MACHEREY-NAGEL

CHROMABOND® PFAS

New solution for the enrichment of per- and polyfluoroalkyl substances

Dr. Max Bielitza, 11. November 2020

Agenda

Introduction

Current solutions and limitations

New product solution

Potential customers/markets/ competitors

Summary

Introduction

Properties – daily use – guidelines

Introduction

Properties

- ~ 4730 compounds known according to OECD*
- All are nonnatural but man-made (used since the 1940s)
- Resistant against aggressive chemicals
- Mostly non-biodegradable (persistent) and accumulate in the environment and the food chain
- Often toxic, some can cause cancer, some are officially banned

* OECD: Toward a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs): Summary Report on Updating the OECD 2007 List of Per- and Polyfluoroalkyl Substances (PFASs), Series on Risk Management, No. 39, ENV/JM/MONO(2018)7.

Hazardous compounds

Introduction

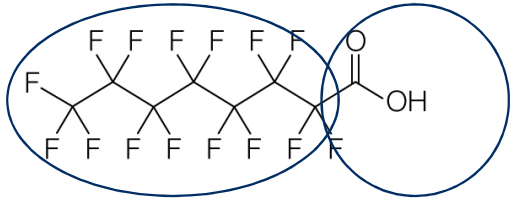
Properties and examples of PFAS

- Organic compounds
- Carbon chain: hydrogen is substituted by fluorine
- Carbon-fluorine bond very strong
- Structure: hydrophobic, lipophobic chain + hydrophilic „head“

→ tensid-like → water-, dirt- and fat-repellent (non-sticky)

Perfluorosulfonic acid

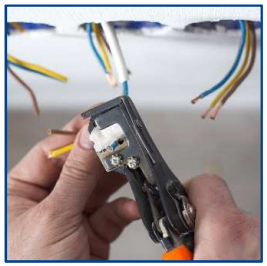
Perfluorooctanoic acid



Introduction

Appearance/daily use

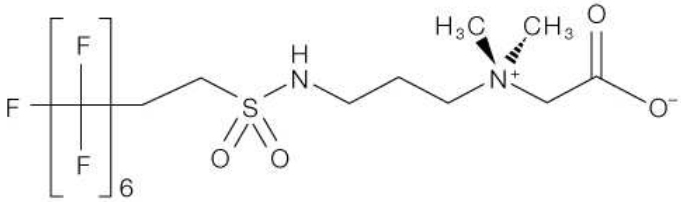
- Fire-fighting foam
- Fiber coating
- Textile coating, e.g. seat covers, carpets, outdoor clothing
- Cookware
- Paper finishing
- Food packaging, e.g. pizza cartons, paper cups
- Building material, e.g. water resistant lacquer



