CREW CENTRE OF EXPERTISE FOR WATERS

Developing risk assessment approaches for PFAS and watch list parameters under the recast Drinking Water Directive

PFAS, 17ß-estradiol, nonylphenol

Carolin Vorstius, John Rowan, Iain Brown, Sarah Halliday, and Sarah Hendry

United Nations
Educational, Scientific and
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Glossary

Term	Definition (source)	Application in the project
Drinking water supply system	Treatment works and its connected supply system (The Public Water Supplies (Scotland) Regulations 2014)	This term covers all parts of the public water supply from catchment to customer tap
Hazard	Biological, chemical, physical or radiological agent in, or condition of water, with potential to cause harm to public health (BS EN 15975-2)	Relates to emerging contaminants of concern - individual PFAS or sum of PFAS; 17ß-estradiol (E2); 4-nonylphenol (NP)
Hazardous event	Event that introduces hazards to, or fails to remove them from, the drinking water supply system (BS EN 15975-2)	Presence of sources for PFAS/E2/NP in the catchment, treatment, or distribution system
Exposure	The (degree of) contact with the hazard	Concentration of PFAS/E2/NP in drinking water
Vulnerability	Propensity or predisposition to be adversely affected (IPCC)	Potential adverse health effects arising from exposure to PFAS/E2/NP
Risk	Combination of the likelihood of a hazardous event and the severity of consequences, if the hazard occurs in the drinking water supply system (BS EN 15975-2)	Likelihood of drinking water concentrations above thresholds (standards/guidance values)
Likelihood	The chance of a specific outcome occurring, where this might be estimated probabilistically (IPCC)	Relative likelihood refers to higher or lower chance for the specific outcome
Consequence	Result or effect, typically undesirable	Effect on human or environmental health from pollution
Risk assessment	Assessment of the drinking water supply system so as to establish whether or not there is a significant risk of supplying unwholesome water (The Public Water Supplies (Scotland) Regulations 2014)	Assessment of the likely presence and concentration of PFAS/E2/NP in the drinking water supply system
Raw water presence potential (RWPP) assessment	Assessment of hazardous events for raw water	Assessment of the relative likelihood for presence of the emerging contaminant of concern (PFAS/E2/NP) in raw water
Source-pathway-receptor model	Concept used in environmental risk assessment describing delivery from source via pathway to receptor	Applied in the context of a catchment
Source	Origin of the hazard	Point or area from which PFAS/E2/NP are released to the environment
Pathway	Mechanisms by which the hazard (contaminant) is transmitted through the environment	Conditions that mitigate or facilitate the movement of PFAS/E2/NP through air, vegetation, soils, rock, and water
Receptor	Who or what is affected by the hazard	Supply source/freshwater body that receives PFAS/E2/NP
Water supply source	The water body from which raw water is abstracted into the treatment system	Reservoir, loch, river, spring or borehole used for drinking water abstraction
Catchment	The area of land from which water flows into a river, lake, or reservoir	Area of land from which water flows into the water supply source
Verification	Routine confirmation, through the provision of objective evidence, that the drinking water supply system is delivering water in accordance with the set objectives and that the risk management approach is effective (BS EN 15975-2)	Comparison of relevant water sampling data to scores derived from risk assessment/assessment of raw water presence potential
Validation	Obtain evidence, assessment, and approval of the capability of the current or proposed control measures (BS EN 15975-2)	Before and after treatment sampling

Executive Summary

Purpose of research

The research project assessed potential presence of per- and polyfluoroalkyl substances (PFAS), 17ß-estradiol, and nonylphenol for drinking water supply sources in Scotland, to identify high risk areas and enable prioritisation of monitoring and additional knowledge generation.

Background

PFAS are a class of synthetic chemicals produced since the 1940s, with broad application such as in packaging, textiles, and firefighting foam. They are persistant, toxic and bioaccumulative and have been linked to detrimental impacts on childhood development, cancers, and immune system disorders. Nonylphenol and 17ß-estradiol are endocrine-disrupting chemicals. Increased exposure to endocrine disruptors are connected to cancer, reduced fertility and obesity. Due to increasing awareness of the widespread occurrence of these substances in the environment, there is concern over their potential presence in drinking water sources and final drinking water.

In January 2023, a new standard for PFAS was introduced for Scottish drinking water, and a watch list established that includes guidance values for 17ß-estradiol and nonylphenol. Drinking water providers therefore need to ensure that the standard for PFAS are adhered to and establish monitoring for the presence of 17ß-estradiol and nonylphenol. For effective monitoring and treatment, understanding of the spatial and temporal patterns of risk for raw water pollution is crucial.

Key findings

Some risk factors for raw water presence potential of PFAS are: manufacturing plants where PFAS are produced or used; waste products and waste management facilities such as landfills, wastewater discharges, and sludge; sites where waste products are applied to land; sites where PFAS containing products are stored or applied; areas where PFAS from the atmosphere are deposited on land and/or surface water. The assessment found areas and catchments with higher potential for presence of PFAS in untreated drinking water especially along the central belt and East of Scotland, reflecting higher population densities.

- Risk factors for raw water presence potential of 17ß-estradiol are sites where concentrated animal or human excretion are emitted, such as wastewater discharges, areas of manure or sludge/biosolid application, and areas/sites with high livestock densities. Areas and catchments with higher potential for presence of 17ß-estradiol in untreated drinking water were identified for the Northeast and South of Scotland, reflecting agricultural land use pressures.
- Risk factors for raw water presence potential of nonylphenol are sites of waste management such as landfills and water treatment, with these sites emitting nonylphenol through leachate and discharge as well as to the atmosphere. Risk factors are thus also atmospheric deposition and application of wastewater treatment products to land. The assessment identified the central belt and Northeast of Scotland as having the highest potential for presence of nonylphenol in untreated drinking water.

Recommendations

1. Monitoring needs to be risk-based, systematic and deductive to allow verification and continuous improvement of risk assessment, and to build an evidence base for the occurrence and concentration of contaminants of concern in Scotland. This is especially important when setting up a monitoring strategy for emerging contaminants as knowledge is generally sparse.
2. Relevant data (from monitoring, registers of import, or applications to land of products containing the chemicals) should, if possible, be made available across agencies and pooled to enable a more complete picture and better analysis options.
3. Targeted sampling and analysis can address specific knowledge gaps to be fed back into risk assessment and provide a basis for regulation and mitigation.
4. Regulatory tools for source control exist in Scotland and can be employed balancing available evidence and precaution.

1 Introduction

1.1. Background and scope

In January 2021, the revised EU Drinking Water Directive (2020/2184 Recast) entered into force. The Scottish Government continues to follow EU legislation and implemented the revision into Scots law through amendment (SSI 2022/387) to the Public Water Supplies (Scotland) Regulations 2014 '(as amended). Among other changes, a new standard for per- and polyfluoroalkyl substances (PFAS) was introduced as a sum of 20 individual PFAS. The recast EU Directive also provides for a watch list of substances and compounds of concern, which was adopted by the European Commission in January 2022 but has not been implemented into Scots law. This list includes guidance values for two parameters, 17ß-estradiol (E2) and nonylphenol (NP).

PFAS are a class of synthetic chemicals produced since the 1940s, with broad applications such as in packaging, textiles, and firefighting foam (Gaines, 2023; Glüge *et al*., 2020). In recent years, concerns have been growing because of their widespread occurrence in the environment (Evich *et al*., 2022). PFAS are not easily degraded and bioaccumulate, and are linked to detrimental impacts on childhood development, cancers, and immune system disorders (Chohan *et al*., 2021). PFAS have been detected in air, wastewater, freshwater, drinking water, soils, plants, animals, food products, and human blood/serum (Bansal *et al*., 2022; Kurwadkar *et al*., 2022; Meegoda *et al*., 2020; Stoiber *et al*., 2020).

NP and E2 are endocrine-disrupting chemicals. E2 is a naturally occurring hormone in mammals and enters the freshwater environment primarily where human or livestock excretions reach surface or groundwater (Ciślak *et al*., 2023). NP is used in plastics or occurs in the environment as a by-product of nonylphenol ethoxylates (NPEO), used e.g. in detergents or pesticides, and enters the freshwater environment through industrial and domestic wastewater discharges and from agricultural runoff (Bhandari *et al*., 2021). Both substances have been detected in wastewater and freshwaters, including in drinking water sources (Carvalho *et al*., 2015; Forghani *et al*., 2018; Gałązka & Jankiewicz, 2022).

Due to the widespread occurrence of these substances in the environment, there is concern over their potential presence above WHO guidelines in Scottish drinking water sources. Although there is no statutory requirement for monitoirng of NP and E2, unless indicated by a risk assessment. The public water supplier has a statutory requirement to monitor presence and concentrations of contaminants in drinking water supplies. To control risk to public health, understanding patterns of contamination is crucial for the management of both public and private drinking water supplies. In the absence of comprehensive analytical data to inform about occurrence and concentration in Scottish freshwaters, a risk-based approach is warranted that includes potential sources of these substances and their likelihood of reaching drinking water supplies. Strategic monitoring based on perceived risks then informs and refines further development of the risk evaluation, leading to a continuously improving knowledge and information base to assess and manage risks.

1.2. Project objectives

The research project conducted Raw Water Presence Potential (RWPP) assessments for PFAS, E2, and NP. These assessments had the purpose to understand the likelihood for presence of the contaminants in Scottish public drinking water supply sources before treatment. This supported identification of high-risk supplies and enabled systematic monitoring and priority setting for additional knowledge generation.

To this end, the project identified risk factors for the presence of the pollutants in surface and groundwater, including direct and indirect contamination sources, and processes involved in transfer to and retention in freshwater systems. The project then evaluated public drinking water abstraction catchments in terms of the presence of the identified risk factors and catchment sensitivity to them. The project discussed gaps in data and knowledge and gives recommendations to support further understanding of contaminant sources and pathways to drinking water sources, and to enable regulation and mitigation. The assessments also serve as a blueprint to discuss how this framework can be developed and applied more generally to emerging contaminants in a drinking water context to support robust, science-led, and strategic risk assessment.

1.3. Structure of the report

Section 2 of the report briefly outlines the methodology of the research carried out, with more details in Appendix A. Section 3 presents the findings by first describing the identified risk factors, (with the detailed results of the literature review provided in Appendix B), and the outcomes of the RWPP assessment for each the three substances or group of substances of interest (3.1 – 3.3). The results are discussed (3.4) and suggestions made for improving the assessments (3.5), leading to broader observations on approaches to risk assessing emerging contaminants in a drinking water context (3.6). Section 4 provides an overview of identified gaps in knowledge and data that need to be addressed to improve preparedness for and management of emerging pollutants through the existing regulatory framework described in Appendix C.

2. Research undertaken

Based on currently available knowledge, the project carried out RWPP assessments for PFAS, E2 and NP for Scottish drinking water sources, with a focus on the public water supply. The following section describes the research approach, which included a literature review, spatial analysis and mapping to represent potential contaminant sources and transfer to surface and groundwater. This provided the basis for understanding likelihood of finding contaminants in drinking water supply sources.

As underpinning concept, the source-pathway-receptor model was used, providing an adaptable framework to describe interactions in complex systems (e.g., Waldschläger *et al*. 2020). This concept was applied in a catchment system context and entailed identifying potential sources of the contaminants, understanding the way they travel through the environment (pathways), and identifying freshwater receptors.

2.1. Literature review

A literature review was carried out to establish the available knowledge base (Appendix A.1). It identified direct and indirect sources, pathways, and freshwater receptors. The findings were encapsulated into risk factors for the presence of PFAS, E2 and NP in surface and groundwater. The available literature was also reviewed to synthesise available information and evidence of occurrence nationally and globally, and to establish current treatment ability. The literature review was enhanced by stakeholder interviews to better understand perception of risk related to these substances, and available information on risks and impacts specifically for Scotland (Appendix A.2).

2.2. Assessment

For each potential contaminant source identified through the literature review, a risk factor map (layer) was created. To create risk factor geospatial layers, data representing these sources were extracted into GIS shapefiles (Appendix A.3). Where possible, open-source, freely accessible data were utilised to enhance the replicability and transferability of the assessment approach. Pathways risk factors that were identified from the literature to facilitate/enable the movement of contaminants to freshwater receptors, were also extracted into relevant geospatial layers (i.e., raster or shapefiles as appropriate). All risk factor layers were created and visualised using QGIS 3.16.15 (Hannover) at a national spatial scale (Table 2.1). This resulted in a geodatabase for each contaminant that included spatial representations for identified sources and pathways with a national (Scotland) coverage.

To conduct the RWPP assessments for public water supply catchments in Scotland, Scottish Water catchment delineations were used. From the created risk factor layers, all risk factor features for each catchment were counted, or the percentage area derived. To achieve comparability across catchments of different sizes, counts and line lengths were transformed into risk factor densities (divided by catchment area).

To achieve comparability of scale between all risk factors, the derived risk factor densities were normalised with min-max normalisation[1]. **This resulted in all risk factors having a range of values between 0-1, with the catchment with the highest density/area percentage receiving a 1, and the one with the lowest receiving a 0**. For the overall risk rating, the normalised scores for all risk factors were added together for a first assessment. To include a pathway consideration, an alternative RWPP assessment was derived by weighting the score more heavily if the feature lay on an identified

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[1] While the majority of risk factors were normalised by its own value range, livestock values were normalised over the value range of some species: Alpacas, llamas and other camelids, deer, donkeys, horses and cattle were normalised over the range of cattle values, sheep and goats were normalised over the range of sheep values, pigs were normalised over the range of pig values and poultry over the range of poultry. This was done as they were seen as having the same impact by animal, rather than by highest density.

Table 2.1: List of risk factor layers prepared for the RWPP assessments per substance.

PFAS	E2	Nonylphenol
Shapefiles (points)		
Airports Electrical infrastructure Fire brigade stations Industrial Estates Landfills Metal recyclers Ore mines Renewable energy sites Septic tanks (modelled) Septic tanks (registered) Ski Infrastructure Telecommunications Waste management discharge points Wastewater discharge points	Agricultural sites Septic tanks (modelled) Septic tanks (registered) Wastewater discharge points	Landfills Septic tanks (modelled) Septic tanks (registered) Waste management discharge points Wastewater discharge points
Shapefiles (lines)		
Roads		
Shapefiles (polygons)		
Arable area Area for biosolid application Area for paper and pulp waste spreading Area for atmospheric deposition around arable land Area for atmospheric deposition around point sources Areas with median soil pH of 6 or above Areas above moderately or highly productive aquifers	Arable area Improved grassland area Livestock counts: • Total cattle • Total alpacas • Total llamas • Total other camelids • Total horses • Total donkeys • Total deer • Total sheep • Total goats • Total pigs • Total poultry • Unspecified Wild deer count Areas above moderately or highly productive aquifers	Area for biosolid application Area for paper and pulp waste spreading Area for atmospheric deposition around point sources Areas above moderately or highly productive aquifers
Raster		
Slopes		Slopes
Rainfall		

condition[2]. The resulting scores were again added for the final score (Figure 2.1).

This method resulted in a relative assessment across the specific set of catchments (i.e., all public water supply catchments as provided by Scottish Water). This means that a score does not relate to an absolute risk (such as a concentrations range or threshold) but allows a ranking of the included catchments. **Due to normalisation, risk factors were assigned equal weight insofar that the highest density/area percentage for risk factors were assumed to be equally impactful**. For example, the catchment with the highest density of airfields would be allocated a risk score of 1 for this risk factor – the same as the catchment with the highest density of wastewater discharges. This is therefore unrelated to the actual density/area percentage but views each risk factor in relation to the rest of the catchments under consideration.

For verification of the assessment, PFAS and NP concentration data were available from Scottish Water monitoring, spanning 01/01/23 to 13/10/23. The samples included source water (no mixing of supply sources or with already treated water), and

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[2] Source risk factors features on pathways risk factor areas were by multiplied a factor of two. Where source features were on both included pathways (soil pH and aquifer productivity), they were multiplied by a factor of three. To achieve comparability for the risk factors excluded from these considerations, their score was automatically multiplied by a factor of three. For the pathway consideration for atmospheric deposition, the score for area of deposition was multiplied by the score for mean slope.

Example catchment: 10 km^2

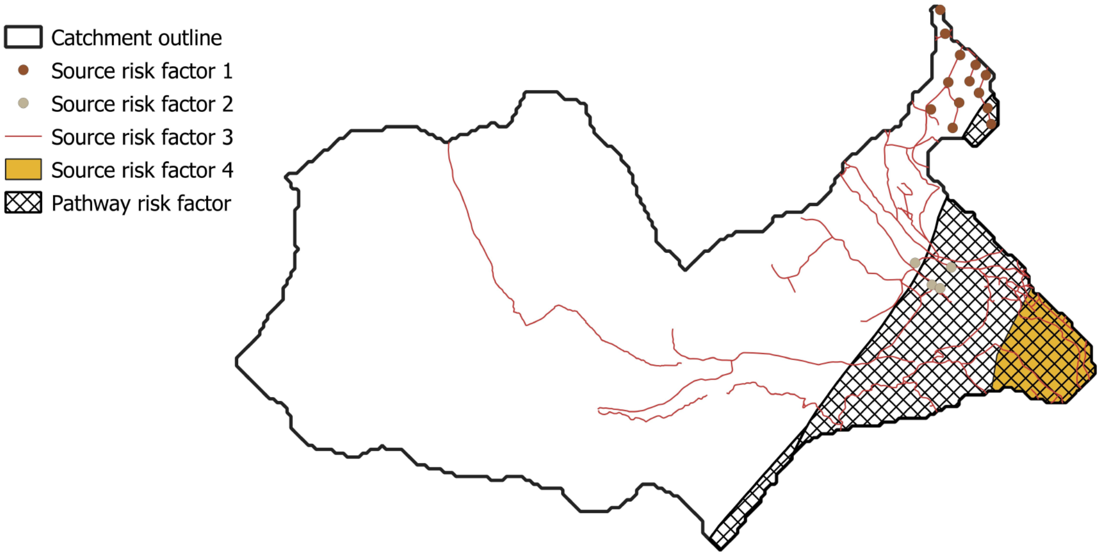


Figure 2.1: Simplified worked example of assessment score calculation. Catchment outline shown with risk factors (points, lines or areas) that are present in the catchment. Numbers for illustration only.

CALCULATION OF ASSESSMENT SCORE:

Equal weight:

- Source risk factor 1:
  Count (*13*) -> covert to density: count/area (*1.3*) -> normalise over range of densities for this risk factor of all catchments: (Catchment value – minimum value)/(Maximum value - minimum value) ((*1.3-0*)/(*2-0*)=***0.65***)
- Source risk factor 2:
  Count (4) -> convert to density (*0.4*) -> normalise ((*0.4-0*)/(*5-0*)=***0.08***)
- Source risk factor 3:
  Sum length (*20*)-> convert to density (*2*) -> normalise ((*2-0.8*)/(*6-0.8*)=***0.23***)
- Source risk factor 4:
  Percentage area (*18*) -> normalise ((*9-0*)/(*100-0*)=*0.09*)
- Add all (*0.65+0.08+0.23+0.09=****1.05***)

Pathway consideration: double weight to source risk factors on pathway risk factor

- Source risk factor 1:
  Count on pathway (2), outwith pathway (*11*) -> convert to density (*0.2/1.1*) -> normalise (*0.1/0.55*) -> multiply and add (*0.1*2+0.55=****0.75***)
- Source risk factor 2:
  Count on pathway (*3*), outwith pathway (*1*) -> convert to density (*0.3/0.1*) -> normalise (*0.06/0.02*) -> multiply and add (*0.06*2+0.02=****0.14***)
- Source risk factor 3:
  Sum length on pathway (*9*), outwith pathway (*11*) -> convert to density (*0.9/1.1*) -> normalise (*0.019/0.21*) -> multiply and add (*0.019*2+0.21=****0.248***)
- Source risk factor 4:
  Percentage area on pathway (*18*), outwith pathway (*0*) -> normalise (*0.09*) -> multiply (*0.09*2=****0.18***)
- Add all (*0.75+0.14+0.248+0.18=****1.318***)

raw water (water entering water treatment works). The sampling for PFAS included 20 substances, sampled for at 194 locations, with a total of 277 samples taken; each sample was then analysed for the 20 PFAS listed in the Regulations and the regulatory parameter Sum of PFAS calculated. NP was sampled 123 times, at 61 locations. There was no recent sampling data available for E2. The sample results were mapped to get a first impression of the capability of the RWPP assessments to identify where the substances may occur in raw water in concentrations above their detection limits. For mapping, the sample locations needed to be matched to a catchment. Therefore, 59 locations were not included in the visualisation as only source water samples and raw water samples that could be matched to a single catchment were considered.

3 Findings

The following sections summarise key points for identifying risk factors to inform the RWPP assessments, and present and discuss the results of the assessments. Details from the review of the literature can be found in Appendices B.1 – B.3. A summary of stakeholder interviews is provided in Appendix B.4.

3.1. PFAS

PFAS are regulated through import, manufacturing and use restrictions, environmental standards and drinking water standards. In the recast EU drinking water directive, an EU standard of 0.1 µg/l is set for a sum of 20 compounds, comprising perfluoroalkylated carboxylic acids (PFCAs) and perfluoroalkylated sulfonic acids (PFSAs) with chain lengths of 4-13 carbons. These compounds are often the end product of other PFAS degrading in the environment, as well as being manufactured and used in their own right (Evich *et al*., 2022). The group of chemicals summarised as PFAS however comprises more than four thousand substances, to which is added by newly created PFAS, and have varying characteristics leading to differences in behaviour in the environment and in impact, both on the environment as well as on human health (Chohan *et al*., 2021).

3.1.1. Identification of risk factors

Source risk factors: Today, PFAS are near ubiquitous in the environment in low concentrations, due to their widespread use and ability to be transported by air, water, and through soils (Meegoda *et al*., 2020). Areas at risk of experiencing elevated concentrations are those with occurrence of:

- Sites of PFAS manufacture, or where PFAS are used in the manufacturing of other products
- Sites where PFAS get concentrated, such as landfills, waste incineration and wastewater treatment plants
- Sites where concentrated waste products, such as biosolids, are applied to land
- Sites where products containing PFAS, such as aqueous film forming foams (AFFF), are stored or applied
- Sites where waste containing PFAS leaks into the environment, such as septic tanks or mines
- Sites where large quantities of products containing PFAS directly emit them onto land or into the atmosphere, for example ski areas (PFAS can be present in ski wax) or wind farms (from PFAS applied to rotor blades), or from use in infrastructure that needs to withstand harsh environmental conditions.
- Some PFAS compounds are volatile and can be emitted into the air, allowing them to travel some distance (>150 km) from the site of emission. PFAS deposition from the atmosphere is mainly by rainfall. Subsequent redistribution and fate of such atmospheric sources is akin to non-point source pollutant transport by river solute and sediment-associated mechanisms.
- Atmospheric deposition of PFAS is likely to be highest in closer proximity to emission sources and concentrations in soil and water will typically reduce with increasing distance. A study by Chen *et al*. (2018) showed that most of the long-chain PFAS compounds (>75%) are deposited within a 5 km range of the source.

The RWPP assessment for PFAS needs to include the above listed sites as point or diffuse sources. Risk is assumed to be higher if sources are present in the catchment, or if sources likely to have PFAS emissions to atmosphere are within close proximity to the catchment boundary which makes it likely that higher amounts of PFAS reach the catchment through atmospheric deposition. Catchments receiving higher rainfall amounts could also be more vulnerable from atmospheric deposition.

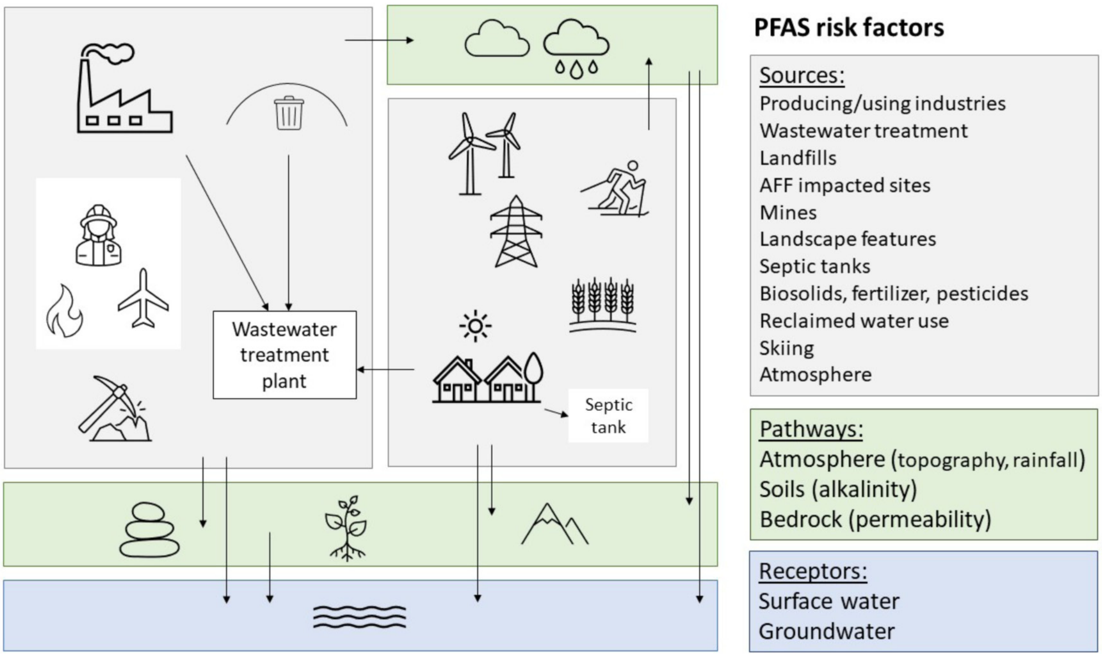


Figure 3.1: Overview of risk factors for the presence of PFAS in drinking water sources, and their relationships.

Pathway risk factors: PFAS can reach the catchment through the atmosphere, or be directly emitted to soils from a source (from where they can travel to surface and ground water), or they are emitted from a source directly into surface water systems. Soil properties, such as e.g., pH, organic matter content, and ionic strength, play a role in PFAS leaching to freshwater (Kabiri *et al*., 2022), but mobility in the environment will depend mainly on PFAS characteristics, with shorter chain PFAS, and PFCAs, typically being more mobile due to differences in aqueous solubility and adsorption potentials (Lyu *et al*., 2022). Catchment characteristics that facilitate movement of PFAS substances through the environment (higher soil pH, higher ground permeability) can thus be included as pathways in the RWPP assessment.

