Alternatives to PFAS in Floor Polish

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Yuning Xu

MPH in Environmental Health Sciences Class of 2022

Jenna Tan

PhD in Chemistry Class of 2022

Tessa Wardle

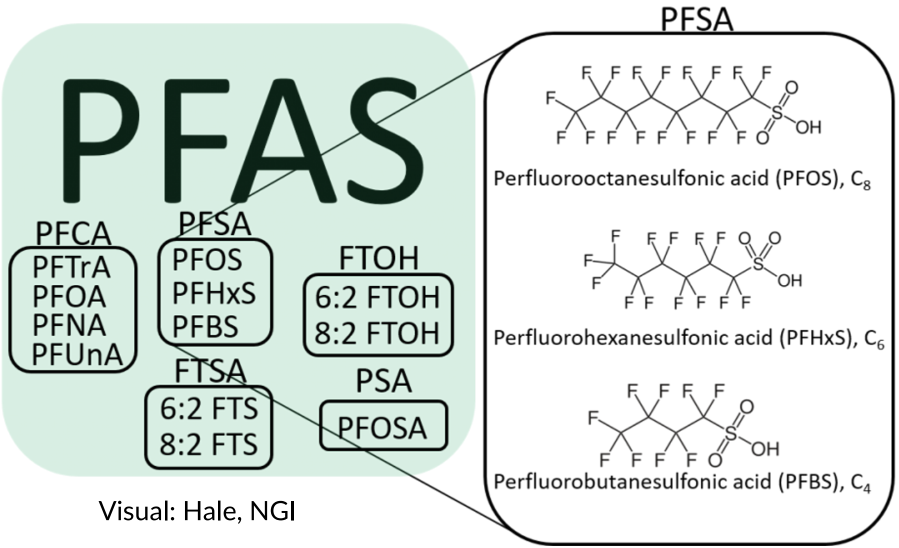
MS in Environmental Health Sciences Class of 2022

Overview

1. Background
    a. PFAS
    b. Current floor polish technology
    c. Approach
2. Strategies
    a. Rhamnolipids
    b. Amino acid surfactants
    c. Technical performance
3. Hazard Assessment
4. Summary
    a. Advantages/disadvantages
    b. Outlook


Freeman, EPIC

Why do we care about PFAS in floor polish?

