Nouvelles applications de la MVA, incluent des Multivariances, Multi-Statistiques, Machine Learning, Clustering (IA) et une grande Banque des données des Spectres Enviro-chimiques des Produits Commerciaux (historiques) PFAS, dégradés et non-dégradés pour l'Identification & la Différenciation des Sources des pollutions par les PFAS

New MVA Applications, including Multivariances, Multi-Statistics, Machine Learning, Clustering (AI) and a large Data-Bank of Enviro-chemical Spectrums of (historical) commercial PFAS Products for Identification & Differentiation of PFAS Contamination Sources

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1. Introduction

Environmental PFAS contaminations and especially Groundwater Pollution Plumes are constituted mostly by multi-contamination Sources. The principal question is which PFAS Contamination Sources are responsibles for which part of the complete PFAS contamination. The following Article is showing the approach of MVA-AI to differentiate the responsibilities for each contamination source's pollution part. This is important, for the Industry, different polluters, Insurance Companies, Authorities and in case of Court Disputes, to share correctly and in Transparency the financial charges for Remediation and pollution Management.

Since the 1960s, PFAS monomers (Per- & Polyfluoro-Alkyl Substances) have gradually become a major environmental and public health problem in industrialized countries, due to their multiple and wide-ranging applications (historical and still current). This threat to the environment and to public health has been gradually coming to the fore since the 2010s and will be considered to a greater extent in 2022 - 2024. As a result, PFAS are now found in the soil at polluted sites, in groundwater, in food, drinking water, in soil gas and in ambient air (volatile PFAS, e.g. FTOH: Fluorotelomer alcohols, etc.). Between 9,000 and 12,000 synthetic PFAS pollutants have been produced, with some publications indicating as many as 15,000 molecules.

Polymeric PFASs such as Teflon (or PFTE etc.) are not very bioavailable and are therefore much less toxic than monomeric PFASs. These monomeric PFAS are the subject of the work presented below. PFASs are known for their toxicological effects as endocrine disruptors, hepatotoxicity, immunotoxicity, effects on fetal development and, in some cases, carcinogenicity (e.g. PFOA).

An important characteristic of PFASs is their behavior in Environmental Chemistry, since only polyfluorinated PFASs are modified by microbiological bio-transformation into perfluorinated PFASs, which remain totally stable and non-degradable, and even bio-accumulable.

Particularly in the case of groundwater pollution by PFAS, it is becoming increasingly important to identify and, above all, differentiate the contribution of each PFAS source to pollution plumes. This need for clarification regarding the contribution of each PFAS source to pollution, e.g. in the vicinity of drinking water wells, etc., is becoming crucial for the protection of water resources, (shared) responsibilities and the search for the (multiple) origins of pollution in the context of legal court expertise.

Sources of pollution by PFAS are varied and can be found on industrial sites that have used these products, sites that have suffered fires or fire training sites where fire-fighting foams have been used. **(AFFF : Anti Fire Fighting Foams or Aqueous Film Forming Foam, e.g. at airports)** have been used. Agricultural land is also a source of PFAS pollution, due to the input of sewage sludge, which contains accumulated PFAS.

The following (historical) activities may be the source of PFAS pollution:

- Fire-fighting training,
- Airport or air base on a military site,
- Fire site and use of AFFF,
- Electrochemical galvanisation,
- Production of waxed paper and cardboard,
- Manufacture of waterproof textiles,
- Sprays, paints, waterproofing lacquers,
- Production and application of Teflons (PTFE, etc.),
- Petroleum and chemical industry sites and/or production and application of paints, dyes, inks, pigments, chemical waxes and polishing products,
- Solvent applications (garages, dry cleaners, laundries, etc.),
- Landfill sites and former municipal landfill sites, etc. (ISDD, ISDND, ISDD, etc.),
- Dyeing & Tanning,
- Carpets, rugs, fabrics and plastics with flame retardants,
- Production of objects and furniture containing surfaces,
- Production of cleaning products,
- Photographic chemistry (laboratories, paper and film production, etc.),
- Production of electronic components,
- Production and application of pesticides and biocides,
- Production of cosmetics,

- Sites receiving WWTP sludge.

2. Environmental chemistry of PFAS

The environmental chemistry of PFAS is particularly important and complicated. There is no group of pollutants with a more complex environmental chemistry than PFAS. In particular, there are **more than 9,000 PFAS substances**, divided into **33 categories of substances**.

The mostly known PFAS are Perfluoroalkane sulphonic acids (PFASs), Perfluoroalkyl carboxylic acids (PFCAs), Perfluoroalkyl phosphates and their esters, Fluorotelomer alcohols (**FTOH**), etc. (including more than 29 other groups …). Some of them, such as the **PFOA :** Perfluorooctanoic acid and **PFOS** : Perfluoro-octane-sulphonate are banned (and **prohibited in EC and USA & Canada**) by the **Stockholm Convention** in the category of **POPs** : Persistent Organic Pollutants. PFOA is carcinogenic. **Commercial products** mainly contain **mixes**.

The reason for the high solubility in water, associated with lipophilicity, is based on the fact that **PFAS** :

- **Anionics** (e.g. sulphonates, sulphates, carboxylates and phosphates),
- **Cationics** (e.g. quaternary ammonium),
- **Amphoteric** (e.g. betaines and sulpho-betaines): base + acid and
- **Non ionic** (e.g. polyethylene glycols, acrylamide oligomers).

It is very important to emphasize that poly-fluorinated PFAS that are not fully fluorinated ('precursors') can be converted by bio-transformation into persistent, fully fluorinated chemicals, per-fluorinated PFAS. The complete microbiological degradation of PFAS has not yet been demonstrated.

In recent AFFFs (since about 2006 – 2015) the part of 6,2-FTAB and 6,2-FTS is very dominant and especial that one of 6,2-FTAB (Capstone B).

Figs. 1a & 1b show an **example of the biotransformation of 6 :2-FTAB & 6 :2-FTS** in soil and water to volatile Fluorotelomer Alcohols (FTOHs) which then migrate into soil gas (vapor) and ambient air. FTOHs are then microbiologically transformed into stable per-fluorinated PFASs. For example, 6:2-FTOH is biotransformed into PFHxA, PFPeA and PFBA and 8:2-FTOH into PFOA,

PFHpA, PFHxA, PFPeA and PFBA. Fig 1c shows the Photolysis pathways of 6:2-FTAB.

In top-soils and in surface waters an additional chemo-transformation happens by UV-based photolysis. In this case the final degradation products could be even ultrashort PFAS, like PFPrA (Perfluoro propionic Acid) and TFA (Trifluoro acetic acid), beside PFHxA, PFPeA and PFBA (Naveed, A. et al 2024, cf. Fig 1c).

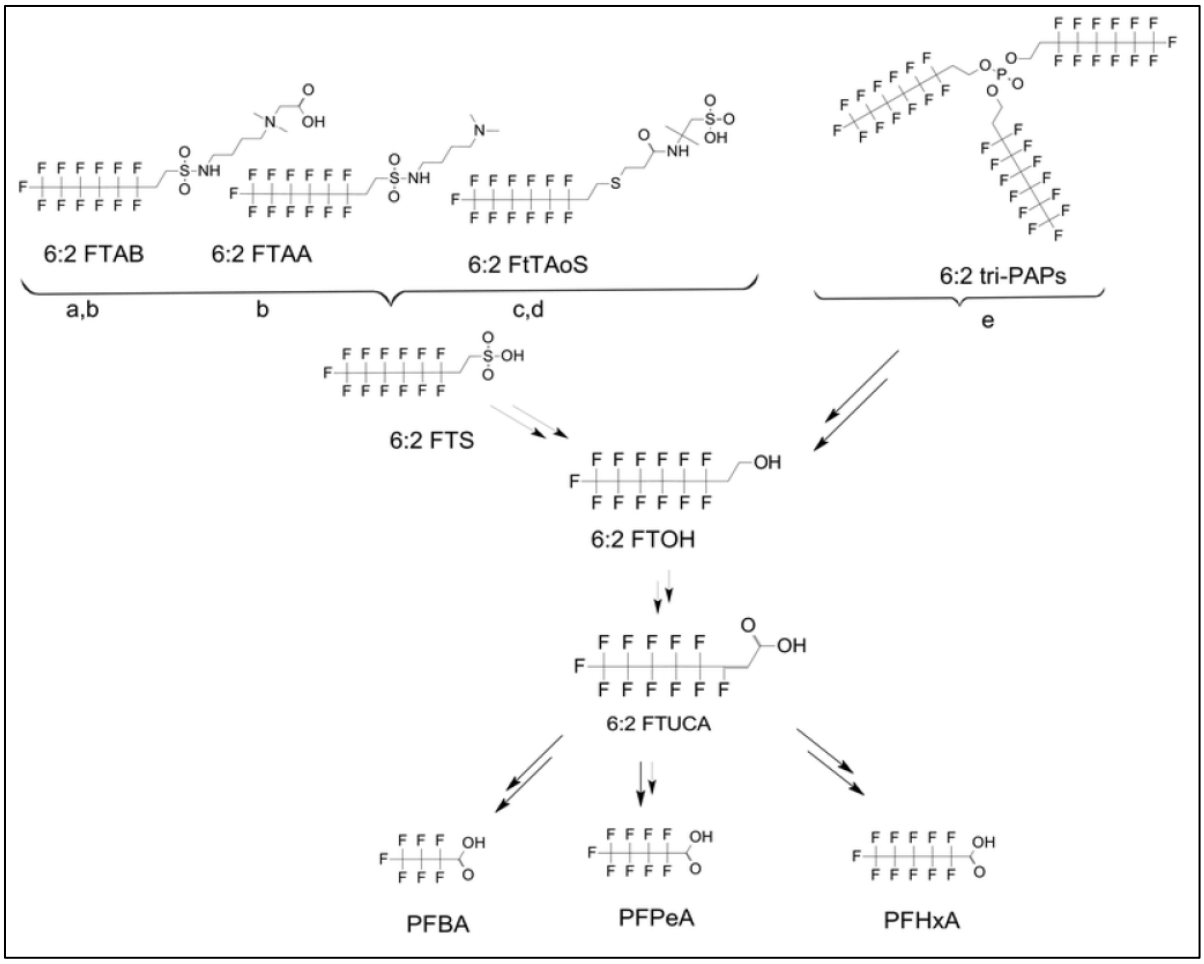

Fig. 1a : Biotransformation scheme of polyfluorinated PFAS (Precursors): Example: 6 :2 FTAB (Capstone B) and its degradation via 6 :2 FTS and 6 :2 FTOH to per-fluorinated PFAS PFBA, PFPeA and PFHxA (LaFond et al. 2023, D.M.J. Shaw et al. 2019,Ying Shi, 2018 and V. Mendeza et. al. 2022)

