

PFAS in Contaminated Land – Scope of Analysis and Soil Risk Relevance

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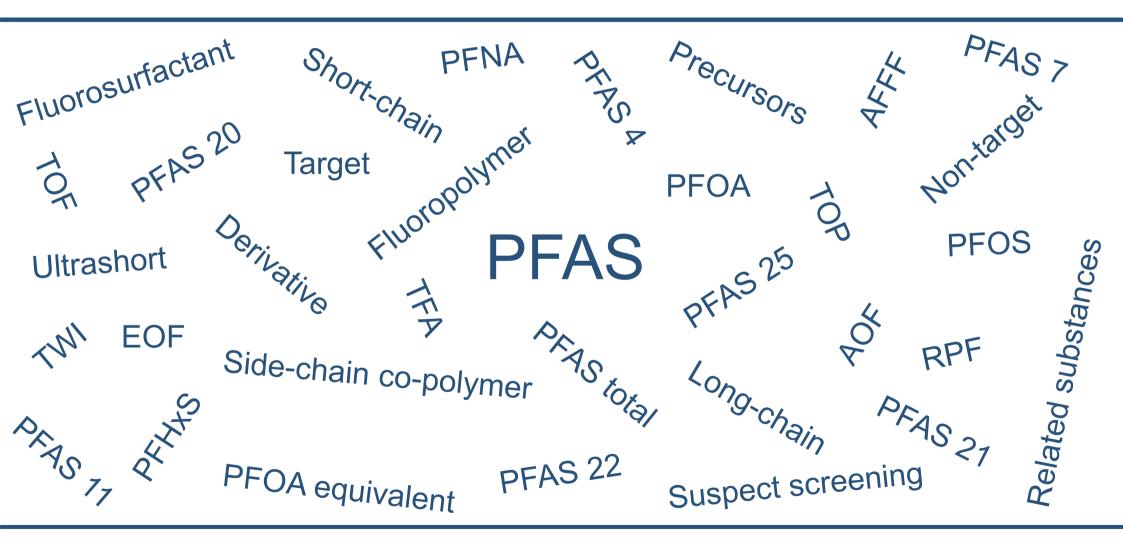
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PFAS – A Complex Issue (Chemistry, Analysis, Risk)







PFAS Precursors

Precursors



- Thousands of PFAS compounds impossible to analyze all
- Known precursors e.g. 6:2 FTS, PFOSA (PreFOS), FTOH, PFHxSA, PFBSA
- In nature, precursors can be broken down to PFCA and PFSA
 - Sulfonamides form PFSA (e.g. PreFOS to PFOS)
 - Telomers form PFCA (e.g. 8:2 FTS to PFOA, PFHpA, PFHxA)
 - Substances with ester, ether, urethane, ethoxylate, phosphate bonds (e.g. FTAC, FTMAC, FTEO and PAP), most often telomers (nowadays)
 - FTSAS, FTAA, FTAB, DPOSA (6:2 FTNO) common in modern AFFF
- Pool of known as well as unknown precursors
- Many questions about time aspects, degradation rates, "final" yields of perfluorinated substances, soil/water conditions etc.
- Which "new" compounds including degradation products (e.g. FTUCA, FTCA, FTOH) are of importance? Leaching?
- TOP (total oxidizable precursors), non-target and suspect screening are methods to "reveal" precursors qualitatively and (semi)quantatively



PFAA

Precursors



PFOA +

other

PFCAs





6:2 FTAB and other AFFF compounds

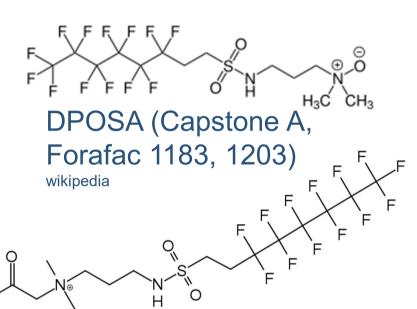
AFFF Content – 6:2 telomer precursors



- Capstone: Chemour (formerly Dupont) family of 6:2 sulphon(amide) based
 - 8 different products are still sold just for AFFF...
 - Not just AFFF.....
 - 6:2 FTAB found in drinking water FR, CA, UK (<0.1-15 ng/l)