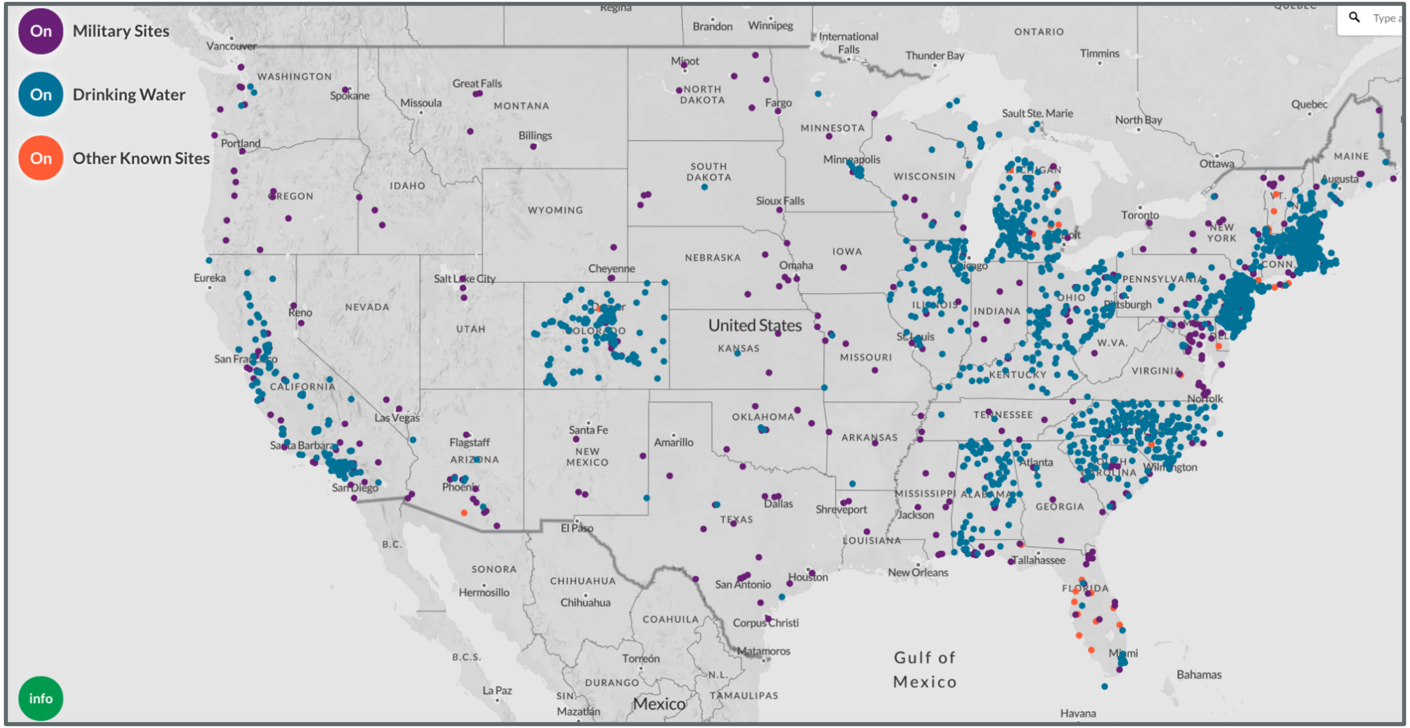


Visual: Hale, NGI

PFAS = Per- and **P**oly-**F**luor**a**lykl **S**ubstances

Why do we care about PFAS in floor polish?

Detected in drinking water sources across the country



Map created by the Environmental Working Group, last updated October 4th, 2021

Why do we care about PFAS in floor polish?

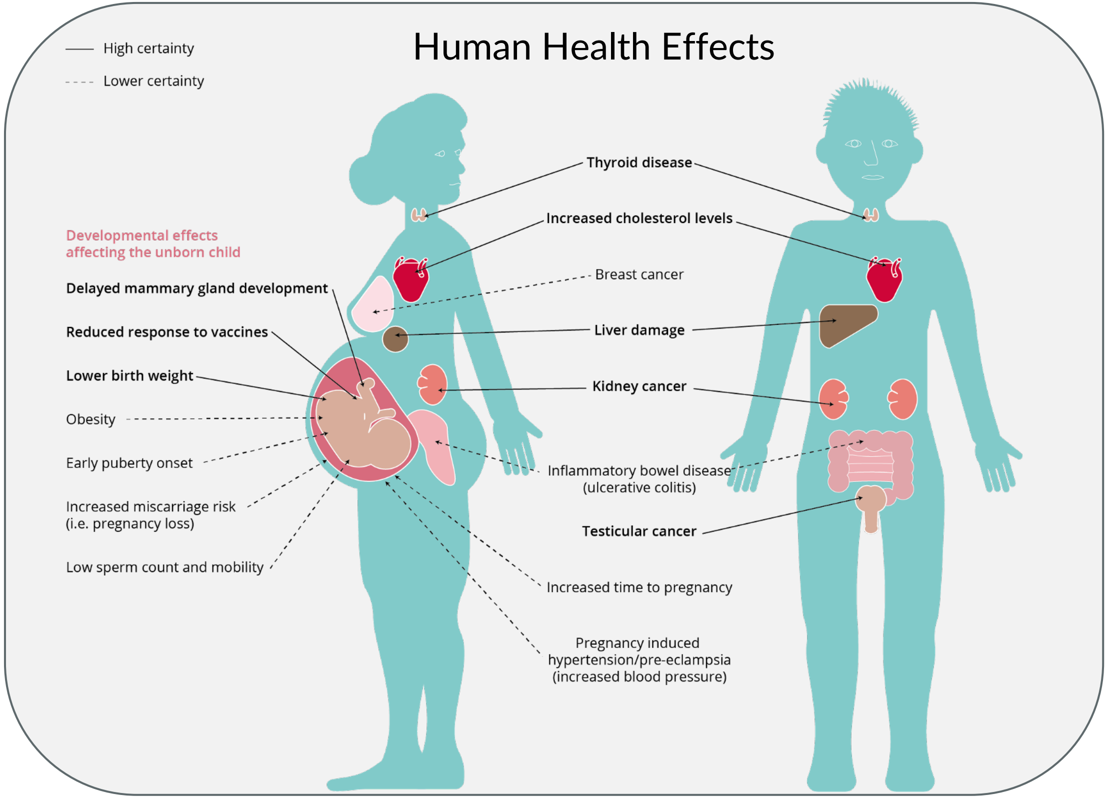
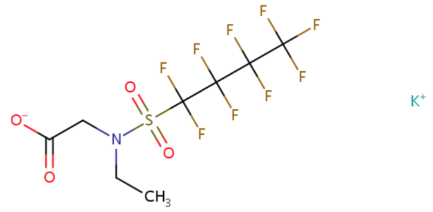


Image: ECHA, "Emerging Chemical Risk in Europe - PFAS", 2019.

