How to Deal with Complexity in the Chemicals Area?

Martin Scheringer
Masaryk University, Brno
Swiss Federal Institute of Technology, Zürich

June 10, 2021

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Introduction Martin Scheringer

- Chemist by training
- Professor of environmental chemistry, Masaryk University, Brno, Czech Republic
- Senior scientist and group leader, ETH Zürich, Switzerland

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scheringer@usys.ethz.ch

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Addressing the Big Picture

- Not: methods and techniques for the hazard and risk assessment of individual chemicals
- But: the big picture of “all” chemicals on the market
- How big is this big picture?

Addressing the Big Picture

- Before REACH: approx. 100’000 chemicals in the EU (listed in EINECS and ELINCS)

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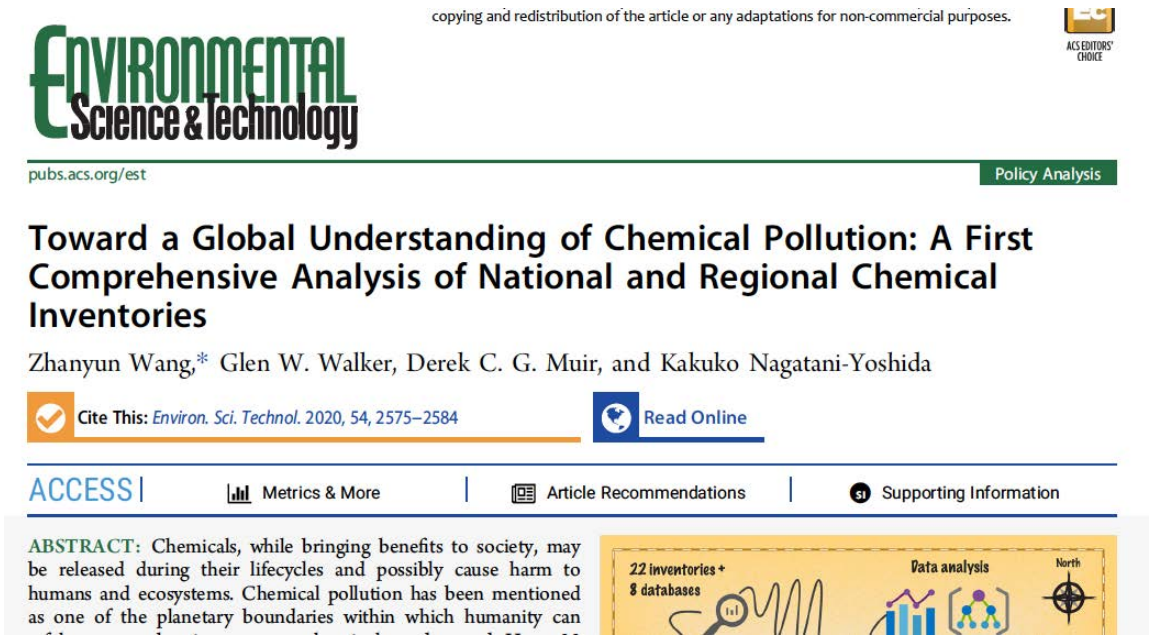
- Wang et al. (2020): more than 350’000 chemicals listed in 22 inventories from 19 countries



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Policy Analysis

Toward a Global Understanding of Chemical Pollution: A First Comprehensive Analysis of National and Regional Chemical Inventories

Zhanyun Wang,* Glen W. Walker, Derek C. G. Muir, and Kakuko Nagatani-Yoshida

Cite This: *Environ. Sci. Technol.* 2020, 54, 2575−2584

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ABSTRACT: Chemicals, while bringing benefits to society, may be released during their lifecycles and possibly cause harm to humans and ecosystems. Chemical pollution has been mentioned as one of the planetary boundaries within which humanity can

Wang et al. (2020) Environ. Sci. Technol. 54, 2575–2584, doi: 10.1021/acs.est.9b06379

