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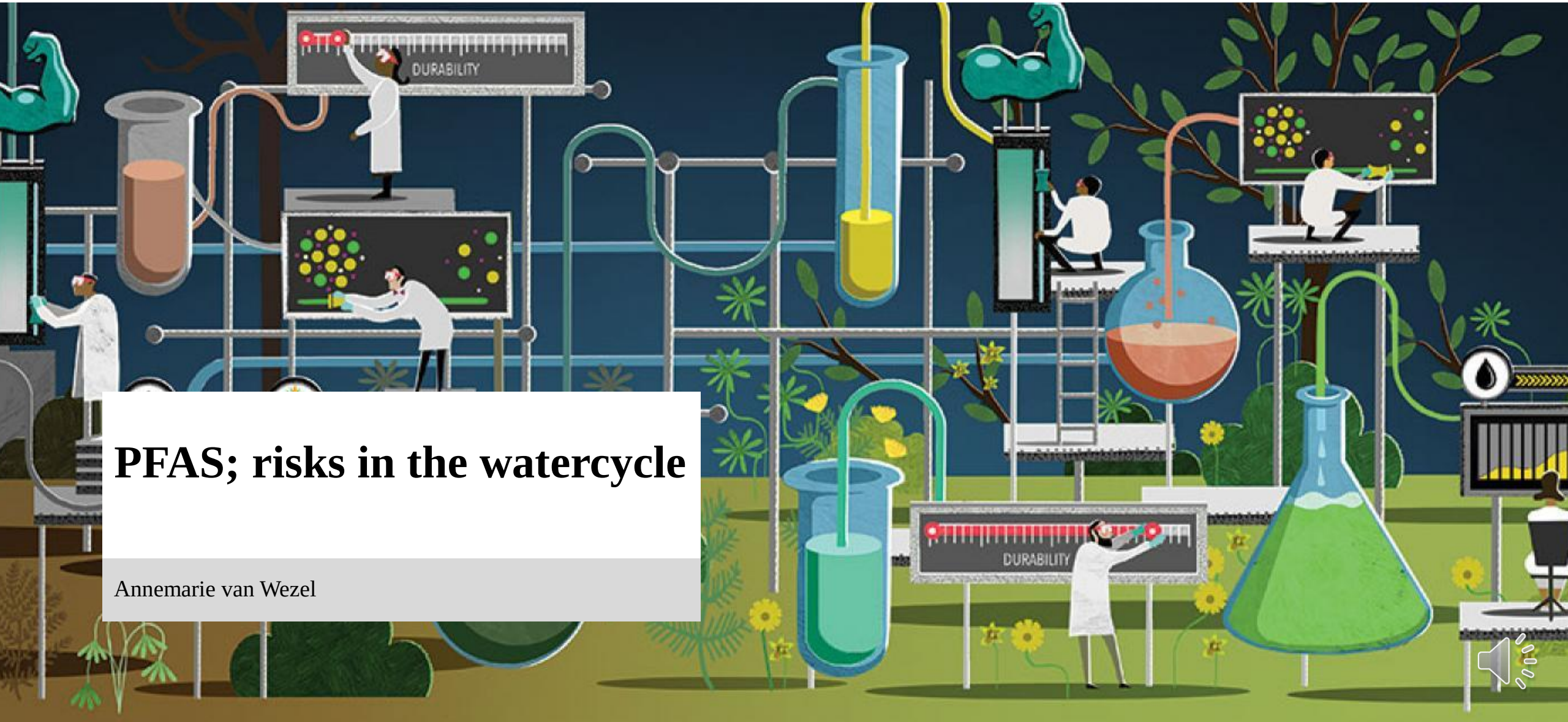
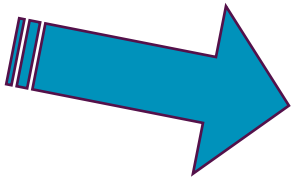