State of the Floor Polish Industry

Chemours™

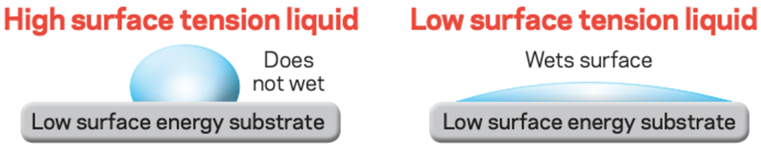
- Fluorochemicals commonly used in floor polish: Capstone FS-60 and FS-65
- 2008 survey revealed that nearly every floor polish on the market contained a fluorochemical
    - Existing drive from within industry to remove PFAS
- Primary commercial users: schools, hospitals, retail and grocery stores



Potassium N-ethyl perfluoro alkane sulfonamidoacetate (N-EtFOSAA)

SBM Industrial Products

PFAS in floor polish highly effective - posing challenge for comparable replacement

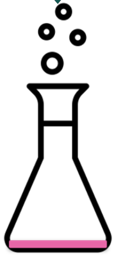


Wetting
Spreads more evenly over floor surface

Leveling
Creates a smooth and even surface

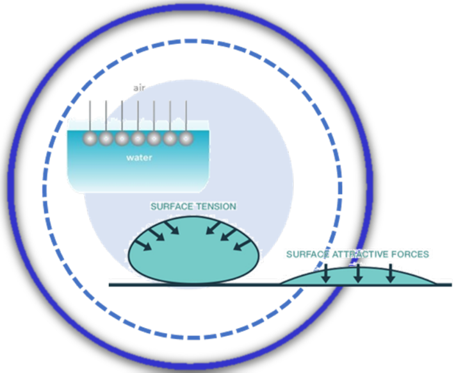
Recoating
Formulations without fluorosurfactant do not perform as well

Low concentration
Doesn't affect the viscosity of the formulation



Chemours Fluorochemicals, "Capstone™ Fluorosurfactants: For High Value-in-Use Applications That Require Maximum Performance."

Criteria for a strong PFAS alternative



Technical

Surfactant performance
Recoatability

Environmental

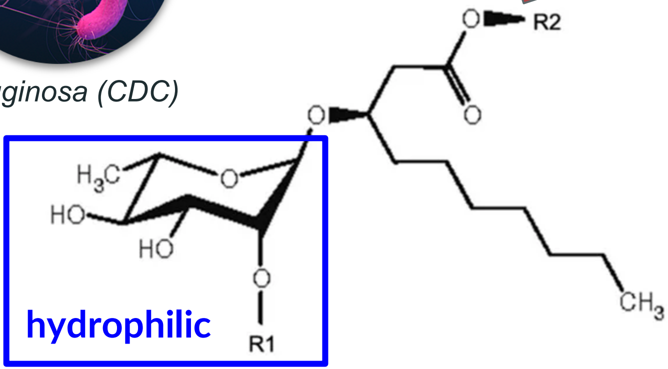
Health

Production → Application → Disposal

Image credits: Biolin Scientific, Clean Freak, Water Quality Products, Phil Roeder

Strategy 1: Rhamnolipids - bacterially produced surfactants

P. aeruginosa (CDC)



- Use renewable feedstocks by fermentation
- Stable in wide range of conditions (pH, temp)
- Biodegradable and low toxicity

Current commercial applications

Pharmaceuticals

Cosmetics

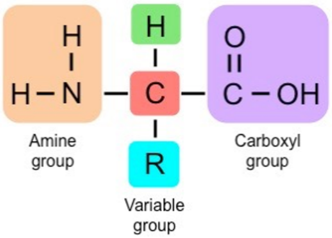
Agriculture

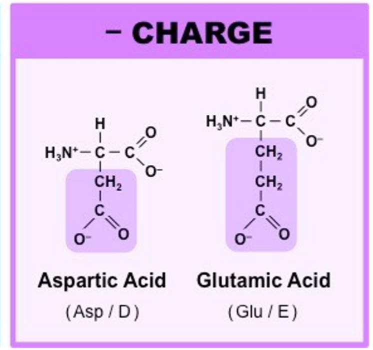
Bioremediation

Liepins, J. *et al.*. Glycolipid Biosurfactant Production from Waste Cooking Oils by Yeast: Review of Substrates, Producers and Products. *Fermentation* **2021**, *7*, 136.