Receptors: PFAS have been found in surface waters as well as groundwater. While it may be possible to distinguish predominant types of freshwater receptors for PFAS depending on source (e.g., wastewater effluent directly discharged into surface water), surface and groundwater connectivity will blur this distinction. Due to this and current limited knowledge about PFAS movement, all types of supplies were treated equally in the RWPP assessment.

An overview of risk factors and their relationships is provided in Figure 3.1.

3.1.2. RWPP assessment

For PFAS, the catchments at the upper end of the relative score spectrum are concentrated especially along the central belt and East of Scotland (Figure 3.2), which reflects that many risk factors are concentrated in this area due higher population densities. The highest risk score (both with and without pathway consideration) however is allocated to a catchment in the South of Scotland with presence of several risk factors, including wastewater discharges and a high number of septic tanks, as well as proximity to potential sources for atmospheric pollution with PFAS. Most of the medium to higher scoring catchments also have a high score for area of atmospheric deposition.

For some individual catchments, their relative score changed significantly when pathway considerations were incorporated into the assessment (Figure 3.3). However, overall, the spatial pattern does not vary substantially between the RWPP assessments with and without pathway considerations. This is likely because a significant proportion of the catchments have few risk factors, and their risk score is therefore mostly unaffected by pathway considerations.

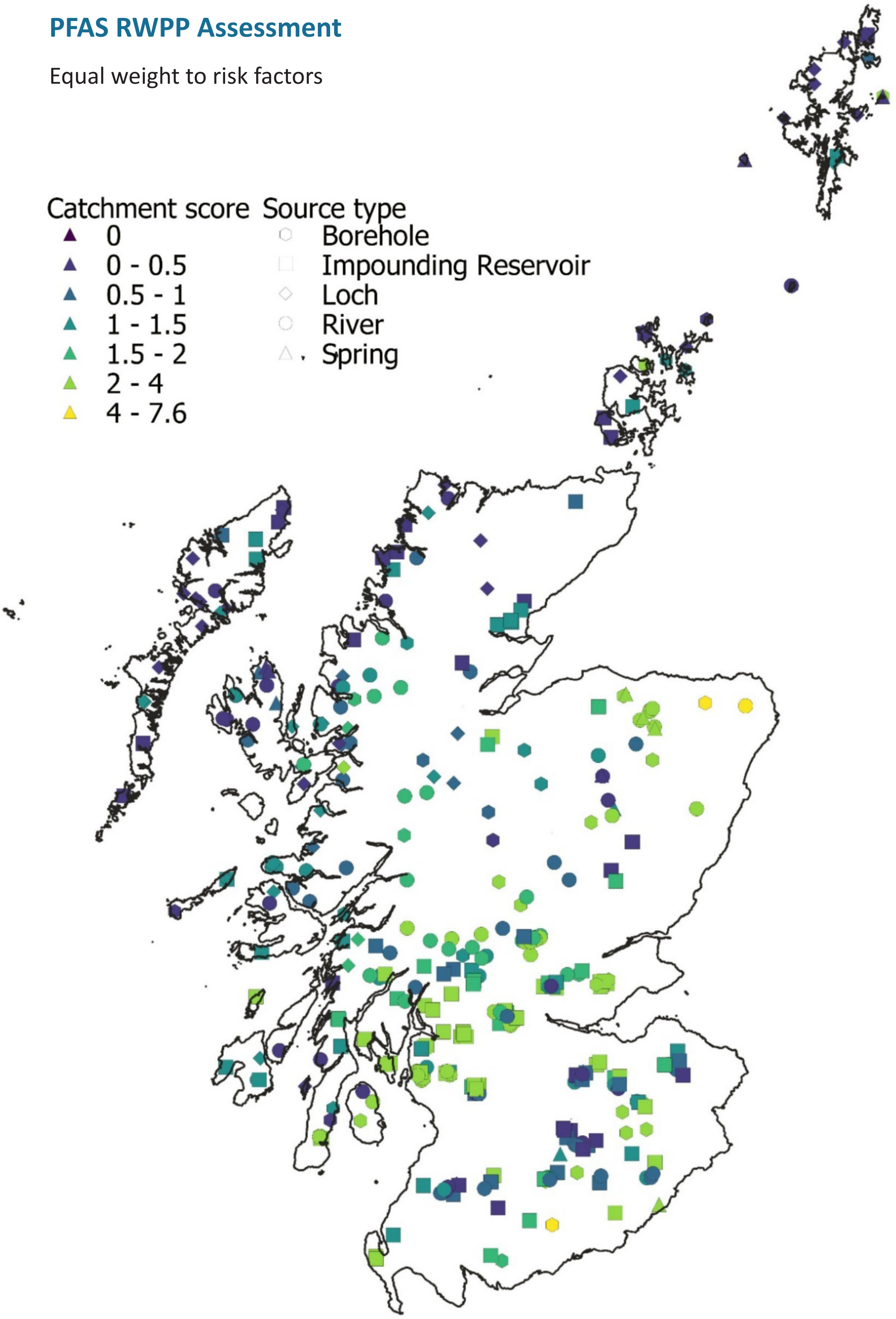


Figure 3.2: PFAS RWPP assessment outcomes when equal weight given to all source risk factors.

PFAS RWPP Assessment

Higher weight to risk factor on moderately or highly productive aquifers and soils with median pH of >6; atmospheric deposition weighted by steepness (mean slope).

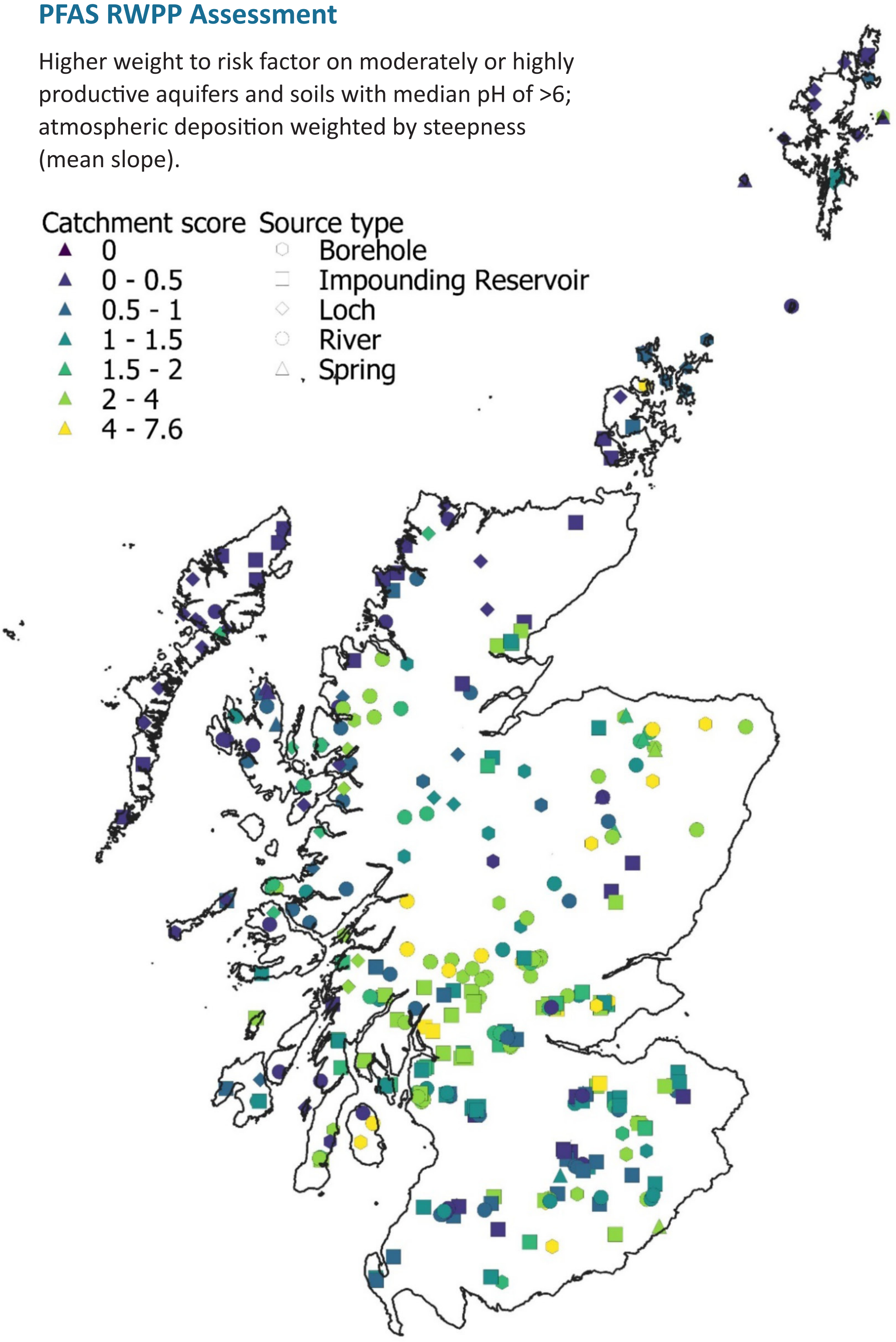


Figure 3.3: PFAS RWPP assessment outcomes when risk factors on identified pathways are attributed higher weight.

3.1.3. Monitoring data

The results of the Scottish Water sampling (from 01/01/23 to 13/10/23) are summarised in Table 3.1 and visualised in Figure 3.4. The most commonly detected PFAS compound was PFBA, followed by PFOA, PFHpA, and PFOS. The highest concentration was detected for PFBA. It was noted that the shorter chain PFAS are detected more often, as well as PFCAs. No clear spatial pattern in detection could be observed.

As the number of samples per each location is very small (many have been sampled only once), and detection has not been consistent at any site, it is unsound to use these to verify or further calibrate the assessment. One interesting point to observe are the relatively elevated PFAS concentrations detected in the Western Isles and the Atlantic seaboard, which were not anticipated in the RWPP assessment. This raises the prospect that one or more risk factors have been overlooked or incorrectly weighted.

Table 3.1: Summary of Scottish Water PFAS sampling data. No. of samples per substance = 277, no. of locations = 194.

Substance	No. of catchments with detection	No. of detections	Maximum concentration detected (µg/l)
Perfluorobutane sulfonic acid (PFBS)	7	20	0.0017
Perfluorobutanoic acid (PFBA)	93	179	0.0062
Perfluorodecane sulfonate (PFDS)	–	–	–
Perfluorodecanoic acid (PFDA)	1	1	0.0003
Perfluorododecane sulfonic acid (PFDoS)	–	–	–
Perfluorododecanoic acid (PFDoDA)	–	–	–
Perfluoroheptane sulfonate (PFHpS)	–	–	–
Perfluoroheptanoic acid (PFHpA)	53	91	0.0012
Perfluorohexane sulfonic acid (PFHxS)	6	11	0.002
Perfluorohexanoic acid (PFHxA)	13	33	0.001
Perfluorononane sulfonic acid (PFNS)	–	–	–
Perfluorononanoic acid (PFNA)	14	20	0.0008
Perfluorooctane sulfonate (PFOS)	33	57	0.0029
Perfluorooctanoic acid (PFOA)	68	123	0.0036
Perfluoropentane sulfonic acid (PFPS)	–	–	–
Perfluoropentanoic acid (PFPA)	12	26	0.0013
Perfluorotridecanoic acid (PFTrDA)	–	–	–
Perfluoroundecane sulfonic acid (PFUnDS)	–	–	–
Perfluoroundecanoic acid (PFUnDA)	1	1	0.0003
Perfluorotridecane sulfonic acid (PFTriS)	–	–	–
Sum of PFAS	105	192	0.0128

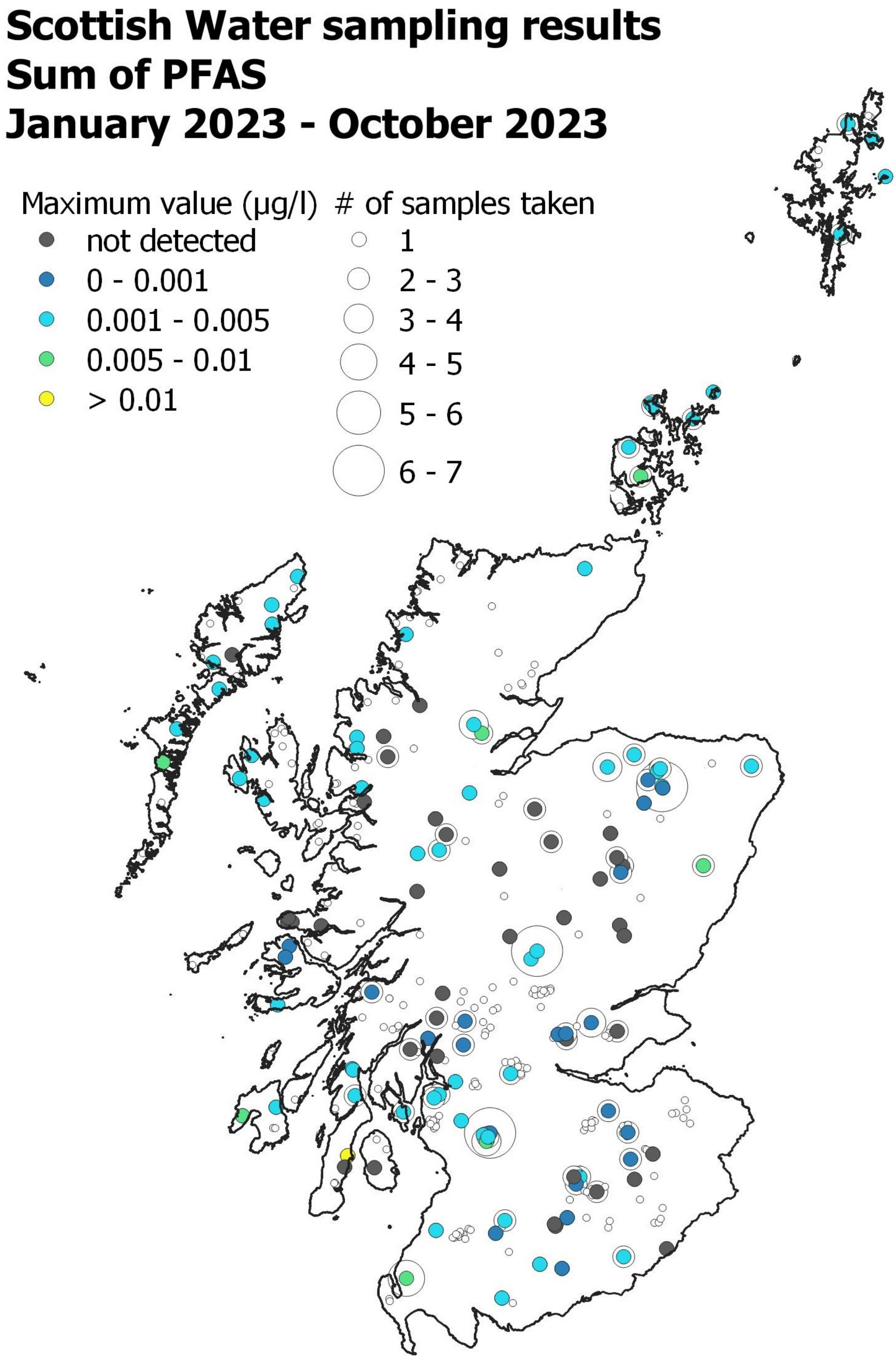


Figure 3.4: Sampling results for Sum of PFAS values from Scottish Water raw water monitoring from 01/01/23 to 13/10/23, with detected maximum concentration (in µg/l) and number of samples taken. Regulatory limit for finished drinking water in Scotland: 0.1 µg/l.

3.2. 17ß-estradiol (E2)

E2 is a natural hormone emitted by humans and animals. The European Commission adopted a watch list of substances in drinking water on 19th January 2022, with E2 one of the two substances included on this first watchlist, next to nonylphenol. The watchlist guidance value for E2 in finished drinking water is 0.001 µg/l. The inclusion of E2 is due to concerns over the effect of human exposure to increased levels of estrogens, which include reduction in male fertility, lower puberty age in girls, obesity, increased rates of breast, ovarian, prostrate and testicular cancer, or endometriosis in humans (Ciślak *et al.*, 2023; Forghani *et al.*, 2018). There are also concerns over effects on wildlife, which include feminization of males, hatch retardation, malformation, growth retardation, or reduced reproductive fitness (Odinga *et al.*, 2022).

3.2.1. Identification of risk factors

Source risk factors: The predominant potential sources of E2 are where human and livestock excretions are concentrated, i.e. wastewater treatment, runoff from fields with high livestock densities and spreading of manure or biosolids (Nazari & Suja, 2016). It has been shown that increased stocking levels of livestock may lead to increased concentrations in freshwater systems (Rechsteiner *et al.*, 2020). Risk factors that can be identified are thus high livestock densities, manure and biosolid application, and farms as point sources.

While E2 can be adsorbed and degraded in wastewater treatment, efficiency varies (Koh *et al.*, 2008). The data available for Scotland seem to indicate some overall effectiveness of wastewater treatment, but also that wastewater effluent presents a potential source of E2 to the environment. Similarly, septic tanks may release E2 to the environment, and due to this typically happening in the subsurface, these systems may present a potential source of E2 especially where they occur at high densities.

Pathway risk factors: Under aerobic conditions, E2 is degraded within a few days, reducing risk of contamination of drinking water supply sources (Johnson *et al.*, 2006). Degradation also reduces the risk of E2 reaching freshwater through runoff from manure and biosolid spreading, although there are also indications that degradation processes might be more complex and slower in the field than laboratory studies suggest (Schoenborn *et al.*, 2015). Higher temperatures increase degradation, and could thus reduce risk. The potential of diffuse sources to contribute to contamination will depend on the hydrologic connectivity to the freshwater source.

Both the hydrological connectivity as well as relationship to temperature are working on a very local level that is difficult to describe through data typically used in a first assessment, so these factors have not been included. The likelihood of reaching groundwater has been included to take account of the fact that E2 is released into the subsurface, has been found in groundwater sources, and may be

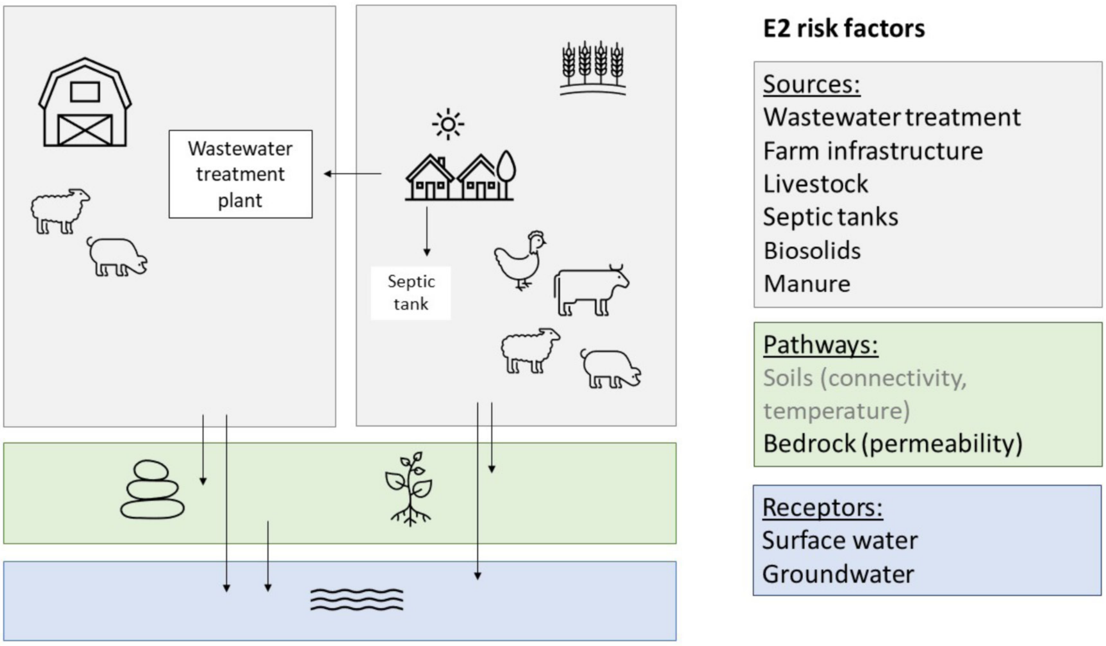


Figure 3.5: Overview of risk factors for the presence of E2 in drinking water sources, and their relationships. Greyed out pathways were identified as important on a local scale but not included in the assessment.

more persistent where groundwater is anaerobic (Ying *et al*., 2003).

Receptors: Due to degradation, groundwater is less likely to be impacted by E2 but all source types have been treated equally for this first assessment. An overview of risk factors and their relationships is provided in Figure 3.5.

3.2.2. RWPP assessment

The highest scoring catchment for E2 is the same Southern catchment as for PFAS. Generally, catchments with the highest scores are found in the Northeast and South of Scotland, as well as on Orkney, presumably reflecting agricultural land use pressures (Figure 3.6).

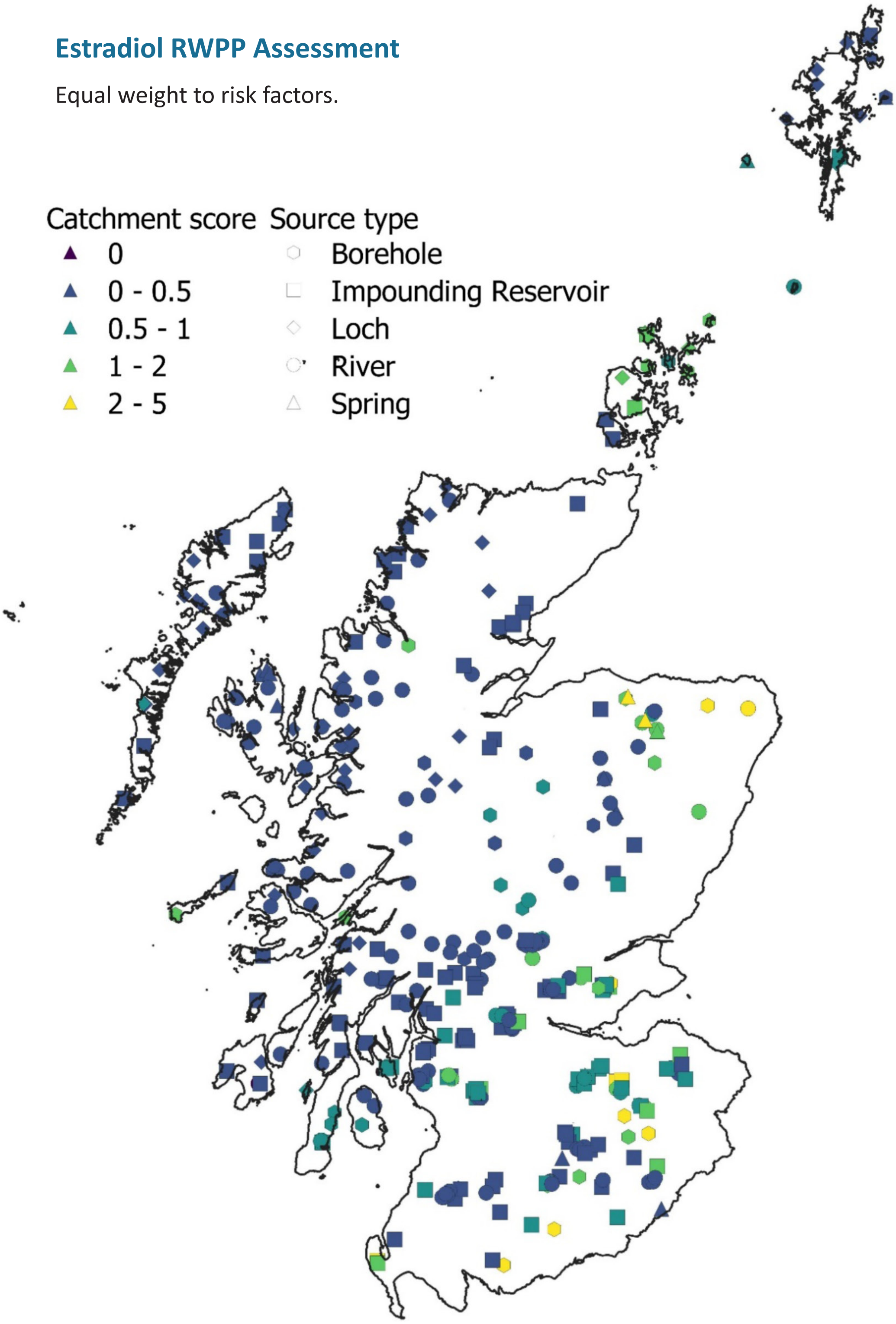
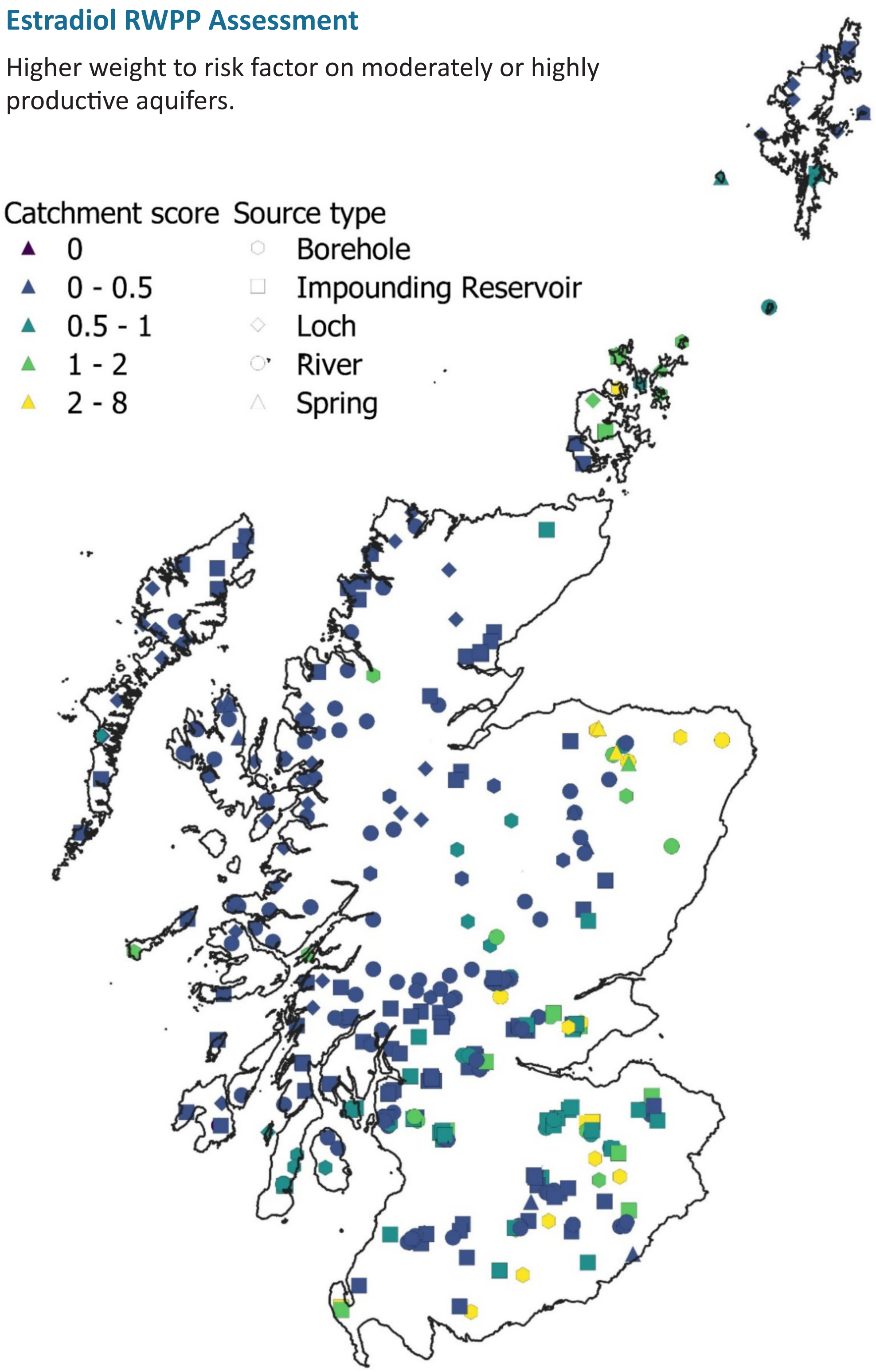


Figure 3.6: E2 RWPP assessment outcomes when equal weight given to all source risk factors.