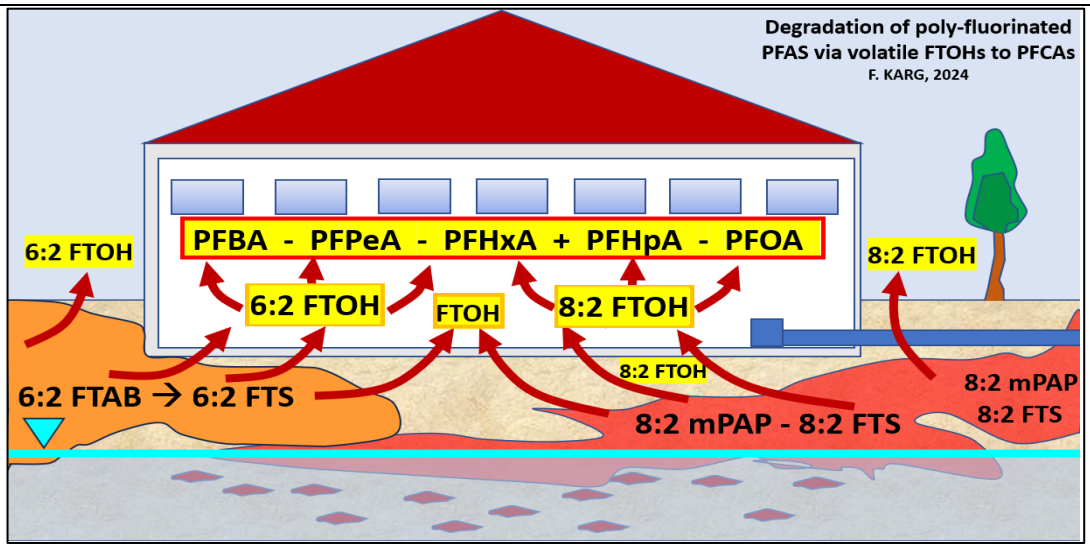

Fig. 1b : Example of the biotransformation of 6 :2 FTAB, 6 :2 FTS, 8 :2 FTS and polyfluorinated alkyl phosphates (PAP) in soil and water to Fluorotelomer alcohols (FTOH) and per-fluorinated PFAS, e.g. to PFOA, PFHpA, PFHxA, PFPeA and PFBA (L. KOPF / HPC, 2017 and F. KARG, 2022 & 2024).

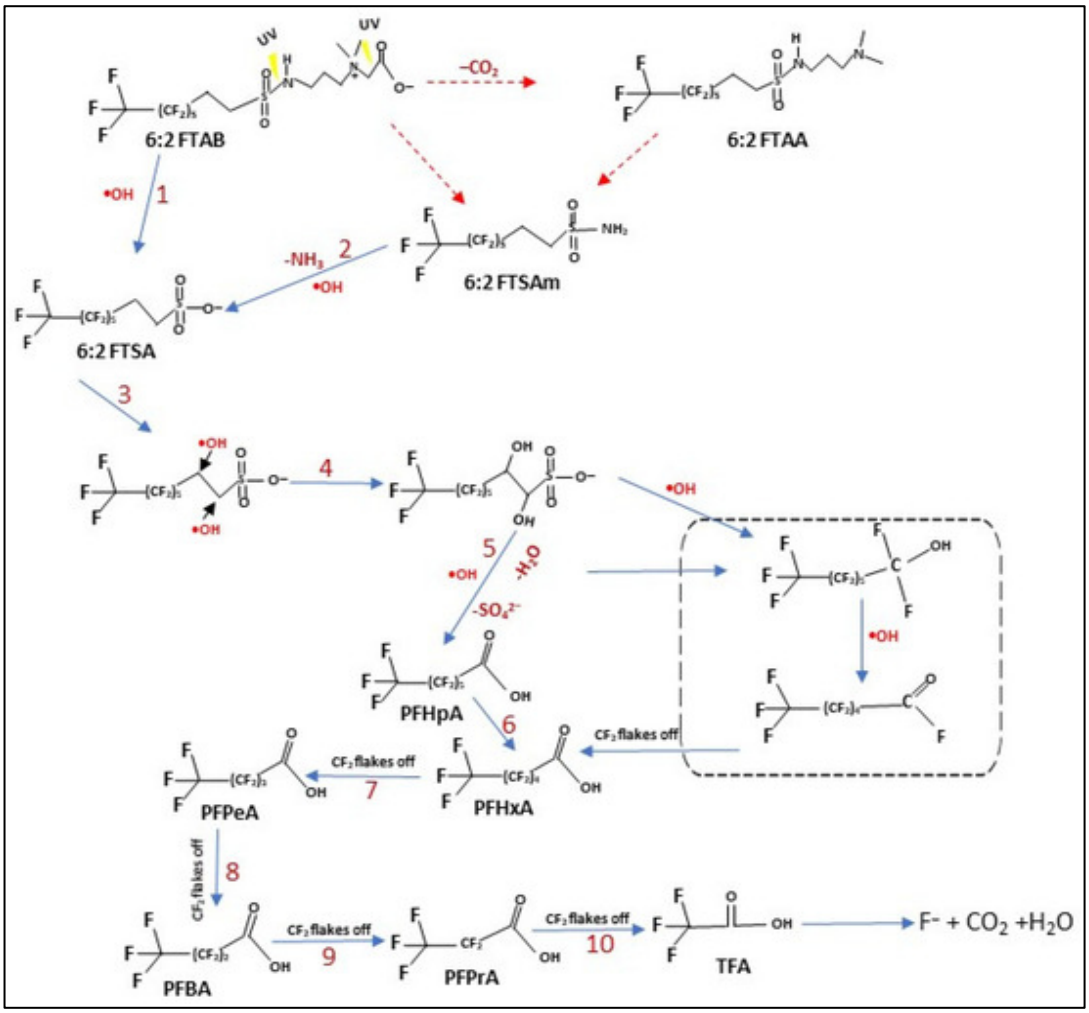

Fig. 1c: Photolysis of 6:2-FTAB to ultrashort PFAS, like PFPrA (Perfluoro propionic Acid) and TFA (Trifluoro acetic acid), beside PFHxA, PFPeA and PFBA (Naveed, A. et al 2024)

In the event of a change in pH, some PFAS may become more or less soluble, which also has an impact on emissions of volatile fluorinated telomers such as FTOH, etc. in soil gas (vapor). Certain precursors could change their solubility (and their extractable properties during chemical analysis procedures). For example, the intrusion of seawater into the aquifer could result in an increase in the basic pH and therefore in the solubility of Capstone B. This was observed in 2022 in the port area of Hamburg/Germany following seawater flooding and groundwater intrusion (see Fig. 2). These effects could result in groundwater concentrations more than 10 times higher than before seawater intrusion into the soil and groundwater.

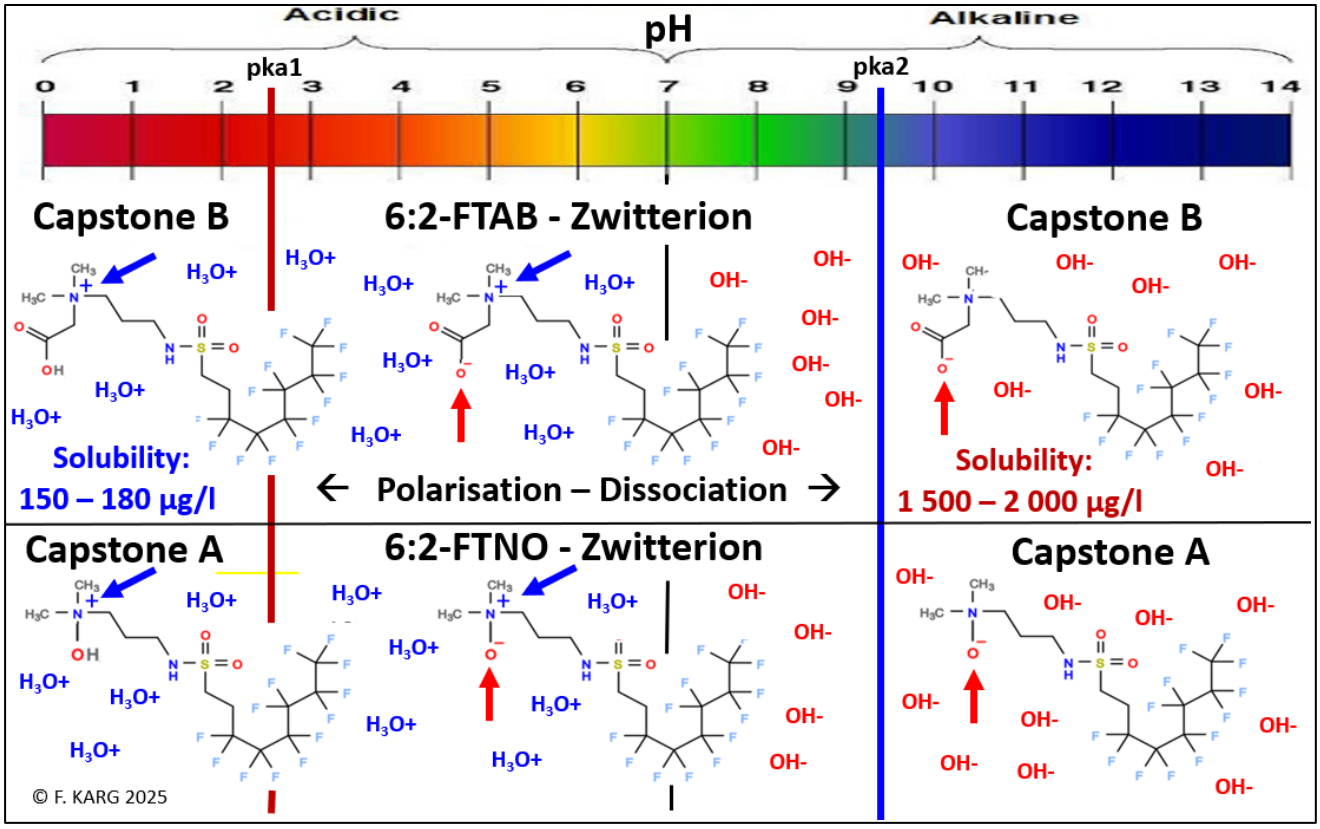

Fig. 2 : Solubility of 6:2-FTAB & 6:2-FTNO according to pH (example: before and after seawater intrusion into an aquifer and change to a slightly alkaline pH)

3. Differentiation of sources of PFAS pollution

Pollution of soil, groundwater and surface water by PFAS is frequently a mixture of several sources of commercial products and sources of pollution. It is possible to carry out complete screening of individual PFAS substances to identify between 9,000 and 12,000 molecules, but in the day-to-day management of pollution in the environment this is not applicable due to the limits of technical and economic feasibility.

For this reason, it is necessary to reduce the number of PFAS compounds to be analysed during environmental assessments by means of **the chemical Identification** of commercial products suspected of being the source of contamination. As PFAS are a family of more than 9,000 compounds, it would be impossible to quantify them all.

Typical sources of pollution caused by PFAS include, for example, applications of fire-fighting foams (AFFF = Aqueous Film Forming Foam or Anti Fire Fighting Foams), for example during fire drills and fires at airports, refineries and oil depots, industries involved in the production and processing of PFAS polymers, galvanizing activities such as chromium plating, the agricultural application of sewage WWTP sludge or fertilizers containing PFAS, the application of water-repellent coatings to paper, cardboard and textiles, etc., but also when they are used as flame retardants in the electrical and electronics industries... The list of sources of PFAS in the environment is long, and there are also volatile PFAS pollutants that can enter indoor air via soil gases, such as fluorotelomer alcohols (FTOH).

One of the current challenges in managing environmental problems linked to PFAS is to identify the various sources of pollution caused by PFAS or their commercial products, for example in the case of major contamination of groundwater by PFAS.