Image credits: PxHere, Pixabay, Flickr, The Science Explorer

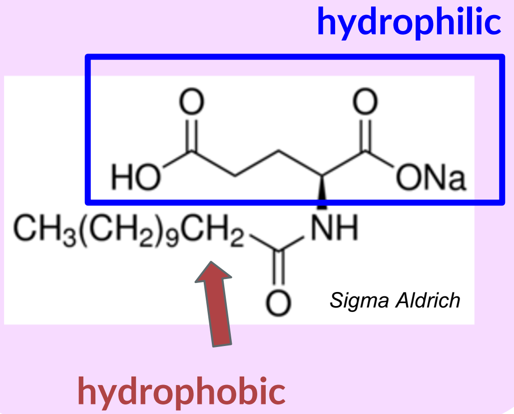
Strategy 2: Amino acids - versatile building blocks to make a variety of surfactants





- Anionic - cleaning
- Cationic - anti-microbial agent

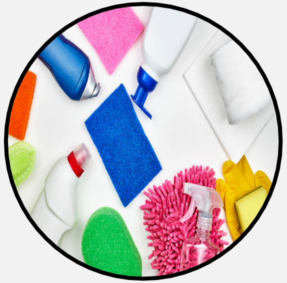
Sodium lauroyl glutamate (SLG)



- Produce from renewable and raw feedstock (e.g. vegetable oils)
- High surface activity
- Low toxicity and quick biodegradation

Current commercial applications

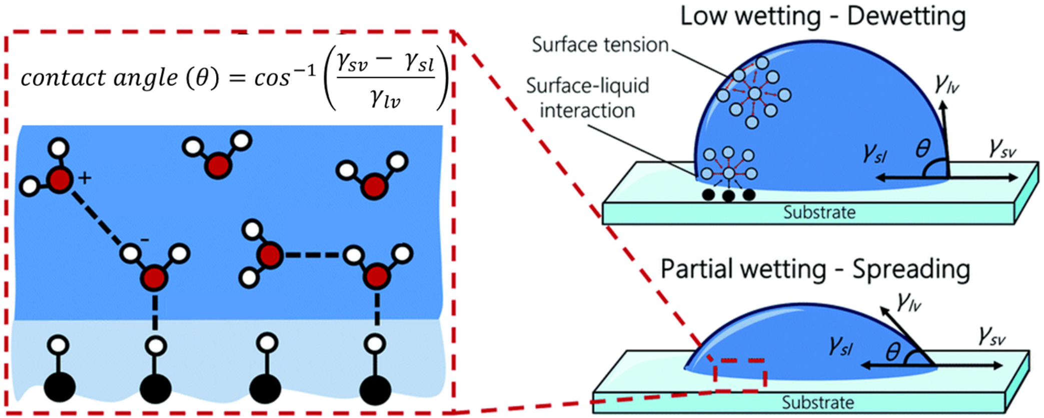
Cosmetics



Cleaning

Image credits: BioNinja, Pixabay, Flickr

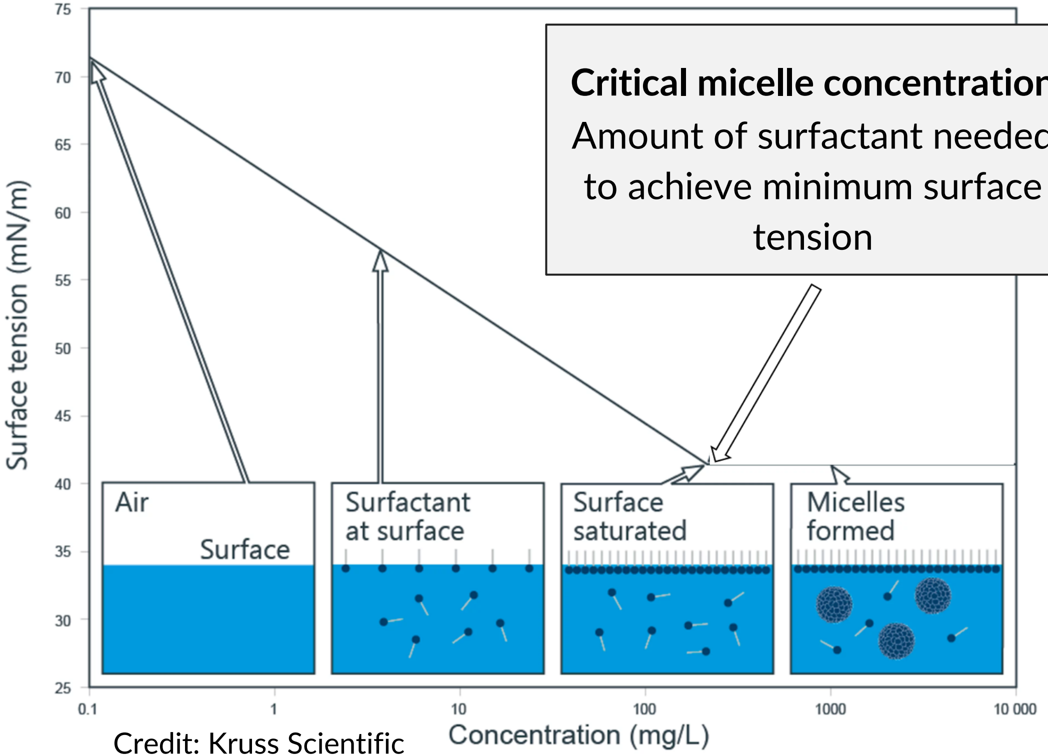
Alternatives will need to reduce the energies at the liquid-substrate and liquid-air interfaces