Abundant in the (global) environment

Distribution of PFAS in the environment-examples

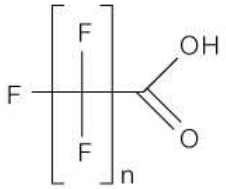
Precursor



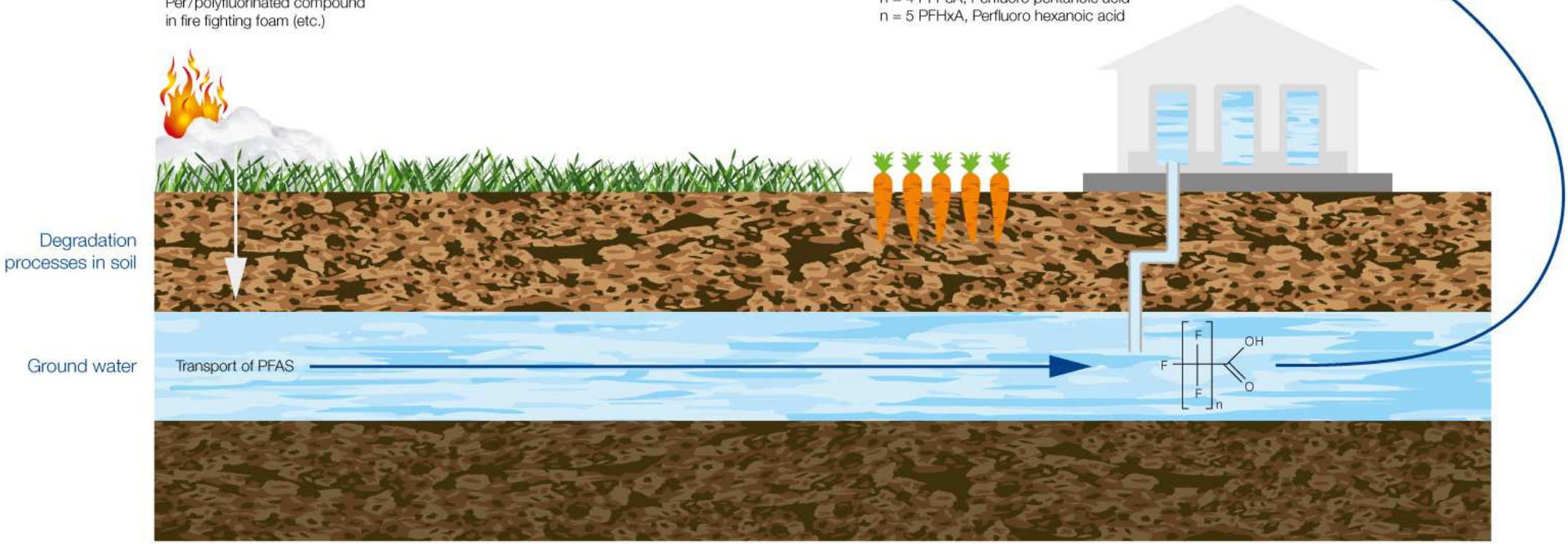
Fire fighting with foam

Per/polyfluorinated compound
in fire fighting foam (etc.)

Dead-end products



n = 3 PFBA, Perfluorobutyric acid
n = 4 PFPeA, Perfluoro pentanoic acid
n = 5 PFHxA, Perfluoro hexanoic acid



Current solutions and limitations

Current solutions and limitations

Guidelines

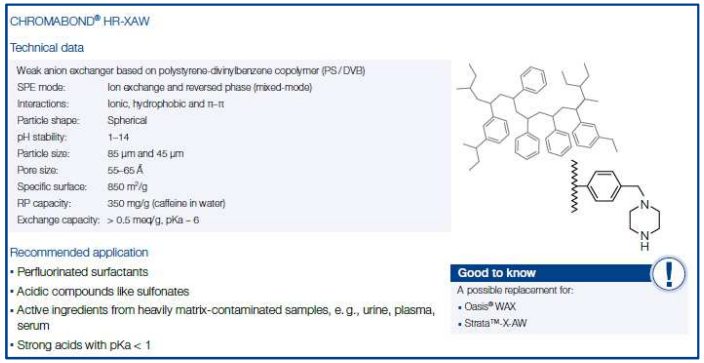
- EPA 533, EPA 537 (**2008**), EPA 537.1 (**2020**)
  - PFAS from water
- DIN 38407-42 or DIN 38414-14 (**2011**)
  - 10 PFAS from water, soil

For now few official methods were developed

Current solutions and limitations

Weak anion exchanger – CHROMABOND® HR-XAW

- Recommended by DIN 38407-42 and EPA 533
- Methods are often sufficient
  for short-chain PFAS with acid functions
- But not for other PFAS substance classes
  - Alcohols
  - Alkyl ethers
  - Sulfonamides etc.