Addressing the Big Picture

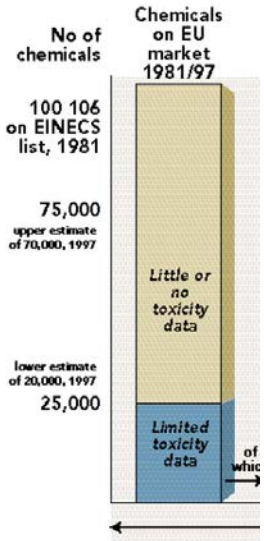
- Before REACH: approx. 100’000 chemicals in the EU (listed in EINECS and ELINCS)

- Wang et al. (2020): more than 350’000 chemicals listed in 22 inventories from 19 countries[1]

- REACH (June 2021): 23’285 substances, 103’310 dossiers[2]

1 Wang et al. (2020) Environ. Sci. Technol. 54, 2575–2584, doi: 10.1021/acs.est.9b06379
2 https://echa.europa.eu/information-on-chemicals/registered-substances

Chemical Risk Assessment Before REACH



HPVC High Production Volume Chemicals, i.e. production over 1,000 tons/year

Little/no toxicity = less than OECD minimum for screening

Limited toxicity data available for OECD/EU screening (e.g. only 20-30% of substances have useable data on cancer or reproduction)

EINECS: European Inventory of Existing Commercial Chemical Substances

IUCLID: International Uniform Chemical Information Data Base

Adequate toxicity for EU risk assessment (including some cancer/ reproductive/neurotoxic data) but inadequate data on consumer or environmental exposures

ELINCS: European List of Notified Chemical Substances (New Substances)

Limited data available for basic toxicity screening

400 risk assessments carried out by Member States (confidential data)

Note: In addition to the EU existing chemicals risk assessment programme, both the OECD and WHO/IPCS have completed detailed risk assessments covering about 200 priority chemicals.

Source: EEA, based on CEC (1996), NRC (1984), EDF (1997) and ECB (1998).

Chemicals in the European Environment: Low Doses, High Stakes;
EEA 1998;
http://www.eea.europa.eu/publications/NYM2

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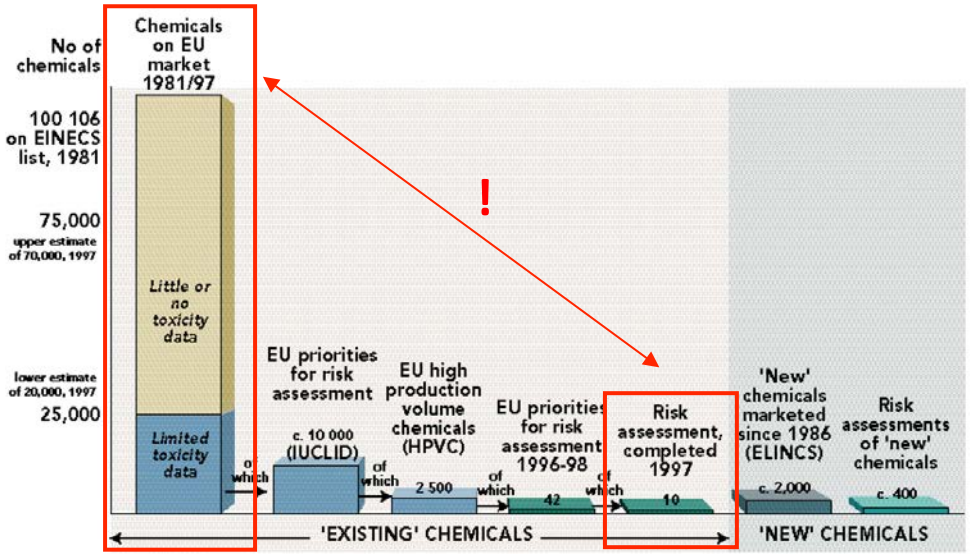
Chemical Risk Assessment Before REACH



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It Is still the Same Task ...

