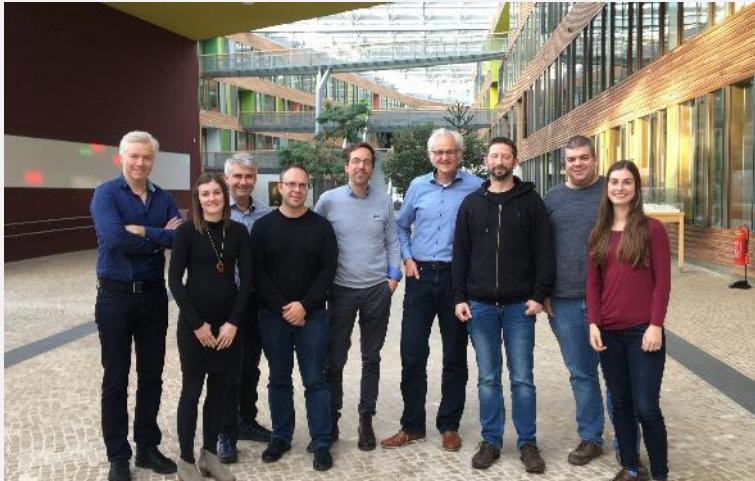
Minimize and Control

Eliminate and remediate

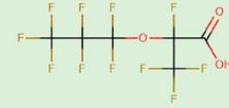


Zero pollution of PM substances

# Thank-you and Happy Spring!



Hans Peter Arp (NGI), Sarah Hale (NGI), Ivo Schliebner (UBA), Vassil Valkov (IWW), Michael Neuman (UBA), Ulrich Borchers (IWW), Karsten Nödler (TZW), Daniel Zahn (HSF), Isabelle Neuwald (HSF)



*PMT/vPvM*

*Rose*

► Hale et al. *Environ. Sci. Technol.* 2020, 54, 23, 14790–14792

► Funding from the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety of Germany (FKZ 3719 65 408 0)

► Thanks to: Sarah Hale (NGI), Michael Neuman (UBA), Ivo Schliebner (UBA), Jona Schulze (UBA), Ulrich Borchers (IWW), Vassil Valkov (IWW), Laura Wiegand (IWW), Karsten Nödler (TZW), Marco Scheurer (TZW), Isabelle Neuwald (HSF), Daniel Zahn (HSF)