6:2 FTS or 6:2 FTSA

wikipedia



6:2 FTAB (Capstone B, Forafac 1157)

wikipedia

8:2 Fluorotelomer stearate (FTS)

The Versatility of Capstone™ Fluorosurfactants

Capstones" fluoresur factants are used in a variety of applications because of their ability to enhance performance and assist in formulating many everyday products, including wetting, surfacing, and leveling Common applications for Capstones" fluorosurfactants include:

Paints and Coatings

Capstone" fluorosurfactants work as multifunctional additives to simplify formulations for paints and coatings especially those formulated with low- or no-VOC chemistry. Capstone" fluorosurfactants:

- Improve substrate wetting
- · Improve pigment wetting and leveling
- Provide anti-blocking for water-based systems
- Extend open-time
- Reduce foaming
- Improve dirt pick-up resistance
- Enhance oily stain removal

Cleaners and Waxes

Capstones" fluorosur factants are cost-effective additives that enhance professional-use cleaners, polishes, and waxes by thoroughly wetting a substrate, allowing the cleaner to further penetrate deep dirt and stains. They also provide improved leveling characteristics and surface properties in floor care formulations.

Adhesives, Sealants, and Caulks

Adhesive applications exist in many forms, such as adhesives for tape, hot-melt, and wood (and other porous surfaces). Adding a small amount of a Capstone" fluorosurfactant improves the adhesive's wetting and penetration into substrate pores to strengthen the bond. Capstone" fluorosurfactants provide reduced surface defects, dynamic surface tension reduction (in combination with existing surfactant package), and increased adhesive penetration.

ilms

For print acceptors, Capstone¹⁴ fluorosurfactants improve

- Wetting and leveling for ink
- Adhesion
- Abrasion resistance
- Reduced ink transfer
- General "printability"

In addition to wetting, Capstone" fluorosurfactants migrate to the top of a coating and thus encourage rewetting in multi-coat operations. Capstone" fluorosurfactants can also provide antistatic properties.

Ink and Graphic Arts

Capstone" fluorosur factants achieve excellent wetting and leveling properties for inles and graphic art coatings without interfering with dispersed phase dyes and pignents. Because Capstone" fluorosur factants rise to the air interface, they reduce "transfer" to the next surface when sheet or roll-type products are stacked.

Primary performance functions include anti-block, ink acceptance, leveling, and wetting.

AFFF Content – 6:2 telomer precursors



- KEMI PM 6/15 (Swe Chem Agency; Anna Kärrman, Örebro Univ)
 - 6:2 FTSAS: Towalex master, Alcoseal 3-6%, Foam AFFF3% (MSB), OneSeven B-AR
 - 6:2 FTAB: Sthamex, Alcoseal 3-6%, Towalex 3% master
 - DPOSA (6:2 FTNO): ARC Environment (+ variant with an O linked to amide group and 6:2 FTAA)
 - 6:2 FTSAS-SO and –SO2 may also be important
 - There should be more... (van Hees, 2025)
 - 6:2 FTSAPr-AmHOPrS, 6:2 FTSHA and 6:2 FTTh-PrAm
 - Possibly 6:2 FTS and 6:2 FTAA

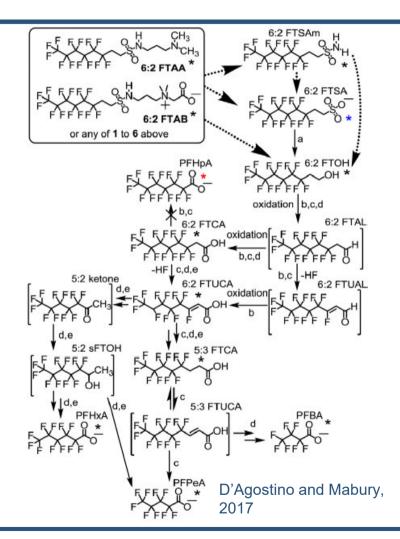
DPOSA "variant" (upper) and 6:2 FTAA (lower)