Chemical Watch

‘Extensive’ improvement still needed on REACH, CLP industry data – Echa

03 June 2021

Five-year report on the regulations reveals shortcomings ahead of Commission reviews

Europe | Substance registration | CLP Regulation | Data reporting | REACH | EU chemicals strategy

After 14 years of REACH, information provided by industry in their registration dossiers "still needs extensive improvement", Echa has said, as the European Commission begins to process stakeholder feedback on proposed widespread changes to the Regulation.

In its third five-year report on the operations of REACH and CLP, published on 1 June, Echa said companies need to improve the way they use information contained in chemical safety reports, safety data sheets (including exposure scenarios), and in classification and labelling, which the agency said are the main vehicles for communicating safe use.

https://chemicalwatch.com/274945/extensive-improvement-still-needed-on-reach-clp-industry-data-echa

It Is still the Same Task ...

Echa checks reveal nearly 90% of REACH dossiers needed more data

25 February 2021

Only 12% passed compliance checks without information requests during 2020

Europe | Substance registration | Data reporting | Substances of concern | REACH

Compliance checks carried out by Echa last year resulted in 88% of REACH dossiers needing additional information, revealing the impact of extra screening the agency has embarked on to identify substances of concern that require further testing.

Echa relies on accurate and relevant safety data in registrations to be able to identify potentially harmful substances for risk control measures.

https://chemicalwatch.com/221713/echa-checks-reveal-nearly-90-of-reach-dossiers-needed-more-data

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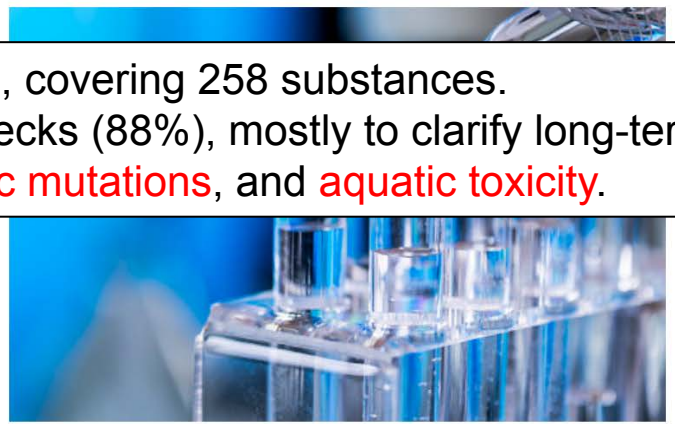
Europe | Substance registration | Data reporting | Substances of concern | REACH

Chemical Watch

Compliance checks carried out by Echa last year

271 full compliance checks carried out in 2020, covering 258 substances.
Further information requested in 240 of the checks (88%), mostly to clarify long-term effects on the development of unborn children, genetic mutations, and aquatic toxicity.



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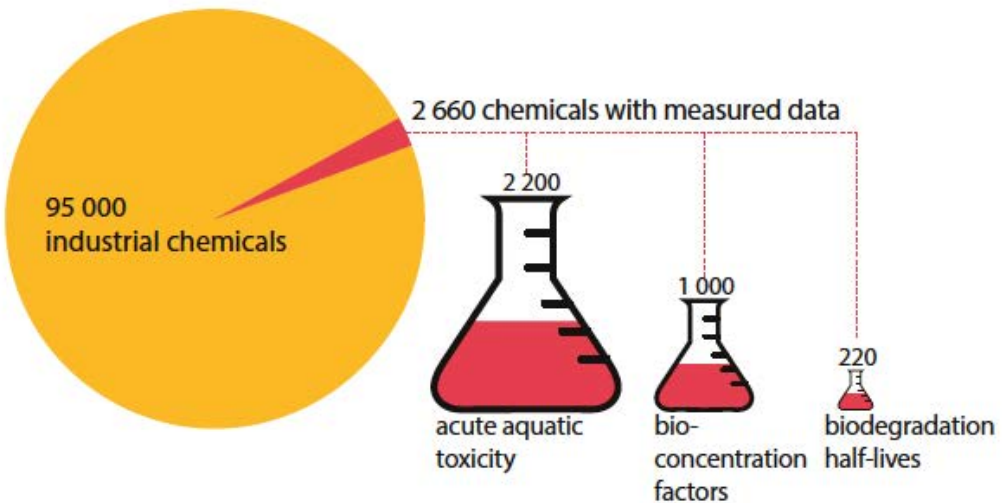
https://chemicalwatch.com/221713/echa-checks-reveal-nearly-90-of-reach-dossiers-needed-more-data