Pathway considerations tend to exacerbate the difference in scores (Figure 3.7).

3.2.3. Monitoring data

No recent monitoring data was available for public water supplies. A risk-based monitoring programme for E2 by Scottish Water is planned to start in the first half of 2024.



Estradiol RWPP Assessment

Higher weight to risk factor on moderately or highly productive aquifers.

Figure 3.7: E2 RWPP assessment outcomes when risk factors on identified pathways are attributed higher weight.

3.3. Nonylphenol (NP)

NP is an alkylphenol, produced since 1940. In the environment, it primarily occurs through degradation of nonylphenol ethoxylates (NPEOs), which have been used in industry as non-ionic surfactants, in households as detergents, and in personal care products (Gałązka & Jankiewicz, 2022). NP is non-soluble with water, oil-repellent, semi-volatile, highly resistant to biodegradation, and bioaccumulative. It is a xenoestrogen, mimics E2, and blocks the effects of androgens, leading to disorders in men, reduced birth weight and premature deliveries, cancer such as breast, ovarian, uterine, pituitary and testicular cancer (Bhandari *et al*., 2021). In aquatic organisms, it can cause feminization, reduce male fertility and survival of young, and it has acute toxicity to phytoplankton, zooplankton, amphibian, invertebrates, and fish (Gałązka & Jankiewicz, 2022). The guidance value for finished drinking water in the EU drinking water watch list is 0.3 µg/l.

3.3.1. Identification of risk factors

Source risk factors: The use of NP and NPEOs has been banned in the UK for several decades, and primary sources (manufacture and use) can be excluded, except for potential small scale legacy industrial productions such as paper and pulp, and plastic and rubber. However, NP is still found in old products as well as wastewater influent and effluent, making sites of waste management the main sources to the environment, including wastewater treatment plants and landfills (Gardner *et al*., 2022; Kurata *et al*., 2008). Both of these sources emit through effluent discharge/leachate, as well as potentially to air (Ferrey *et al*., 2018). The sludge from wastewater treatment also contains NP and thus represents a diffuse source if spread to land (Marshall & Yates, 2022).

Pathway risk factors: NPs have been detected in the air especially in urbanised areas and associated with sewage treatment plants. They return to aquatic and terrestrial ecosystems with rainfall, but have no significant long-range transport (Soares *et al*., 2008). Due to absence of evidence of range, the same distance for increased likelihood of atmospheric deposition from potential sources was chosen as for PFAS. Additionally, as with PFAS and E2, ground permeability was considered as facilitating transport to freshwater systems.

Receptors: All source types were again treated equally for this first assessment. An overview of risk factors and their relationships is provided in Figure 3.8.

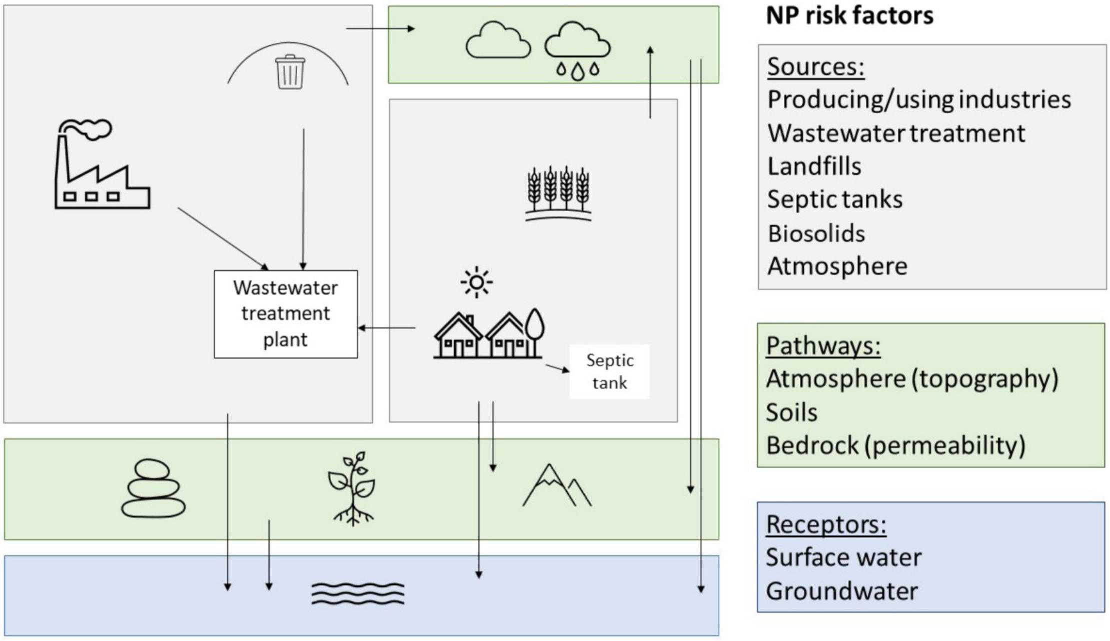


Figure 3.8: Overview of risk factors for the presence of NP in drinking water sources, and their relationships.

3.3.2. RWPP Assessment

For NP, only few catchments show a comparatively high relative score (Figure 3.9). There are fewer risk factors included in this RWPP assessment compared to the PFAS assessment. Therefore, a high score in one risk factor will push up the overall score, with the highest-ranking catchments each having a score of 1 for one or more particular risk factors (wastewater discharges and septic tanks, landfills, and biosolid application potential). Due to catchments having very few risk factors, pathway considerations exacerbate the difference in scores but do not change the general pattern (Figure 3.10).

3.3.3. Monitoring data

Scottish Water monitoring data (from 01/01/23 to 13/10/23) is visualised in Figure 3.11. Samples were available from 61 catchments, with different numbers of samples available. 123 samples were taken altogether, with NP being detected 18 times at 16 sites.

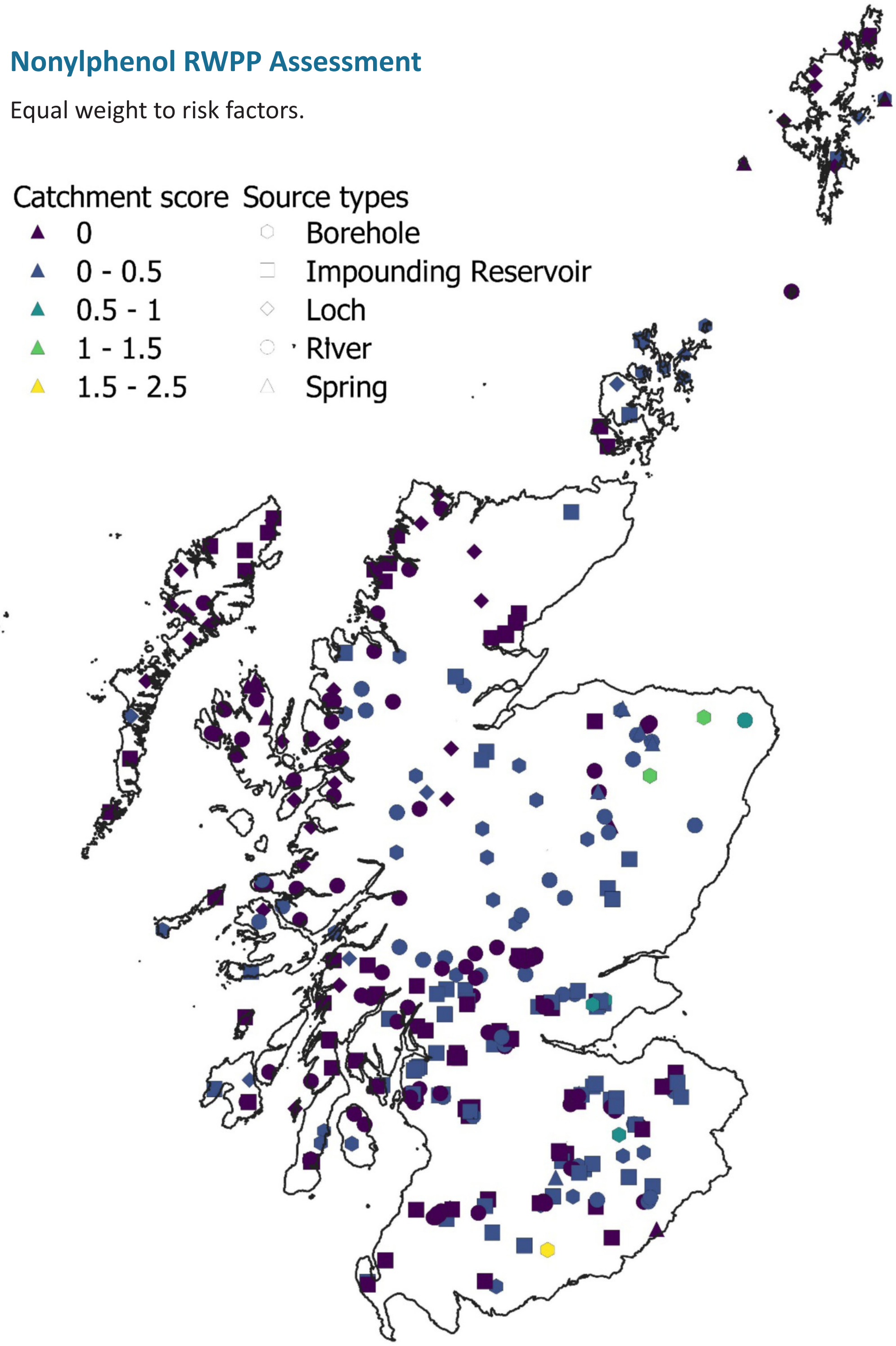


Figure 3.9: NP RWPP assessment outcomes when equal weight given to all source risk factors.

There is no sampling data for the catchments that have been allocated the highest risk score. Catchments where comparatively higher concentrations have been measured, the assessment has allocated lower or median risk scores, indicating that risk factors have been missed.

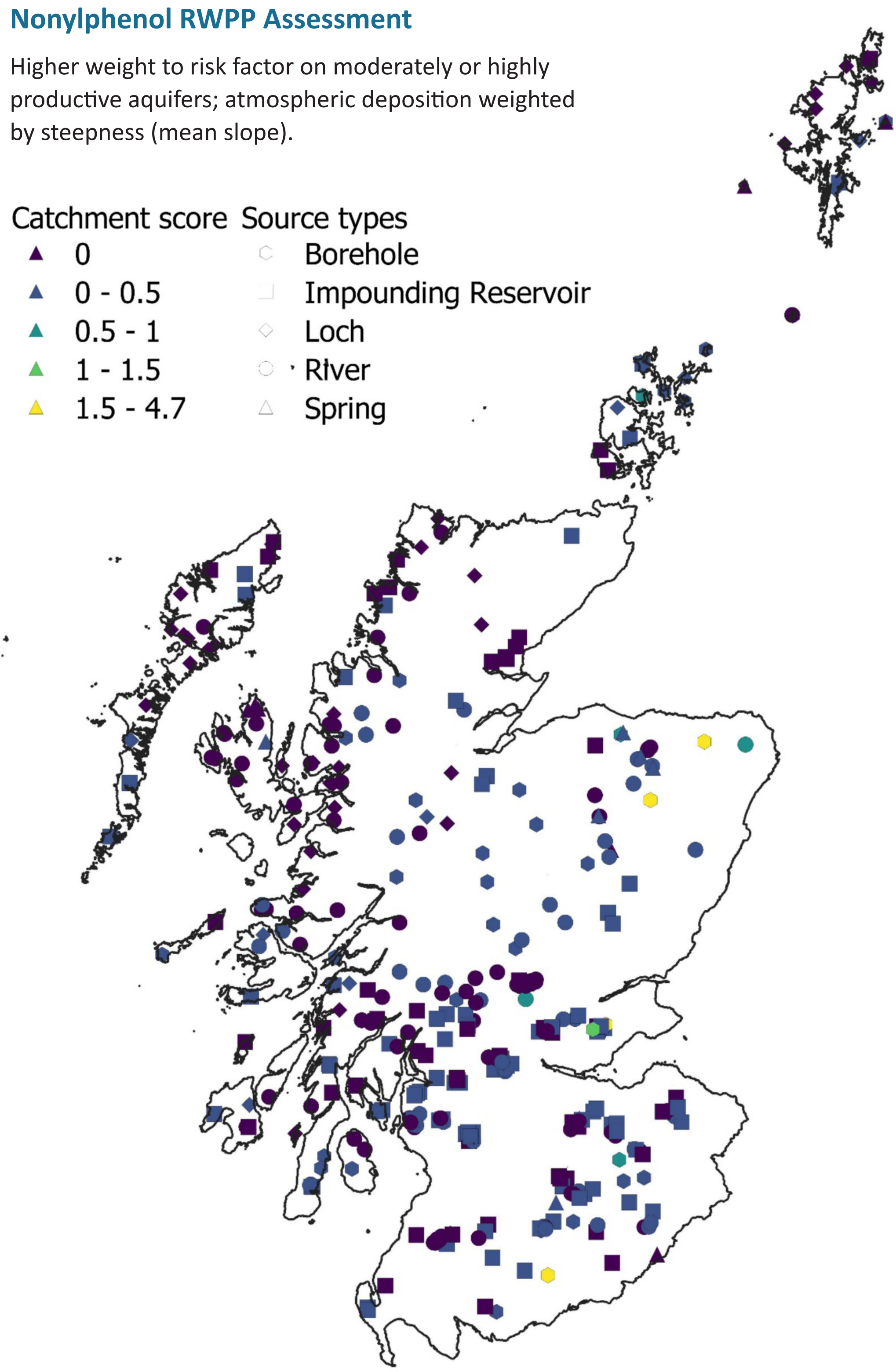


Figure 3.10: NP RWPP assessment outcomes when risk factors on identified pathways are attributed higher weight.

Scottish Water sampling results

Nonylphenol

January 2023 – October 2023

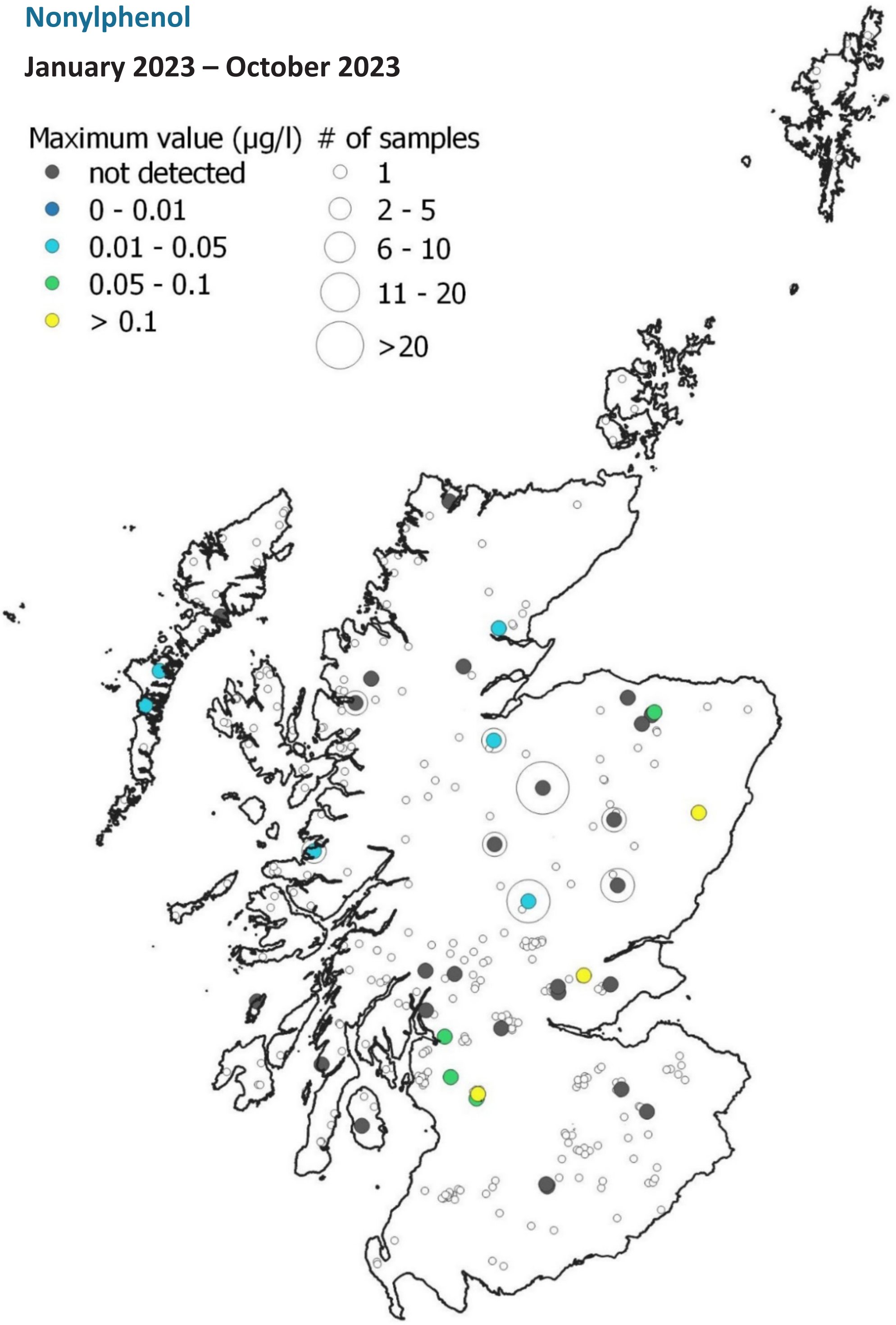


Figure 3.11: Sampling results for NP values from Scottish Water raw water monitoring from 01/01/23 to 13/10/23, with detected maximum concentration (in µg/l) and number of samples taken. EU drinking water watch list guidance value for finished drinking water: 0.3 µg/l.

3.4. Discussion

It is in the nature of contaminants of emerging concern that many facets of their release into and travel through the environment are unknown, and to encounter limits to data quality and availability. These aspects are core limitations of risk assessment approaches.

In the context of drinking water quality, it is important to err on the side of caution, so the RWPP assessments include source risk factors even if their significance is currently uncertain. Pathways can diminish or amplify exposure, and these first assessments used pathway factors to identify increased risk. Receptors can be used to tailor the assessments (e.g., creating different scoring systems depending on type of water body) if there are distinct pathways, but it was judged not to be the case here. Similarly, there may be a lack of data to directly represent risk factors, in which case proxies were used if available.

In the presented assessments, some of the datasets used are a good representation of the risk factors as they directly reflect the pressure, e.g., wastewater discharges or landfill sites. A judgement had to be made on which categories, e.g., discharge types, to include, again based on identified potential for pollution from the literature review. OS Mastermap provided some up-to-date information for sites e.g., industry or landscape features. For some risk factors, their size was not taken into account, e.g., industrial estates, although this might vary and reflect potential impact. Additionally, sites that are no longer in use are not included. The only historical sites that are included are landfill sites, going back to 1978.

The dataset used for renewable energy includes all energy forms rather than only wind turbines. This was preferred over a dataset representing areas for onshore windfarm proposals, to achieve better completeness, and to recognise that other forms of renewable energy generation may also present a source of PFAS.

Livestock densities are summarised over a 2 km by 2 km grid. This cannot capture whether livestock are localised rather than dispersed across the catchment, so the RWPP assessment assumes a general pressure from livestock. For other agricultural pressures, proxies were identified, e.g., arable area for the extent of area treated with fertilizers and pesticides, or arable area and improved grassland cover as area treated with manure/slurry. Area with potential biosolid application was derived from several datasets combining three conditions (under arable agriculture, soil pH above 5, and proximity to a wastewater treatment facility; Crooks & Litterick, 2020), which again presents a rough approximation.

Area impacted by atmospheric deposition was assumed to be a 5 km radius around the point source. This was based on estimates available from the literature, although it is known that PFAS, especially shorter chain compounds, can be deposited beyond that range. Mean long-term annual rainfall was used as a proxy for long-term deposition, due to PFAS predominantly falling out as wet deposition.

Transport of pollutants through the environment is very complex and pathway representation is therefore very simplified. A dataset was available for median topsoil pH, while potential contamination of groundwater was chosen to be represented by aquifer productivity. An existing dataset with national coverage for Scotland covers groundwater vulnerability and would be a better fit to represent this, but it was not available for this project. Thresholds for pH and permeability were arbitrarily set and could be adjusted with increasing knowledge of pathways as related to the underlying processes.

The quality of representation of risk factors and the confidence in the ability to accurately reflect pressures varies, but a balance had to be achieved between inclusion of all relevant risk factors in the assessment and confidence of accurate representation of these. If datasets become available that improve on those used, or better knowledge on the risk factors develops, datasets could be replaced or refined.

As the importance of risk factors with regard to their impact on raw water quality is not yet clear, they were all given equal weight in the assessments. This could be changed over time as understanding improves and as more monitoring data allows specific risk factors of significance to be identified. Similarly, all types of water bodies were treated equally, however with more insight into pathways it might be possible to tailor the assessments to receptors.

While limited in scope, the monitoring data available so far for PFAS and NP provide first insights into the extent and spatial scale of contamination and point towards gaps in understanding. For example, for some catchments, PFAS were detected but the RWPP assessment has not allocated a high score, suggesting that important risk factors may not yet have been identified and included, or that critical risk factors may not have been weighted appropriately. This is the case for some catchments on the West coast, where a more in-depth look at the area can confirm if identified risk factors were missed (not included in the dataset), if historical sites of identified risk factors are present, or if there are potential sources that were generally not identified in the RWPP assessment. As an example for the latter, a first hypothesis could be that due to the catchments proximity to the coast, sea salt aerosols could transport PFAS into these catchments (Sha *et al*., 2022). Similarly, if catchments were identified as high risk but there are consistently no detections, it should be investigated which risk factors led to the high score, and if the factors are not actual sources, or if the amount of PFAS emitted is very low, or if environmental conditions mitigate transport to freshwater.

3.5. Improving the assessments

The RWPP assessment carried out in this project focused on the public water supply catchments to provide a demonstration case for the approach. The assessments can be refined and enhanced in several ways through collecting further water quality data.

3.5.1. Verifying the RWPP assessments

With more data being collected by Scottish Water, adding to the number of samples available, further verification of the RWPP assessment will be possible. The sampling already carried out indicates that source factors have been missed (with detections being made at sites that were assessed in this project as low likelihood), so a more strategic sampling to support verification would be required to refine the assessment and increase confidence in the scoring. The set-up of a systematic and deductive verification sampling should consider several aspects:

- Sampling across the score spectrum to cover catchments from the highest to the lowest score
- Sampling across risk factors, ideally covering all risk factors included in the assessment
- Sampling across Scotland
- Sampling across known water quality profiles, e.g. covering catchments with different water quality issues (e.g., organic material, pathogens, nutrients, pesticides)
- Ensuring adequate sampling frequency to capture different seasons and environmental conditions

The verification sampling should help to determine if the RWPP assessment can identify catchments with detectable concentrations of the contaminants, and start relating relative scores to detected concentrations. It could start by confirming if high scores indeed relate to higher raw water concentrations. In order to do this, enough samples from each location need to be collected to allow confidence of detections being representative, and provide meaningful mean/median, minimum and maximum values. Sampling should therefore also span at least one year to cover variations throughout the year, with sufficient frequency to provide robust inferences.

3.5.2. Completing the risk assessments for the supply system

To understand the fate of the contaminants in the different treatment processes at Scottish Water's water treatment works, raw water as well as treated water samples would need to be collected. There should be samples to cover a variety of treatment methods and set-ups.

For PFAS, currently assumed effective treatment methods are activated carbon, anionic exchange resins, and membrane (nano)filtration (Crone *et al*., 2019; Meegoda *et al*., 2020). Activated carbon is thought to be effective, especially for longer-chain PFAS, while nanofiltration also returns high removal for shorter-chain and new generation PFAS. Treatment efficiency can also vary depending on conditions (e.g., pH or presence of natural organic matter). Different compounds and conditions should therefore be considered in validating treatment. Removal of PFAS however creates a problematic concentrated waste stream.