6:2 FTSAS KEMI PM 6/15

AFFF Content – Biodegradation



- Biodegradation of 6:2 AFFF molecules
 - Research field that is developing
 - (Highly) likely that 6:2 FTAB is biodegraded to PFCAs (C4-C6/7) as final products
 - FTAB may be more resistant than e.g. DPOSA or 6:2 FTSAS
 - In most experiments with 6:2 AFFF molecules, degradation with sludge/soil/liquid incubation, typically 100 days – few % recovered as PFCA
 - No or limited amounts of 6:2 FTS formed at biotic degradation of 6:2 FTAB, but more from 6:2 FTSAS and 6:2 FTAA (?)
 - Composition of N head group and chain length (adsorption) may influence biodegradation rate
 - Estimation of degradation in the field several decades

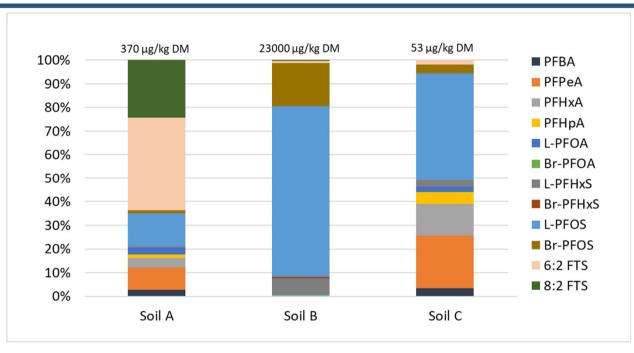




PFAS Content in Soil and Guideline Values

PFAS sums vs PFAS composition in soil





Three soils from	different areas at a
Swedish airport (AFFF contaminated)

- Varying concentration and composition: approx.
 15%, 90%, and 50% PFOS
- Soil composition, leads to varying proportion of PFAS4, 20, 22 (DK22: DWD20 + 6:2 FTS + PFOSA)
- Very different increases after TOP. Original PFAS, before ox. corresponds to 3% or 95–98%
- Relative difference can become even greater after TOP
- EFSA PFAS4 completely "misses" degradation products from 6:2 fluorotelomer (FT) AFFF, and a large part of those from 8:2 FT
 - In addition to risk assessment, it is also important to understand composition in relation to remediation goals and remediation techniques

μg/kg DM			
	5540/	PFAS	45504
	PFAStot	TOP	ΔPFCA
Soil A	370	12600	12200
Soil B	23200	23600	2900
Soil C	53	56	6

	Before TOP			
	PFAS4	PFAS7	PFAS20	PFAS22
Soil A	18%	31%	38%	75%
Soil B	97%	98%	97%	100%
Soil C	49%	91%	95%	97%

After TOP		
PFAS4	PFAS20	
0.5%	0.5%	
95%	95%	
46%	90%	

Need for knowledge about original precursor (AFFF content) - interpretation of TOP + further analysis

AFFF composition in soil



μg/kg DM	Airport 1		Airport 2	Airport 3	Airport 4	PFAS structure
	Soil A	Soil B				
6:2FTAB	8124	5200	2000	900	780	6:2 FT
8:2FTAB	7885	99	n.d	59	tr	8:2 FT
10:2FTAB	1156	18	n.d	7,3	tr	10:2 FT
12:2FTAB	142	2,6	n.d	0,8	n.d.	12:2 FT
14:2FTAB	4,2	n.d	n.d	n.d	n.d.	14:2 FT
DPOSA (6:2 FTNO)	75	n.d	n.d	n.d	n.d.	6:2 FT
5:1:2 FTB	1,4	n.d	n.d	n.d	n.d.	FT
6:2 FTSHA-sulfoxide	402	740	n.d	n.d	n.d.	6:2 FT
N-AmCP-FHxSA	205	5,1	n.d	1,9	0,15	C6-SA
N-AP-FHxSA	n.d.	8.6	2.4	10	0,30	C6-SA
N-CMAmP-FHxSA	n.d.	18	17	46	10	C6-SA
N- CMAmP -FOSA	n.d.	55	nd	210	5,8	C8-SA
N- HOEAMP - FHxSAPS	n.d.	28	nd	1.3	0,67	C6-SA
N- HOEAmP - FHxSE	1.0	66	4.0	11	n.d.	C6-SA
N-HOEAmP-FPeSA	n.d.	50	16	13	0,13	C5-SA
N-TAmP-FHxSA	n.d.	35	21	17	10	C6-SA
N- TAMP -FOSA	n.d.	26	nd	7.7	0,20	C8-SA
CI -PFOS	n.d.	4.8	nd	nd	0,28	PFSA
Ether-PFNS	n.d.	2.9	nd	n.d	n.d.	PFESA
F5S-PFHpS	n.d	3.2	n.d	n.d	0,13	PFSA
F5S-PFHxS	n.d	6.4	n.d	n.d	0,37	PFSA
F5S-PFNS	n.d	41	n.d	1.9	n.d.	PFSA
F5S-PFOS	1.5	150	3.0	7.4	0,12	PFSA