Not Just in the EU

- A merged dataset from EU and US databases (EINECS, ELINCS, Smilecas)
- 95’000 chemicals – P, B and T data?



UNEP Year Book 2013, p. 44, from Strempel et al. (2012)
https://wedocs.unep.org/handle/20.500.11822/8222

Strempel et al. (2012) Environ. Sci. Technol. 46, 5680–5687
doi: 10.1021/es3002713

Chemicals Abound: Humans

- 30 mother-child pairs
- 55 chemicals not previously reported
- 42 unknown origin
- 10 plasticizers

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Article

Suspect Screening, Prioritization, and Confirmation of Environmental Chemicals in Maternal-Newborn Pairs from San Francisco

Aolin Wang,[+] Dimitri Panagopoulos Abrahamsson,[+] Ting Jiang, Miaomiao Wang, Rachel Morello-Frosch, June-Soo Park, Marina Sirota, and Tracey J. Woodruff*

Cite This: *Environ. Sci. Technol.* 2021, 55, 5037–5049

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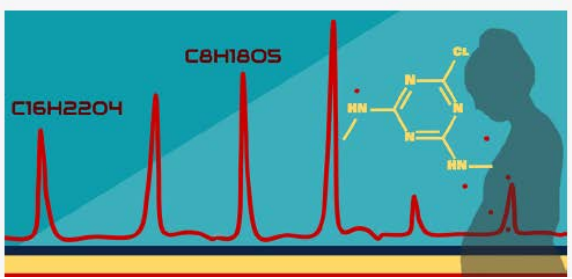
ABSTRACT: Our proof-of-concept study develops a suspect screening workflow to identify and prioritize potentially ubiquitous chemical exposures in matched maternal/cord blood samples, a critical period of development for future health risks. We applied liquid chromatography–quadrupole time-of-flight tandem mass spectrometry (LC-QTOF/MS) to perform suspect screening for ~3500 industrial chemicals on pilot data from 30 paired maternal and cord serum samples (n = 60). We matched 662 suspect features in positive ionization mode and 788 in negative ionization mode (557 unique formulas overall) to compounds in our



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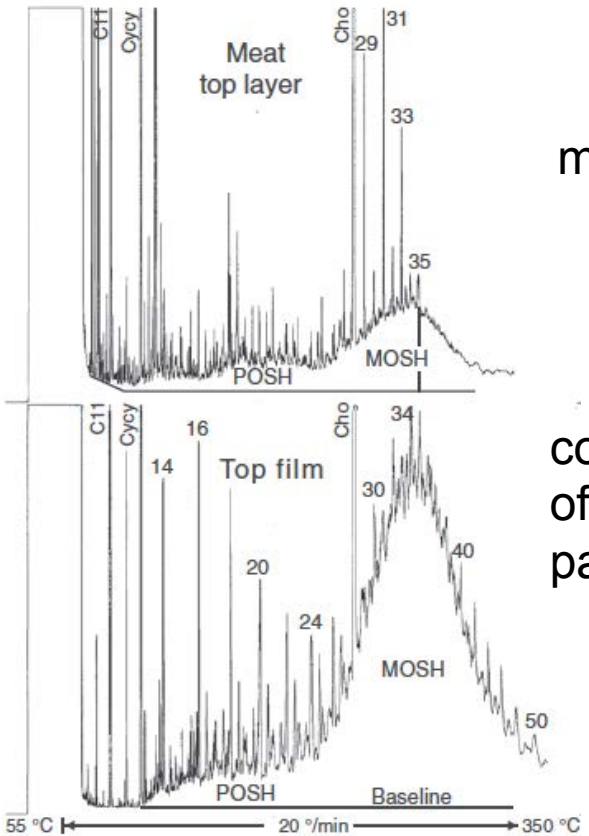
Wang et al. (2021) Environ. Sci. Technol. 55, 5037–5049, doi: 10.1021/acs.est.0c05984