For E2, coagulation alone does not significantly remove estrogens (Schenck *et al*., 2012). While chlorination can reduce estrogen concentration, there is also the potential of chlorinated by-products (Shao *et al*., 2018), which may have reduced or increased estrogenic activity (Tang *et al*., 2023). Activated carbon, nanofiltration, chemical treatment or advanced oxidation are suggested for reduction of estrogens in drinking water.

NP can be biodegraded by bacteria, fungi and microalgae. Removal of NP through conventional drinking water treatment is only partially effective; promising techniques are adsorption to activated carbon, membrane bioreactor or nanofiltration, reverse osmosis, advanced oxidation or cell immobilization (Bhandari *et al*., 2021).

3.5.3. Enhancing the assessments

There are many uncertainties about sources and pathways of the contaminants, and their fate in environmental waters. Increasing our understanding would support a refinement of the assessment. We consider the following aspects the most feasible and with most potential to improve the assessment:

1. The current RWPP for PFAS as well as nonylphenol includes potential for atmospheric deposition from pollution point sources and uses a radial distribution of 5 km. The representation of atmospheric deposition as a risk factor in this way makes an important change to many catchments with otherwise lower risk factor presence, pushing these up into the mid-range for the RWPP scoring. Checking the suitability of the 5 km threshold, (including for different PFAS compounds), the possibility to switch to a distance-based weighting, or take predominant wind direction into account, would increase confidence in the assessment. Additionally, the contribution of atmospheric deposition to pollution compared to other sources would also significantly improve the assessment.
2. A more systematic analysis through already existing data and through systematic sampling of the contaminants in influent wastewater, wastewater discharge, sludge, and biosolids, to support understanding of 1) factors influencing concentrations in untreated wastewater, 2) how wastewater treatment effects the presence and concentration of the pollutants in these products (decrease or increase), and 3) their entry to the environment via these sources.
3. The distance of the source risk factor to the point of the raw water intake is likely to play a role. If the source is higher up in the catchment, the likelihood of contamination may be reduced compared to where a source is close to the intake. Apart from the estimation of atmospheric deposition range, a distance decay consideration was not included in the assessments due to insufficient information to estimate appropriate thresholds. Aspects of distance dependency to study could be: changes in concentration from a wastewater discharge point downstream; the release radius from landscape features such as wind turbines, electrical and telecommunication masts; etc.
4. The role of sea spray aerosols in contamination especially of coastal catchments should be considered as a risk factor and its importance further investigated. PFAS contamination of the marine environment from terrestrial sources contributes to the global distribution of PFAS compounds and their presence even in remote areas. Sea spray aerosols have been shown to contain PFAS and are hypothesised to be an important contributor to PFAS in the atmosphere (Sha *et al.*, 2022), with significant modelled deposition ranges inland, especially for Ireland and Scotland (Johansson *et al.*, 2019).
5. Examining the fate of the pollutants in different types of water bodies, e.g., rivers, reservoirs, and different types of groundwater. This could help tailor the assessment as well as provide more insight into additional factors potentially facilitating or mitigating presence in raw water.
6. A systemic examination and review of PFAS substances imported to and used in the UK/Scotland would significantly advance our understanding of which substances to monitor, observe for trends, and research further in terms of behaviour in the environment and for health implications. However, a successful compilation may be hampered by incomplete or inaccessible information on import and use (e.g., no requirement to register imports of low amounts), and on decomposition compounds.
7. A better understanding of source risk factors and their relative contribution to pollution would enable a better weighting, e.g., by giving greater weight to some risk factors; giving different weight depending on the type/context of individual sources; or improving weighting according to pathway considerations. For PFAS, better evidence on differences in behaviour depending on chemical structure and properties could lead to more accurate assessments for individual compounds.

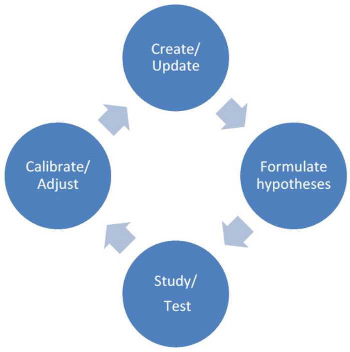


Figure 3.12: Cycle of continuous improvement of risk assessment.

3.6. Approaches for risk assessments of emerging contaminants

Risk assessing emerging contaminants means that there is limited data on occurrence and concentrations available to calibrate and verify a risk assessment. Therefore, they have to be based on available knowledge on sources and how they end up in the freshwater receptors. The source – pathway – receptor model provides a useful framework to identify different roles of risk factors and to guide how to combine them.

3.6.1. Increasing preparedness and anticipatory capacity

Apart from our limited knowledge about sources and behaviours of the substances, knowledge is also evolving around their impacts on human health and the environment, and especially linking those to concentrations. It is therefore possible that standards or guidance values will change with growing insights, including standards tightening. A thorough understanding of the overall range of concentrations therefore increases preparedness to changing standards.

Due to the nature of emerging contaminants, a first risk assessment, or risk screening, mainly serves the purpose to guide a monitoring and sampling strategy to be able to systematically identify areas where these substances are detected, and in which concentrations. It also identifies knowledge gaps and can support finding the most important areas for further studies. Insights gained can then in turn inform the risk assessment and lead to its refinement, improving its reliability (Figure 3.12).

Once an understanding of current potential patterns of contamination is established, the primary focus of risk assessment shifts towards identifying those areas where pressures may lead to changes, especially increases in concentration, so identifying potential areas of pollution rather than actual. This distinction in stage and primary focus of the assessment is important, as it can guide the choice of data used in the risk assessment. For example, the RWPP assessments used potential for biosolid application. It is possible to gather data where biosolids have been applied in the past, so moving from potential to actual sources. This may be more useful in the first phase of the risk assessment, as together with verification monitoring, it can help to understand the role of the risk factor in contributing to concentrations of the pollutant in raw water. However, in a later phase of the risk assessment, using potential sources rather than actual would indicate which areas would need to be monitored more frequently despite pollutants not being detected, or detected in low concentrations, in the past. Especially where this concerns activities that water suppliers may not be aware of or not be informed of in time (e.g. construction, application of material to land), regular assessment of these areas would improve the ability to timely detect new pollution.

Next to the degree of scientific understanding of underlying processes, the quality of the risk assessment largely relies on the quality of used data. Incomplete datasets will lead to presence or importance of risk factors being overlooked – this may happen especially where datasets are not updated regularly or frequently enough. New types of data, e.g., satellite-derived imaging, could provide sources to augment data quality for risk factors. Additionally, sharing data (water quality as well as risk factors) from across different agencies, would augment the available data pool and allow a more complete picture – provided the data is suitable for sharing, which would require appropriate protocols and forethought.

In addition to collecting data that will in time allow more advanced analysis, e.g., of trends in concentrations, increasing understanding of behaviour and underlying processes increases our ability to project trends under changing environmental conditions, such as climate change. This understanding is crucial as climate change will create unprecedented conditions for which past trends may not hold. Especially for catchment derived pollutants, a thorough understanding of catchments, their processes and similarities (both in catchment characteristics and produced water quality) would support anticipatory capacity. This is not only true for assessing impacts of future changes on known water quality issues, but could provide a head-start for assessing other emerging contaminants if they are shown to display similar behaviour to known contaminants.

3.6.2. Supporting private water supply risk assessment and a national assessment

Methods applied for the RWPP assessments of the public water supply are transferable globally. Additionally, within a Scottish context, the prepared risk factors maps can be used without further preparation for different sets of areas/catchments. Combining the source and pathway risk factor maps e.g., over a national grid covering the whole of Scotland, areas can be identified with the highest potential exposures (Figure 3.13 – Figure 3.15). Private water supplies could thus be targeted for further investigation, starting with those in areas of highest assessed potential for pollution. The national maps also indicate areas of highest freshwater pollution potential and thus are more widely interesting from an environmental point of view. Applying the assessment across Scotland would also allow using a wider pool of data for verification, e.g., SEPA's monitoring data.

The method is also applicable to other environmental media if risk factors are adjusted and/or added to accordingly. For example, presence potential in crops grown in Scotland, or in air could be assessed in a similar way. Assessing and mapping potential exposure also supports risk assessment for e.g., freshwater, marine or terrestrial species. The areas of recommended further research/ investigation would of course also benefit these assessments.

Risk factor layers could form part of a basis for a GIS-based risk assessment tool that flexibly combines data describing risk factors with algorithms to combine them according to a preferred method. Such a tool could be developed and adjusted to complete first-tier risk assessments for any emerging contaminant.

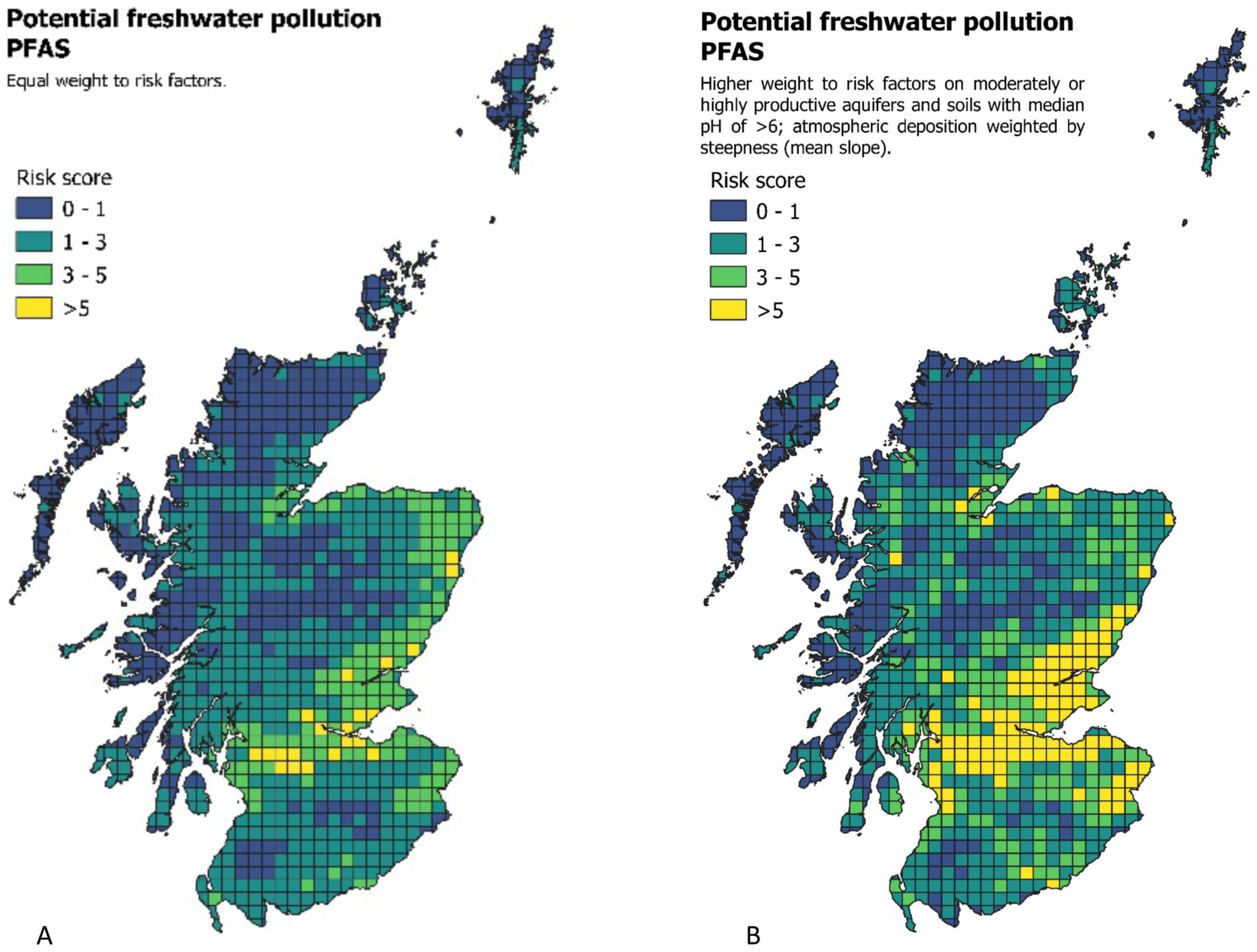


Figure 3.13: National assessment for freshwater PFAS contamination potential, using the RWPP assessment approach outlined in 2.2, run over a 10 by 10 km grid for Scotland.

A. All source risk factors have been included without a pathway consideration. B. Source risk factors weighted according to pathway.

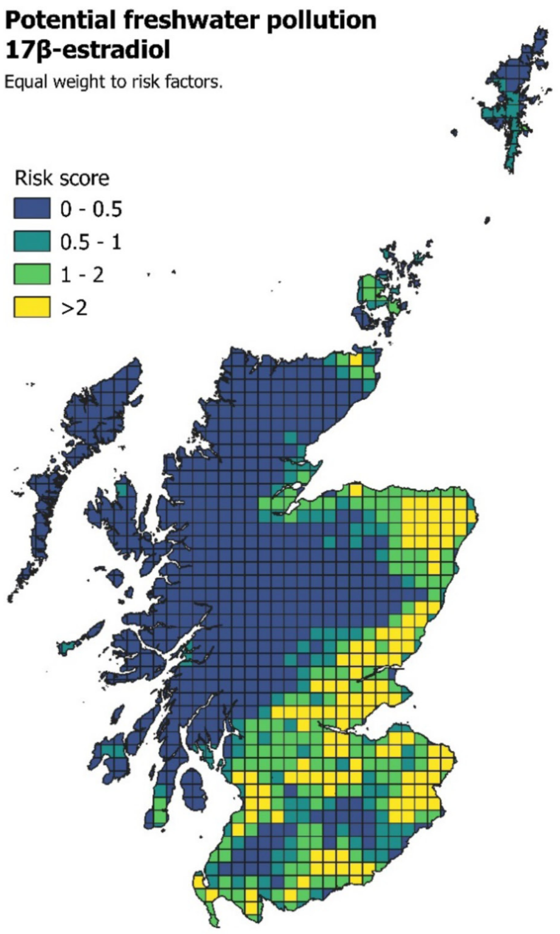


Figure 3.14: National assessment for freshwater E2 contamination potential, using the RWPP assessment approach outlined in 2.2, run over a 10 by 10 km grid for Scotland.

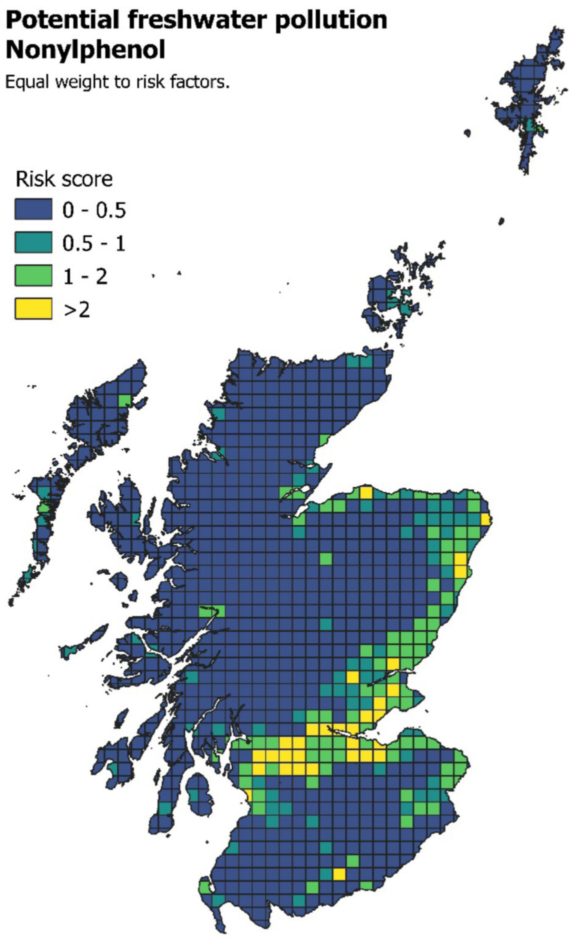


Figure 3.15: National assessment for freshwater NP contamination potential, using the RWPP assessment approach outlined in 2.2, run over a 10 by 10 km grid for Scotland.

4. Recommendations

Recommendations following from the project revolve around two main strands: improving the evidence base to improve understanding of occurrence and behaviour of pollutants, and regulatory controls to manage and mitigate pollution. An overview of identified gaps in data and knowledge is provided in Table 4.1.

4.1. Building an evidence base for Scotland

Risk-based sampling, guided by principles of testing our understanding of patterns and relationships between risk factors and pollution detection, is especially important for emerging contaminants, for which the evidence base is yet sparse. Monitoring and targeted sampling to answer key questions provide evidence for the presence and concentrations of the contaminants (detection), while also supporting knowledge generation of their origin, movement, and impact (attribution). Understanding underlying processes enables a prediction of their presence and thus a projection how patterns of exposure may change with changes in drivers. This in turn is crucial for the identification of effective risk control and mitigation measures (Figure 4.1).

As the RWPP assessment within this project was focused on the public water supply, monitoring recommendations for verification sampling are necessary for public water supply sources; however, a wider network of monitoring is available and should be used to complement this sampling. SEPA's water quality monitoring data, or monitoring carried out under the Chemicals Investigation programme (CIP) could be used for verifying an assessment with national coverage and provide additional and/or further insight into the questions as outlined in this document. Pooling of these different datasets would also provide better statistical robustness.

4.2. Regulation and source control of emerging contaminants

Due to the environmental impacts of the contaminants, their complex pathways, and costs for and limitations of treatment, mitigation should start at the source. There are many knowledge gaps concerning e.g., actual vs. potential sources, contribution of sources, etc. An overview over regulatory tools that could be used for source control of contaminants is given in Appendix C.1. Current regulatory regimes provide potential to further restrict, monitor, and mitigate the use and release of the pollutants into the environment. However, regulation often requires evidence of pollution and severity of impacts, which is usually lacking for emerging contaminants. With increasing awareness by the public of the problems posed by emerging contaminants, public pressure and consumer behaviour may come to influence policy as well as market developments.

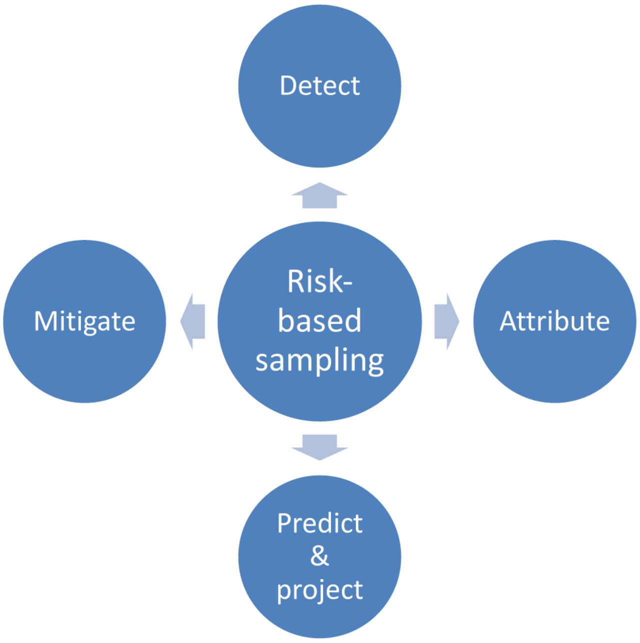


Figure 4.1: Monitoring guided by risk assessment supports moving from detection to attribution, prediction and projection and effective mitigation that increases in effectiveness as understanding and risk assessment evolves.

Table 4.1: Overview of data and knowledge gaps and action to address them

	Purpose	Substance	Recommendation	Rationale/Aim	Organisation
	Verify assessment of raw water presence potential (RWPP) and risk assessment for the public water supply				
1	Verify current RWPP assessment	All	Collect raw water samples at strategic locations spanning high RWPP sites to low RWPP sites; sampling frequency should allow robust statistical inferences and seasonal observations	Collect enough samples per sites to allow confidence in detections being consistent and validate sampling and analytical protocols	Scottish Water
2	Understand relationship of the identified relative score to concentrations			Span enough time and conditions to allow some confidence in mean/median concentrations and concentration ranges	
3	Understand/confirm fate of contaminants in treatment		Take water samples before and after treatment, under different conditions (e.g. flow, temperature, organic material)	Compare efficiency of treatment which may vary depending on other water quality parameters	
4	Understand/confirm fate of contaminants in the remainder of the supply chain		Take water samples at strategic points after treatment (water storage, water supply zone, customers' taps)	Check for evidence to determine whether water is re-contaminated in the distribution network	
	Improve RWPP assessment				
	Test hypotheses made under the current assessment, e.g.:				
5	Atmospheric deposition range (current threshold 5 km)	PFAS & NP	Identify several sources of PFAS/NP emission, sample soil/surface water at different locations around the point source	The threshold set in the current assessment is based on a limited amount of studies. Confirming the distance travelled of different PFAS substances/NP under different conditions could help to either confirm the suitability of the threshold, find a more suitable threshold, develop a distance-dependent scoring, and/or consider factors like wind-direction. Additionally, depending on the set-up, the study could allow to study the amount of PFAS/NP emitted by different sources, and fate of PFAS/NPs under different environmental conditions.	Scientific study
	Improve quality of (proxy) data used in the current assessment, and/or move from potential to actual source, e.g.:				
6	Biosolid application	PFAS & NP	Collect data on sites where biosolids have been applied, or where sludge has been used for site restoration	The current assessment uses three conditions to identify areas with the highest potential for biosolid application. Using areas where biosolids have been applied enhances the assessment from potential to actual source.	Scientific study/ Data (partly) held by Scottish Water and SEPA
7	Sites of AFFF storage and application	PFAS	Collect data on sites where AFFF have been applied/ stored over the past decades	The current assessment used sites/areas where AFFF would be applied in case of a fire (roads and industrial settings), or known to be stored (fire stations, airfields). This excludes disused sites, and does not allow to differentiate actual areas of application and storage.	Scientific study/ Data could be obtained from records of relevant fires and storage

Table 4.1: Overview of data and knowledge gaps and action to address them

	Purpose	Substance	Recommendation	Rationale/Aim	Organisation
	Improve quality of (proxy) data used in the current assessment, and/or move from potential to actual source, e.g.:				
8	Inclusion of historical sites	PFAS & NP	Compile dataset that includes sites that are/may be legacy sources	This could include disused airfields, old military bases, etc., that released contaminants in the past which are still detectable in freshwater.	
	Understand importance of risk factors/sources				
9	Concentration of contaminants in wastewater and wastewater discharges	All	Collect available data on concentrations found at different locations	Some data is available on concentrations found in municipal wastewater for the substances. Additional data needed also for industrial discharges and domestic wastewater systems, to better understand differences in concentrations depending on discharge type and overall contribution.	Scientific study/ Data available e.g., through CIP
10	Concentration of contaminants in biosolids	All	Analyse biosolid samples for concentrations of the substances spanning different conditions and locations (e.g., treatment methods, sites) Analyse soil and water concentrations on and around the site of application.	This would allow to understand the possible concentrations in sludge/biosolids that will reach the land. In combination with testing around the application site, it would help to relate these concentrations to outcomes for land and water.	Scottish Water monitoring/ Scientific study
11	Concentrations of PFAS in sea spray aerosols (SSA), travel distances and deposition mechanisms	PFAS	Analyse the concentrations of PFAS substances in SSA. Study concentrations of PFAS in different proximities to coast in soils and analyse correlation to SSA.	This would support understanding of SSA as a source of contamination relative to terrestrial sources and which areas are mainly affected.	Scientific study
12	All identified sources	All	Sample sources and distance/strategic points around sources to measure and understand emissions of contaminants	This would allow the assessment to take into account which sources are of more importance, and which conditions influence this.	Scientific study
	Understand movement through the environment and facilitating/mitigating conditions, e.g.				
13	Soil characteristics and dependency to leaching	PFAS	Measure soil concentrations and leachate concentrations, either in vitro or in vivo, from different soils, and for different compounds	This could serve to either improve the thresholds set in the current assessment or develop a scale, or to characterise pathways by soil types/mixture of characteristics to better represent complexities	Scientific study
14	Distance dependency	All	Measure concentrations from source to intake/reference distance	Estimate distance – concentrations dependency and form hypotheses about fate in the environment	Scientific study
15	Fate in different water body types (reservoirs, lochs, rivers, boreholes, springs, etc.)	All	Measure concentrations at different locations and in sediment throughout the year	Understand what happens to the substances and if they get trapped/remobilised	Scientific study/ Scottish Water/ SEPA
16	Seasonal variability	All	Measure concentrations throughout the year		Scottish Water/ SEPA
17	Surface water-groundwater relationships	All		This may support differentiating between and tailoring to different receptors	

Table 4.1: Overview of data and knowledge gaps and action to address them

	Purpose	Substance	Recommendation	Rationale/Aim	Organisation
	Understand movement through the environment and facilitating/mitigating conditions, e.g.				
18	Degradation rates	E2	Examine the conditions and time under which degradation occurs.	Support understanding of conditions that would mitigate risk due to rapid degradation, and vulnerability of groundwater sources.	
	Further understanding of substances in the environment and their trends				
19	Compile a register of substances imported to Scotland	PFAS	Collate and examine relevant documents, e.g., UK REACH applications, patents, etc.	This would give a clearer picture about the amount of different substances that could potentially end up in the Scottish/UK environment, and enable better alertness to emerging substances.	Scientific study/Scottish government
20	Include more compounds in the sampling	PFAS	Include new generation PFAS compounds and branched isomers in the analysis.	Not including substances that have been in increasing use over the past years makes it likely that total PFAS concentrations are not represented.	Scottish Water/ SEPA
21	Develop a method for screening for total PFAS	PFAS	Identify PFAS parts to screen	This would allow assessment of total PFAS rather than individual PFAS	Ongoing[3]
22	Investigate correlation with other contaminants	All	Analyse water quality data for correlations	Understanding typical combinations could not only support formulating hypotheses about sources and pathways, but also deliver important information for risk control.	Scottish Water/ SEPA/ Scientific studies
	Understand the impacts of contamination				
23	Interaction with other contaminants	All	Research/Keeping up with guidance		Scientific studies
24	Interaction with other environmental pressures (e.g., climate change, invasive species, habitat loss)				
25	Toxicity levels for plants, animals, humans				
26	Most vulnerable groups				

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[3] See EPA 2022, Lanciki 2021

5. Conclusions

The report describes RWPP assessments for PFAS, E2 and NP. The assessments highlight risk factors and areas with higher densities of risk factors, leading to higher risk of the presence of the substances in raw water supplies. Sampling data from the public water supplier, Scottish Water, indicates that there are still risk factors that are being missed in the assessments. Moreover, the transport pathways for these contaminants from their original sources to potentially reach drinking water resources are complex and variable (spatially and temporally) and remain to be better understood. The literature review and assessments highlight areas of knowledge gaps that need to be addressed to improve our understanding of risk from these pollutants.