Experience and assessments of more than 800,000 PFAS analyses in soil, groundwater and surface water show the presence of various PFAS clusters and substances, such as perfluorinated carboxylic acids (PFCAs), perfluorinated sulphonic acids (PFSAs) and others, which are typical of certain industrial sectors. Other important PFAS groups are fluorotelomer sulphonic acids (FTS), fluorotelomer alcohols (FTOH) and fluorinated sulfo-betaines (FTAB), from a total of 33 different PFAS groups.

When identifying and differentiating PFAS sources, various relative concentration distributions, relationships with perfluorinated carboxylic acids (PFCAs) and with various poly-fluorinated PFASs as 'precursors', as well as various statistical distribution models, are taken into account.

Commercial PFAS products are examined using non-target analyses to identify as many individual PFAS substances as possible present in PFAS products. To this end, percolation tests to simulate the ageing of 'fresh' commercial PFAS products are being carried out on lysimeters, with bacteriological degradation allowing the biotransformation of poly-fluorinated PFAS (precursors) to per-fluorinated PFAS, and to identify the chromatographic effects of soils (F. Karg et al.: 2023 and 2024).

The purpose is to record the resulting mixtures of individual PFAS molecules by HR-MS (high-resolution mass spectrometry). The results obtained are typical fingerprints of fresh and degraded commercial PFAS products for the complete database of parent mixtures of PFAS products.

PFAS sources can be identified from this database using standard analyses and a multivariate statistical identification program. Multi-Vector-Analysis (MVA) is carried out in several dimensions using artificial intelligence (machine learning), so that PFAS sources can also be determined in the event of groundwater pollution containing a mixture of several different PFAS sources.

The next figure shows:

- the different MVA program applications of Several Statistical QT Technology Back- & Front-End Models & Identification of composition Similarities between Chemical PFAS Spectrums of (historical) commercial PFAS Products and their biotransformed & degraded Forms of the created dedicated Data Bank and environmental Soil & Groundwater Sample Analyses.
- Chemical Clustering Models & Modules*: Evolutive Programs, based on « Machine Learning » & Artificial Intelligence (AI) Differentiation & Identification of PFAS Sources.
- Associated Geostatistical Programs & Mapping and Hydro-chemical & Hydro-geological Programs & Modelling for Chromato-graphical Soil + Aquifer Effects and Bio-reactivities & Photolysis.

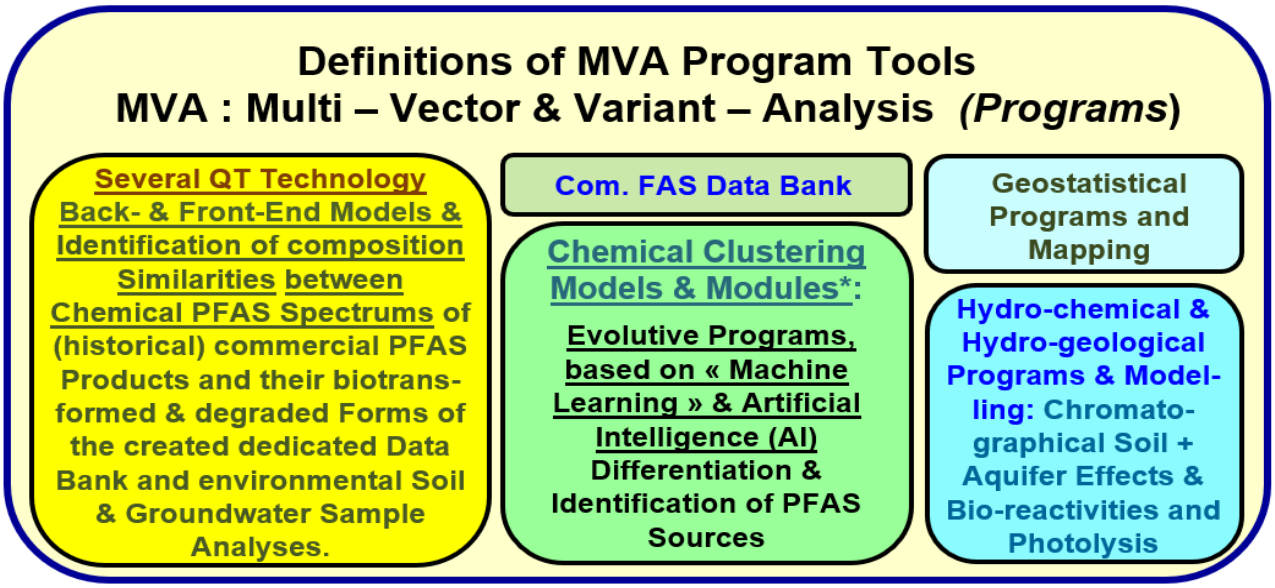

Fig.: Definitions of MVA Program Tools: Multi – Vector & Variant – Analysis (Programs)

In addition to the use of standard environmental analyses of polluted sites for MVA identification of the different sources of PFAS pollution, other analytical tools may also be applicable, such as the 'Top Assay' (Houtz & Sedlak: 2012, Glöckner et al.: 2021) to best determine the mass of poly-fluorinated precursors present, which can be oxidized to perfluorinated carboxylic acids (PFCAs) (see Fig. 3). In addition, measurements of isotope ratios between PFAS source areas and plume areas can be carried out to determine PFAS sources (Quian et al. 2023), as well as the use of comprehensive 'untargeted analyses', in which hundreds of individual PFAS molecules can be identified and at least semi-quantified.

Such applications are more time-consuming and expensive than the normal standard PFAS analysis for polluted sites, which is mainly used to identify PFAS sources. The MVA application can avoid this and be more cost-effective.

More than 9 000 – 12 000 PFAS have been polluting the environment and our health for decades. This also includes volatile PFAS, such as fluorotelomer alcohols (6:2 or 8:2 FTOH, etc.). The problem in investigating PFAS-contaminated sites lies mainly in the huge quantity of poly-fluorinated PFASs, which are biotransformed into per-fluorinated PFASs over time. Individual poly-fluorinated PFASs may also be relatively resistant in the environment and transform only very slowly into perfluorinated PFASs (such as Capstone B - FTAB, FTS or FTOH). In order to improve transparency and knowledge of this large number of PFAS pollutants, there are several approaches to the investigation, risk assessment and remediation of PFAS.

An important characteristic of PFASs is their chemical behavior in the environment, as poly-fluorinated PFASs (precursors) are converted to stable perfluorinated PFASs by biotransformation. The risk assessment of individual cases via a QSRA* (or RRA*) can estimate the future risks of most of the "precursors", since an analysis based on 28 to 70 individual PFASs is carried out before and after examination by the 'Top Assay' test (see Fig. 3). In the Top Assay, poly-fluorinated PFAS are converted into stable per-fluorinated PFAS by oxidation via persulphate, into which they are generally biotransformed after a certain residence time in the environment (see also Fig. 2a & b). Thanks to the 'Top Assay' test, investigations and risk assessments include almost all transformable 'precursors' as well as the remaining per-fluorinated PFAS end products.

(*EQRS & *ARR: Quantitative Health Risk Assessment and Residual Risk Analysis).

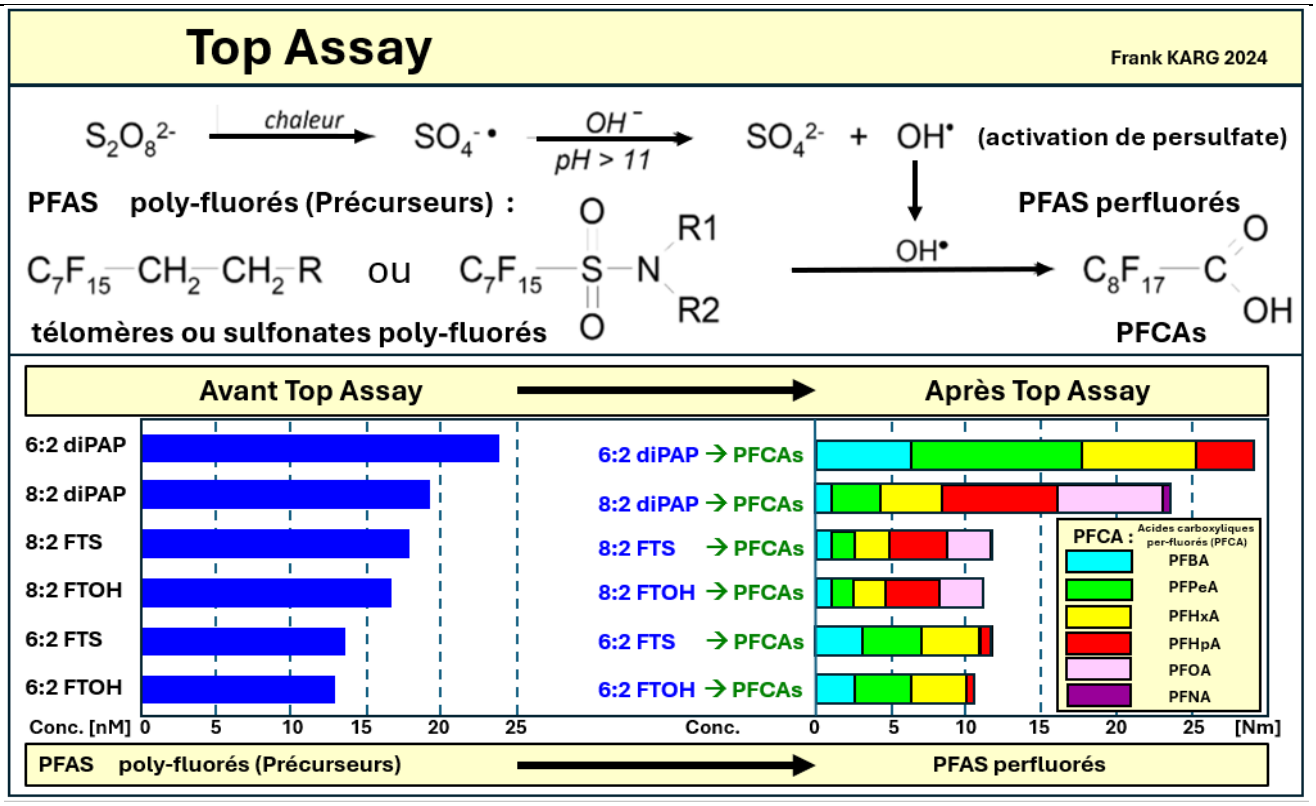

Fig. 3 : *Top Assay (Total Oxidizable Precursor method) to quantify oxidizable poly-fluorinated PFAS, transformable into per-fluorinated carboxylic acids (F. Karg 2015, Houtz & Sedlac 2012, Glöckner et al.: 2021).*

The following examples illustrate some of the ways in which sources of PFAS can be identified and differentiated using certain standard analyses, taking into account experience of MVA (Multi-Vector-Analysis) applications based on artificial intelligence in Europe (EU) and the United States.

Typical sources of PFAS include areas that have experienced fire and fire training events, civil and military airports (anti fire-fighting foams / AFFF), but other activities can also cause PFAS contamination in soils and groundwater.

These activities include, for example, the spreading of sewage sludge from wastewater treatment plants, galvanic chromium plating, landfill leachates, paper production, textile impregnation, the electrical and electronics industries, paint companies, cleaning products and fluor-polymer production, etc.