CHROMABOND® HR-XAW

Technical data

Weak anion exchanger based on polystyrene-divinylbenzene copolymer (PS/DVB)	
SPE mode:	Ion exchange and reversed phase (mixed-mode)
Interactions:	Ionic, hydrophobic and π–π
Particle shape:	Spherical
pH stability:	1–14
Particle size:	85 µm and 45 µm
Pore size:	55–65 Å
Specific surface:	850 m^2/g
RP capacity:	350 mg/g (caffeine in water)
Exchange capacity:	> 0.5 meq/g, pKa ~ 6

Recommended application

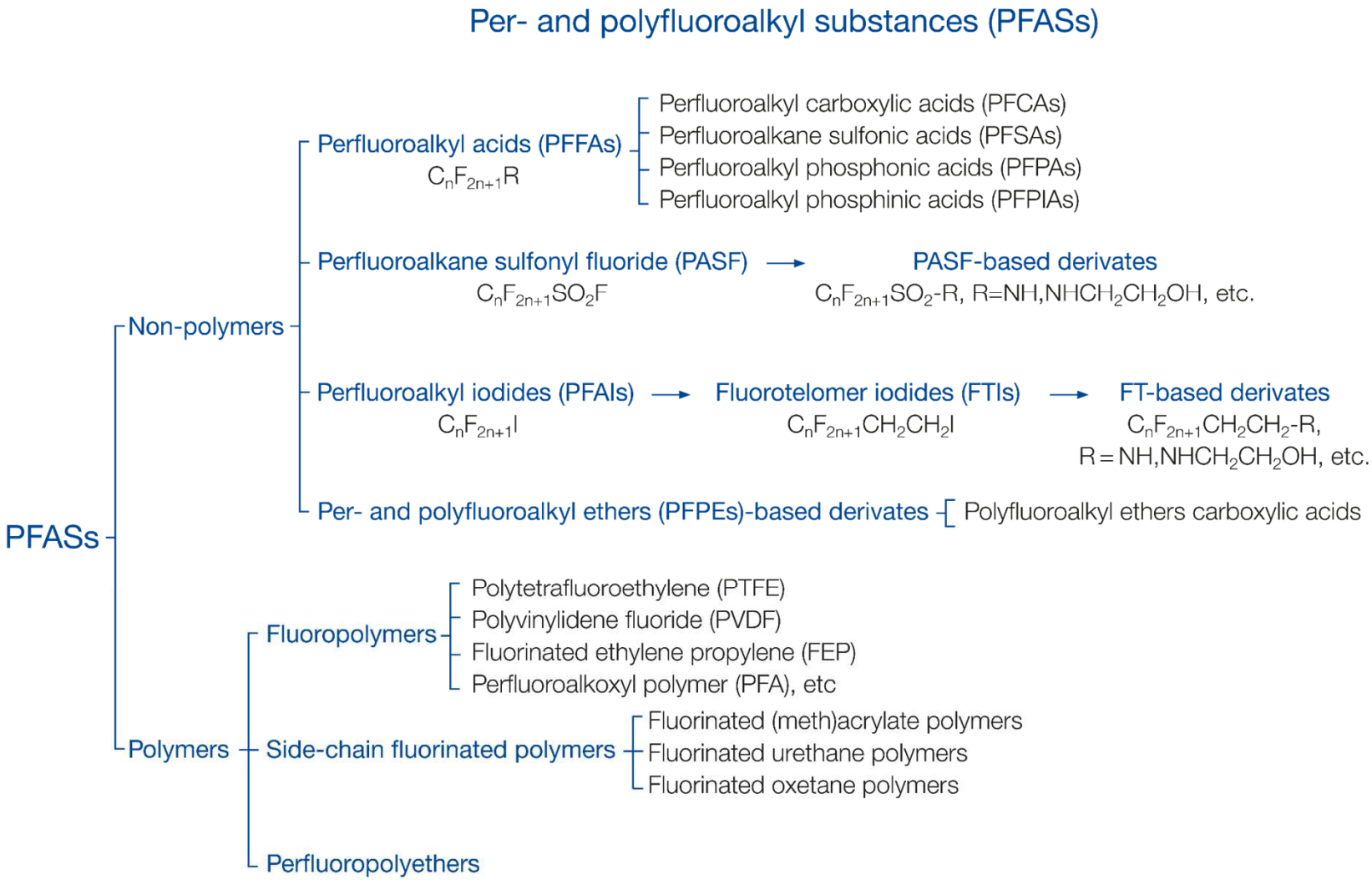
- Perfluorinated surfactants
- Acidic compounds like sulfonates
- Active ingredients from heavily matrix-contaminated samples, e.g., urine, plasma, serum
- Strong acids with pKa < 1