The research highlights the need and the requirements for a more strategic, risk-based sampling programme to build up the evidence base for occurrence and concentration of the contaminants in Scotland. Such sampling informs risk assessment and how this gradually leads to better preparedness for rapid developments in this field. Closing knowledge gaps and providing evidence of occurrence and impact will also inform mitigation options and their potential effects, and help to shape and implement regulatory steps.

Monitoring and research need to be adequately funded to provide much needed answers. Due to the complexity of regulation, gaps in our knowledge about occurrence of the contaminants, and the scale of potential impacts both for the environment and for humans, it is important that agencies work together to pool available information and ensure effective use of resources. In view of current international developments towards tighter restrictions on import and use, tighter standards for drinking water, and more monitoring obligations, a better understanding of the situation in Scotland is especially important to allow moving from reaction towards anticipatory precautionary measures that are grounded in the evolving evidence base.

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Public Water Supplies (Scotland) Amendment Regulations 2022 SSI 2022/387

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Regulatory Enforcement and Sanctions Act 2008

Regulatory Reform (Scotland) Act 2014

Sludge Directive, Council Directive 86/278/EEC of 12 June 1986 on the protection of the environment, and in particular of the soil, when sewage sludge is used in agriculture

The Controls on Nonylphenol and Nonylphenol Ethoxylate Regulations 2004

The Sludge (Use in Agriculture) Regulations 1989/1263

UK REACH, SI 2019/758 as amended, SI 2021/904

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Urban Waste Water Treatment Directive, Council Directive of 1991 concerning waste water treatment

Urban Waste Water Treatment (Scotland) Regulations 1994 SI 1994/2842

Water Environment (Controlled Activities (Scotland) Regulations 2011 SSI 2011/208

Water Environment (River Basin Management Planning: Further Provision) (Scotland) Regulations 2013 SSI 2103/323, as amended, 2015 SSI 2015/211

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Water Industry Act 2002

Water Supply (Water Quality) Regulations 2016 SI 2016/614

Water Supply (Water Quality) Regulations 2018 SI 2018/647 (W 121)

Appendices

A. Methods

1. Literature review

Four web-based search engines (Google Scholar, PubMed, ScienceDirect and Wiley Online Library) were used to identify relevant scientific literature. As a first step, searches with each of these were carried out separately for PFAS, E2 and nonylphenol along three guiding questions:

1. What are sources, pathways, and receptors of the contaminant?
2. What do we currently know about the distribution, occurrence and concentration of the contaminant and their sources (in Scotland)?
3. What is the current evidence base related to effective treatment methods?

Search terms were identified and combined as in Figure A.1 and Table A.1. Due to a high number of search results, only the first 100 papers of each run, sorted automatically by the search engine by relevance, were included for further analysis.

In the next step, the identified papers of each search run were checked for duplicates and titles and abstracts scanned for evaluation of relevance. Duplicates and irrelevant papers were removed. The remaining papers were tagged according to topic (Table A.2) and formed the initial body of literature used in the reviews (B-3.1 – B-3.3). A small number of papers were added later through identification of relevant sources when reading these papers. A limited targeted search for grey literature, focusing on reports published in languages accessible to the research team (English, German, French) from European research institutes or environment agencies on monitoring results for the substances, was performed, yielding a literature source for each France, Denmark, Switzerland, and the EU, and two from Norway. Finally, literature suggested or provided by stakeholders (e.g. reports from the Chemical Investigation Programme) complemented the reviewed information.

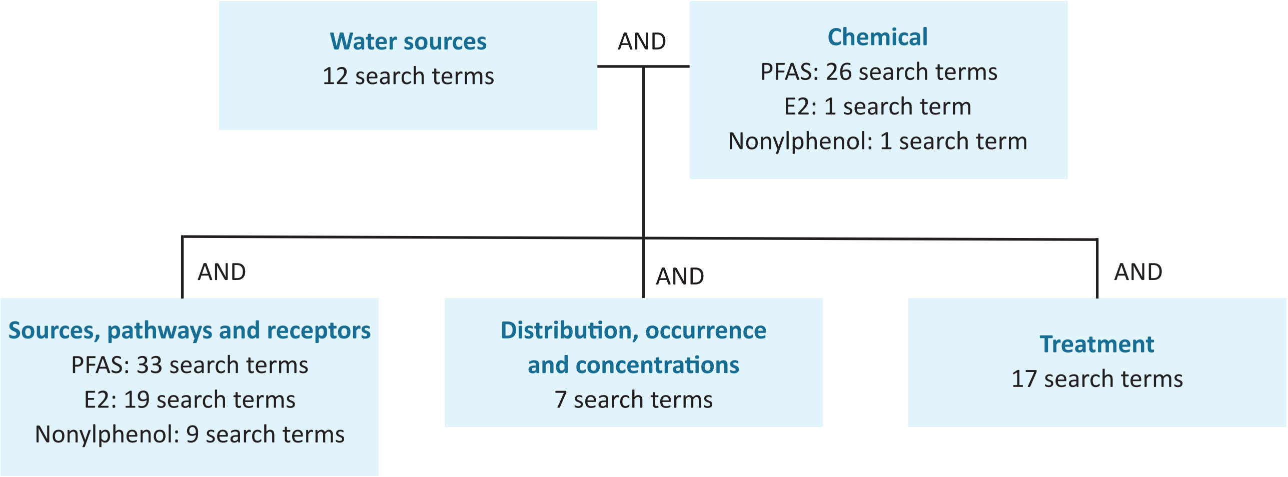


Figure A.1: Combination of search terms for web-based search engines.

Table A.1: Search terms used in the web-based search	
Water sources	reservoir OR river OR stream OR lake OR loch OR groundwater OR spring OR borehole OR surface water OR freshwater OR raw water OR source water
Chemical: PFAS	PFAS OR persistent organic pollutant OR forever chemical OR PFOS OR PFOA OR Per- and polyfluoroalkyl substances OR Perfluorobutanoic acid OR Perfluoropentanoic acid OR Perfluorohexanoic acid OR Perfluoroheptanoic acid OR Perfluorooctanoic acid OR Perfluorononanoic acid OR Perfluorodecanoic acid OR Perfluoroundecanoic acid OR Perfluorododecanoic acid OR Perfluorotridecanoic acid OR Perfluorobutane sulfonic acid OR Perfluoropentane sulfonic acid OR Perfluorohexane sulfonic acid OR Perfluoroheptane sulfonic acid OR Perfluorooctane sulfonic acid OR Perfluorononane sulfonic acid OR Perfluorodecane sulfonic acid OR Perfluoroundecane sulfonic acid OR Perfluorododecane sulfonic acid OR Perfluorotridecane sulfonic acid
Chemical: 17ß-estradiol	Beta-estradiol
Chemical: nonylphenol	Nonylphenol
Sources, pathways and receptors: PFAS	Source OR pathway OR mobilisation OR transfer OR receptor OR transport OR route OR pollution OR process OR industry OR biosolid OR wind farm OR fire OR foam OR airport OR airfield OR wastewater OR discharge OR effluent OR sewer OR septic tanks OR chromium OR paper OR cardboard OR carpet OR textile OR cosmetic OR packaging OR landfill OR sludge OR historic OR latent OR legacy
Sources, pathways and receptors: 17ß-estradiol	Source OR pathway OR mobilisation OR transfer OR receptor OR transport OR route OR pollution OR process OR livestock OR manure OR slurry OR biosolid OR wastewater OR effluent OR septic tank OR sewer OR discharge OR hospital
Sources, pathways and receptors: nonylphenol	Source OR pathway OR mobilisation OR transfer OR receptor OR transport OR route OR pollution OR process
Distribution, occurrence and concentrations	Occurrence OR concentration OR source OR Scotland OR England OR Wales OR UK
Treatment	Drinking water OR treatment OR clarification OR sand filtration OR microfiltration OR ultrafiltration OR ozonation OR chlorine OR UV OR disinfection OR adsorption OR techniques OR activated carbon OR natural organic material OR nanofiltration OR reverse osmosis OR ion exchange

Table A.2: Number of papers identified through the web-based search.

	Sources, pathways and receptors	Distribution, occurrence and concentrations	Treatment
PFAS	158	110	162
E2	97	114	110
Nonylphenol	67	104	76

2. Stakeholder interviews

To complement and enhance the findings of the literature review and draw on the institutional knowledge of relevant stakeholder organisations across Scotland a number of interviews were carried out with 'key informants'. This is a recognised social science survey approach to augment documentary evidence and can be used to reveal knowledge and levels of activity in seeking to manage contaminants of emerging concern. Ethical approval for the interviews was obtained from the University of Dundee's Research Ethics Committee as well as participants' consent to conducting and recording the interview.

Participants were chosen due to their expertise in the field and ability to represent their institution's perspective. Interviews were conducted with nine participants, representing eight stakeholder institutions: the Scottish Government, the Drinking Water Quality Regulator (DWQR), Scottish Water, the Water Industry Commission for Scotland (WICS), the Scottish Environment Protection Agency (SEPA), a Local Authority (Perth & Kinross Council), NatureScot, and Public Health Scotland. Zero Waste Scotland were also approached but it was not possible to secure a representative in the time available.

Interviews were semi structured around five core questions (Box A.1) and conducted online. Recordings and transcripts were summarised by the interviewer and the summaries were shared with and approved by the interviewee. These summaries were used in further analysis. Individually, and collectively these interviews afforded a synthesis of the key issues for Scotland, providing a holistic view of perception of risk and previous work and data relevant to this project.

Box A.1: Interview questions guiding the semi-structured interviews.

1. How concerned is (your organisation) about (PFAS/E2/nonylphenol) in the environment?
2. How would you describe the extent of knowledge about (PFAS/E2/nonylphenol) within (your organisation)?
3. How do you use this information within (your organisation)?
4. What else would you like to know about (PFAS/E2/nonylphenol) to support (your organisation's) work?
5. What would (your organisation) like to see happening to reduce (PFAS/E2/nonylphenol) in the environment.

3. Data preparation

Datasets were sourced from open sources or where accessible to the authors via licencing (Table A.3). Datasets were subset according to relevant features to create layers for source risk factors (Table A.4). Source risk factor layers related to organic material application to land were created from several datasets (Table A.5). Pathway risk factors layers were created by subsetting datasets as for source risk factors (Table A.6).

Table A.3: Datasets used for describing risk factors.

Dataset	Source	Licence
SEPA data publication: Water discharges	Environmental data | Scottish Environment Protection Agency (SEPA)	Open Government Licence
SEPA waste sites and capacity tool	sepa.org.uk/data-visualisation/waste-sites-and-capacity-tool/	Open Government Licence
OS Mastermap Points of Interest	Points of Interest | Data Products | Ordnance Survey	Licenced
OS Mastermap Highway Network	OS MasterMap Highways Network - Roads | Data Products | Ordnance Survey	Licenced
Renewable Energy Sites - Scotland	https://data.spatialhub.scot/dataset/renewable_energy_sites-is	Open Government Licence
Agricultural census	[ARCHIVED CONTENT] Agriculture and Fisheries - Publications (nrscotland.gov.uk)	Accessed via Digimap under the Agcensus licence of UoD
JHI topsoil pH	Scotland's Soil Data | Soils@Hutton | The James Hutton Institute	JHI Open Data Licence
Scotland DTM	OS Terrain 50 | Data Products | Ordnance Survey	Open Government Licence
BGS hydrogeological maps of Scotland	Hydrogeological maps of Scotland - British Geological Survey (bgs.ac.uk)	Licenced – £0.4/km^2
UKCEH Land cover 2021	Land Cover Map 2021 - EIDC (ceh.ac.uk)	UKCEH licence – free
NatureScot Deer count deer density	Deer Counts Deer Density | NatureScot Spatial Data Hub	Open Government Licence
Septic Tanks	Septic Tanks – Scotland – Septic Tanks – Spatial Hub Scotland	Open Government Licence
Septic Tanks modelled	Provided by SEPA/JHI	
UK Met Office: 30 year mean annual rainfall (1991-2020)	HadUK-Grid Gridded Climate Observations on a 1km grid over the UK, v1.2.0.ceda (1836-2022), CEDA Archive Web Browser	Open Government Licence

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Wastewater discharge	SEPA data publication: Water discharges	Vegetable raw materials			
		Municipal waste-water treatment plants with the capacity of 15,000 population equivalent and not exceeding 100,000 population equivalents	x	x	x
		Municipal waste-water treatment plants with the capacity of 100,000 population equivalents	x	x	x
		Opencast mining	x		
		Installations for the disposal of non-hazardous waste	x		x
		Installations for the intensive rearing of poultry, exceeding 40,000 places.		x	
		Installations for the building of, and painting or removal of paint from ships	x		
		Intensive aquaculture with a production capacity not exceeding 1,000 tonnes of fish per year			
		Intensive aquaculture with a production capacity of 1,000 tonnes of fish or shellfish per year			
		Treatment and processing of milk		x	
		Thermal power stations and other combustion installations	x		
		Activities at Premises with Non-Nuclear Authorisation under the Radioactive Substances Act 1993 Fees and Charging (Scotland) Scheme 2004			
		Intensive aquaculture			
		Salts, such as ammonium chloride, potassium chlorate, potassium carbonate, sodium carbonate, perborate, silver nitrate			
		Installations using a chemical or biological process for the production on an industrial scale of basic pharmaceutical products	x		
		Installations for the intensive rearing of pigs, exceeding 2,000 pigs (over 30kg)		x	
		Animal raw materials (other than milk)		x	
		Installations for the disposal or recycling of animal carcasses and animal waste		x	
		Landfills (excluding landfills of inert waste)	x		x
		Installations for the recovery or disposal of hazardous waste	x		x
		Slaughterhouses		x	
		Installations for the surface treatment of substances, objects or products using organic solvents, in particular for dressing, printing, coating, degreasing, waterproofing, sizing, painting, cleaning or impregnating	x		
		Industrial plants for the production of paper and board and other primary wood products (such as chipboard, fibreboard and plywood)	x		x
		Mineral oil and gas refineries	x		

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Wastewater discharge	SEPA data publication: Water discharges	Independently operated industrial waste-water treatment plants which serve one or more activities of this annex	x		x
		Industrial plants for the production of pulp from timber or similar fibrous materials	x		x
		Industrial plants for the production of pulp from timber or similar fibrous materials	x		x
		Installations for the manufacture of glass, including glass fibre	x		
		Plants for the pretreatment (operations such as washing, bleaching, mercerization) or dyeing of fibres or textiles	x		
		For the smelting, including the alloying, of non-ferrous metals, including recovered products (refining, foundry casting, etc.)	x		
		Simple hydrocarbons (linear or cyclic, saturated or unsaturated, aliphatic or aromatic)	x		
		Cement clinker in rotary kilns	x		
		Synthetic rubbers	x		x
		Chemical installations for the production on an industrial scale of basic plant health products and of biocides	x		
		Installations for the incineration of non-hazardous waste	x		x
		Installations for the intensive rearing of pigs, exceeding 750 places for sows		x	
		Acids, such as chromic acid, hydrofluoric acid, phosphoric acid, nitric acid, hydrochloric acid, sulphuric acid, oleum, sulphurous acids	x		
		Non-metals, metal oxides or other inorganic compounds such as calcium carbide, silicon, silicon carbide	x		
		Gases, such as ammonia, chlorine or hydrogen chloride, fluorine or hydrogen fluoride, carbon oxides, sulphur compounds, nitrogen oxides, hydrogen, sulphur dioxide, carbonyl chloride	x		
		Activities at Premises with Nuclear Authorisation under the Radioactive Substances Act 1993 Fees and Charging (Scotland) Scheme 2004			
		Oxygen-containing hydrocarbons such as alcohols, aldehydes, ketones, carboxylic acids, esters, acetates, ethers, peroxides, epoxy resins	x		
		For the production of non-ferrous crude metals from ore, concentrates or secondary raw materials by metallurgical, chemical or electrolytic processes	x		
		Dyes and pigments	x		
		Installations for the manufacture of ceramic products by firing, in particular roofing tiles, bricks, refractory bricks, tiles, stoneware, or porcelain	x		
		Installations for gasification and liquefaction	x		

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Wastewater discharge	SEPA data publication: Water discharges	Installations for surface treatment of metals and plastic materials using an electrolytic or chemical process	x		
		Plants for the tanning of hides and skins	x		
		Chemical installations for the production on an industrial scale of basic organic chemicals, such as:	x		
		Hot-rolling mills	x		
		Nitrogenous hydrocarbons such as amines, amides, nitrous compounds, nitro compounds or nitrate compounds, nitriles, cyanates, isocyanates	x		
		Chemical installations for the production on an industrial scale of phosphorous-, nitrogen- or potassium-based fertilizers (simple or compound fertilizers)	x		
		Smitheries with hammers			
		Municipal waste-water treatment plants	x	x	
		Basic plastic materials (polymers, synthetic fibres and cellulose-based fibres)	x		x
		Installations for the production on an industrial scale of explosives and pyrotechnic products	x		
Landfills	SEPA waste sites and capacity tool	Landfill (not operational)	x		x
		Landfill	x		x
		Civic amenity			
		Other treatment			
		Composting			
		Transfer station			
		Incineration			
		Co-incineration			
		Anaerobic digestion			
		Metal recycler	x		
Sites of storage of AFFF	OS Mastermap Points of Interest	Airports and landing strips	x		
	OS Mastermap Points of Interest	Fire brigade stations	x		
Sites of application of AFFF	OS Mastermap	Roads	x		
	OS Mastermap Points of Interest	Industrial estates	x		
Mines	OS Mastermap Points of Interest	Ore mining	x		

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Landscape features	OS Mastermap Points of Interest	Electrical features	x		
	OS Mastermap Points of Interest	Telecommunications features	x		
	Renewable Energy sites – Scotland	All renewable energy sites	x		
Agricultural discharges/ point sources	SEPA data publication: Water discharges			see above	
	OS Mastermap Points of Interest: Farming	Animal breeders (not horses)		x	
		Arable farming			
		Dairy farming		x	
		Horse breeders and dealers		x	
		Livestock farming		x	
		Mixed or unspecified farming		x	
		Poultry farming, equipment, and supplies		x	
		Beekeepers			
		Fish and shellfish			
		Fruit, flower, and vegetable growing			
		Forestry			
Biosolid/sludge application	*see Table A.5*		x	x	x
Application of waste from card, paper and pulp production	*see Table A.5*		x		x
Fertiliser and pesticide application	UKCEH Land cover 2021	Arable area	x		
Ski infrastructure	OS Mastermap Points of Interest	Ski infrastructure and aerial cableways	x		
Livestock	Agricultural census 2019	Total cattle		x	
		Female beef cattle under 1 year			
		Female dairy cattle under 1 year			
		Female beef cattle aged 1-2 years			
		Female dairy cattle aged 1-2 years			

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Livestock	Agricultural census 2019	Female beef cattle with offspring aged 2 years and over			
		Female dairy cattle with offspring aged 2 years and over			
		Female beef cattle without offspring aged 2 years and over			
		Female dairy cattle without offspring aged 2 years and over			
		Male cattle under 1 year			
		Male cattle aged 1-2 years			
		Male cattle aged 2 years and over			
		Sows in pig			
		Gilts in pig			
		Other sows for breeding			
		Barren sows for fattening			
		Gilts 50kg and over expected to be used for breeding			
		Boars for service			
		Other pigs 110 kg and over			
		Other pigs 80 kg-under 110 kg			
		Other pigs 50 kg-under 80 kg			
		Other pigs 20 kg-under 50 kg			
		Other pigs under 20 kg			
		Total pigs		x	
		Breeding ewes			
		Rams for service			
		Other breeding sheep 1 year and over			
		Other non-breeding sheep 1 year and over			
		Lambs			
		Total sheep		x	
		Total goats		x	
		Laying flock hens in 1st season			
		Laying flock moulted hens			
		Laying flock pullets for laying			
		Breeding flock layer chicks			

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Livestock	Agricultural census 2019	Breeding flock table chicks			
		Breeding flock cocks			
		Broilers and other table fowls			
		Ducks			
		Geese			
		Other poultry incl. turkeys			
		Total poultry		x	
		Deer		x	
		Horses used in agriculture			
		All other horses			
		Total horses		x	
		Donkeys unraised		x	
		Unspecified livestock		x	
		Alpacas unraised		x	
		Llamas unraised		x	
		Other camelids unraised		x	
Manure application	*see Table A.5*			x	
Atmospheric deposition	OS Mastermap Points of Interest:	Carpets, flooring, rugs, and soft furnishings	x		
		Clothing, components, and accessories	x		
	Manufacturing and production	Footwear	x		
		Furniture	x		
		Hobby, sports, and pastime products	x		
		Leather products	x		
		Luggage, bags, umbrellas, and travel accessories	x		
		Cosmetics, toiletries, and perfumes	x		
		Curtains and blinds	x		
		Cutlery and tableware	x		
		Photographic and optical equipment	x		
		Refrigeration and freezing appliances	x		
		Tents, marquees and camping equipment	x		
		Adhesives and sealants	x		

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Atmospheric deposition	Manufacturing and production	Aeroplanes	x		
		Bricks, tiles, clay, and ceramic products	x		
		Cable, wire, and fibre optic	x		
		Cleaning equipment and supplies	x		
		Concrete products	x		
		Cooling and refrigeration	x		
		Electrical components	x		
		Electronic equipment	x		
		Industrial coatings and finishings	x		
		Marine equipment including boats and ships	x		
		Medical equipment, supplies and pharmaceuticals	x		
		Metal manufacturers, fabricators, and stockholders	x		
		Packaging	x		
		Paints, varnish, and lacquers	x		
		Radar and telecommunications equipment	x		
		Pesticides	x		
		Road maintenance equipment	x		
		Rubber, silicones, and plastics	x		
		Fertilisers	x		
		General construction supplies	x		
		Textiles, fabrics, silk, and machinery	x		
		Wood products including charcoal, paper, card and board	x		
		Workwear	x		
	SEPA waste sites and capacity tool	Landfill (not operational)	x		
		Landfill	x		
		Civic amenity			
		Other treatment			
		Composting			
		Transfer station			
		Incineration	x		

Table A.4: Preparation of source risk factor layers

Source	Dataset	Categories	PFAS	E2	NP
Atmospheric deposition	SEPA data publication: Water discharges		see above		see above
	Biosolid application		x		x
	Pesticide and fertilizer application		x		
	SEPA waste sites and capacity tool	Co-incineration	x		
		Anaerobic digestion			
Wildlife	NatureScot Deer count deer density	Total count		x	
Septic tanks	SEPA modelled dataset	Total count	x	x	x

Table A.5: Preparation of risk factor layers relating to organic material spreading.

Material	Considerations	Factor	Metric	Dataset	Categories
Sludge/biosolids	Spreading of sewage sludge is regulated on agricultural land through the Sludge (Use in Agriculture) Regulations 1989, and in other areas through the Waste Management Licensing Regulations. In agriculture, sludge may not be spread on areas with soils with a pH below 5. It can be used prior to growing cereals, grass, fodder, sugar beet, oilseed rape and similar crops, fruit trees, soft fruit, potatoes, vegetables, and nursery stock. Sewage is spread typically in a 30 km radius of the sewage plant due to transportation costs, although may be spread further.	Soil pH	pH >5	JHI topsoil pH	
		Land cover	Percentage	UKCEH Land cover 2021	Arable area
		Distance to source	Area within a 30 km radius of a sewage plant	SEPA data publication: Water discharges	Municipal waste-water treatment plants with the capacity of 15,000 population equivalent and not exceeding 100,000 population equivalents
					Municipal waste-water treatment plants with the capacity of 100,000 population equivalents
					Municipal waste-water treatment plants
Manure	The majority of organic material spread to land is manure (86%). There are restrictions on the spreading of organic material: on land with <40 cm average soil depth overlying gravel or fissured rock, on land within 10 m of a waterbody or wetland, on land that is sloping, in excess of the nutrient need of the crop. It is likely that there will be additional constraints in areas e.g. that have a conservation designation, that are in a nitrate vulnerable zone, etc.	Land cover	Percentage	UKCEH Land cover 2021	Arable area
					Improved grassland
Waste from card, paper and pulp production		Paper mills	Arable area within a 30 km radius of a mill	SEPA data publication: Water discharges/ OS Mastermap Points of Interest	Industrial plants for the production of pulp from timber or similar fibrous materials/Wood products including charcoal, paper, card and board

Table A.6: Preparation of pathways risk factor layers.

Pathway	Factor	Dataset	Categories	Metric	PFAS	Estradiol	Nonylphenol
Soil & Bedrock	Alkalinity	JHI topsoil pH	pH median	Set threshold (>6)	x		
	Aquifer productivity	BGS hydrogeology	Very low	Include/exclude			
			Low				
			Moderate		x	x	x
			High		x	x	x
			Very high		x	x	x
Atmosphere	Topography	Scotland DTM	Mean slope	n/a	x		x

B. Findings

1. Literature review: PFAS

PFAS are a large group of synthetic compounds, manufactured for several decades. The simplest perfluorocarbon, tetrafluoride, was first produced in 1886, and PFAS with functional groups have been made since the 1940s and used in industry at least since the 1950s (Gaines, 2023). Today, there are more than 200 industrial uses for PFAS, including food packaging, weather-proof clothing, anti-stain fabrics, fire-suppressing foams, etc. Uses are continuing to expand along the development of more and new PFAS compounds, creating a group of thousands of unique chemicals with a highly stable fluorinated carbon chain (Evich *et al.*, 2022).

There is no globally agreed definition for PFAS. The OECD defines PFAS as “fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it), i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group (–CF3) or a perfluorinated methylene group (–CF2–)” (OECD, 2021). This definition is adopted in the EU REACH restriction proposals, but the HSE has adopted a narrower working definition, excluding compounds with only a single isolated methylene group, as these have been shown to biodegrade (HSE, 2023). The list of PFAS Chemicals on the US EPA CompTox Chemicals Dashboard (US EPA, 2023) currently lists 10,776 structures (updated August 2021). The OECD global database of PFAS lists 4730 substances.