Various statistical analyses and visualizations, based on experiments and PFAS clusters from over 800,000 soil and groundwater analyses (NAS: 2023, F. Karg: 2024), help to identify PFAS sources.

The methodology for differentiation of PFAS sources can be divided into three main categories:

I. Analysis of data and (historical) information available that can be used to identify potential sources of PFAS at different sites (specific industrial sites airports, landfills, etc.).

II. Laboratory methods for analyzing PFAS in environmental samples.

III. Advanced forensic investigations to identify potential sources of PFAS more precisely.

Category I. includes the following phases :

- Historical investigation of potential sources of PFAS from suspect areas. The objective is to list and map the areas of potential sources of PFAS pollution.
- Study the hydrogeological zones above the suspected areas to determine whether there are (or have been) activities that use (or have used) PFAS.
- To obtain a detailed understanding of the geology, hydrogeology, hydrology, stormwater infrastructure and surface water run-off of the sites. This also includes the nature of the soil, the location and depth of nearby wells, and the depth and direction of surface and groundwater flow.
- Prepare a conceptual plan of the site concerning PFAS sources, transfer paths and exposure paths to targets.

Categories II and III focus on :

- Evaluation of PFAS chemical analysis data as a screening step to determine whether indications or evidence of source differentiation can be identified.
- Analysis of advanced PFAS forensics on selected samples to differentiate potential sources of PFAS (e.g. by structural isomerism, isotopic studies, Top Assay, MVA applications, etc.).

The general differences between PFAS's commercial products can be identified, for example, through the following distinctions:

- Modern anti fire-fighting foams (AFFF) are based on fluoro-telomers, mainly with C6-PFAS molecules. Although these firefighting foams do not contain PFOA or PFOS, when emitted into the environment they can degrade to other shorter-chain PFAS, such as perfluoro-

hexanoic acid (PFHxA), perfluoro-pentanoic acid (PFPeA), buntanonic acid and 5:3 fluorotelomer carboxylic acid (FTCA).

- In the early 2000s (following general requests from the US and European authorities), the chemical industry began to phase out anti fire-fighting foams based on C8-PFAS, as PFOS and PFOA were classified as being “too toxic”. Producers of fluorotelomer-based firefighting foams then turned to the use of short-chain forms of PFAS with six fluorinated carbons (called C6-PFAS), which did not contain PFOS or PFOA (and could not be broken down into these products either). These C6-PFAS firefighting foams can also contain PFHxA, PFPeA and 6:2-fluorotelomersulphonate (6:2-FTS) as well as fluorotelomers, which can be transformed over time into their end groups, perfluoro carboxylic acids with less than six carbon atoms. The exact period of transition from C8-PFAS fire-fighting foams to C6-PFAS fire-fighting foams varies according to the application site (civil or military airports, fire training areas, oil sites, etc.).

- Before 2016, many firefighting foams contained PFAS with eight fluorinated carbon chains. Some of these long-chain firefighting foams, or C8 PFASs, contained PFOS until the early 2000s, and PFOA and other long-chain PFCAs until around 2015, when these products were withdrawn from the market.

- Analyses of the molecular chemical structures of PFASs can be useful in relation to existing information such as origin, period and likely use. Structural differences include, for example, structural isomerism (linear and branched isomers, etc.). For example, if a particular cyclic PFAS with an eight-carbon chain, such as perfluoroethyl-cyclohexane sulphonate (PFECHS: CAS 335-24-0) is observed, it could originate from a corrosion inhibitor used in aircraft hydraulic fluids (MPART: 2020). PFECHS is not known to be a component of fire-fighting foams.

- Specific PFASs can be used as markers in the production of fluoropolymers, food packaging and paper coatings, as well as cosmetics. They are not currently thought to be related to fire-fighting foam products.

- Some PFASs can be chemically biotransformed (i.e. broken down into smaller, stable chemicals), but these poly-fluorinated PFASs (precursors) often transform into other PFASs, particularly per-fluorinated PFAAs.

Identifying and differentiation of PFAS Contamination Sources:

The standard environmental analyses used during investigations of sites polluted by PFAS can, in principle, be used to identify and differentiate sources of PFAS. Between 30 and 70 individual PFAS substances are analyzed. The analytical data obtained can be very complex due to the presence of many different PFAS in an environmental sample and pose a challenge in interpreting the data. For this reason, a computerized MVA application with artificial intelligence is required.

Because of this complexity, large amounts of data need to be interpreted on the basis of statistical experience gained from large amounts of analysis in multi-vector analysis (MVA or poly-topic analysis) with artificial intelligence, so that the sources of PFAS can be identified and differentiated with a very high probability. This can only be done as part of a parallel analysis of different pieces of evidence, as each analysis on its own is generally not sufficiently significant. The basis for this are 'target' (and 'non-target') analyses as well as the 'Top Assay', total organic fluorine (TOF) or **AOF (adsorbable total organic fluorine) and isotopic analyses.**

The following Experiences can be applied for Identifying and differentiation of PFAS Contamination Sources:

- **TOF or Total Organo Fluorine is measuring PFAS Monomers & Polymers and other organo-fluorine Compounds, like Pesticides, Pharmaceuticals, etc. No Compound Identification is realized. The use of TOF can't be really recommended for PFAS analysis appreciation.**
- **AOF: Adsorbable Organic Fluorine is only measuring compounds which were priorly adsorbed in Water samples. AOF is measuring PFAS Monomers, small PFAS Polymer particles and other organo-fluorine Compounds, like Pesticides, Pharmaceuticals, etc. No Compound Identification is realized. The use of AOF can't be really recommended for PFAS analysis appreciation.**
- **NTA: Non-Target Analysis is the semi-quantitative Identification of up to 12 000 Compounds of PFAS Monomers. The costs and time needs are very important.**
- **QTA: Quantitative Target Analysis of up to 500 – 700 Compounds of PFAS Monomers (in general 20 – 70 compounds).**
- **QTA + TA: Quantitative Target Analysis after Top Assay of 20 - 200 Compounds PFCA Monomers (in general 20 – 70 compounds). Only per-fluorinated PFAS are analyzed, including poly-fluorinated PFAS after transformation to PFCA by persulfate.**

Recommended are QTA: Quantitative Target Analysis of about 70 choosen compounds before and after Top Assay. Its important to analyse via the QTA also the ultrashort PFCA, like TFA (trifluoro-acetic acid), PFPrA (perfluoro-propanoic acid), TFMS (trifluoro-methane-sulfonic acid), PFES (perfluoro-ethane-sulfonic acid) and PFPrS (perfluoro-propane-sulfonic acid).

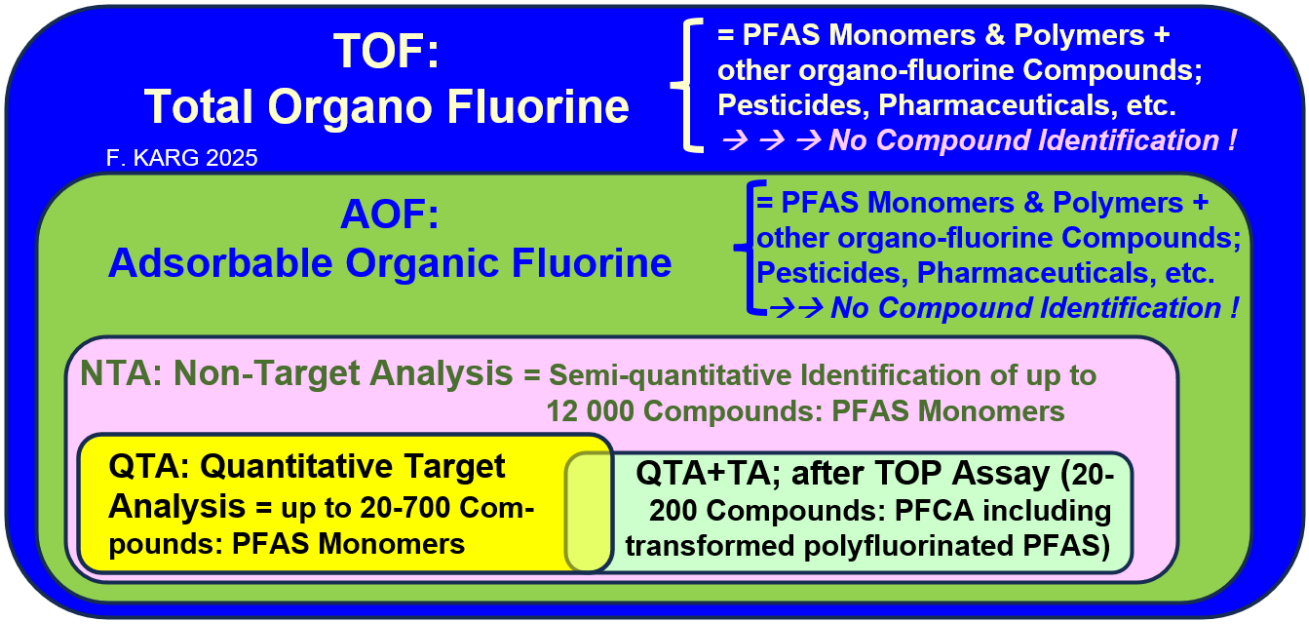

Fig. 4 : Analytical procedures for the identification and differentiation of PFAS sources using multi-vector analysis (MVA or poly-topic analysis) with artificial intelligence.

Figure 5 shows the procedure for identifying and differentiating potential sources of PFAS using MVA based on artificial intelligence (e.g. AFFF fire-fighting foams, sewage sludge, electroplating activities, textile and paper industries, waste dumps, etc.).

The procedure principles for identifying and differentiating potential PFAS Sources are the following:

A. **Lots of different Statistical Comparisons of Sample analyses with registered Standards** of chemical PFAS Spectrums on about 70 analyzed compounds from commercial PFAS Products (AFFF, Galvanic products, Paper related production Products, Surfactants mixtures, etc.).