Good to know

A possible replacement for:

- Oasis® WAX
- Strata™-X-AW

Not sufficient for all PFAS substance classes



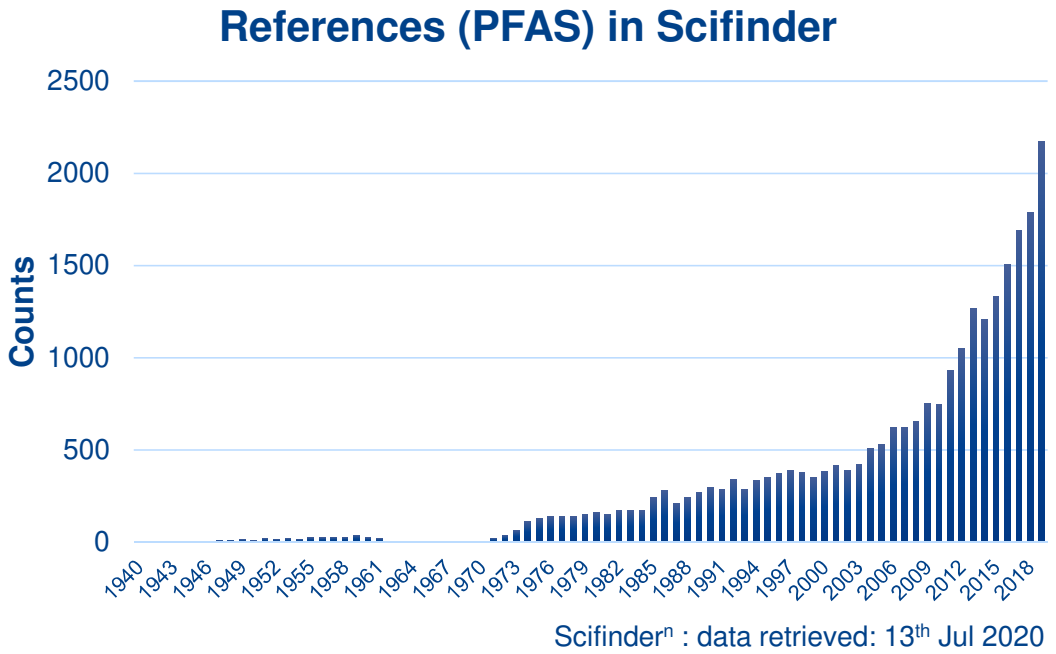
Per- and polyfluoroalkyl substances (PFAs) Source:
Buck, R.C.; Franklin, J.; Berger, U.; Conder, J.M.; Cousins, I.T; Voogt, P.d.; Jensen, A.A.; Kannan, K.; Mabury, S.A; Leeuwen, S.P.v (2011) Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification, and Origins. Integr.Environ.Assess.Manag Vol. 7 No. 4 pg. 513-541.
OECD, 2013, OECD/UNEP Global PFC Group, Synthesis paper on per- and polyfluorinated chemicals (PFCs), Environment, Health and Safety, Environment Directorate, OECD. (http://www.oecd.org/env/ehs/riskmanagement/PFC_FINAL-Web.pdf, retrieved: 01 Jul 2020

Current solutions and limitations

Increasing interest

Continuous research on:

- Health effects
- Occurance
- Metabolism
- Reactant and Reagent
- **Analytical methods**