There are different categories of PFAS, polymeric and non-polymeric (Figure B.1). Non-polymeric PFAS have a core structure of a carbon chain attached to multiple fluorine atoms with different end functional groups. Polymeric PFAS have at least one per- or polyfuoroalkyl moiety. Fluoropolymers have a carbon only backbone with fluorine atoms attached, whereas side-chain fluorinated polymers have a non-fluorinated polymer backbone with fluorinated side-chains attached. They can be sources of non-polymeric PFAS due to detaching of side-chains, or from manufacturing impurities. During direct fluorination, uncontrolled chemical reactions such as carbon chain shortening and rearrangement lead to by-products such as cyclic and branched isomers. Functional moieties of starting materials may also further react to yield different pathways. Final products may therefore contain a number of intermediates and degradation products (Evich *et al.*, 2022).

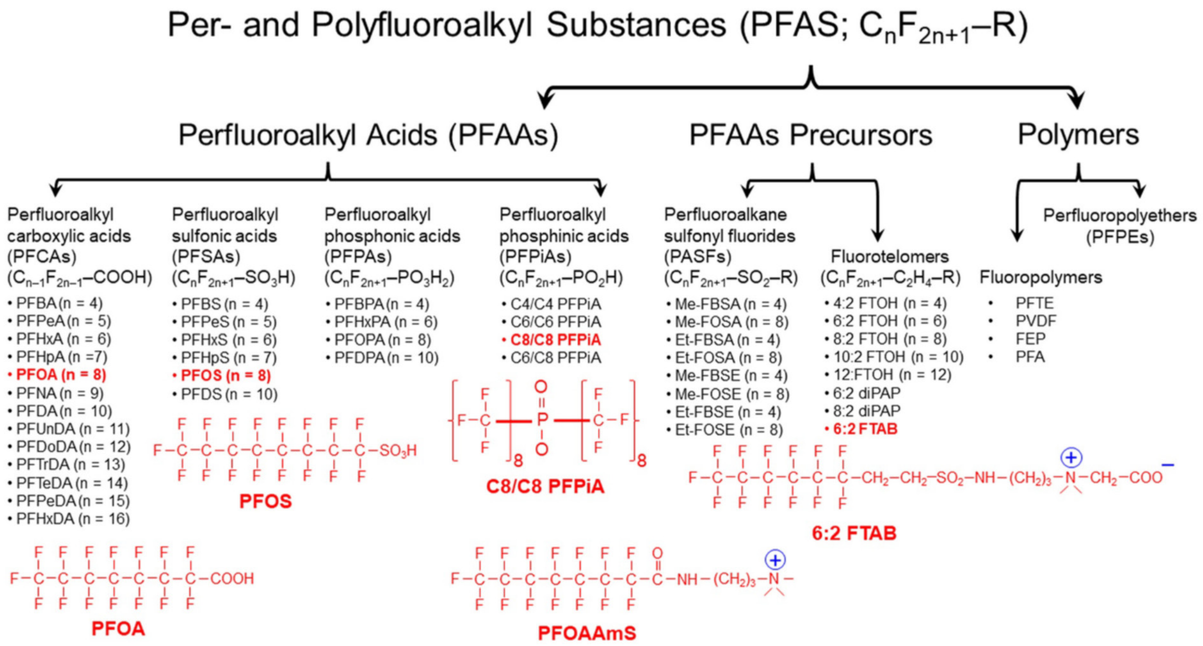


Figure B.1: PFAS family tree, with example compounds and structures, taken from Lyu et al. (2022).

Polyfluoroalkyl substances have the potential to be transformed into perfluoroalkyl substances, while some PFAS degrade in the environment, usually with perfluoroalkylated acids (PFAA) as end products. These are usually separated into perfluoroalkylated carboxylic acids (PFCAs) with a carboxyl group (-COOH; Figure B.2), and perfluoroalkylated sulfonic acids (PFSAs) with a sulfonyl hydroxide (-SO_3H; Figure B.3). PFAAs are long- or short-chained; PFCAs are referred to as long-chain if they have an eight carbon alkyl chain or more, and PFSAs are referred to as long-chain if they have a perfluoroalkyl chain of six or longer.

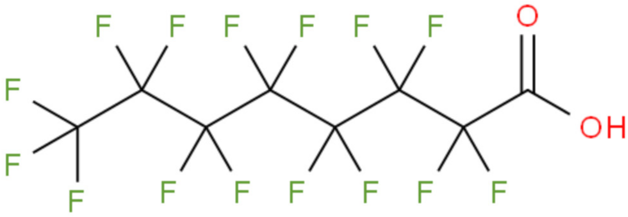


Figure B.2: Structure of PFOA as an example of a PFCA, taken from Sorokin et al. (2019)

Figure B.3: Structure of PFOS as an example of a PFSA, taken from Çelik et al. (2013)

1.1. Regulation

PFAS regulation in the UK is fragmented, with legal requirements spread across different regimes, including UK REACH, the EU POPs Regulation, and water quality standards.

1.1.1. UK REACH

PFAS are mostly industrial and consumer chemicals and as thus fall under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) Regulation of the European Union (Regulation (EC) No 1907/2006). Manufacturers and users of chemicals are obliged to register the substances if they exceed 1 tonne per year per company, and companies must identify risks from the substances. Substances posing high risks can be banned. The UK has retained the regulation in national law (UK REACH, SI 2019/758 as amended, SI 2021/904).

Under EU REACH, PFCAs with a carbon chain of nine or more fall under ANNEX XVII, which places restrictions on the manufacture, placing on the market and use of the included substances. PFCAs, their salts and related substances may not be manufactured or placed on the market since February 2023 (Commission Regulation (EU) 2021/1297). It is also prohibited to use or place them on the market as a constituent, mixture, or article if the concentration exceeds a certain threshold, with some exceptions (e.g., for aqueous film forming foams (AFFF) in some circumstances). PFOS and related compounds and PFOA are also regulated under UK REACH.

The information on volume and use of PFAS in the UK is incomplete, due to a number of factors related to registration obligations under EU and UK REACH, e.g., no registration requirement for imports <1 t/y, long lead-times for submitting transitional registrations for low tonnage (<10t/y), and no obligation to register polymers. An initial investigation by HSE (2023) identified 40 PFAS imported to the UK from the EU, and 182 PFAS in the EU REACH database (ECHA, undated). Highest tonnages (1000-15,000 t/y) are reported under UK REACH for polyfluoroalkyl substances comprising hydrofluorocarbons (HFCs), -ethers (HFEs), and -olefins (HFOs), and perfluoroalkenes.

1.1.2. EU POPs Regulation

Persistent organic pollutants are regulated internationally under the Stockholm Convention and the Aarhus Protocol, which are implemented by the Regulation (EU) 2019/1021 of the European Parliament and of the Council of 20 June 2019 on persistent organic pollutants (EU POPs Regulation), which still applies in the UK as retained EU law and is implemented by the Persistent Organic Pollutants Regulations 2007. Under the Regulations, PFOS and related compounds and PFOA and its salts and related compounds, are banned, with some exceptions for specific usage.

1.1.3. Water Framework Directive

The European Commission published a proposal for a directive amending the Water Framework Directive, the Groundwater Directive, and the Environmental Quality Standards (EQS) Directive in October 2022 (COM (2022) 540 final). This would update the lists of priority substances for surface water and groundwater, and introduce standards for the sum of 24 PFAS (including PFOA, PFOS, PFHxS, PFNA, PFBS, PFHxA, PFBA, PFPeA, PFPeS, PFDA, PFDoA, PFUnA, PFHpA, PFTriA, PFHpS, PFDS, PFTeDA, PFHxDA, PFODA, HFPO-DA/GenX, Propoanoic Acid, 6:2 FTOH, 8:2 FTOH, Acetic acid).

1.1.4. Drinking water

Standards for PFAS in drinking water vary (Table B.1). The WHO is in the process of developing drinking water guidance values for PFAS which are predicted to be 0.1 µg/l for each PFOA and PFOS and 0.5 µg/l for total PFAS, based on the 29 compounds reliably measured with the EPA's analytical methods. However, the WHO has been criticised over these guidelines being far above values suggested by scientists linking PFAS exposure to adverse health effects (Southerland & Birnbaum, 2023).

The recast EU Drinking Water Directive (Directive (EU) 2020/2184) introduced standards for PFAS that were implemented in Scotland through the Public Water Supplies (Scotland) Amendment Regulations 2022 with a standard for the sum of 20 PFAS compounds at 0.1 µg/l at consumers' taps, from January 2023. The 20 compounds include short- and long-chain perfluoroalkyl carboxylic acids and sulphonic acids. Sampling needs to be carried out for all these substances if the risk assessment establishes a risk of PFAS presence in raw or final water.

In Scotland, sampling needs to be carried out for all these substances in line with the assessed risk to the raw water sources and the representativeness of the sampling points in relation to the water entering the downstream water treatment works (DWQR, 2022). A risk assessment, and monitoring if there is a risk to the wholesomeness of the supply, should also be carried out for other PFAS substances if there is a risk of those contaminating drinking water sources. If concentrations above 0.01 µg/l are detected for any PFAS substance, monitoring frequency has to be between quarterly and monthly or more if it is predicted that concentrations may breach 0.1 µg/l (DWQR, 2022).

There is limited information about sampling frequency for other countries. Reports from Australia suggest monthly sampling, the EPA sampling is in line with the Unregulated Contaminant Monitoring Rule sampling frequency and timeframe, which is 4 times during a consecutive 12-month monitoring period, with 3 months apart for surface water, and 2 times during a consecutive 12-month monitoring period, with 5-7 months apart for groundwater.

PFAS are measured by solid phase extraction followed by a liquid chromatograph coupled to tandem mass spectrometry (LC/MS/MS). The developed methods are applied to test for specific PFAS compounds. EPA has developed methods (533, 537, and 537.1; EPA, 2019; Shoemaker *et al*., 2009; Shoemaker & Tettenhorst, 2020) for 29 PFAS (see Table B.2). Detection limits vary per compound – detection limits for PFOA and PFOS are 0.00053 µg/l and 0.0011 µg/l, respectively, using method 537.1.

Table B.1: Overview of drinking water standards (black) or other PFAS standards (grey).

Country	PFOA (µg/l)	PFOS (µg/l)	Other (µg/l)
Australia	0.56	0.07 (combined with PFHxS)	
China	0.08	0.04	
Canada	0.2	0.6	Screening values for PFBA, PFBS, PFHxS, PFPeA, PFHxA, PFHpA, PFNA, 6:2 FTS, 8:2 FTS
Denmark			Sum of PFOA, PFOS, PFNA and PFHxS: 0.002
England & Wales			Monitoring of 47 PFAS[1], action triggered at 0.1 µg/l for any substance
EU EQS			Sum of 24 PFAS1: 0,0044 µg/l as PFOA equivalent; annual average value
EU Drinking Water			Sum of 20 PFAS1: 0.1 Total PFAS: 0.5 (from 2026)
Germany			Sum of PFAS (as EU): 0.1 (from Jan 2026) Sum of PFHxS, PFOA, PFOS, PFNA: 0.02 (from 2028)
Japan	0.05 (combined)		
Scotland			Sum of 20 PFAS (as EU): 0.1 µg/l
REACH Annex XVII			Ban on 5 PFAS[1]
EU POPs	ban	ban	
USA (EPA) - proposed	0.004 (with a goal of 0)	0.004 (with a goal of 0)	PFHxS, PFNA, PFBS, HFPO-DA (GenX) (combined): 1.0 (unitless) Hazard index
WHO – proposed guidance	0.1	0.1	Total PFAS (29 compounds)1: 0.5

[1] See Table B.2

Table B.2: List of PFAS compounds that are covered by different regulations.

Name	Abbrev.	Formula	Regulated under								CAS No.
			EU/ Scotland	England	EU EQS	EU POPs	REACH Annex XVII	US EPA	Canada DW	WHO guidance	
Short-chain PFCAs											
Perfluorobutanoic acid	PFBA	C_3F_7COOH	x	x	x				x	x	375-22-4
Perfluoropentanoic acid	PFPeA	C_4F_9COOH	x	x	x				x	x	2706-90-3
Perfluorohexanoic acid	PFHxA	$C_5F_{11}COOH$	x	x	x				x		307-24-4
Perfluoroheptanoic acid	PFHpA	$C_6F_{13}COOH$	x	x	x				x	x	375-85-9
Long-chain PFCA											
Perfluorooctanoic acid	PFOA	$C_7F_{15}COOH$	x	x	x	x		x	x	x	335-67-1
Perfluorononanoic acid	PFNA	$C_8F_{17}COOH$	x	x	x		x	x	x	x	375-95-1
Perfluorodecanoic acid	PFDA	$C_9F_{19}COOH$	x	x	x		x			x	335-76-2
Perfluoroundecanoic acid	PFUnA	$C_{10}F_{21}COOH$	x	x	x		x			x	2058-94-8
Perfluorododecanoic acid	PFDoA	$C_{11}F_{23}COOH$	x	x	x		x			x	307-55-1
Perfluorotridecanoic acid	PFTriA	$C_{12}F_{25}COOH$	x	x	x		x			x	72629-94-8
Perfluorotetradeconoic acid	PFTeDA	$C_{13}F_{27}COOH$		x	x					x	376-06-7
Perfluorohexadeconoic acid	PFHxDA	$C_{15}F_{31}COOH$		x	x						67905-19-5
Perfluorooctadecanoic acid	PFODA	$C_{17}F_{35}COOH$		x	x						16517-11-6
Short-chain PFSA											
Perfluorobutane sulfonic acid	PFBS	$C_4F_9SO_3H$	x	x	x			x	x	x	375-73-5
Perfluoropentane sulfonic acid	PFPS	$C_5F_{11}SO_3H$	x	x	x					x	2706-91-4
Long-chain PFSA											
Perfluorohexane sulfonic acid	PFHxS	$C_6F_{13}SO_3H$	x	x	x			x	x		355-46-4
Perfluoroheptane sulfonic acid	PFHpS	$C_7F_{15}SO_3H$	x	x	x					x	375-92-8
Perfluorooctane sulfonic acid	PFOS	$C_8F_{17}SO_3H$	x	x	x	x		x	x	x	1763-23-1
Perfluorononane sulfonic acid	PFNS	$C_9F_{19}SO_3H$	x	x							98789-57-2
Perfluorodecane sulfonic acid	PFDS	$C_{10}F_{21}SO_3H$	x	x	x						335-77-3
Perfluoroundecane sulfonic acid	PFUnS	$C_{11}F_{23}SO_3H$	x	x							749786-16-1
Perfluorododecane sulfonic acid	PFDoS	$C_{12}F_{25}SO_3H$	x	x							79780-39-5
Perfluorotridecane sulfonic acid	PFTriS	$C_{13}F_{27}SO_3H$	x								791563-89-8

Table B.2: List of PFAS compounds that are covered by different regulations.

Name	Abbrev.	Formula	Regulated under								CAS No.
			EU/ Scotland	England	EU EQS	EU POPs	REACH Annex XVII	US EPA	Canada DW	WHO guidance	
New generation PFAS											
Ammonium perfluoro (2-methyl-3-oxahexanoate) / hexafluoropropylene oxide dimer acid	HFPO-DA/ GenX	$C_5F_{11}OCOOH$		x	x			x		x	13252-13-6
Hexafluoropropylene oxide trimer acid	HFPO-TA	$C_8F_{17}O_2COOH$		x							13252-14-7
Propanoic Acid / Ammonium 2,2,3-trifluoro-3-(1,1,2,2,3,3-hexafluoro-3- (trifluoromethoxy) propoxy)propanoate / ammonium 4,8-dioxa-3H-perfluorononanoate	ADONA	$C_7H_4F_{13}NO_4$		x	x					x	919005-14-4
Perfluoro-4-oxapentanoic acid/ Perfluoro-3-methoxypropanoic acid	PFMOPrA/ PFMPA	C_3F_7OCOOH		x						x	377-73-1
Perfluoro-4-methoxybutanoic acid	PFMOBA	C_5HF_9O								x	863090-89-5
Perfluoro-3,6-dioxaheptanoic acid	NFDHA	$F_3OCF_2CF_2O$ CF_2COOH		x						x	151772-58-6
Perfluoro-5-oxahexanoic acid	PFMOBA	$C_5HF_9O_3$		x							863090-89-5
Perfluoroethylcyclohexane Sulfonate	PFECHS	$C_8HF_{15}O_3S$		x							646-83-3
3-Perfluoropropyl propanoic acid (3:3)	3:3 FTCA			x							356-02-5
3-Perfluoropentyl propanoic acid (5:3)	5:3 FTCA			x							914637-49-3
3-Perfluoroheptyl propanoic acid (7:3)	7:3 FTCA			x							812-70-4
Perfluoro-(2-ethoxyethane)-sulfonic acid	PFEESA			x						x	113507-82-7

Table B.2: List of PFAS compounds that are covered by different regulations.

Name	Abbrev.	Formula	Regulated under								CAS No.
			EU/ Scotland	England	EU EQS	EU POPs	REACH Annex XVII	US EPA	Canada DW	WHO guidance	
Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate	6:2 Cl-PFESA/ 9Cl-PF3ONS			x						x	756426-58-1
Potassium 11-chloroeicosafluoro-3-oxaundecane-1-sulfonate	8:2 Cl-PFESA/ 11Cl-PF3OUdS			x						x	763051-92-9
Sodium 1H,1H,2H,2H-perfluorohexane sulfonate (4:2)	4:2 FTSA/ 4:2 FTS			x						x	757124-72-4
Sodium 1H,1H,2H,2H-perfluorooctane sulfonate (6:2)	6:2 FTSA/ 6:2 FTS			x					x	x	27619-97-2
Sodium 1H,1H,2H,2H-perfluorodecane sulfonate (8:2)	8:2 FTSA/ 8:2 FTS			x					x	x	39108-34-4
Perfluoro-1-butanesulfonamide	FBSA	$C_4F_9SO_2NH_2$		x							30334-69-1
Perfluoro-1-hexanesulfonamide	FHxSA	$C_6F_{13}SO_2NH_2$		x							41997-13-1
Perfluoro-1-octanesulfonamide	FOSA	$C_{13}H_{13}F_{17}N_2O_2S$		x							13417-01-1
N-methylperfluoro-1-octansulfonamide	MeFOSA/ N-MeFOSA			x							2355-31-9
N-ethylperfluoro-1-octanesulfonamide	EtFOSA/ N-EtFOSA			x						x	2991-50-6
2-(N-methylperfluoro-1-octanesulfonamido)-ethanol	MeFOSE	$C_{11}H_8F_{17}NO_3S$		x						x	24448-09-7
2-(N-ethylperfluoro-1-octanesulfonamido)-ethanol	EtFOSE	$C_{12}H_8F_{17}NO_4S$		x							
N-methylperfluoro-1-octanesulfonamidoacetic acid	NMeFOSAA/ MeFOSAA	$C_{11}H_6F_{17}NO_4S$		x							1400690-70-1
N-ethylperfluoro-1-octanesulfonamidoacetic acid	NEtFOSAA/ EtFOSAA			x							2991-50-6
Acetic acid / 2,2-difluoro-2-((2,2,4,5-tetrafluoro-5-(trifluoromethoxy)1,3-dioxolan-4-yloxy)-		$C_6H_4F_9NO_6$			x						1190931-27-1

Table B.2: List of PFAS compounds that are covered by different regulations.

Name	Abbrev.	Formula	Regulated under								CAS No.
			EU/ Scotland	England	EU EQS	EU POPs	REACH Annex XVII	US EPA	Canada DW	WHO guidance	
Precursors											
6:2 Fluorotelomer alcohol	6:2 FTOH	$F(CF_2)_6CH_2CH_2OH$			x						647-42-7
8:2 Fluorotelomer alcohol	8:2 FTOH	$F(CF_2)_8CH_2CH_2OH$			x						678-39-7

1.1.5. National and international developments

In October 2023, a class action was started in the US, with two cases in Connecticut against water companies together supplying about 1 million people (*Hoffnagle et al. v. Connecticut Water Company, Vincent v. Aquarion Water Company*). The complaints are interesting for their narration of the properties of PFAS and PFOA, for which the EPA has just introduced standards for drinking water quality, the narration of the potential harms, the allegation that the suppliers knew of the presence of PFAS and the potential harm, and the identification of water treatments that would have alleviated the problem (activated carbon, ion exchange and reverse osmosis). The complainers base their claims inter alia on breach of duty, negligence, and failure to warn, and are seeking medical monitoring and statutory punitive damages.

In the UK, the Royal Society of Chemistry (RSC, 2023) has recommended that in England, there should be a regulatory limit of 0.01 µg/l for each PFAS and a total limit of 0.1 µg/. The RSC notes that PFAS are a priority area for UK REACH (HSE, 2023). They also suggest that permits for landfills and for industrial activities should include conditions on PFAS; that PFAS should be priority substances for water services providers; that water treatment plants should manage waste (e.g., from filters) that may contain PFAS; that biosolids should be tested; and that manufacturers using PFAS should be audited and be required to report on their emissions.

1.2. Processes (sources, pathways and receptors)

1.2.1. Manufacturing and use

PFAS are relatively costly to produce and tend to be used where other substances are not reaching the same performance or if only small amounts of PFAS are necessary to achieve the required result (Glüge *et al.*, 2020). Because the C-F bond is very strong, PFAS can resist chemical attack and withstand high temperatures, and are typically oil and water repellent. They are widely used in different industries, mainly where very stable and non-reactive substances, or where both hydrophobic and oleophobic characteristics are required. Attempts have been made to comprehensively list all uses (Gaines, 2023; Glüge *et al.*, 2020). Some of the main uses are described in Table B.3. HSE (2023, p. 27) reports as the result of a GB call for evidence that “fluoropolymers and fluoroelastomers are particularly important to the industrial, automotive, aerospace and defence sectors, where uses include membranes, diaphragms, gaskets, seals and pipe linings. Side chain (C6) fluorinated polymers are used in coatings for textiles, upholstery, leather, carpets and paper. F-gases are of particular importance to the refrigeration, air conditioning and heat pump (RACHP) sector, and for foam blowing in the production of polyurethane foams. F-gases are also used in anaesthesia (sevoflurane, isoflurane) and in a number of specialist medical applications. Short-chain PFAS may be used at low concentrations (<0.1%) in household paints as fluorosurfactants.”

1.2.2. Sources to the environment

PFAS have been found in the atmosphere globally due to the volatile nature of some PFAS (e.g., perfluoroalkane sulfonamido ethanols, perfluoroalkane sulfonamides, fluorotelomer alcohols), which are precursors to PFAAs (Faust, 2023). PFAS have been shown to disperse as far as 150 km by air (D’Ambro *et al*., 2021), leading to a background concentration of PFAS in soils (Mattias *et al*., 2022). Elevated soil concentrations indicate additional local or regional contamination sources. Local sources of PFAS can be point sources or diffuse sources. Table B.4 provides and overview over point and diffuse source potentially relevant for Scotland.

Point sources include industrial sites where PFAS are produced or used in manufacturing, e.g., for electric or electronic products, paper, or metal plating (Garg *et al*., 2020; Glenn *et al*., 2021; Helmer *et al*., 2022; Langberg *et al*., 2021). These sites can emit PFAS into the atmosphere, leading to contamination of soils and surface water around the sites (Galloway *et al*., 2020), or through effluent discharge into surface water. Measurements of PFAS in air revealed quickly decreasing concentrations of longer chain PFAS within 5 km of two PFAS manufacturing plants in China, but shorter chain PFAS concentrations stayed elevated over a longer distance. Similarly, overall PFAS concentrations in surface water declined by >75% within the first 5 km downstream of the plant, although shorter chain PFAS concentrations remained elevated in surface water even 38 km downstream, and were detected in reservoirs 5 and 12 km upstream (Chen *et al*., 2018).

While PFAS are found in many items in domestic and commercial settings, their main route from these into the environment are through disposal, either in wastewater or in landfills. Wastewater discharge points are sources of PFAS to the

Table B.3: Selected industries using PFAs and examples of areas of application (Gaines, 2023; Glüge et al., 2020).