B. Identification and Differentiation of PFAS Clusters by MVA on Artificial Intelligence via Clustering.

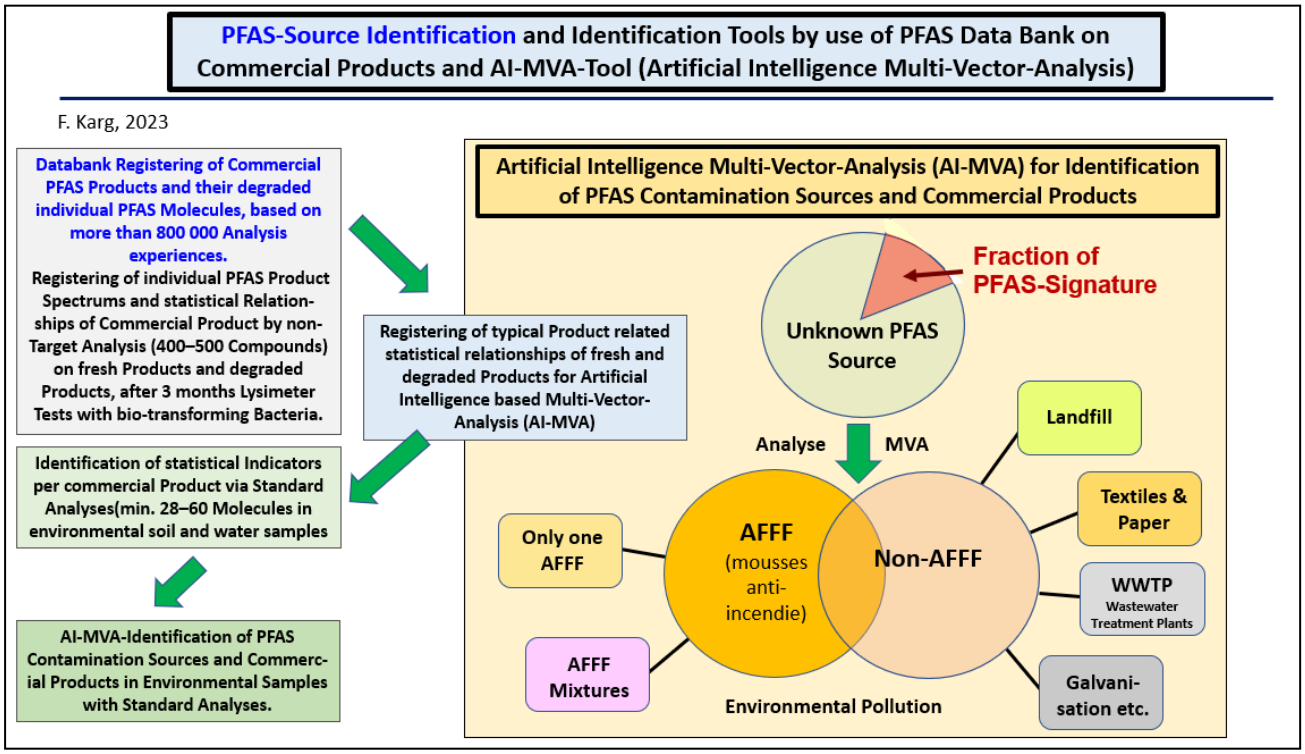

Fig. 5 : MVA analysis approach based on artificial intelligence to identify and differentiate sources of PFAS (e.g. AFFF fire-fighting foams, sewage sludge, galvanic activities, textile and paper industries, waste dumps, petroleum sites, etc.) (F. Karg et al.: 2023 & 2024).

Because of the many individual PFASs within this chemical family, 'non-target analysis' also offers the possibility of identifying unknown molecules, as the result is open-ended without any limitation on a standard list of pre-calibrated pollutants. Hundreds of individual compounds can be identified. The disadvantage is that non-targeted analysis is relatively expensive and time-consuming. Figure 6 shows the differences compared with standard analysis of selected PFAS parameters.

Figure 6a shows different AFFFs in Soil samples and the 6:2-FTAB & 6:2-FTS domination. The similarity of these analytical results needs the MVA-Application for product identification. In Fig. 6b Biolysimeter-Tests are shown for obtaining different intermediary AFFFs' bio-transformation steps under aerobic and anaerobic conditions. Figure 6c shows different stages of AFFF bio-transformation, example of "H4 (Hydral 3)".

Figures 7 and 8 show PFAS cluster analyses to differentiate between several PFAS sources and Figure 9 shows PFAS Cluster Sources Overlapping and percentage parts of Groundwater pollution plume participation.

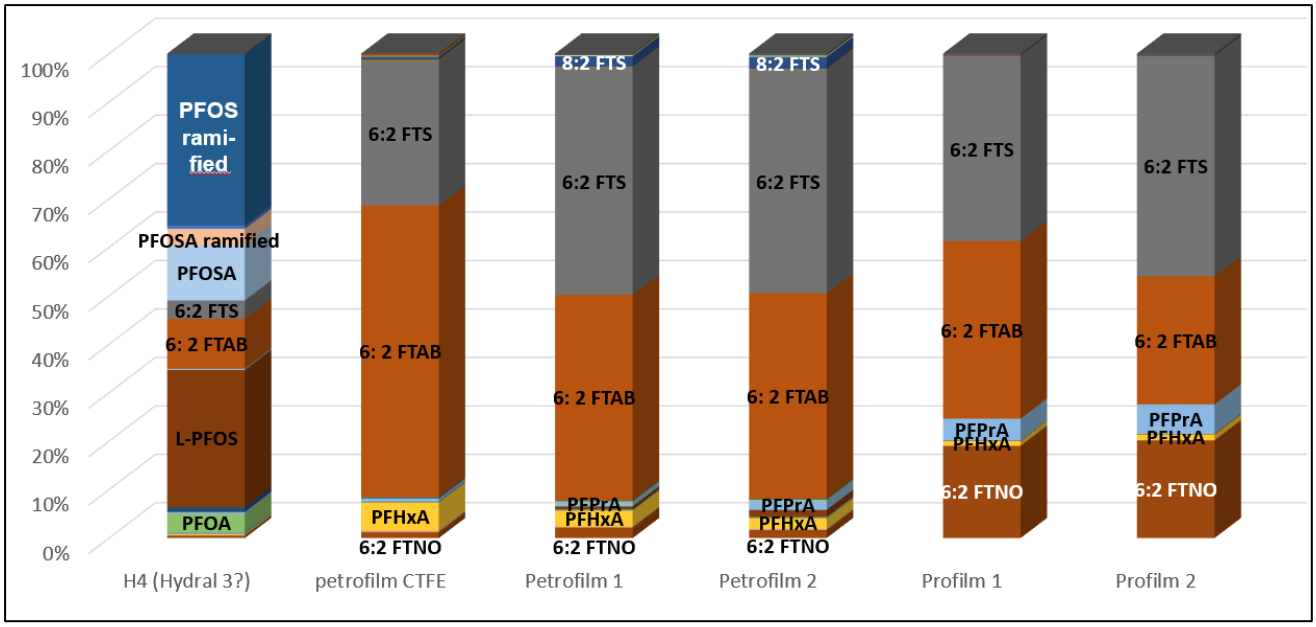

Fig. 6a: Different AFFFs in Soil samples and the 6:2-FTAB & 6:2-FTS domination.

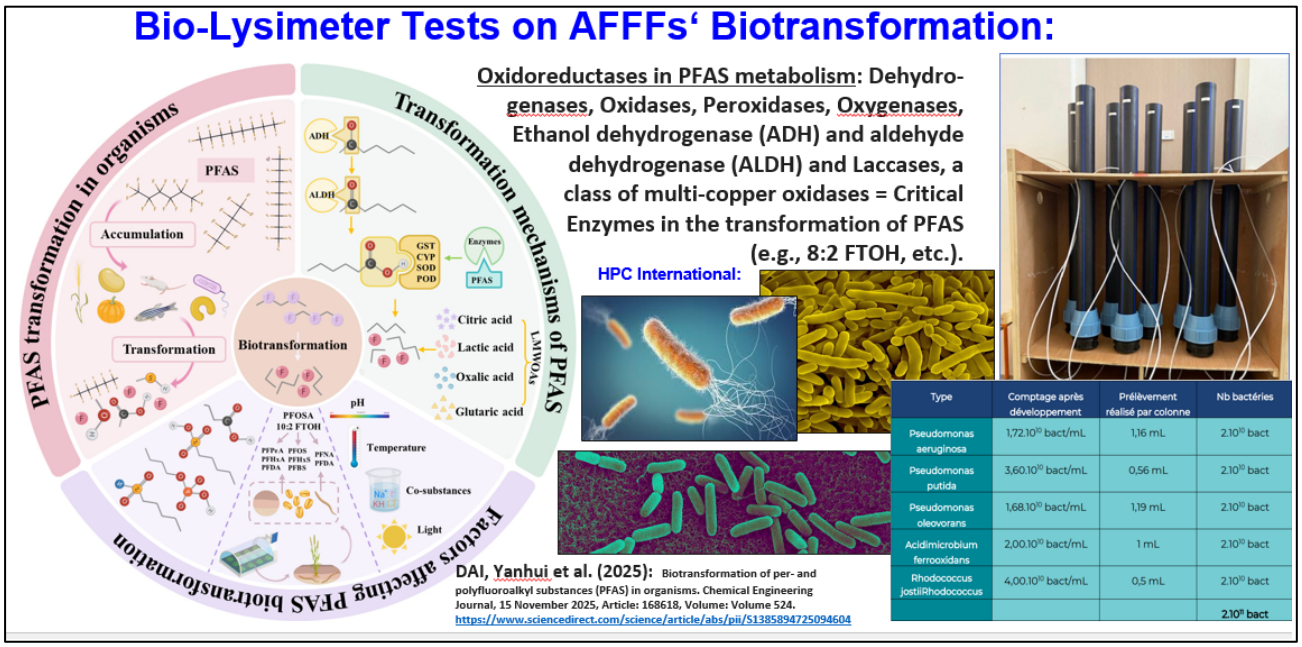

Fig. 6b: Biolysimeter-Tests for obtaining different intermediary AFFFs' bio-transformation steps under aerobic and anaerobic conditions.

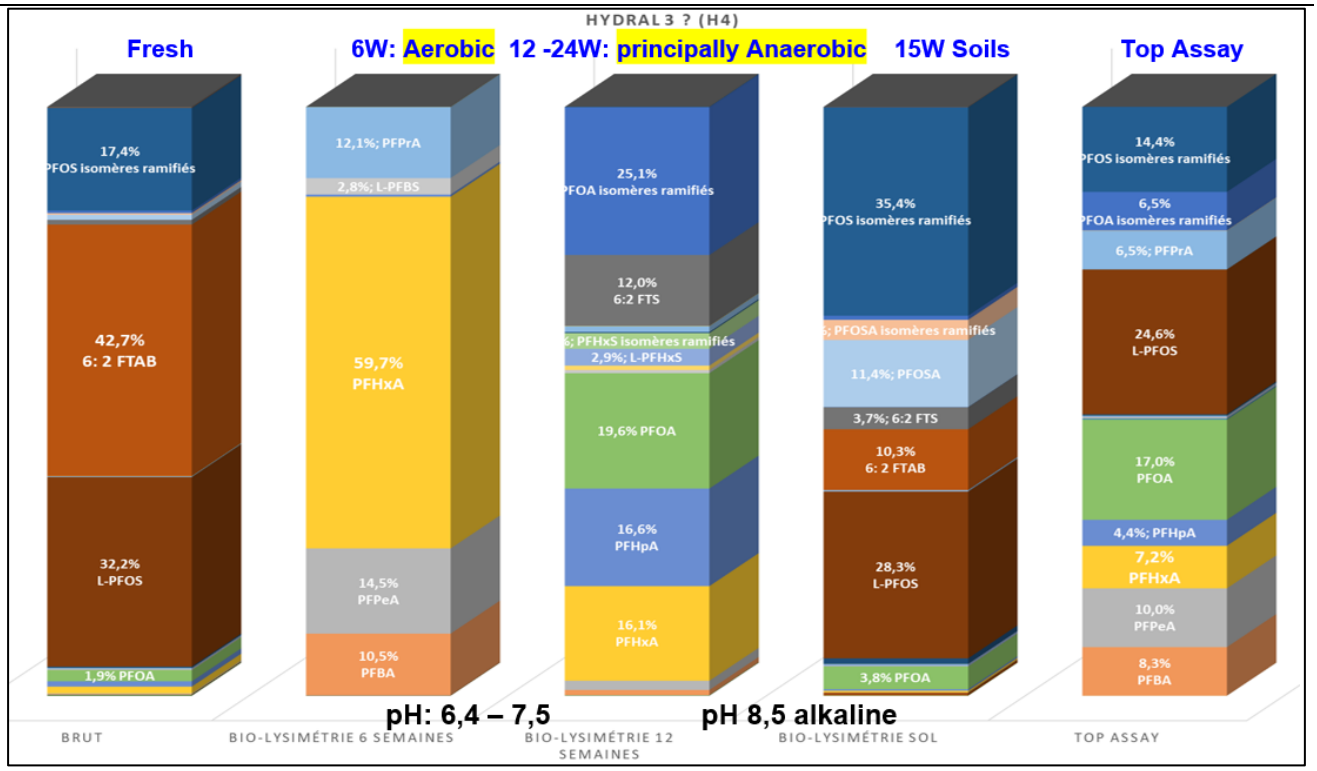

Fig. 6c: Different stages of AFFF bio-transformation, example of AFFF “H4 (Hydral 3)”.