Chemicals Abound: Materials

- An additional problem: non-intentionally added substances (NIAS



meat

cover of polyethylene package

POSH: polyolefin oligomeric saturated hydrocarbons

MOSH: mineral-oil saturated hydrocarbons

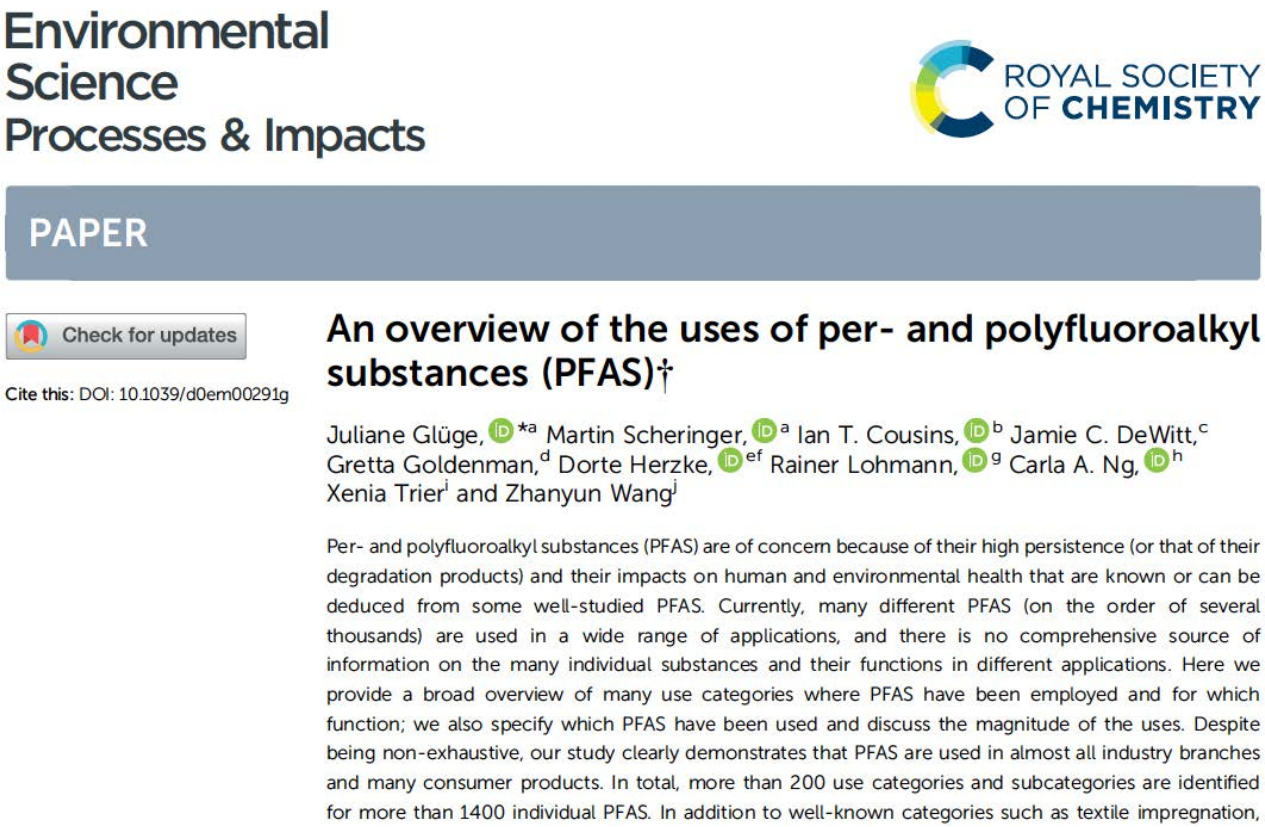
Biedermann-Brem et al. (2012) Food Additives & Contaminants: Part A, 29, 449–460

What Can Be Done?