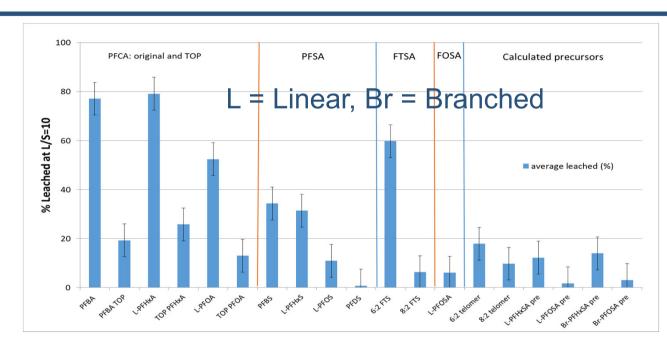
Five soils from four Swedish airports

- " Selected " suspect screening
 - Few standards, largely semi-quantified
- Airport 2 and 3 included in SGI government assignment
- "Common" PFAS not included in table
- 6:2 based AFFF (+8:2) can have very high levels that are not "visible" in target analysis
- Higher content of 6:2 FTAB in Arpt 1-soil A, Arpt 2, 3 and 4 than PFOS
- Good qualitative and in "right order" quantitative comparison vs TOP
- 6:2/8:2 FT and C6/C8-Sulphonamides are important precursors
 - 7 of 9 ECF sulphonamides have quaternary (alkyl)
 N head (or terminal) groups
 - The same for 7 of 8 FT substances (incl betaine)
- Can never guarantee that there is nothing else to be found.....

FT = fluorotelomer SA = sulphonamide PFSA = perfluorinated sulphonic acid PFESA = perfluoro ether sulphonic acid

Results Leaching – PFAS and TOP





Leaching test L/S=10

	log Koc (n=5/6)
6:2 FTAB	2.9±0.2
PFOS	3.2±0.1
6:2 precursors TOP	2.9±0.1
6:2 FTS	2.2±0.3

- Leaching test batch (L/S=10), 5 and 6 soils (2 data sets)
- % Leached 1-79% (picture)
- TOC 0.3-18% and pH 6.8-8.1 across data sets
- Generally lower % leached for longer PFAS, especially >6C
- Tendency for lower Koc for Br-PFSA, Br-FOSA
- Correlation C and log Koc above ≥C6, log Koc ~ +0.35-0.5 per C
- 6:2 FTAB lower Koc than PFOS
 - Comparable Koc to TOP calculated 6:2 precursors (6:2 FTAB major 6:2 FT)
 - Negative correlation Koc vs 6:2 FTAB (300-8000 μg/kg), less obvious for PFOS
 - Zwitterionic (6:2 FTAB) vs anionic (PFOS)?
 - pH of soil?
 - Saturated vs unsaturated conditions, airwater interface?

Summary and Conclusions



- PFAS is a complex issue (risk assessment, structure/chemistry, analysis) – differs in several ways from other pollutants
 - How many PFAS should one choose (vs guideline values, vs occurrence etc)?
 - PFAS4 or 20 etc constitute a limited part of PFAS pollution in many cases. Do we explain 0.5 or 95%?
 - PFAS4 completely misses all contributions from 6:2 FT AFFF
- There is a need to address PFAS precursors (in AFFF and soil)
 - TOP is one method to "visualize", suspect screening with semiquantification another. Extended target analysis of AFFF components
 - 6:2 FTAB has become a representative for this group
 - Biodegradation of AFFF, especially FT, needs to be assessed. What are the major degradation products? Rates?
 - Need to know more about adsorption characteristics
 - How should we evaluate PFAS precursors in the risk assessment?
 Toxicity, groundwater protection etc

Thanks!



Thanks for listening!
Welcome to contact me!
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