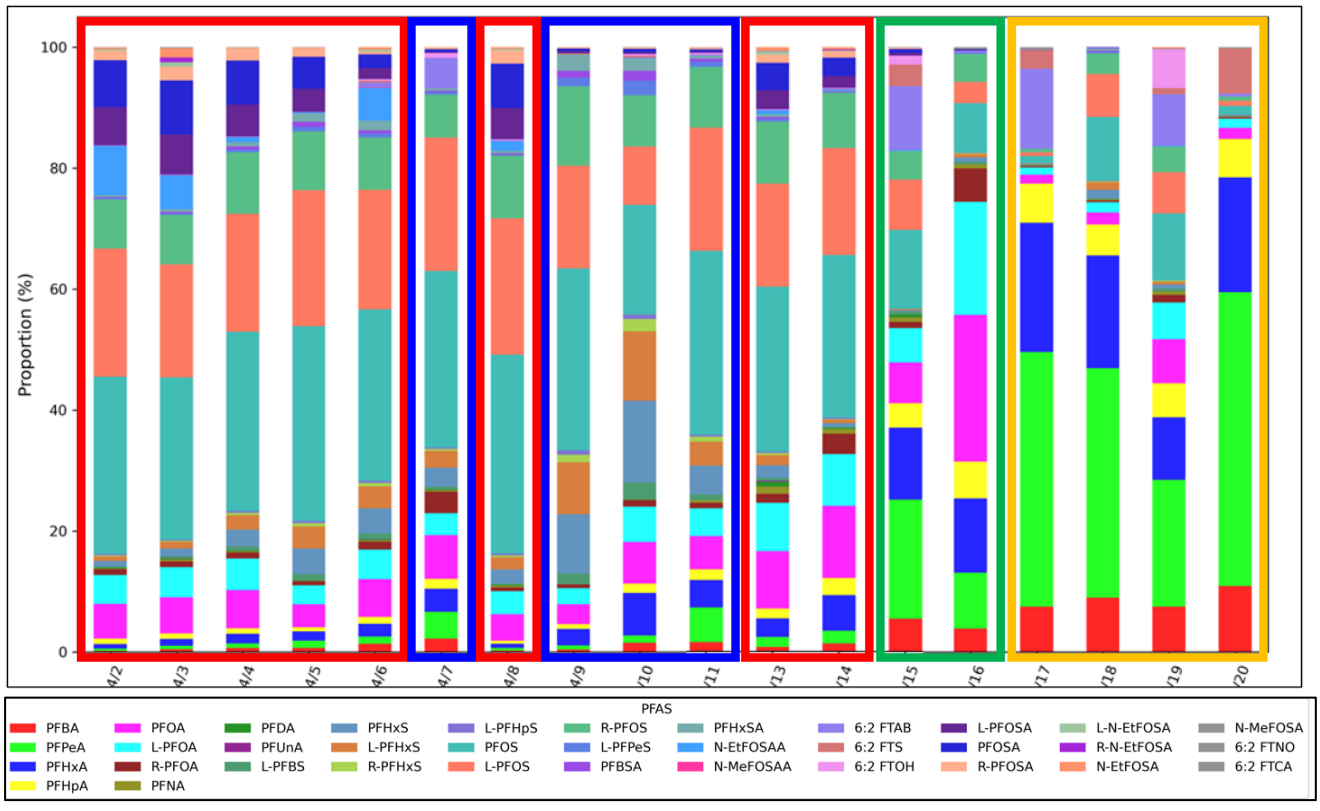

Fig. 7: Various PFAS Clusters and Cluster Mix, identified to determine the sources of PFAS

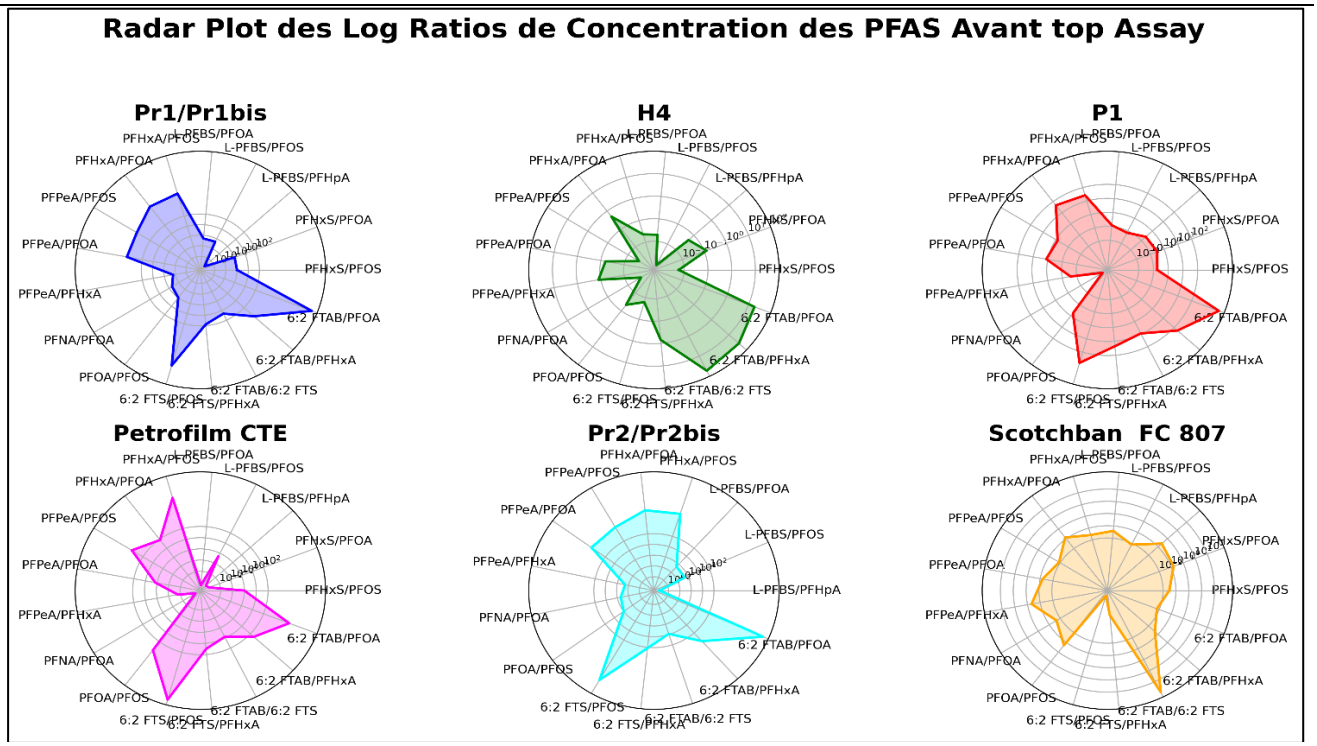

Fig. 8 : Various PFAS Clusters:Commercial PFAS Products and their chemical signature in Radargrams

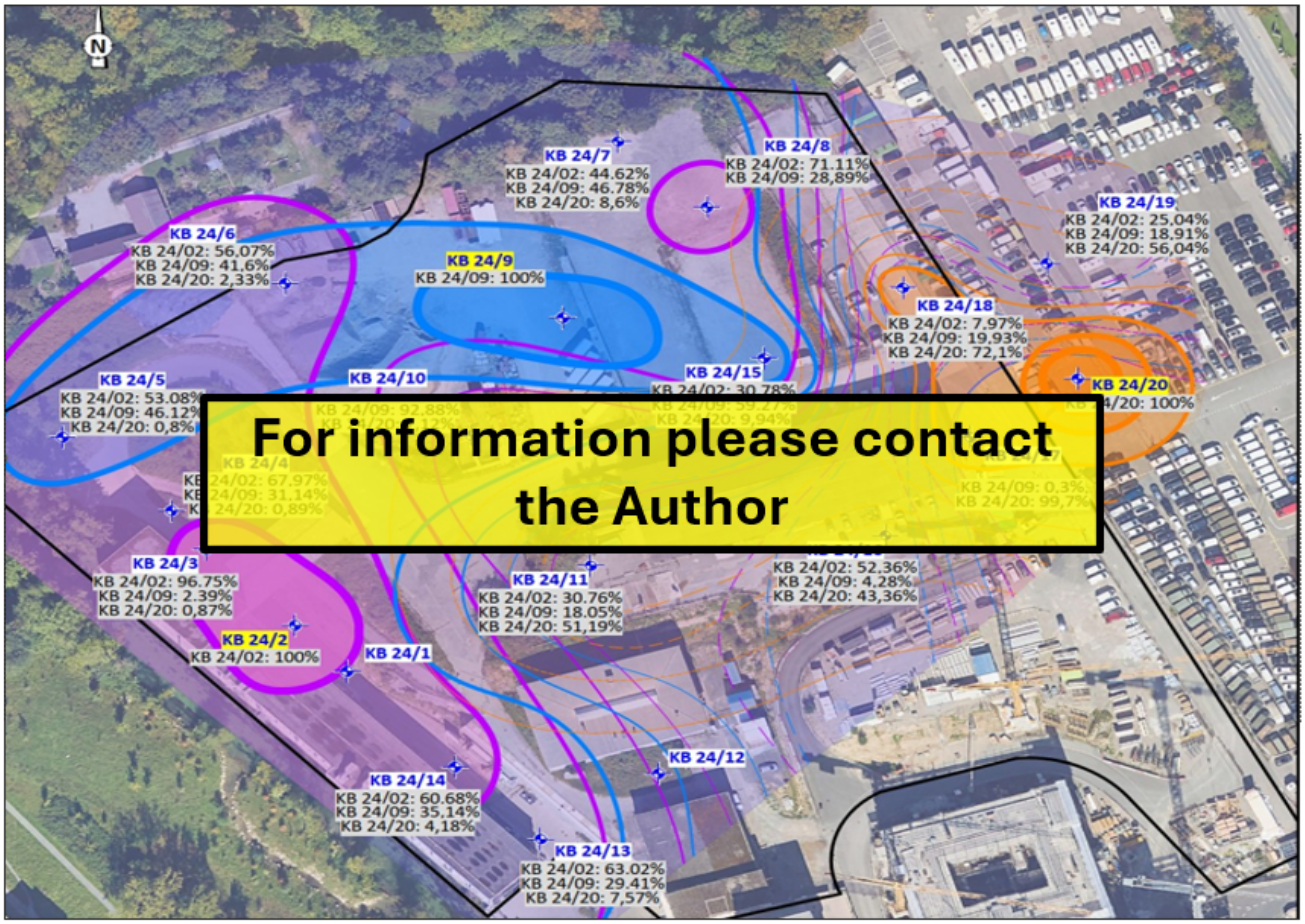

Fig. 9 : Identification and differentiation of 4 different Sources of 3 different PFAS Clusters and commercial

PFAS products on the basis of groundwater analysis and MVA-AI.