Scifinder^{n} : data retrieved: 13th Jul 2020

Need for advanced analytical methods and product solutions for monitoring

New product solution

Product and application note

New product solution

Special phase - CHROMABOND® PFAS

- Polymer-based combination phase with weak anion exchange functionality
  - Combines the advantages of different sorbents by using several retention mechanisms (dipole-dipole, ionic, hydrophobic, H-bond)
- Advantages
  - Solution for various PFAS substance classes
  - 28 PFAS can be enriched
  - Sorbent retention mechanisms according to DIN 38407-42, EPA 537.1 and 533 guidelines
  - High capacity
  - High recovery rates

New product solution

- One type of column:
  - 6 mL PP column
  - 300 mg adsorbent weight

- Standard packaging size: pack of 30

→ REF 730283

- BIGpack: pack of 250 (5 x 50 columns)

→ REF 730283.250

- Samples available

→ REF 730283.Muster

New product solution

CHROMABOND® PFAS – application note

- PFAS from water

New product solution

Chromatographic conditions

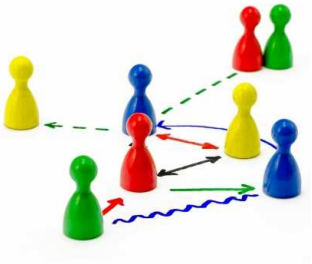
- Solid phase extraction
  - Column: CHROMABOND® PFAS, 6 mL, 300 mg
  - Conditioning: 10 mL 0.1% NH_3 in methanol, 10 mL methanol, 10 mL water
  - Sample application: 150 mL water sample with a flow rate of 5 mL/min
  - Washing (optional): 5 mL of 25 mM $(NH_4)^+$ acetate buffer (pH 4.0) water with flow rate of 3 mL/min
  - Drying: 1 min with vacuum
  - Elution: 10 mL 0.1% NH_3 in methanol
  - Eluent exchange: dissolve: Evaporate eluate to dryness at 40 °C under a stream of nitrogen and residue in 0.5 mL water / methanol (40:60, v/v)
- Subsequent analysis: LC-MS/MS with NUCLEOSHELL® RP 18plus (2.7 µm)

New product solution

Recovery rates

- For most PFAS: **80 – 100 %**
- Lower for
  - FOSA (sulfonamide) lower due to high polarity/low ionic interaction
  - PFTrDA, PFTeDA, PFDoA due to solubility issues and adsorption effects on surfaces

Good and reproducible recovery rates for most analytes



Potential customers/markets/competitors

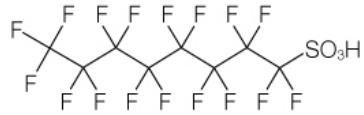
Potential customers/markets/competitors

- Contract laboratories (environmental)
- Textile and paper industry
- Chemical industry, producers of:
  - Fire extinguisher foams
  - Lubricants, emulsifying agents
  - Impregnation agents, etc.
- Galvanic industry
- Aviation
- Photo and semi-conductor industry
- …

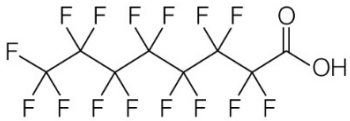
Summary

Summary

- PFASs are persistent, tensid-like, harzardous compounds
- Commonly used because of their non-sticky properties
- Introduced by textiles, fire extinguisher foams, paper cups etc.
- Used since the 1940s, but long-time neglected
- Found in the environment (water, foods, soil, animals and humans)



Perfluorosulfonic acid



Perfluorooctanoic acid

- **Current analytical methods for monitoring are limited**

Summary

- **CHROMABOND® PFAS**:
  - Solution for the enrichment of a broad range of different PFAS (32) from water
  - Several sorbent retention mechanisms according to DIN 38407-42, EPA 537.1 and 533 guidelines
  - High reproducibility and recovery rates
  - Application note available

- Samples available
- Customers: contract laboratories (environmental); textile, paper and chemical industry, etc.

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Thank you for your attention!

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