PFAS; risks in the watercycle

Annemarie van Wezel

PFAS are used a lot for their nice properties



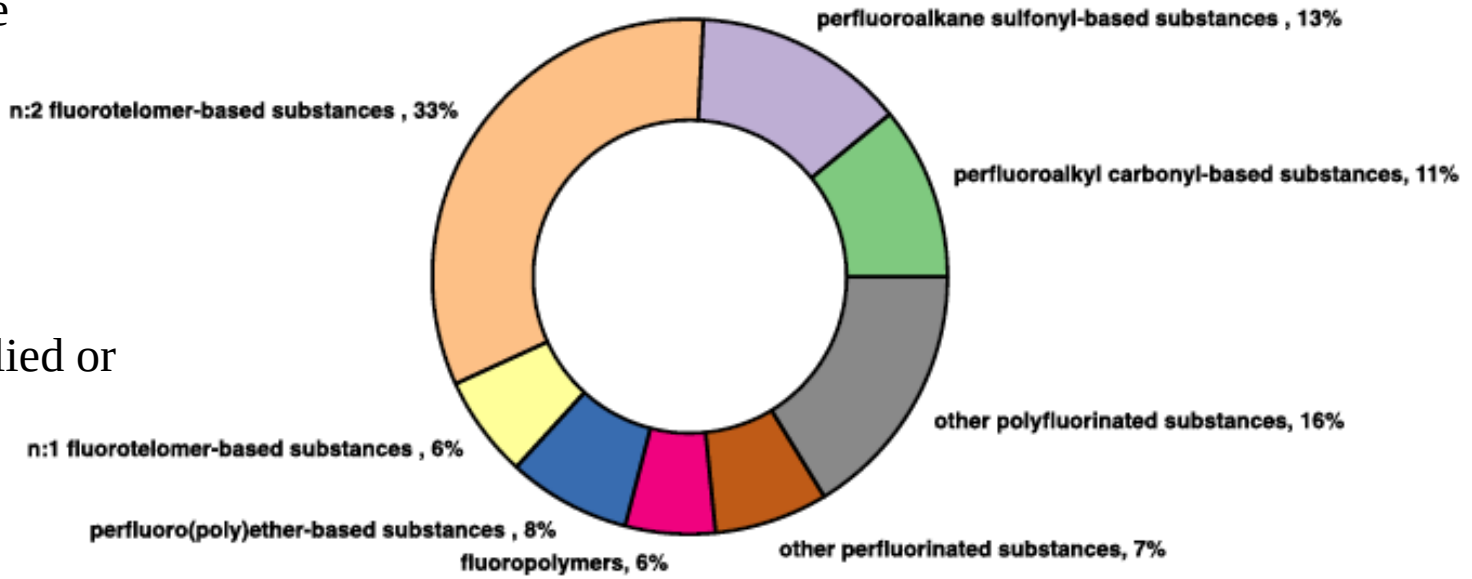
OECD list; 4730 PFAS

New PFAS often shorter C-chains and thus more mobile.

Ca. 1000 preregistrered and 107 registered in REACH, 2 as pesticides.

All other PFAS should not be made, traded, applied or used.

Severe scarcity on emission data!

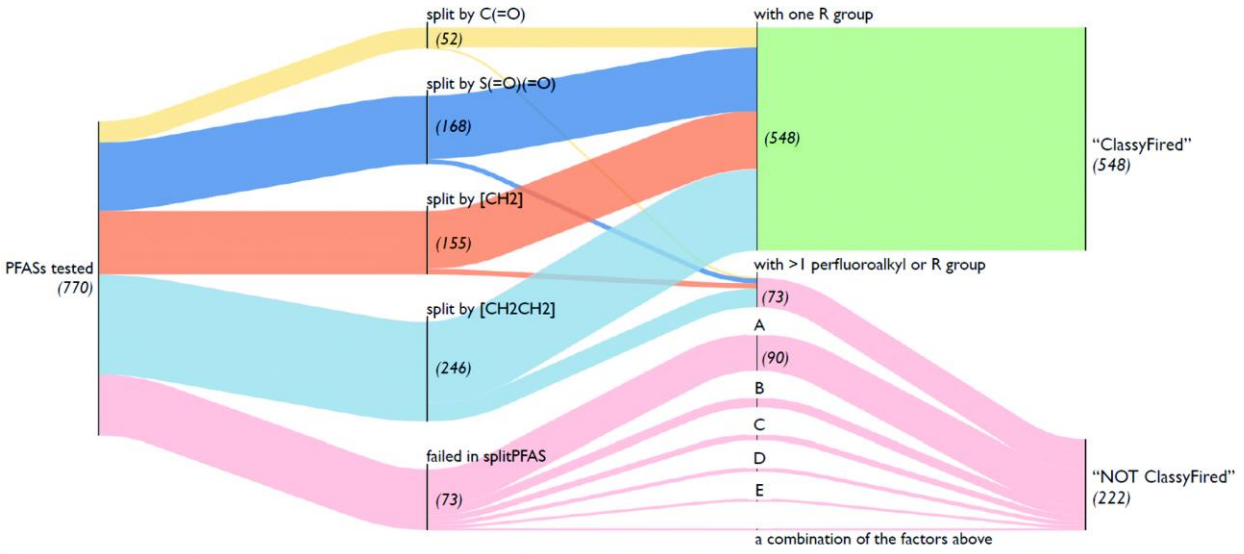


OECD 2018

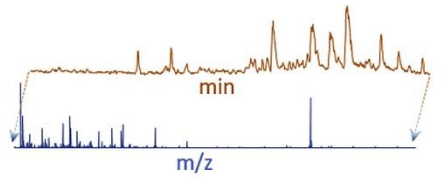
Analytical methods

High resolution MS, combined with suspect lists (eg NORMAN PFAS list)