- Reduce complexity of portfolio of chemicals on the market
- Reduce chemical complexity of materials
- Where to start?
- Hazardous substances, Substances of Very High Concern

Example: PFAS

- 200 uses of 1400 PFAS
- Which ones can be removed?



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ROYAL SOCIETY OF CHEMISTRY

PAPER

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Cite this: DOI: 10.1039/d0em00291g

An overview of the uses of per- and polyfluoroalkyl substances (PFAS)†

Juliane Glüge, *[a] Martin Scheringer, [a] Ian T. Cousins, [b] Jamie C. DeWitt,[c] Gretta Goldenman,[d] Dorte Herzke, [ef] Rainer Lohmann, [g] Carla A. Ng, [h] Xenia Trier[i] and Zhanyun Wang[j]

Per- and polyfluoroalkyl substances (PFAS) are of concern because of their high persistence (or that of their degradation products) and their impacts on human and environmental health that are known or can be deduced from some well-studied PFAS. Currently, many different PFAS (on the order of several thousands) are used in a wide range of applications, and there is no comprehensive source of information on the many individual substances and their functions in different applications. Here we provide a broad overview of many use categories where PFAS have been employed and for which function; we also specify which PFAS have been used and discuss the magnitude of the uses. Despite being non-exhaustive, our study clearly demonstrates that PFAS are used in almost all industry branches and many consumer products. In total, more than 200 use categories and subcategories are identified for more than 1400 individual PFAS. In addition to well-known categories such as textile impregnation,

Environ. Sci.: Processes Impacts, 2020, 22, 2345–2373
https://doi.org/10.1039/d0em00291g

Example: PFAS

- Many non-essential uses
  - carpets
  - dental floss
  - ski wax
  - climbing ropes
  - baking paper
  - bicycle lubricants
  - skin cream
  - household cleaning agents
  - ...

Environmental Science Processes & Impacts

ROYAL SOCIETY OF CHEMISTRY

CRITICAL REVIEW

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Cite this: DOI: 10.1039/c9em00163h

The concept of essential use for determining when uses of PFASs can be phased out

Ian T. Cousins, †*[a] Gretta Goldenman,[b] Dorte Herzke,[c] Rainer Lohmann, [d] Mark Miller,[e] Carla A. Ng, [f] Sharyle Patton,[g] Martin Scheringer, [h] Xenia Trier,[i] Lena Vierke,[j] Zhanyun Wang [k] and Jamie C. DeWitt[l]

Because of the extreme persistence of per- and polyfluoroalkyl substances (PFASs) and their associated risks, the Madrid Statement argues for stopping their use where they are deemed not essential or when safer alternatives exist. To determine when uses of PFASs have an essential function in modern society, and when they do not, is not an easy task. Here, we: (1) develop the concept of "essential use" based on an existing approach described in the Montreal Protocol, (2)

Environ. Sci.: Processes Impacts, 2019, 21, 1803–1815
https://doi.org/10.1039/C9EM00163H

Conclusions (I)

- Many chemicals not “under control”:
  - poorly characterized or properties just unknown
  - found in human bodies
  - found in materials, food, water, ...
  - make recycling difficult or impossible (only down-cycling)

Conclusions (II)

- After decades of increasing chemical sophistication, **chemical simplification** should be a goal of innovation.

- Putting the Chemicals Strategy for Sustainability into practice!

Thank You
for Your Attention

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scheringer@usys.ethz.ch

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