Category	Application examples
Building and construction	Air emission filters, cement tiles, concrete mixtures, greenhouse/conservatory windows, house doors, house shutters, house sidings, house windows, marine structures, roofing, roof fabrics, skyscraper metal walls coating, solar application films
Electronic industry	Aerospace applications, automotive, cables and wired with communication facilities, cell phones, circuit boards, coaxial cable insulation, computer cables and networks, digital cameras, disk drives, electrical wiring insulation, floppy disks, lithium batteries, low-frequency plenum cables, magnetic recording devices, magnetic tapes, optical fibres, printed circuit boards, printers, radar systems, satellite communication systems, scanners, solar collectors coating, zinc batteries
Metal production	Decorative chrome plating (historical), hard chrome plating, nickel, cadmium, lead plating, metal plating on plastics, alkaline zinc plating, copper electroless plating, coating baths for nickel-boron layers, copper, nickel and tin electroplating, aluminium foil
Plastics and rubber production	Raw material, processing aids or manufacturing intermediate in fluoropolymer production
Coatings, wax, paint, varnish, ink	For anticorrosive, water and oil repellent, antifog characteristics, e.g., for use on stony material, marble, tiles, cement, glass, metals, to prevent fogging in humid environments such as in the bathroom, or of eyeglass lenses, windshields, greenhouses, skis, or in agriculture; paints and inks used in automotive coatings
Cleaning products	Types of items for cleaning: alkaline cleaners, ATVs, automobile waxes, bicycle chains, blades and bits, cams and pulleys, car wash products, carpet spot cleaners, concrete, conveyor belts, countertops, denture cleaners, dishwashing liquid, floor polish, floors, glass, hard surfaces, hinges, masonry, metal surfaces, motorcycle chains, power tools and equipment, rollers, shampoos, slides, winches, wood
Flame retardant and extinguishing agents	AFFF, used at airports, train yards, ships, oil refineries, oil platforms, etc.
Packaging, paper, and cardboard	Anticorrosion paper, baking paper, butter wrappers, carbonless forms, coated raw paper, folding cartons, food plates & bowls, general liner and flute, kraft paper, masking paper, microwave popcorn bag susceptors, neutral liner, neutral white role paper, paper combined with metal, pet food bags, pizza boxes, paper food straws, raw paper for plaster boards, take-out food containers and wraps, wallpaper, wood-containing paper
Cosmetics and personal care products	Acne treatment, blush/highlighter, brow products, creams, dental floss, dental plaque remover, eye cream, eyeshadow, foundation, hair conditioner, hair creams, shampoo, hand sanitizer, lip balm, lotions, mascara, nail polish, shaving cream, sunscreen, wax
Medical and scientific use	Pharmaceuticals, medical diagnostics (MRI, ultrasounds, PET, multimodal contrast agents), medical devices (e.g., implantable material, devices, parts and components, such as bags, blood substitutes, soft tissue replacement, catheters, contact lenses, needles, oral tablets, shunts, stents, inhalers, wound care)
Mining	Copper and gold, uranium, aluminium, and vanadium ore separation
Oil and gas	Well drilling, completion, or workover operations; controlling oil spills
Pesticides and fertilizers	Active or inactive component of pesticides, coating for fertilizers to reduce dust
Textiles	Automobile interior, awning textiles, carpets, clothing, fire fighters protective clothing and gear, gloves, home textiles, industrial environment textiles, jackets, leather, medical garments, outdoor textiles, sails, shoes, tents, umbrellas, upholstery
Other	Dry cleaning, etching, explosives, propellants and ammunition, photography and lithography, recycling and material recovery, refrigerants, semiconductors, energy and nuclear sector, watchmaking, wood industry, conservation of books and manuscripts, cook- and bakingware, floor coverings, glass, leather, music instruments, optical devices, sport equipment such as tennis racquets and skis

Table B.4: Summary of potential PFAS sources and their primary receptors in the environment.	
Source	**Primary receptor**
Point sources	
Industrial discharges, e.g., from • Paper production • Metal plating • Textiles • Plastic and rubber production • Building material production and storage	Surface water
Wastewater discharges	Surface water
Landfills	Soils and groundwater, surface water
Sites of storage and application of AFFF • Airports/airfields • Fire stations • Major fire incident sites	
Septic tanks	Soils and groundwater
Mines	Groundwater
Landscape features • Electrical infrastructure, incl. power stations • Telecommunication infrastructure • Wind farms	Soils and surface water
Diffuse sources	
Atmospheric deposition • Manufacturing • Waste incineration • Biosolid, fertilizer and pesticide application	Soils and surface water
Biosolid/sludge application to land	Soils and groundwater
Fertilizer and pesticide application to land	Soils and groundwater
Irrigation	Soils and groundwater
Ski areas	Soils and groundwater

freshwater environment if wastewater treatment is inadequate at removing PFAS. PFAS fate in wastewater treatment depends not only on the design, capacity, and operating conditions of the treatment plant (e.g., hydraulic and sludge retention time, temperature, flow rate etc.), but also on climatic conditions, types of wastewater and types of PFAS substances (Lenka *et al*., 2021). The primary factor of removal of PFAS from the effluent is adsorption onto sludge, especially for longer-chain PFAS. Biological remediation techniques can increase concentrations of PFAAs due to transformation of precursors (Lenka *et al*., 2021). Adsorption (e.g., anion exchange resins, activated carbon), nanofiltration, and reverse osmosis have been found to have some efficiency in removing PFAS from wastewater (O'Connor *et al*., 2022). Work carried out under the Chemical Investigations Programme for PFOA and PFOS (Campitelli *et al*., 2022) shows that concentrations in influent and effluent at WWTW are variable, in line with findings from Denmark and Germany that also observed very variable concentrations within the same WWTWs (Becker *et al*., 2010; Larsen & Giovalle, 2015). Nevertheless, it seems clear that WWTWs can add to the PFAS load (overall mean influent PFOS concentrations were 0.002 µg/l, while overall mean effluent concentration was 0.01 µg/l; see also a review by Lenka *et al*., 2021). This might be due to their physiochemical properties but also due to transformation of polyfluoroalkyl substances to PFAAs. This can lead to substantial increases in concentrations downstream of wastewater treatment works (Comber *et al*., 2022). Especially treatment plants that have a high industrial component tend to have higher effluent PFAS concentrations (Cookson & Detwiler, 2022).

Wastewater sludge can concentrate PFAS, and thus become a diffuse pollution source to land if it is applied to land in agricultural settings (Garg *et al*., 2023; Johnson, 2022). In an analysis of biosolid samples from Scotland, concentrations of several contaminants, including PFOS, were measured, finding concentrations significantly lower than previously reported in literature (Stutt *et al*., 2019). This seems to indicate a relatively low risk from biosolids, as PFOS is widely found in UK biosolid samples, in contrast to PFOA and PFBS (Marshall & Yates, 2022). Fertilizers and pesticides can include PFAS and their application to land thus also represents a potential diffuse source.

Houses that are not connected to a sewer system operate septic tanks that receive the wastewater. These septic tanks then become potential sources of PFAS to the surrounding groundwater and surface water. Schaider *et al*. (2016) analysed water samples from domestic drinking water wells in the US and found several PFAS compounds at comparatively high concentrations in areas with onsite wastewater treatment systems. They suggest nitrate concentrations as an indicator substance for organic wastewater compounds.

Landfill leachate poses a point source to soils and eventually groundwater (Eschauzier *et al*., 2013; Garg *et al*., 2020; J. Li *et al*., 2023; T. Liu *et al*., 2022). It has been shown that operating municipal landfills leach higher PFAS levels than closed and historical ones, and landfills with construction and demolished material leach higher levels than municipal ones (Abunada *et al*., 2020). Biological leachate treatment can increase PFAS concentration, and bioreactor landfills have shown to have higher PFAS concentrations than non-bioreactor landfills (Meegoda *et al*., 2020). Additionally, it has been shown that landfill ambient air contains elevated PFAS concentrations (Hamid *et al*., 2018).

It has also been shown that sites where AFFF have been stored (Anderson *et al*., 2021), such as fire stations and training sites, airfields (M. Liu *et al*., 2022), or military bases (Eschauzier *et al*., 2013), or where they were applied due to major fire incidents (Alghamdi *et al*., 2022; Marchiandi *et al*., 2021), are sources for PFAS to soils and groundwater (Hatton *et al*., 2018). PFSAs are more frequently detected in AFFF impacted sites than PFCAs (Wilkinson *et al*., 2022).

Mines are beginning to be identified as local sources of PFAS, with some low-level impacts (Barfoot *et al*., 2022). They are used in the extraction of ores and minerals as acid mist suppressing agents, wetting agents, hydrocarbon foaming agent, and in ore floating (Keyte *et al*., 2021). Disused mines could be a source of PFAS if PFAS compounds were used while they were operational. Ski wax contains PFAS and Carlson and Tupper (2020) show that it can locally be a major source of PFAS to soils and water sources.

Box B.1: Physiochemical properties of PFAS substances.

Carboxyls degrade more easily than sulfonates when the same chain length. Transformation also depends on environmental conditions, such as soil sorption, pH, temperature, or microbial population, leading to variation in half-life of specific PFAS compounds. For example, biodegradation of N-ethyl perfluorooctane sulfonamido ethanol was found to be slower in marine sediments, ultimately leading to higher concentrations in marine environments (Benskin *et al*., 2013). Similarly, anaerobic conditions slow down biotransformation, so some compounds that are usually intermediary may become terminal under reducing conditions, found for example at landfills. As many PFAS are co-compounds in a mixture, also with non-PFAS contaminants, this can influence degradation (Evich *et al*., 2022).

PFAS have different mechanisms of interacting with the environment (H. Li *et al*., 2023). The C-F bond is hydrophobic, meaning hydrophobic groups can aggregate and PFAS can be adsorbed on hydrophobic media such as natural sediments and organic matter. Especially longer chained PFAS, having more C-F bonds, can therefore be retarded in hydrophobic media.

Functional groups dissociate into ionic forms in aqueous solutions under appropriate conditions, forming either anions, cations or zwitterions. In normal environmental conditions (pH between 4 and 9), most PFAS are in their anionic form. Anions are less likely to be adsorbed to soils than cations. Anions will be retained in positively charged media but negatively charged media will decrease retention and retardation. Sorption to soils is thus also dependent on pH, for example high soil pH can suppress anion sorption to soils and increase leaching especially for longer chain PFAS (Kabiri *et al*., 2022). PFAS anions may be adsorbed on the surface of metallic minerals such as iron and aluminium, meaning PFAS can be retained in metallic mineral-rich media (H. Li *et al*., 2023).

Due to the hydrophobic nature of PFAS, they can get retarded at the air-water interface in unsaturated zones, especially longer chain PFAS. A similar effect occurs with non-aqueous phase liquids (NAPLs, such as oil, petroleum), which is important for PFAS mobility at sites polluted with NAPLs (H. Li *et al*., 2023).

Table B.5: Physiochemical characteristics of PFAS, according to group (short- vs. long-chain and carboxyl vs. sulfonamide head). – indicates lower potential, + indicated higher potential. Blank cells indicate no known difference.

Property	Short-chain PFAS	Long-chain PFAS	Carboxyl	Sufonamide
Degradation in the environment			+	–
Water solubility	+	–		
Soil adsorption	–	+	+	–
Adsorption to hydrophobic media	–	+		
Mobility in soil and water	+	–		
Bioaccumulation potential - terrestrial plants	+	–	–	+
Bioaccumulation potential – aquatic plants	–	+		
Bioaccumulation potential - animals	–	+		
Expected toxicity	–	+		

1.2.3. Pathways to the aquatic environment

Despite high stability, approximately 20% of PFAS undergo transformation in the environment, usually degrading to PFCAs and PFSAs, which contribute up to 86% of total PFAS identified in wastewater-treatment sludge (Evich *et al*., 2022).

Physiochemical properties of different PFAS compounds are determined by carbon chain length and functional group (sulfonates, carboxyls, and hydroxyls) and influence PFAS interaction with the environment and thus the pathways the different compounds take (Box B.1, Table B.5). There are competing influences leading to complex mobility behaviour. In soils, migration gets slowed by sorption on NOM, minerals, and at fluid-fluid interfaces. Key influences in retaining PFAS in the soil are therefore organic matter content, minerals, saturation, pH, and ionic strength, generally with increasing retardation from high organic matter content, low water saturation, low pH, and high ionic strength (H. Li *et al*., 2023). Some of the findings are ambiguous and influences are complex, for example the influence of organic matter: organic matter content above 15% has been shown to retard PFAS in the soils (especially longer-chain PFAS), but lower organic matter content (<5%) could facilitate PFAS mobility especially for shorter-chain compounds due to competition with for interaction sites on the media surface (H. Li *et al*., 2023). A significant positive retardation effect was observed along a pH 10 to 5 gradient. These effects are especially pronounced for longer chain PFAS (Kabiri *et al*., 2022), which are more likely to attach to soil particles, but can thus present a long potential contamination source. Shorter-chain PFAS are likely to more rapidly leach into deeper soil and groundwater (Lyu *et al*., 2022). Kabiri *et al*. (2022) summarise that leaching was mainly controlled by PFAS chemical properties, rather than soil physiochemical properties, with the functional group (PFAS with carboxylate heads leaching more easily than those with a sulfonate or sulfonamide head) also playing a role, next to carbon chain length.

Plants tend to take up PFAS through roots, with shorter chain PFAS being taken up more easily (Adu *et al*., 2023), whereas microinvertebrates accumulate longer-chain PFAS more easily (Evich *et al*., 2022). Plant uptake increases with increasing temperatures, but reduces with increasing soil organic carbon content, probably due to lower bioavailability from adsorption to soil particles (Adu *et al*., 2023). In aquatic environments, aquatic vegetative leaf accumulation increases with increasing chain length, which is mirrored for uptake in aquatic macroinvertebrates (Evich *et al*., 2022).

Few studies examine variations in PFAS concentrations depending on season and underlying mobilisation processes. Nguyen *et al*. (2022) studied two catchments in Sweden, one impacted by a civilian airport, the other by a military airport and wastewater effluents. The sites demonstrated contrasting seasonal behaviour, with the site showing predominantly positive correlations of flow and concentration, the second showing high concentrations at low flow. This indicates two different processes, ***mobilisation***, and ***dilution,*** that govern PFAS concentration patterns. The study also indicates that PFAS concentrations correlate to total organic carbon concentrations especially for longer chain PFAS compounds at the mobilisation-governed site. A complicating factor in seasonal patterns for PFAS concentrations is connectivity of ground and surface waters (Tokranov *et al*., 2021), which can cross-contaminate (Pétré *et al*., 2022; Sharma *et al*., 2016).

Table B.6: Summary of SEPA surface water monitoring for PFAS in 2018. Total number of smples per PFAS compound = 61.

Compound	No. of detections	Maximum concentration (µg/l)	Site of max. concentration
PFBS	39	0.0107	River Almond (Lothian)
PFDA	2	0.00078	River Clyde
PFHpS	12	0.00035	River Almond (Lothian) & River Don
PFHpA	7	0.00417	River Almond (Lothian)
PFHxS	37	0.00116	River Almond (Lothian)
PFHxA	14	0.0182	River Almond (Lothian)
PFNA	8	0.00105	River Almond (Lothian)
PFOS	43	0.00311	River Carron
PFOA	31	0.00437	River Almond (Lothian)

1.2.4. Branched isomers and new generation PFAS

While the linear isomers of PFAS compounds are the desired product and predominant result of manufacturing processes of PFAS, branched isomers occur as co-products. There is little known about different effects to humans and animals, although studies indicate that while the linear isomers tend to dominantly accumulate in animals, the branched isomers are found in slightly higher percentages in humans (Schulz *et al*., 2020). Branched isomers also adsorb to a lesser extend to soil and sediment, and some studies have found branched isomers in surface waters at the same concentrations or higher than their linear counterparts. The lower adsorption to soil could make branched isomers more likely to reach groundwater, but groundwater studies have shown very variable distribution of concentrations between linear and branched isomers (Schulz *et al*., 2020).

With the phase-out of PFOS and PFOA, and increasing awareness of toxicity of long-chain PFAS and assumed lesser toxicity of short-chain PFAS, manufacturing and use has shifted to shorter chain PFAS alternatives, which are now found in greater prevalence in the environment, such as PFBA, PFBS, and PFHxS. Further, new generation PFAS have started to be in widespread use, belonging to the groups of perfluoroalkyl ether sulfonic and carboxylic acids (PFESAs and PFECAs), including hexafluoropropylene oxide dimer acid (HFPO-DA, or GenX), 6:2 chlorinated polyfluorinated ether sulfonate (6:2 Cl-PFESa), and ammonium 4,8-dioxa-3H-perfluorononanoate (ADONA); or fluorotelomer sulfonic and carboxylic acids (FTSA and FTCA). Another alternative is perfluoroethylcyclohexane sulfonate (PFECHS), an 8-carbon cyclic PFAS. There is limited knowledge about the behaviour of these substances in the environment and their toxicity, but it is believed they behave similarly to the substances they have replaced (Mahoney *et al*., 2022). They are being increasingly found in surface and groundwater (Wang *et al*., 2019), as well as wildlife (Herzke *et al*., 2023), and studies indicate they may be harder to remove from water (Heidari *et al*., 2021; Hopkins *et al*., 2018).

Table B.7: Summary of SEPA groundwater monitoring for PFAS from 2013-2016. Total number of smples per PFAS compound = 40.

Compound	No. of detections	Maximum concentration (µg/l)
PFBS	4	0.0143
PFDA	0	–
PFDoA	0	–
PFHpA	1	0.00689
PFHpS	0	–
PFHxS	0	–
PFOA	3	0.0328
PFOS	3	0.0147
PFOSA	0	–
PFPeA	6	0.0292
PFUnA	0	–

1.3. Occurrence and concentration in freshwater

1.3.1. Scotland and the UK

The information about presence and prevalence of PFAS compounds in the Scottish freshwater environment is limited. The Scottish Environment Protection Agency (SEPA) carried out some limited surface and groundwater sampling for PFAS (Table B.6). Available surface water samples span 22 locations sampled app. monthly between July and October 2018 for nine different PFAS compounds (PFDA, PFHpA, PFHxA, PFNA, PFOA, PFBS, PFHpS,

Table B.8: Summary statistics of concentrations (µg/L) in inland surface waters across Europe from the datasets the JRC collected, reproduced from Niegowska et al., 2021).

Substance	Min	Mean	Median	P90	P95	Max	No. of EU member states with information
PFOS	0.0005	24.2	11.6	36.9	63.0	50.0	5
PFUnA	0.001	15.1	1.0	25.2	100	118	5
PFPeA	0.15	11.2	5.0	18.0	38.0	974	2
PFHxA	0.2	17.6	5.0	28.0	65.0	89.2	8
PFDoA	0.02	2.43	1.0	5.0	5.0	100	4
PFOA	0.001	53.4	12.0	68.0	140	12,000	13
PFDA	0.001	8.18	5.0	5.0	12.5	2,500	8
PFDS	5.0	5.0	5.0	5.0	5.0	5.0	1
PFHxS	0.0002	7.58	5	10.0	21.0	980	3
PFBA	0.5	208	5.0	23.0	52.3	235,000	2
PFBS	0.15	22.6	5.0	29.9	57.3	4,330	8
PFHpA	0.25	11.7	5.0	16.0	82.4	1,000	10
PFHpS	2.5	4.97	5.0	5.0	5.0	5.0	1
PFNA	0.0004	4.91	5.0	5.0	8.0	320	11
PFTriA	1.25	1.25	1.25	1.25	1.25	1.25	1

PFHxS, PFOS). The highest detection was made for PFHxA at the River Almond (Lothian) in October 2018 (0.0182 µg/l). In the same sample, PFBS was detected with 0.0107 µg/l. Both substances were detected at this location also in August and September, albeit at lower concentrations (0.00226 – 0.00314 µg/l). PFOS and PFOA were also found in all samples for the River Almond (Lothian), at concentrations between 0.00124 and 0.00437 µg/l. Five further detections were made for >0.005 µg/l: at the River Kelvin, also in October, for PFHxA and PFBS, and the remaining for PFHxA at Water of Leith, Dighty Water and River Leven. PFBS was found in all samples from the River Kelvin, and PFHxA was found in all samples from the River Leven and Dighty Water, with concentrations between 0.00243 µg/l and 0.00425 µg/l. PFOS and PFOA were also detected a the Dighty Water, and PFOS at the River Carron in samples from August, September and October, at low concentrations.

Groundwater samples span 17 locations sampled app. annually or less between 2013 and 2016, for 11 compounds (PFDA, PFPeA, PFHpA, PFOA, PFUnA, PFDoA, PFBS, PFHpS, PFHxS, PFOS, Perfluorooctanesulfonamide (PFOSA); Table B.7). Some detections were for PFBS, PFHpA, PFOA, PFOS, and PFPeA. Only two samples showed detections for more than one compound (one sample for PFHpA, PFOA, PFOS and PFPeA, and one for PFOA and PFOS). The highest detection overall was made for PFOS (0.0328 µg/l), but PFPeA was detected most often (six times) with concentrations up to 0.0292 µg/l. This dataset was used in the previous assessment of risk to private water supplies in Scotland (Akoumianaki & Coull, 2018).

A report is available on results of the more extensive sampling of English waters by the Environmental Agency between 2014 and 2019, which comprised fully quantitative sampling for PFOS and PFOA and semi-quantitative sampling for 15 PFAS compounds (Pemberton, 2021). The report concludes that PFAS are likely to be widespread in English surface and groundwater. The longer chain PFAS such as PFUnA and PFDoA are rarely detected, whereas the more mobile PFAS such as PFBS, PFHxS, PFHxA, PFPeA are detected at the highest percentage of sites. PFAS are more frequently detected in surface waters (e.g., PFOS, PFOA and PFBS were detected are 95% or more of the sampled surface water sites, but only at 26, 29, and 39% of groundwater sites, respectively). Mean concentrations per site in surface freshwater ranged from below the minimum reporting value (MRV) to 0.61 µg/l for PFOS and below the MRV to 0.073 µg/l for PFOA.

1.3.2. International

A report by the Joint Research Centre (Niegowska *et al.*, 2021) gives an overview over semi-quantitative and fully quantitative PFAS inland surface water monitoring data collected from several EU member states between 2006 and 2014. Data was collected for 15 substances, with nine of them (PFOS, PFOA, PFBS, PFDA, PFHpA, PFHxA, PFNA, PFUnA, PFDoA) being reported from four or more member states. Concentrations are summarised in Table B.8.

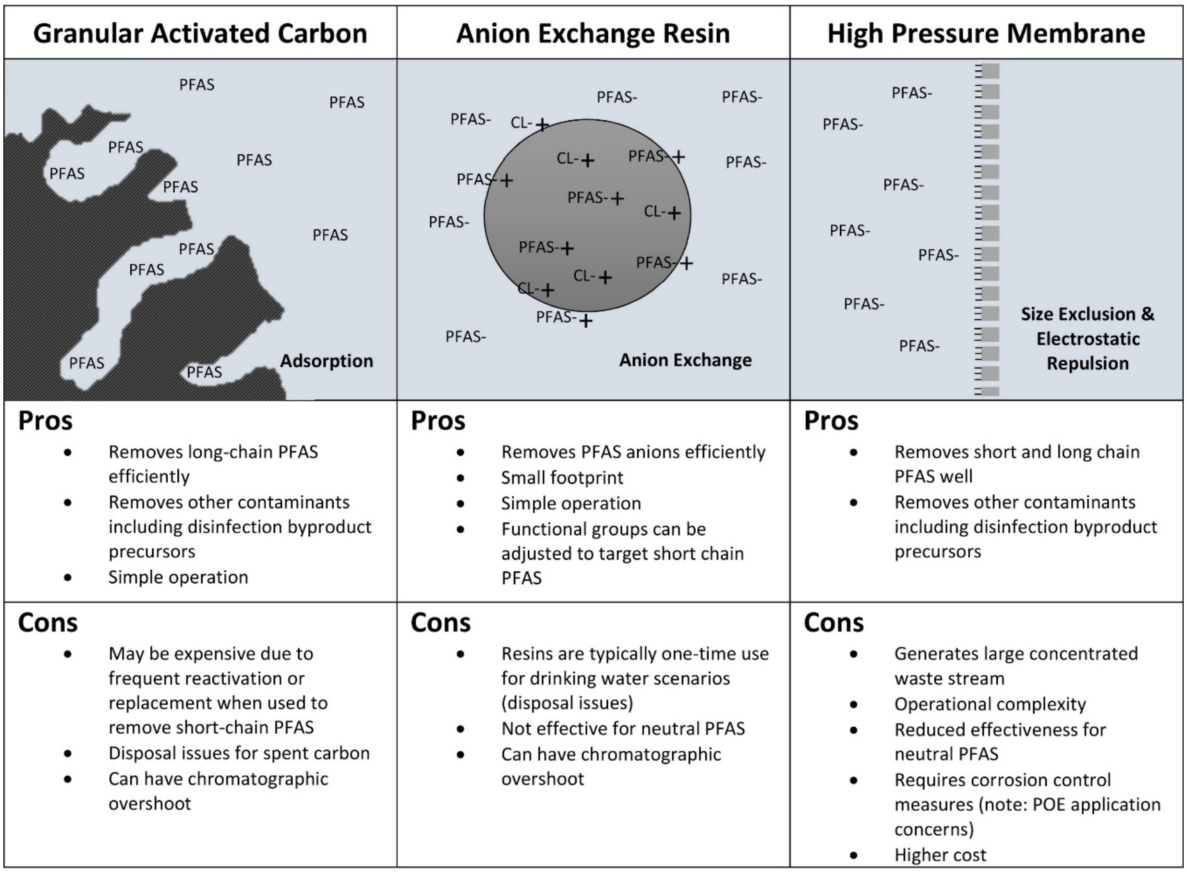
Kurwadkar *et al*. (2022) review studies from around the world to collect information on concentrations of PFAS, focusing on PFOA and PFOS. Across European countries, concentration patterns are similar, with PFAS concentrations generally higher in densely populated and industrialised areas. Podder *et al*. (2021) review studies on the occurrence and concentration of PFAS according to decade (pre-2000, 2001-2010, and post 2010). They report a decrease in PFOS concentrations after 2010, but occurrences of elevated PFOS concentrations remain, and an increase of short-chain PFAS.

The USEPA's third Unregulated Contaminant Monitoring Rule (UCMR3), which collects comprehensive data from drinking water suppliers, ran until 2015 and included 6 PFAS compounds (PFOS, PFOA, PFNA, PFHxS, PFHpA, PFBS). Crone *et al*. (2019) summarise the results, finding that PFOS and PFOA were most frequently detected. Maximum concentration for PFOS was 7 µg/l. PFBS was only found with low frequency but with high mean concentrations (0.212 µg/l and 0.136 µg/l, in large (more than 10,000 population served) surface and groundwater systems, respectively). PFHxS concentrations occurred more often in larger groundwater systems but mean concentration was higher in small groundwater systems. PFNA mean concentration was higher in large systems. Mean total PFAS concentrations were higher in groundwater systems than in surface water. In about half the samples, multiple PFAS compounds were found, with some substances correlating, such as PFOS and PFHxS. There were also correlations with non-PFAS contaminants, e.g. 1,4-dioxane, chlorodifluoromethane, hexavalent chromium, chlorate 1,1-dichloroethane (Crone *et al*., 2019).

1.4. Drinking water treatment

There are many reviews available on current and emerging methods to treat PFAS (Ahmed *et al*., 2020; Barisci & Suri, 2021; Crone *et al*., 2019; Ji *et al*., 2020; Leung *et al*., 2022; Meegoda *et al*., 2020; Verma *et al*., 2021). The main established treatment technologies that are discussed are activated carbon, anion exchange resins, and membrane filtration (Figure B.4). Further research is into emerging and optimum treatment of PFAS is ongoing (e.g., Smaili and Ng (2023)).