→ more than 750 PFASs, belonging to more than 130 diverse classes, found in strategically selected environmental samples, biofluids or commercial products



(1) HRMS full-scan data



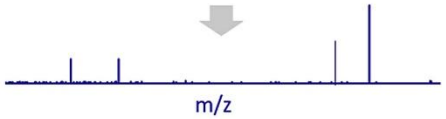
(2) prospective PFAS feature identification

- feature reduction
- mass defect filtering
- homologous series searching
  - e.g. CF_2-normalized mass defect plots
- study design
  - e.g. case-control
- diagnostic fragments or neutral losses
  - e.g. data-dependent acquisition
    - data-independent acquisition
    - all-ion-fragmentation
    - in-source fragmentation
- parallel HRMS & F-detection instruments

(3) molecular formula assignment

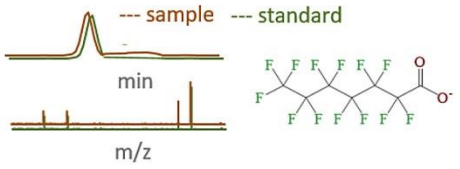
$C_7F_{13}O_2^-$ 0.8 ppm
$C_{10}F_{11}H_2S^-$ -2.4 ppm
...

(4) structural characterization by MS^n (n≥2)