The multi-vector analysis (MVA) computer tool with artificial intelligence to identify and differentiate the sources of PFAS clusters was created on real commercial PFAS Product and environmental analyses.

The basis is, among others, the experiences of the US Airport Cooperative Research Program (ACRP), the Airports Council International - North America (ACI-NA), the American Association of Airport Executives (AAAE), the USA National Academy of Sciences Guide (NAS: 2023), as well as chemical cluster determinations of fresh commercial PFAS products and aged commercial PFAS products (according to degradation procedures applied by HPC International; F. Karg et al. 2023 - 2024) as standards for the MVA-PFAS database. The ageing of commercial PFAS products was carried out using bio-lysimetric tests in 2024 & 2025 with exposure to degrading bacteria for biotransformation of poly-fluorinated PFAS into per-fluorinated PFAS (F. Karg et al. 2023 – 2024, NAS, 2023).

The analysis of PFAS clusters takes into account the environmental chemistry of PFAS and in particular the metabolism or biotransformation of poly-fluorinated PFAS into stable per-fluorinated PFAS, e.g. the metabolism of poly-fluorinated PFAS into stable per-fluorinated PFAS, for example 6 :2 FTAB → 6:2-FTS → 6:2-FTOH → PFHxA + PFPeA + PFBA etc. to determine the 'precursors' and final products in the event of environmental contamination by mixtures of PFAS through the biotransformation chain.

Site-specific investigations and the identification and differentiation of PFAS sources include the following multi-criteria applied in the MVA tool. All the criteria are always applied at the same time:

A. **Concentration ratios between PFAS:** this is a simple first screening technique, where one or more concentration ratios between two or more different PFAS compounds can be applied. For example, PFHxS/PFOS ratios within a certain range have been used as an indicator of a source of fire-fighting foam (McGuire et al. 2014), and PFHxS/PFOA ratios have been identified as markers of other sources of industrial PFAS production (Guelfo and Adamson 2018).

B. **Circular diagrams and other data visualizations:** These are statistical graphs showing **the relative contribution of several molecules** to the total PFAS concentration in the same study area.

They can help identify compositional differences between PFAS mixtures in different samples to determine whether there are chemical clues or evidence from different PFAS sources. It can also identify the mixing of different PFAS sources or changes in source signatures along a transport pathway (e.g. migration in groundwater) and also reveal biotransformations and soil chromatography effects.

C. **Isomer ratios:** Individual PFAS can exist in **different isomeric forms** and the relative abundance of different isomers in a sample can be used to infer the source of PFAS (Charbonnet et al. 2021). **The presence of branched isomers (structural isomers) in a sample can be measured using standard methods** (which analyse around 60 to 70 individual substances). **The two different PFAS production processes, ECF (electrochemical fluorination) and telomerisation, result either in a mixture of branched and linear PFAS (ECF) or in isomers of purely linear PFAS.**

This information could be useful as evidence to identify sources of PFAS. **Branched isomers indicate that PFAS come from the specific electrochemical fluorination (ECF)** manufacturing process**.** The proportion of branched isomers in ECF products falls within a relatively narrow range (ITRC 2022 a&b). If the proportion of branched isomers in a sample is below this range, this may indicate that products containing PFAS generated by telomerisation-based manufacturing processes are also present.

Modern firefighting foams (AFFFs) contain PFASs that are produced solely by telomerization processes. Older AFFF blends may contain PFAS produced by ECF manufacture or telomerization. In the USA and somewhat later in Western Europe, the production of AFFF mixes using ECF production was discontinued in the early 2000s.

Another important fact is that branched isomers of some PFAS (e.g. PFOS) propagate more rapidly in groundwater than linear isomers of the same compound (different chromatographic effects in soil) due to the different interactions of the isomers with the soil. This can lead to enrichment of **ramified isomers** in groundwater hydro-geologically downstream of a PFAS source (Nickerson et al. 2020).

D. Analysis of the main components of PFAS and hierarchical classification study of PFAS clusters: These statistical methods are used to analyze data associated with many variables (e.g. measured PFAS) in order to identify differences between clusters of PFAS that can be visualized graphically. This data analysis facilitates the identification of different groups (or clusters) of PFAS mixtures (each of which may come from different sources or commercial PFAS products (see Figs. 7 & 8), which clusters may overlap).

E. Research methods (screening): identification and characterization of sources of PFAS :

- **Frequency of detection:** Experimental statistics (from over 800,000 individual analyses from different PFAS source locations) on the relative detection of individual PFAS (in each analysis data set) help to distinguish between different PFAS sources. The absence (or low frequency of detection) of specific PFAS in samples from one type of site can also be used in the same way. Experiments with over 800,000 individual analyses of samples from various PFAS source locations show very clearly these differences depending on the PFAS source (NAS: 2023).

- **Concentration distributions:** These data help to determine the relative distribution of individual PFAS found in environmental samples from different locations. The average concentration of individual PFAS from the samples examined is used in the MVA assessment (see Fig. 7a - d). These data provide information on the relative proportion of different PFAS sources in a given site type, as well as the relative presence of PFAS associated with different sources.

- **PFAS composition ratios:** These ratios show the general distribution of PFAS within the sample groups. This includes the percentage of perfluoroalkyl carboxylic acids (PFCAs), perfluoroalkyl sulphonic acids (PFSAs) and non-perfluoroalkyl acids (non-PFAAs) relative to the total of overlapping PFAS mixtures (e.g. present in groundwater). The application of this methodology also includes the quantification of concentration ratios between frequently detected individual PFASs.

- **Statistics for identifying and characterizing sources of PFAS using multi-vector analysis (MVA):**

The results of the PFAS source determination are presented in five different types of statistical visualizations of PFAS source categories. These five types of MVA are:

- **MVA1 : PFAS composition circular diagrams,**
- **MVA2 : Boxplot distribution of concentrations and PFAS histograms,**
- **MVA3 : Average PFAS concentrations and detection frequency: Heat-Maps,**
- **MVA4 : Average PFAS concentration and detection frequency: 'Cross-plots',**
- **MVA5 : Report of PFAS logarithmic average concentrations: Relative and radial point diagrams.**

Additionally AI based Clustering is used for cartographical visualization of geographical PFAS Clusters.

Figure 10 shows a summary of the parameters evaluated for the identification and differentiation of AI-MVA (artificial intelligence-based multi-vector analysis) PFAS sources.

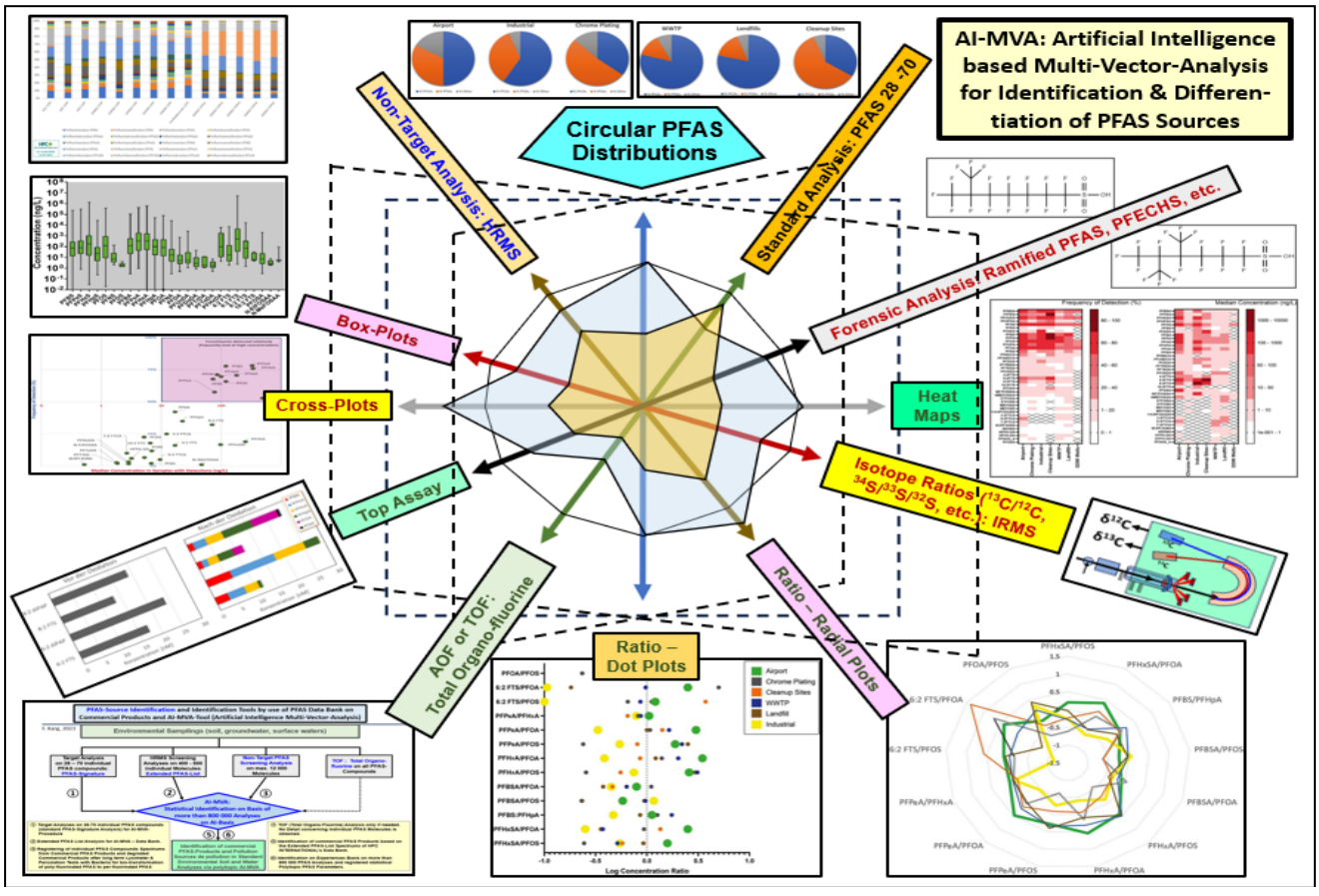

Fig. 10 : Parameters evaluated for the identification and differentiation of PFAS sources additional to AI-Clustering using AI-MVA (artificial intelligence-based multi-vector analysis),

Difficulties:

Some PFAS shows severe problems of laboratory extraction & analysis capabilities, for ex. the perfluoro PFAS of PEFCHS speciations, typical for Aviation Hydraulic oils. The reasons are the different polarities, according the PH Environments, cf. Fig. 11. In this case environmental samples should be treated by extractions under different pH conditions (alkaline, acid and neutral) before analyses.