Jarray, Ahmed, et al. "Systematic approach for wettability prediction using molecular dynamics simulations." *Soft matter* (2020): 4299-4310.

Wetting	**Contact angle (θ)** Liquid-substrate interface	**Good if <90° on PVC**
Levelling	**Surface tension (γ_{lv})** Liquid-air interface	**Good if <36 mN/m**

We will also compare levelling and wetting performance by amount of surfactant needed and potential for recoating



Credit: Kruss Scientific

Critical micelle concentration
Amount of surfactant needed to achieve minimum surface tension

100 - 275 ppm
for N-EtFOSAA
= 2 - 7 mM

Recoatability ~ Oleophobicity
Octanol- water partition coefficient ($\log K_{ow}$)
Want values < 5

Technical performance is highly dependent on concentration and surface choice

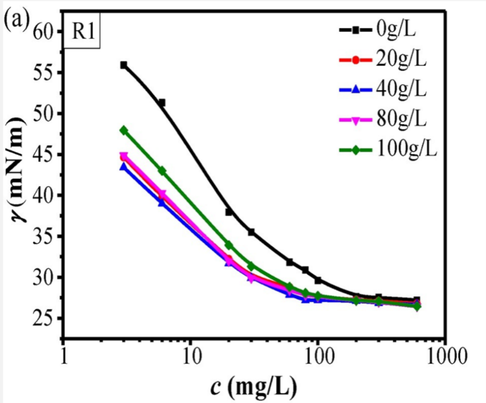
	Baseline Surfactants			Alternative Surfactants	
Technical properties	FS-60	FS-65	Sodium dodecyl sulfate (SDS)	Rhamnolipid	Sodium lauroyl glutamate (SLG)
Water contact angle (°)	**M** ~51-56°*		**H** ~20° at 3.48 mM on PVC	**M** ~20° at 1.5 mM on PVC	**L** 138.69° on sericite (mineral)
Surface tension (mN/m)	**H** 19 at 0.05%	**H** 18 at 0.05%	**H** 23.8 - 34.6	**H** 26-29	**H** <30
Critical micelle concentration (mM)	**H** 0.23*		**M** 8-8.5	**H** 0.41	**H** 0.48
LogKow (octanol water partition coefficient)	**M** 2.51 (0.276 - 5.99)*		**H** 1.69	**L** 5.77 (4.22 - 7.38)	**H** 0.597*

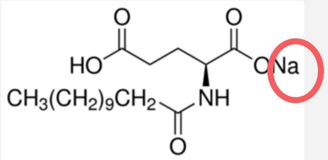
High efficacy **(H)** | Moderate efficacy **(M)** | Low efficacy **(L)** | * = data for similar compound

The surfactant has assistance in floor polish formulas!

Tune technical properties with the salt counterion concentration or gemini surfactants

Salt Counterion

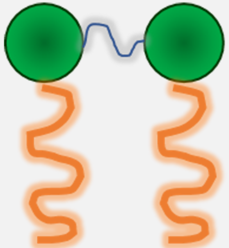


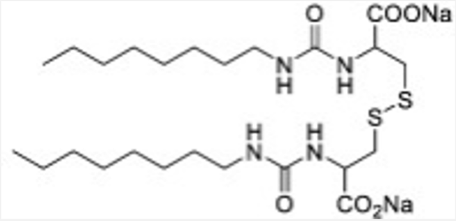


- Different salts with PFAS change surface tension
- Example: changing [Na^+] for rhamnolipid

Wu, L. *et al.* Comparative studies on the surface/interface properties and aggregation behavior of mono-rhamnolipid and di-rhamnolipid. *Colloids and Surfaces B: Biointerfaces* **181**, 593–601 (2019).