(5) Structural proposal & confirmation

- based on MS^n profiles
- matching to database suspects
- standard comparison

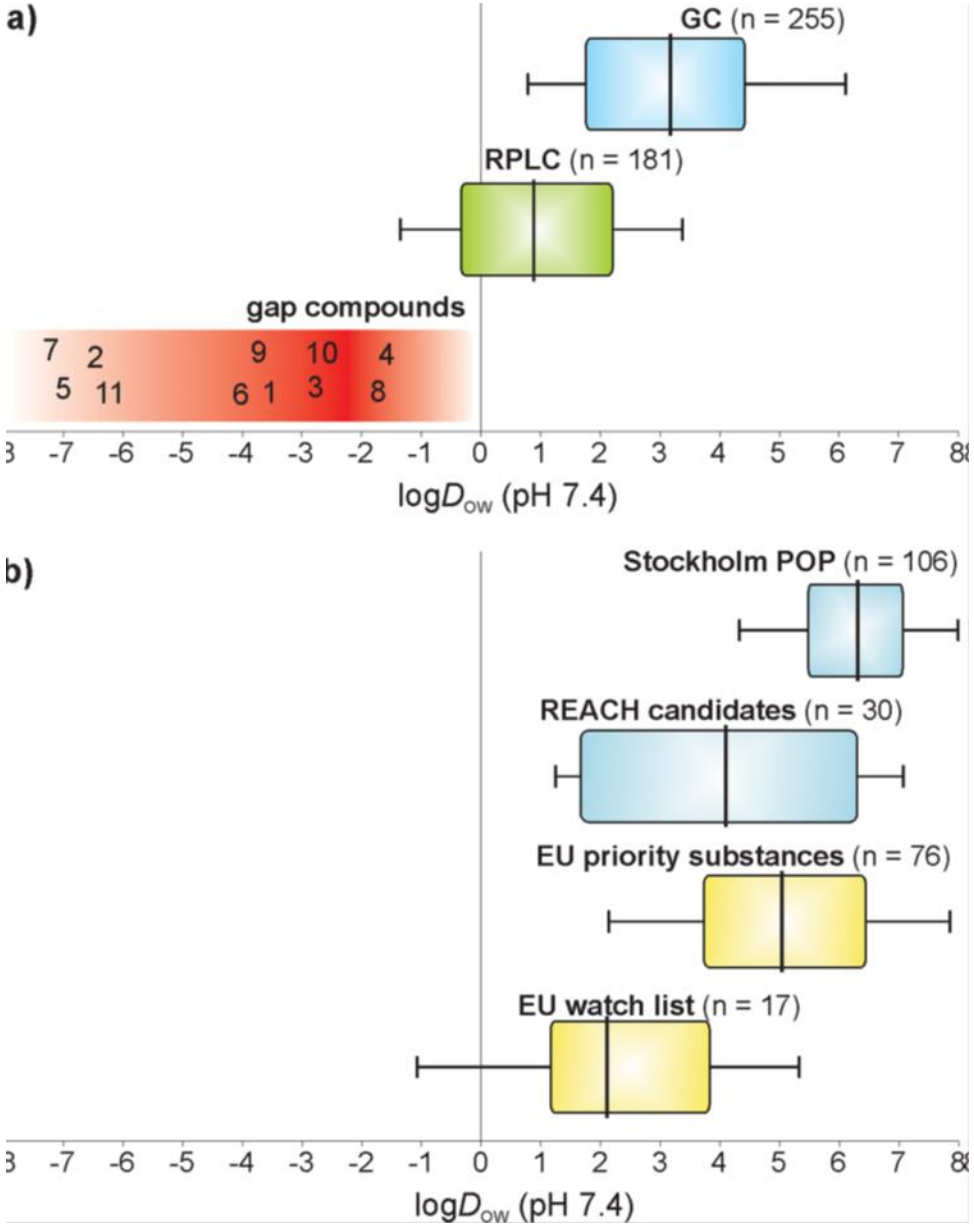


Liu et al TrAC 2019, Sha et al 2019

PFAS are PMT compounds
Mind the gap!

More polar chemicals are;

- Less regulated
- Less easy to measure analytically
- Less easy to remove in water treatment



Reemtsma et al 2016

Concentrations in tap water

Sampling location	Concentrations of PFCAs (ng/L)							
	PFPeA	PFHxA	PFHpA	PFOA (lin/Σbranched)	PFNA	PFDA	PFUnA	PFDoA
1. Stockholm University, Sweden	nd	2.86	1.09	6.18 (92/8)	0.433	0.506	nd	<MLQ
2. Institute for Environment and Sustainability, Ispra, Italy	<MLQ	2.1	1.19	4.92 (90/10)	0.522	0.612	nd	<MLQ
3. University of Antwerp, Belgium	1.39	3	0.996	2.70 (100/0)	0.339	0.182	nd	<MLQ
4. University of Amsterdam, The Netherlands	0.734	3.06	1.47	8.56 (80/20)	<MLQ	<MLQ	nd	<MLQ
5. VU University, Amsterdam, The Netherlands	2.69	5.15	1.91	5.66 (65/35)	<MLQ	<MLQ	nd	<MLQ
6. Norwegian Institute for Air Research, Tromso, Norway	<MLQ	0.806	0.434	2.20 (100/0)	<MLQ	0.094	<MLQ	<MLQ
7. Fraunhofer Institute, Schmallenberg, Germany	<MLQ	<MLQ	<MLQ	0.302 (100/0)	<MLQ	<MLQ	nd	<MLQ

Health effects

Associations between PFAS exposure and health effects; eg obesitas after prenatal exposure, lipid metabolism, immune system, liver failure, renal function, thyroid hormone – important for cognative development.

Worldwide PFAS found in environmental organisms.

For most PFAS no well established risk assessment and ADI derived.

Policy responses

Continued use → increased environmental concentrations
Therefore current call for evidence on broad PFAS restriction, with a possible date of entry in 2025.
Two PFAS groups are identified as SVHCs, based on PMT, i.e. GenX and perfluorobutane sulfonic acid (PFBS), replacers of PFOA and PFOS respectively

Provisional agreement by the European Parliament and the Council in December 2019 on the recast of the Drinking Water Directive includes a limit of 0.5 µg/l for all PFAS, in line with a grouping approach for all PFAS. Currently subject to formal approval by the European Parliament and the Council. Following approval, the Directive will be published in the EU's Official Journal and enter into force 20 days later.

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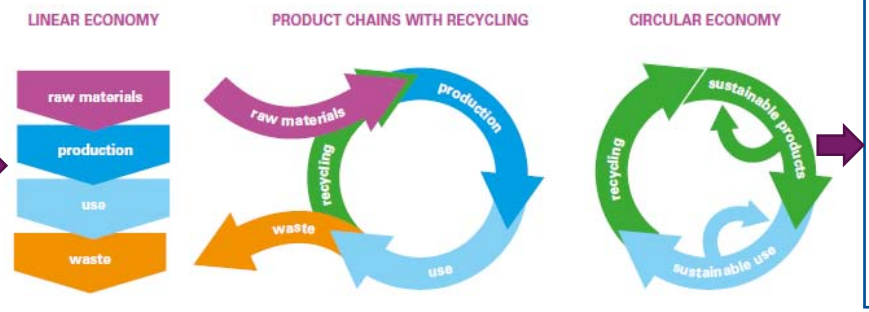
Essential elements for a Chemicals strategy for sustainability

Legislation (OS-OA), chemical design & essentiality, technology

Essentiality & benign-by-design

Necessary for health, safety or critical for societal functioning

No available technically and economically feasible non-chemical alternatives



Equal/better functionality
Less hazardous
Less persistant/More durable
Lower emissions

Dec 2019: EU Green Deal