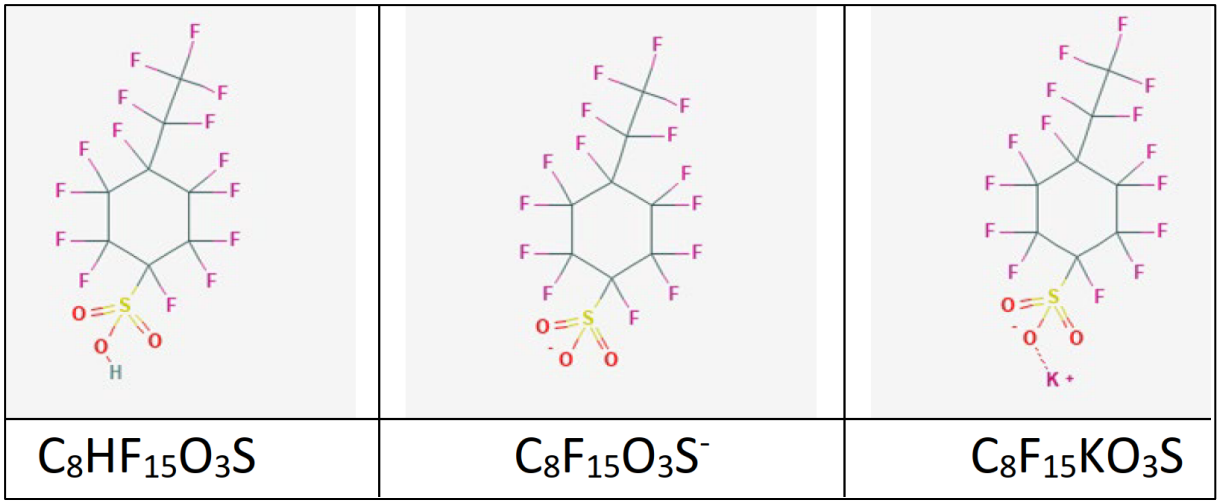

Fig. 11: The perfluoro PFAS speciations of PEFCHS, typical for Aviation Hydraulic oils under different pH conditions (alkaline, acid and neutral) before analyses.

Table 1a & b shows the recommended standard analysis parameters for using the multi-vector analysis (MVA) computer tool with artificial intelligence to identify and differentiate sources of PFAS.

PFAS	LQ Eaux		CAS	VTR	Dir. CE EP2020/ 2184	AM 20/06/23 France
PFBA (acide perfluorobutanoique)	ng/l	1	375-22-4			
PFPeA (acide perfluoropentanoique)	ng/l	5	2706-90-3			
PFHxA (acide perfluorohexanoique)	ng/l	1	307-24-4			
PFHpA (acide perfluoroheptanoique)	ng/l	1	375-85-9			
PFOA linéaire (acide perfluorooctanoique)	ng/l	1	335-67-1			
PFOA ramifié (acide perfluorooctanoique)	ng/l	1	335-67-1			
PFOA totale (acide perfluorooctanoique)	ng/l	1	335-67-1			
PFNA (acide perfluorononanoique)	ng/l	1	375-95-1			
PFDA (acide perfluorodecanoique)	ng/l	1	335-76-2			
PFUnDA (acide perfluoroundecanoique)	ng/l	1	2058-94-8			
PFDoDA (acide perfluorododecanoique)	ng/l	2	307-55-1			
PFTrDA (acide perfluorotridecanoique)	ng/l	1	72629-94-8			
PFTeDA (acide perfluorotetradecanoique)	ng/l	1	376-06-7			
PFHxDA (acide perfluorohexadecanoique)	ng/l	2	67905-19-5			
PFODA (acide perfluorooctadecanoique)	ng/l	1	16517-11-6			
PFBS (acide perfluorobutane sulfonique)	ng/l	1	375-73-5			
PFPeS (acide perfluoropentane sulfonique)	ng/l	1	2706-91-4			
PFHxS linéaire (acide perfluorohexane sulfonique)	ng/l	1	355-46-4			
PFHxS ramifié (acide perfluorohexane sulfonique)	ng/l	1	355-46-4			
PFHxS totale	ng/l	1	355-46-4			
PFHpS (acide perfluoroheptane sulfonique)	ng/l	1	375-92-8			
PFOS linéaire (acide perfluorooctane sulfonique)	ng/l	1	1763-23-1			
PFOS ramifié (acide perfluorooctane sulfonique)	ng/l	1	1763-23-1			
PFOS totale (acide perfluorooctane sulfonique)	ng/l	1	1763-23-1			
PFDS (acide perfluorodecane sulfonique)	ng/l	1	335-77-3			
4:2 FTS (acide 4:2 fluorotelomer sulfonique) H4-PFOS	ng/l	1	757124-72-4			
6:2 FTS (acide 6:2 fluorotelomer sulfonique)	ng/l	1	27619-97-2			
8:2 FTS (acide 8:2 fluorotelomer sulfonique)	ng/l	1	39108-34-4			
10:2 FTS (acide 10:2 fluorotelomer sulfonique)	ng/l	1	120226-60-0			
MePFOSAA (acide N-méthylperfluorooctane sulfonamide acétique)	ng/l	1	2355-31-9			
EtFOSAA (acide N-éthylperfluorooctane sulfonamide acétique)	ng/l	1	2991-50-6			
PFOSA linéaire (perfluoro-n-octanesulfonamide)	ng/l	2	754-91-6			
PFOSA ramifié (perfluoro-n-octanesulfonamide)	ng/l	2	754-91-6			
PFOSA totale (perfluoro-n-octanesulfonamide)	ng/l	2	754-91-6			
MeFOSA linéaire (N-méthylperfluorooctanesulfonamide) (MePFOSA)	ng/l	1	31506-32-8			
6:2-FTAB (6 :2 fluorotelomer sulfonamido propyl betaine) Capstone B	ng/l	10	34455-29-3			

Table 1a: Recommended standard analysis parameters for using the multi-vector analysis (MVA) computer tool with artificial intelligence to identify and differentiate sources of PFAS.

PFAS	LQ Eaux		CAS	VTR	Dir. CE EP2020/ 2184	AM 20/06/23 France
MeFOSA ramifié (N-méthylperfluoro-n-octanesulfonamide) (MePFOSA)	ng/l	1	31506-32-8			
MeFOSA totale (N-méthylperfluoro-n-octanesulfonamide) (MePFOSA)	ng/l	1	31506-32-8			
8:2 DiPAP (8:2 polyfluoroalkyl phosphate diester)	ng/l	1	678-41-1			
HFPO-DA (acide hexafluoropropyleneoxide dimer) Gen X	ng/l	1	13252-13-6			
EtFOSA linéaire (N-éthylperfluorooctanesulfonamide) (EtPFOSA)	ng/l	1	4151-50-2			
EtFOSA ramifié (N-éthylperfluorooctanesulfonamide) (EtPFOSA)	ng/l	1	4151-50-2			
EtFOSA totale (N-éthylperfluorooctanesulfonamide) (EtPFOSA)	ng/l	1	4151-50-2			
MeFBSAA (perfluorobutanesulfonamide(N-méthyl)acetate)	ng/l	5	159381-10-9			
5:3-FTCA: 5:3 acide carboxylique fluorotélomère)	ng/l	1	914637-49-3			
6-2-FTCA: 6:2 acide carboxylique fluorotélomère	ng/l	5	53826-12-3			
8:2 FTUCA (acide 2H-perfluoro-2-décenoique)	ng/l	1	70887-84-2			
DONA (acide 4,8-dioxa-3H-perfluorononanoique)ADONA	ng/l	1	919005-14-4			
MeFBSA (n-méthylperfluorobutanesulfonamide)	ng/l	1	68298-12-4			
PFBSA (perfluorobutanesulfonamide)	ng/l	1	30334-69-1			
PFECHS (acide perfluoro-4-éthylcyclohexanesulfonique)	ng/l	1	646-83-3			
PFNS (acide perfluorononane sulfonique)	ng/l	1	68259-12-1			
PFDoDS (acide perfluorododecane sulfonique)	ng/l	1	79780-39-5			
6:2 diester de phosphate fluorotélomérique. 6:2 diPAP	ng/l	10	57677-95-9			
6:2 8:2 diester de phosphate fluorotélomérique. 6:2 8:2 diPAP	ng/l	10	943913-15-3			
PFHxSA (perfluorohexanesulfonamide)	ng/l	1	41997-13-1			
PFUnDS (acide perfluoroundecane sulfonique)	ng/l	2	749786-16-1			
PFTrDS (acide perfluorotridecane sulfonique)	ng/l	2	791563-89-8			
EtFOSE (2-(N-ethylperfluoro-1-octanesulfonamido)-ethanol)	ng/l	5	1691-99-2			
MeFOSE (2-(N-methylperfluoro-1-octanesulfonamido)-ethanol)	ng/l	5	24448-09-7			
NFDHpA (Nonafluoro-3,6-dioxaheptanoic acid)	ng/l	1	151772-58-6			
PFMPA (Perfluoro-3-methoxypropanoic acid)	ng/l	1	377-73-1			
PFMBA (perfluoro-4-methoxybutanoic acid)	ng/l	1	863090-89-5			
C6O4 (Perfluoro([5-methoxy-1,3-dioxolan-4-yl]oxy)acetic acid)	ng/l	10	1190931-41-9			
6:2-FTOH (6:2 fluorotelemer alcohol) FHET	ng/l	20	647-42-7			
8:2-FTOH (8:2 fluorotelemer alcohol) FOET	ng/l	10	678-39-7			
PFAS Ultrashorts :						
TFA (trifluoroacetic acid)	ng/l	10				
PFPrA (perfluoropropanoic acid)	ng/l	10				
TFMS (trifluoromethanesulfonic acid)	ng/l	10				
PFES (perfluoroethanesulfonic acid)	ng/l	10				
PFPrS (perfluoropropanesulfonic acid)	ng/l	10				

Table 1b: Recommended standard analysis parameters for using the multi-vector analysis (MVA) computer tool with artificial intelligence to identify and differentiate sources of PFAS.

Summary

In the context of groundwater pollution by PFAS, it is becoming increasingly important to identify and, above all, to differentiate the contribution of each PFAS source to pollution plumes. This need for clarification of the contribution of each PFAS source to pollution, e.g. in the vicinity of catchments (for drinking water, etc.), is becoming increasingly crucial for the protection of water resources, (shared) responsibilities and the search for the (multiple) origins of pollution in the context of legal expertise.

Some PFAS shows severe problems of laboratory extraction & analysis capabilities, for ex. the perfluoro PFAS of PEFCHS speciations, typical for Aviation Hydraulic oils. The reasons are the different polarities, according the pH Environments. In this case environmental samples should be treated by extractions under different pH conditions (alkaline, acid and neutral) before analyses.

To conclude, it is now possible (using comprehensive statistical, graphical & chemical-mathematical studies, including Artificial Intelligence based Clustering with Machine Learning) to use the Multi-Vector-Analysis (MVA) in several dimensions to identify and differentiate the sources of PFAS pollution in soils, groundwater and surface water, and in some cases even to identify the commercial PFAS products causing the pollution.

The procedure principles for identifying and differentiating potential PFAS Sources are the following:

A. Lots of different Statistical Comparisons of Sample analyses with registered Standards of chemical PFAS Spectrums on about 70 analyzed compounds from commercial PFAS Products (AFFF, Galvanic products, Paper related production Products, Surfactants mixtures, etc.).

B. Identification and Differentiation of PFAS Clusters by MVA on Artificial Intelligence via Clustering.

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