Gemini surfactants





- CMC can be up to 2x smaller than monomeric form
- Possibly lower surface tension
- Tunable viscosity
- Increased chemical stability → biodegradation?

Morán, M.C., et al. ""Green" amino acid-based surfactants." *Green Chemistry* (2004): 233-240.

Pinazo, Aurora, et al. "Amino acids as raw material for biocompatible surfactants." *Industrial & Engineering Chemistry Research* 50.9 (2011): 4805-4817.

Lifecycle Overview

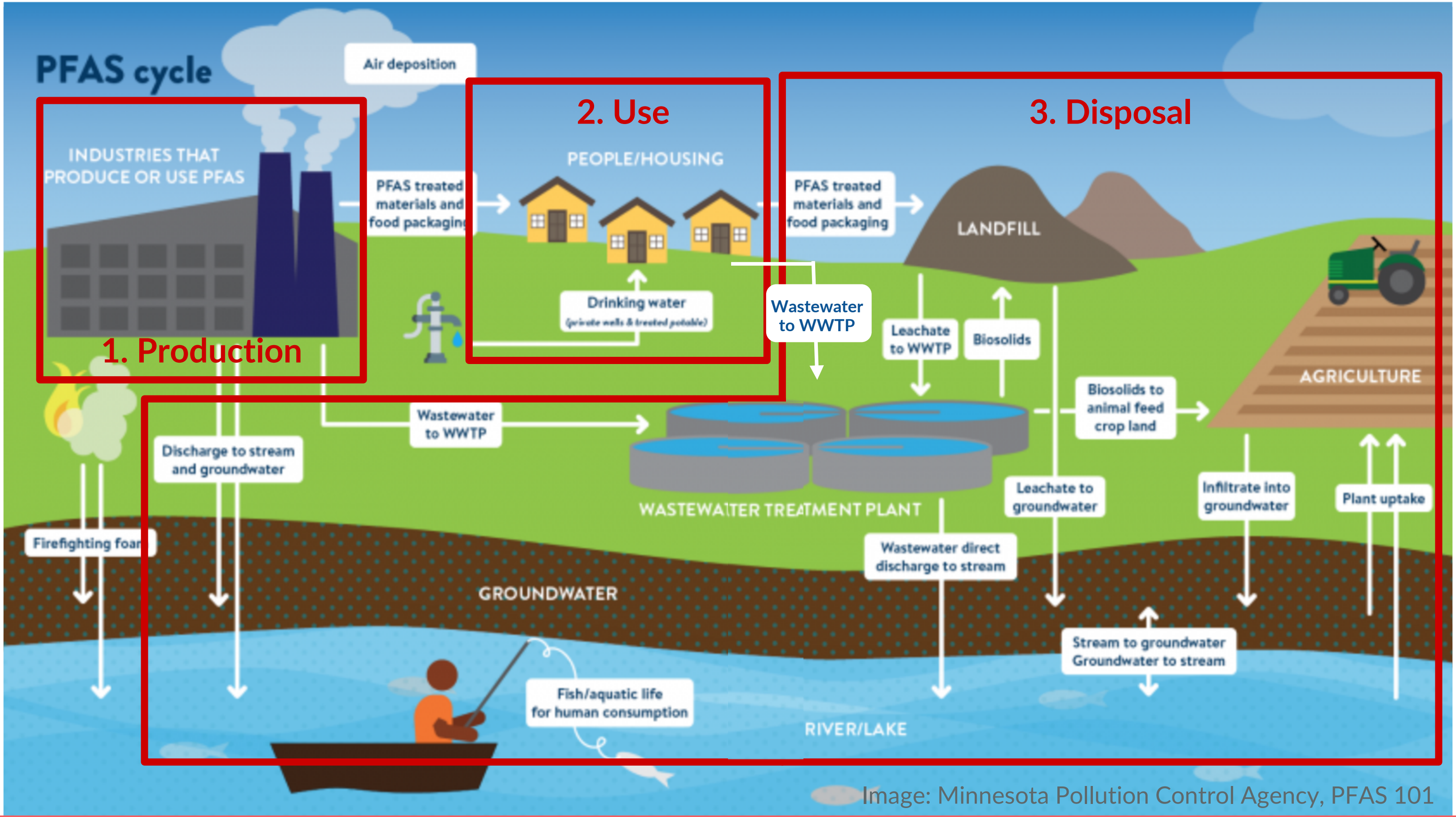


Image: Minnesota Pollution Control Agency, PFAS 101

Hazards During the Life Cycle: Production

N-EtFOSAA

- More likely to have occupational exposure
- Data gaps

Carcinogen	3
Mammalian Toxicity	4
Respiratory Toxicant	DG
Skin irritation	PC
Eye irritation	DG

PFBS*

- Skin and eye irritation hazard concerns

Carcinogen	3
Mammalian Toxicity	2
Respiratory Toxicant	PC
Skin irritation	1
Eye irritation	2

Rhamnolipids

- Low health concerns during production
- Some data gaps
- More eco-friendly: requires less energy during production

Carcinogen	5
Mammalian Toxicity	4
Respiratory Toxicant	4
Skin irritation	4
Eye irritation	1

Sodium Lauroyl Glutamate

- Low health concerns during production
- Some data gaps

Carcinogen	DG
Mammalian Toxicity	5
Respiratory Toxicant	LC
Skin irritation	2
Eye irritation	2

1	2	3	4	5	LC	PC	DG

1 = Very hazardous, 2 = Hazardous, 3 = Moderate, 4 = Low, 5 = Very low

*degradation product of N-EtFOSAA

DG = Data Gap, LC = Low Concern, PC = Potential Concern

Hazards During the Life Cycle: Application

N-EtFOSAA

- Environmental hazard concerns
- Data gaps

Carcinogen	3
Repro/Dev	DG
Endocrine disruptor	DG
Mammalian Toxicity	4
Neurotoxicity	DG
Respiratory Toxicant	DG
Skin irritation	PC
Eye irritation	DG

PFBS

- Consumer exposure risks
- Eco toxicity & fate concerns
- Inhalation exposure

Carcinogen	3
Repro/Dev	2
Endocrine disruptor	1
Mammalian Toxicity	2
Neurotoxicity	3
Respiratory Toxicant	PC
Skin irritation	1
Eye irritation	2

Rhamnolipids

- Environmental (aquatic) hazard concern
- Eye irritation concerns
- Possess antimicrobial

Carcinogen	5
Repro/Dev	DG
Endocrine disruptor	DG
Mammalian Toxicity	4
Neurotoxicity	DG
Respiratory Toxicant	4
Skin irritation	4
Eye irritation	1

Sodium Lauroyl Glutamate

- Consumer exposure risks
- Eye/skin irritation concerns

Carcinogen	DG
Repro/Dev	PC
Endocrine disruptor	DG
Mammalian Toxicity	5
Neurotoxicity	DG
Respiratory Toxicant	LC
Skin irritation	2
Eye irritation	2

1 = Very hazardous, 2 = Hazardous, 3 = Moderate, 4 = Low, 5 = Very low

DG = Data Gap, LC = Low Concern, PC = Potential Concern

Hazards During the Life Cycle: Disposal

N-EtFOSAA

- Persistence in environment brings in relevance of Group 1 endpoints hazard concerns

Carcinogen	3
Repro/Dev	PC
Endocrine disruptor	DG
Aquatic Toxicity	2
Persistence	1
Bioaccumulation	PC

PFBS

- Hazards are particularly relevant during disposal as the degradation product

Carcinogen	3
Repro/Dev	2
Endocrine disruptor	1
Aquatic Toxicity	3
Persistence	1
Bioaccumulation	PC

Rhamnolipids

- Ability to biodegrade makes Group 1 endpoints less concerning

Carcinogen	5
Repro/Dev	DG
Endocrine disruptor	DG
Aquatic Toxicity	2
Persistence	5
Bioaccumulation	PC

Sodium Lauroyl Glutamate

- Appears to be safer than bad actor in disposal phase
- Some data gaps

Carcinogen	LC
Repro/Dev	PC
Endocrine disruptor	DG
Aquatic Toxicity	LC
Persistence	5
Bioaccumulation	DG

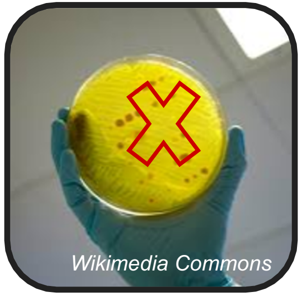
DG = Data Gap, LC = Low Concern, PC = Potential Concer

1 = Very hazardous, 2 = Hazardous, 3 = Moderate, 4 = Low, 5 = Very low

Rhamnolipids and amino acids form environmentally friendly surfactants.

Advantages

Biodegradation



Anti-microbial

Bioremediation

Disadvantages

Production costs

Solvent use in production

Feedstock could be food

Potentially pathogenic

Both, Rhamnolipids only

Outlook

Implementing PFAS alternatives

Wikimedia Commons

- Final performance in floor polish formulation
- Scaling up production

Rethinking floor polish application

Construction Specifier

- Necessity of polishing floors
- Different floor materials

Overall formulation

Compact Appliance

- New paradigm to achieve floor polish effects
- Other toxic ingredients

Acknowledgements

DEFEND OUR HEALTH

Solutions for a Toxic-Free Tomorrow

Patrick MacRoy

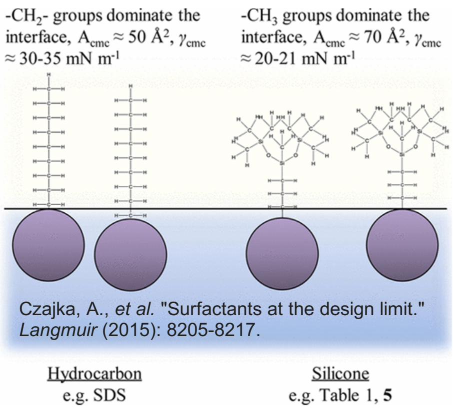
scJohnson PROFESSIONAL A family company®

Carmine Savaglio

- Peer mentor: Ned Antell
- Greener Solutions instructional team: Meg, Kim, Billy

Thank you for listening!

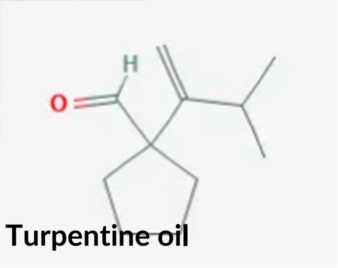
Additional alternatives considered

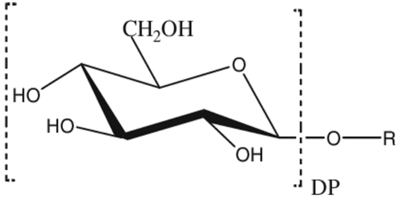


Czajka, A., *et al.* "Surfactants at the design limit." *Langmuir* (2015): 8205-8217.

Siloxanes/silicones

- Higher surface activity than hydrocarbons (lowers surface tension to values similar to fluorosurfactants)
- But persistent, bioaccumulative, and toxic





Sułek, M.W., et al. "Alkyl polyglucosides as components of water based lubricants." *Journal of surfactants and detergents* (2013): 369-375.

Alkyl Polyglucosides

- Can be low-cost and low-ecological impact
- Current commercial applications
- Has been tested by floor polish industry and is not successful when mixed into formulation

Pine oil

Active component: turpentine oil

- Low mammalian toxicity
- Current application in detergents/cleaning products
- Concern with skin and eye irritation/corrosivity
- Mixture of chemical constituents

Hazard Table

		N-EtFOSAA	PFBS	PFOS	Rhamnolipid	Sodium lauroyl glutamate	
		67584-51-4	375-73-5	1763-23-1	4348-76-9	29923-31-7	Key
Group I endpoints	Carcinogen	*3*	*3*	**2**	5	DG	LC = Low concern
	Mutagen	LC	LC	*3*	*4*	LC	PC= Potential concern
	Repro/Dev	DG	*2*	**1**	DG	PC	*prediction based on similar compounds
	Endocrine disruptor	DG	1	*1*	DG	DG	Color scale:
Group II endpoints	Mammalian Toxicity	*4**	2	*4*	4	5	1= Very High Hazard
	Systemic Toxicity	DG	2	**1**	LC	LC	2= High Hazard
	Neurotoxicity	DG	*3*	*1*	DG	DG	3 = Moderate Hazard
	Respiratory Toxicant	DG	PC	PC	*4*	LC	4 = Low Hazard
	Skin irritation	PC	*1*	LC	*4*	2	5 = Very Low Hazard
	Eye irritation	DG	2	2	*1*	2	LC = Low Concern
Eco toxicity	Aquatic Toxicity	*2**	*3*	2	*2*	LC	PC = Potential Concern
Fate	Persistence	*1**	1	**1**	5	5	**Bold** = confidence in score
	Bioaccumulation	PC*	PC	**1**	PC	PC	*Italicized* = potential score