One of the cheaper, relatively effective ways of treating PFAS is through adsorption on activated carbon, e.g., granular activated carbon (GAC),



	Granular Activated Carbon	Anion Exchange Resin	High Pressure Membrane
Pros	• Removes long-chain PFAS efficiently • Removes other contaminants including disinfection byproduct precursors • Simple operation	• Removes PFAS anions efficiently • Small footprint • Simple operation • Functional groups can be adjusted to target short chain PFAS	• Removes short and long chain PFAS well • Removes other contaminants including disinfection byproduct precursors
Cons	• May be expensive due to frequent reactivation or replacement when used to remove short-chain PFAS • Disposal issues for spent carbon • Can have chromatographic overshoot	• Resins are typically one-time use for drinking water scenarios (disposal issues) • Not effective for neutral PFAS • Can have chromatographic overshoot	• Generates large concentrated waste stream • Operational complexity • Reduced effectiveness for neutral PFAS • Requires corrosion control measures (note: POE application concerns) • Higher cost

Figure B.4: Summary and comparison of major PFAS treatment technologies, taken from Crone *et al*. (2019).

powered activated carbon (PAC), biochar, ash, carbon fibres, or carbon nanotubes (Grieco *et al*., 2021; He *et al*., 2022; Huang *et al*., 2022; Liu *et al*., 2021; Ramos *et al*., 2022). Generally, GAC works especially well for long-chained PFAS due to higher hydrophobicity, but is less effective for short-chain PFAS, and less effective for PFCAs than for PFSAs (Kempisty *et al*., 2022; Kucharzyk *et al*., 2017). pH plays an important role in the adsorption capacity, with lower pH being conducive to adsorption. Natural organic matter (NOM) presence also influences effectiveness, and could either reduce effectiveness, especially in the presence of hydrophilic NOM, or increase effectiveness in the presence of hydrophobic NOM. One of the disadvantages of GAC treatment is the need to dispose of, or reactivate, spent activated carbon, which could become a hazardous waste management concern (Abunada *et al*., 2020). In order to destroy adsorbed and volatile PFAS, heating to high temperatures of at least 500°C or even 1000°C is recommended (Crone *et al*., 2019; Sonmez Baghirzade *et al*., 2021). It is also suggested that branched isomers are less effectively removed in GAC treatment (McCleaf *et al*., 2017).

Anion exchange resins vary in their effectiveness for PFAS removal, depending on the hydrophobicity of the compound, and usually being more efficient for long-chain PFAS and PFSAs. They also produce a concentrated waste stream and regeneration may not be possible (Crone *et al*., 2019). However, anion exchange resins seem to be able to be adapted to work better with short chain PFAS and possibly new generation PFAS, such as GenX, which are harder to remove through GAC (Dixit *et al*., 2022; Heidari *et al*., 2021; Hopkins *et al*., 2018). Boyer *et al*. (2021) provide a very detailed review of available evidence for PFAS removal in anion exchange resins.

Another effective method for removal of PFAS high pressure membranes like nanofiltration, also in combination with reverse osmosis (Jin, Peydayesh, & Mezzenga, 2021; Lee *et al*., 2022; C. Liu *et al*., 2022). They have been shown to have more than 90% removal rate for shorter chain PFAS, and are hypothesised to be effective with newer generation PFAS (Hopkins *et al*., 2018; Liu & Sun, 2021). However, this method produces concentrated waste streams, and membrane fouling from accumulation of PFAS will reduce flux, meaning high PFAS concentrations lead to high maintenance effort (Abunada *et al*., 2020; Crone *et al*., 2019).

Several other treatment methods have been suggested but fuller evidence is still lacking on their effectiveness and optimisation potential. These include e.g., advanced oxidation methods, sonochemical methods, redox reactions, plasma treatment, or hydrothermal and supercritical treatment (Abunada *et al*., 2020; Ahmed *et al*., 2020; Barisci & Suri, 2021; Biswas *et al*., 2022; Buckley *et al*., 2022; Dehghani *et al*., 2022; Duinslaeger & Radjenovic, 2022; Endo & Funazukuri, 2023; Esfahani *et al*., 2022; Groele *et al*., 2021; Jiang *et al*., 2022; Jin, Peydayesh, Joerss, *et al*., 2021; Khan *et al*., 2022; Krause *et al*., 2022; Li *et al*., 2022; F. Liu *et al*., 2022; Meegoda *et al*., 2020; Palma *et al*., 2022; Ryan *et al*., 2021; Santiago *et al*., 2022; Sharma *et al*., 2022; Verma *et al*., 2021; Wang *et al*., 2023; Yin & Villagrán, 2022; Z. Zhang *et al*., 2021). Designing passive treatment wetland systems has also been suggested (Arslan & El-Din, 2021).

2. Literature review: 17ß-estradiol

E2 is a natural hormone and the most potent of steroid hormones, or estrogens. It is produced primarily in the ovaries, but also by the adrenal cortex, testes, and the placenta of humans and other mammals (Ciślak *et al*., 2023). It controls the development and maintenance of female sex characteristics. It is prescribed for several conditions when E2 is reduced, for treatment of symptoms related to the menopause, and it can be a component of the oral contraceptive pill. Effects of increasing estrogen exposure include reduction in male fertility, decreasing puberty age in girls, obesity, increased rates of breast, ovarian, prostrate and testicular cancer, or endometriosis (Ciślak *et al*., 2023; Forghani *et al*., 2018).

In wildlife, estrogens are problematic due to their endocrine disrupting abilities, and their effects have been studied in fish (Jobling *et al*., 2006). They include feminization of male fish, hatch retardation, malformation, growth retardation, or reduced reproductive fitness (Odinga *et al*., 2022). Similar effects have been observed in amphibians and reptiles, as well as adverse effects in mammals and birds leading to reductions in reproductive success and disturbed immune function (Forghani *et al*., 2018).

Other natural steroidal hormones are estrone (E1), estriol (E3) and estetrol (E4). They differ in the amount and arrangement of the hydroxyl group (Figure B.5). A synthetic steroidal hormone is ethinylestradiol (EE2). To measure the effect of multiple estrogens, total estrogenity is used as the total estrogenic response in a sample, and can be expressed as E2 equivalents. Total estrogenicity in a river of more than 0.01 µg/L E2 equivalents is linked to high intersex incidence and severity, while concentrations below 0.0001 µg/L E2 equivalents are associated with minimal intersex expressions (Arlos *et al*., 2018).

2.1. Regulation

E1, E2 and EE2 are on the watch list of substances for European Union-wide monitoring in the field of water policy. Under the proposal for the amendment of the WFD, all these three substances would be included as priority substances for surface waters, with a standard of an annual average of 0.00018 µg/l for E2.

The European Commission adopted a watch list of substances in drinking water on 19th January 2022 (Commission Implementing Decision (EU) 2022/679). E2 is one of the two substances included on this first watchlist, along with NP. While not yet in Scottish legislation, drinking water will have to be monitored more closely for the presence of these two substances, and measures taken to reduce the concentrations below the guidance value if necessary. The guidance value for E2 is 0.001 µg/l, based on the WHO recommendation, but without a suggestion for a possible analysis method.

In the US, E2 has been identified as a contaminant on the Contaminant Candidate List (CCL) since 2009. The CCL is a list of contaminants that are currently not subject to any proposed or promulgated national primary drinking water regulations but are known or anticipated to occur in public water systems. Contaminants listed on the CCL may require future regulation under the Safe Drinking Water Act (SDWA). In Australia, limiting values were established for natural and synthetic estrogens in regulations concerning reuse water intended for human supply, with the E2 value set at 0.175 µg/l.

An analysis method is established and used by Scottish Water to analyse for steroid estrogens in wastewater using liquid chromatography and a triple quadra pole MS/MS detector (personal communication, Scottish Water).

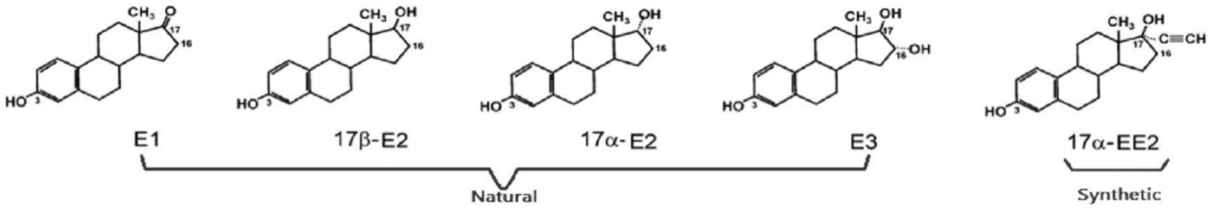


Figure B.5: Structure of natural and synthetic estrogen hormones, taken from Adeel et al. (2017).

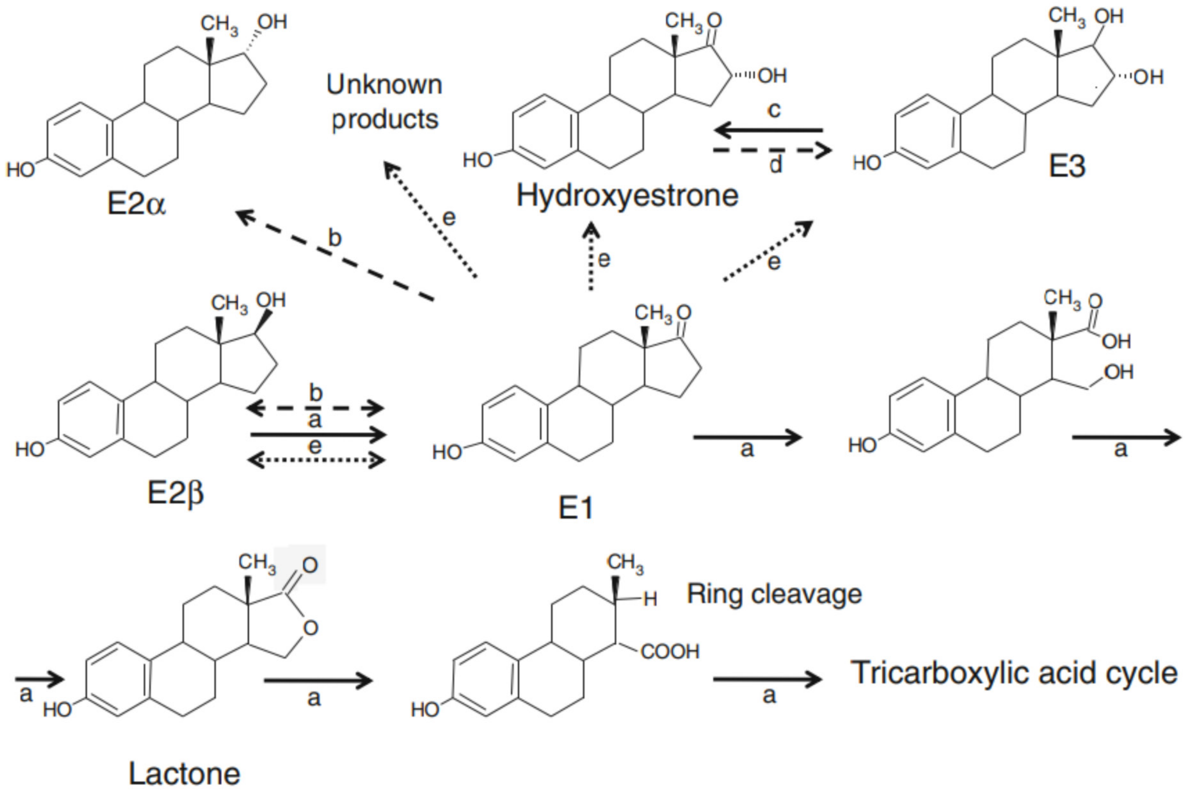


Figure B.6: Proposed degradation pathways of estrogens by bacteria under aerobic (solid line), anoxic or anaerobic conditions (dashed line), and by algae (dotted line). Taken from Combalbert & Hernandez-Raquet, 2010.

2.2. Processes (sources, pathways and receptors)

Human and animal excretions are natural source of estrogens. Q.-Q. Zhang *et al*. (2021) estimated global steroid emissions and calculated that of a total emission of 20,440 t of steroids, more than 70% originated from livestock, predominantly cattle. If looking only at estrogens, animals are responsible for 98% of emissions, as human waste is more commonly treated before being released into the environment (Ciślak *et al*., 2023).

Estrogens are relatively rapidly degraded in the environment (Figure B.6). Due to lower solubility in water and stronger hydrophobicity than other agricultural pollutants, such as herbicides, Johnson *et al*. (2006) conclude they are less likely to be found in runoff, although there are indications that intensive livestock can increase estrogen concentrations in surface waters. Higher concentrations are especially likely after storm-events shortly after manure spreading (Schoenborn *et al*., 2015). However, Schoenborn *et al*. (2015) also find some instances of increased concentrations 14 to 28 days after manure application and in dry weather, indicating higher persistence in soils than laboratory studies indicate.

Main sources of estrogens, including E2, to the environment are therefore insufficiently treated wastewater or runoff from fields (Nazari & Suja, 2016). This includes areas treated with slurry, although good practice can reduce runoff (Rechsteiner *et al*., 2020). As estrogens accumulate in wastewater sludge, application of sludge as a fertilizer can also present a source to the environment (Forghani *et al*., 2018), although due to microbial degradation, concentrations by the time of applications might be very low (Koh *et al*., 2008). The potential for estrogens to reach groundwater is low, as they remain bound to the upper surface layer of the soil (Jurado *et al*., 2019; Nazari & Suja, 2016). However, groundwater contamination with estrogens can occur e.g., through septic tanks (Swartz *et al*., 2006), and degradation is slower under anaerobic conditions (Ying *et al*., 2003).

2.3. Occurrence and concentration in freshwater

2.3.1. Scotland

The database on pharmaceuticals in Scotland's environment (SEPA, undated) collects samples for E2 from different sources, originating mainly from Scottish Water in the context of the second phase of the Chemical Investigations Programme (CIP2) from 2015-2018, but also from SEPA for different locations and periods, including 2013, 2015/2016, 2016-2019, and 2019. The maximum concentration for surface waters included in this dataset is 0.012 µg/l, at a site located downstream of a wastewater treatment plan. With one exception, all concentrations >0.003 µg/l have been measured downstream of wastewater treatment plants.

The highest concentration of E2 was measured for wastewater influent, at 0.2014 µg/l. Other concentrations for samples between 2015 and 2022 vary between <LOD and <0.1 µg/l. Wastewater effluent concentrations are lower, with a maximum concentration of 0.0453 µg/l.

2.3.2. International

Ciślak *et al*. (2023) review estrogen concentrations in European surface, groundwater and sediments and summarise that in Western European countries, observed concentrations mainly oscillate between the values of 0.0001-0.01 µg/l. The authors also observe that in Belgium, a significant decrease in concentrations could be observed over the past 20 years, which they attribute to an increasing percentage of the population connected to a wastewater treatment plant – a pattern that is reflected more generally in Europe, with higher concentrations of estrogens observed in countries with a lower percentage of people connected to the wastewater system (e.g., Italy, Slovenia, Poland).

2.4. Water treatment

Due to wastewater treatment being one of the primary sources of estrogens to the environment, many studies focus on wastewater treatment to reduce environmental loads. Wastewater treatment can effectively remove estrogens, with the main factors being adsorption to sludge and biodegradation. However, efficiency varies depending on hydraulic retention time, solid retention time, organic charge, and redox conditions (Koh *et al*., 2008; Nguyen *et al*., 2021).

E2 is degraded under aerobic, but not under anaerobic conditions. Sludge retention time is a critical factor in degradation of E2 – a low retention time leaves insufficient time for E2 to be degraded. Clara *et al*. (2005) report that at 10°C, a retention time of 10 days is sufficient to almost completely degrade E2. Similarly, a longer hydraulic retention time allows more time for E2 to be adsorbed to sludge and be biodegraded. Due to metabolic rates of bacteria being influenced by temperature, higher temperatures increase biodegradation (Nazari & Suja, 2016).

Activated sludge systems remove the majority of E2 (>66%; Koh *et al*., 2008). In systems where higher solid retention times and hydraulic retention times are not feasible, membrane bioreactors have been suggested (Koh *et al*., 2008; Nguyen *et al*., 2021).

Further to secondary treatment removal, tertiary treatment such as activated carbon, nanofiltration, chemical treatment or advanced oxidation (e.g., ozonation, ultraviolet degradation, manganese oxide, sonolysis) could further enhance estrogen removal (Baynes *et al*., 2012; Broséus *et al*., 2009; Castellanos *et al*., 2022; Cheng *et al*., 2021; Han, 2015; Heo *et al*., 2020; Kim *et al*., 2015; Kovacic *et al*., 2018; Li *et al*., 2012; McCallum *et al*., 2008; Qin *et al*., 2019; Sanches *et al*., 2016; Torres *et al*., 2021). Shallow constructed wetlands have also been shown to further reduce estrogen concentrations (Nguyen *et al*., 2021; Song *et al*., 2009).

For drinking water treatment, coagulation alone does not significantly remove estrogens (Schenck *et al*., 2012). While chlorination can reduce estrogenity, there is also the potential of chlorinated by-products (Shao *et al*., 2018). However, many of the suggested tertiary wastewater treatment options are also established processes in and equally applicable to drinking water treatment. Nazari and Suja (2016) and Silva *et al*. (2012) give good overviews over function and removal efficiency of these additional treatment processes.

3. Literature review: Nonylphenol

Nonylphenol is an alkylphenol, produced since 1940. It consists of a phenolic ring and a chain of nine carbon atoms (Gałązka & Jankiewicz, 2022). The phenol ring can be differently attached to the nonyl group, at the so called meta-, ortho- and para-positions, and the nonyl group can be branched or linear, so that there are several isomers of nonylphenol (Figure B.7). The most common commercial form is 4-nonylphenol, with the fourth carbon atom of the phenol ring attached to a branched nonyl group (Metcalfe *et al.*, 2022).

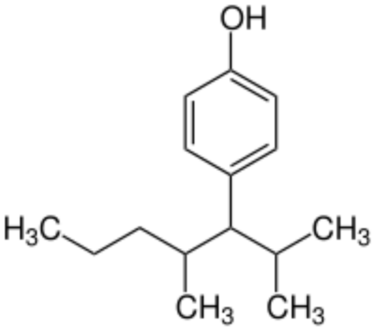


Figure B.7: Structure of a typical nonylphenol

In the environment, nonylphenol primarily occurs through degradation of nonylphenol ethoxylates (NPEOs). NPEOs have been used in industry as non-ionic surfactants, in households as detergents, and in personal care products (Gałązka & Jankiewicz, 2022).

Nonylphenol is liquid at room temperature, non-soluble with water, lipophobic, semi-volatile, highly resistant to biodegradation and bioaccumulative. It is a xenoestrogen and mimics 17ß-estradiol, although the estrogenic activity depends on its structure, and not all isomers are capable of inducing estrogenic activity (Gałązka & Jankiewicz, 2022). NP also has anti-androgenic effects, leading to disorders in men, and reduced birth weight and premature deliveries when women in the second trimester of pregnancy are exposed. It also causes cancer such as breast, ovarian, uterine, pituitary and testicular cancer (Bhandari *et al.*, 2021). In aquatic organisms, it can cause feminization, reduce male fertility and survival of young, and it has acute toxicity to phytoplankton, zooplankton, amphibian, invertebrates and fish (Gałązka & Jankiewicz, 2022).

3.1. Regulation

As an organic chemical persistent in the environment, Nonylphenol falls under similar regulatory regimes as PFAS.

3.1.1. EU REACH & UK legislation

Nonylphenol and NPEOs are on Annex XVII of the EU REACH. Nonylphenol and NPEOs may not be placed on the market or used in concentrations equal to or greater than 0.1% by weight for the purpose of: industrial and institutional cleaning (with some exceptions); domestic cleaning; textiles or leather processing unless there is no wastewater released or wastewater is treated; emulsifier in agricultural teat dips; metal working except in controlled systems with recycling of washing liquid; manufacturing of pulp and paper; cosmetic products; other personal care products; co-formulants in pesticides and biocides. These controls on Nonylphenol and NPOEs were already effective before REACH through Directive 2003/53/EC, which was implemented in the UK through The Controls on Nonylphenol and Nonylphenol Ethoxylate Regulations 2004. Since 2021, NPEOs may also not be contained in textile articles if it will likely be washed out during the product's life cycle. This restriction includes textiles imported from outside the EU.

3.1.2. Water Framework Directive

Nonylphenol is on the list of priority substances of the Water Framework Directive and the Environmental Quality Standards Directive sets a standard of an annual average of 0.3 µ/l for inland freshwaters. Under the proposal for the amendment of the WFD, the standard would go down to an annual average of 0.037 µ/l and a maximum allowable concentration of 0.0018 µ/l for or inland surface waters.

3.1.3. Drinking water

NP is the second substance on the EU drinking water watchlist, with a guidance value of 0.3 µg/l. The suggested analysis method follows ISO 18857-2, specifying a gas chromatographic-mass spectrometric (GC-MS) determination of selected alkylphenols, their ethoxylates and bisphenol A in non-filtered samples of drinking, ground, surface, and waste waters following solid-phase extraction and derivatisation (ISO, 2020).

The method is applicable in a working range from 0.03 µg/l to 0.2 µg/l for 4-nonylphenol (mixture of isomers). ISO 24293:2009 specifies a method for the determination of selected individual isomers of nonylphenol in non-filtered samples of drinking water, waste water, ground water and surface water. The method is applicable in concentrations between 0.001 µg/l and 0.1 µg/l for individual isomers and from 0.01 µg/l to 0.2 µg/l for the sum of 4-nonylphenol (mixture of isomers). Depending on the matrix, the method is also applicable to wastewater in concentrations between 0.1 µg/l and 50 µg/l.

The EPA developed method 559 to determine nonylphenol in drinking water by solid phase extraction and liquid chromatography/tandem mass spectrometry (LC/MS/MS). The Minnesota Department for Health (MDH) developed a guidance value of 20 µg/L for nonylphenols. In Australia, the recommended drinking water guideline is 500 µg/l. The Bureau of Indian Standards (BIS) has set standards for phenolic compounds in drinking water (1 µg/l) and surface water (500 µg/l). However, at present, there are no standards exclusively for nonylphenols in drinking and surface waters in India.

3.2. Processes (sources, pathways and receptors)

Potential sources of nonylphenol are sites where nonylphenol and NPEOs are manufactured, and where nonylphenol and NPEOs are used in processes to manufacture other products. These include resins, plastic stabilisers, polymers, textiles and leather, agricultural products, paints, metal finishes, and paper. In a report for the DWI, Fretwell *et al*. (2021) list potential uses and sources for nonylphenol and NPEOs for the EU and estimate their relevance in the UK. They conclude that manufacture within the UK should have ceased by 2006 at the latest, and that uses in various industries and agriculture should also have been phased out before 2003. Therefore, due to the tight regulation of nonylphenol in Europe and the UK, it is likely that there are few active primary sources of relevance in the UK. However, nonylphenol is still found in wastewater (Gardner *et al*., 2022), and it is thought that the main source of nonylphenol to the freshwater environment is through sewage treatment effluent (e.g., Fairbairn *et al*. (2016)). Sewage sludge and biosolids applied to land are also a potential source; nonylphenol was found in all biosolid samples in an investigation carried out for England and Wales, at most sites with a median concentration of >20 mg/kg (Marshall & Yates, 2022). Leachate from landfills is another potential source for nonylphenol (Kurata *et al*., 2008).

Nonylphenol can bind to aerosols, and re-enter aquatic and terrestrial habitats with rain and snowfall (Gałązka & Jankiewicz, 2022). However, as no primary manufacturing sites are thought to be left in the UK, atmospheric deposition is unlikely to be a major source. However, wastewater, and spreading of sludge, may be a source of nonylphenol to the atmosphere, and thus cause wider spread of these substances (Ferrey *et al*., 2018).

Nonylphenol in water is present as dissolved or adsorbed on suspended solid particles (Hong *et al*., 2020). Due to its high hydrophobicity and low solubility, nonylphenol accumulates in soils and sediments (C. C. Lee *et al*., 2013). It degrades relatively quickly under aerobic, but not under anaerobic conditions (Ying *et al*., 2003). C. C. Lee *et al*. (2013) found that nonylphenol concentrations in rivers correlated with total organic carbon, ammonia-nitrogen, nitrate-nitrogen and *E. coli*, again suggesting high concentrations in wastewater influenced reaches. There are indications that nonylphenol concentrations increase in sediments with higher organic carbon content, although the proximity to primary sources, such as wastewater discharges, may be a more important factor (C.-C. Lee *et al*., 2013).

Nonylphenol concentrations show seasonality with higher concentrations detected in spring and summer (Fairbairn *et al*., 2016). This could be due to increased microbial degradation of NPEOs in wastewater treatment in the warmer season (Gao *et al*., 2017), or from additional agricultural inputs (Fairbairn *et al*., 2016).

Nonylphenols are also used as heat stabilizers in PVC (Hahladakis *et al*., 2018), and thus occur in PVC plumbing, increasing concentrations in drinking water (Cheng *et al*., 2016; Mohammadi *et al*., 2022), although in a study in Finland, nonylphenol was only rarely found and in low concentrations (Rajasärkkä *et al*., 2016).

3.3. Occurrence and concentration in freshwater

3.3.1. Scotland

SEPA carried out some sampling for nonylphenol and NPEOs at 173 sites, mainly taken between 2008 and 2019, but there are also some samples from

1996, 1998, 2000, 2003, and 2007. This includes rivers and lochs, coastal waters, transitional waters, some springs and boreholes, sewage treatment effluent, and very few samples from landfill leachate.

Concentrations of NPEOs in river and loch samples span <LOD to 9.8 µg/l. This maximum value was measured in February 2016 in a sample from the River Clyde. Concentrations of nonylphenol lay between <LOD to 5.8 µg/l, the maximum concentration being in a sample from the River Irvin in April 2011. All together, 243 out of 2471 samples had concentrations above 0.3 µg/l, at 126 different sites.

In coastal and transitional waters, 24 out of 355 samples had concentrations for nonylphenol above 0.3 µg/l, with a maximum of 1.9 µg/l at the Clyde estuary in September 2012. For NPEOs, the maximum concentration of 4.3 µg/l was measure in December 2017 in the Forth estuary, but the majority of samples were <LOD. The same applies to the groundwater samples, although there is a marked outlier of 10 µg/l. Nonylphenol at a concentration above 0.3 µg/l were found in 6 of those samples, from 4 sites, with a maximum of 0.89 µg/l.

Landfill leachate showed no concentrations higher than these. Wastewater treatment effluent however showed concentrations magnitudes higher, with a maximum for nonylphenol of 100 µg/l, and 499 samples out of 993 having concentrations above 0.3 µg/l. Maximum concentrations for NPOE was 13 µg/l.

Gardner *et al*. (2022) report UK-wide mean concentrations of nonylphenol in wastewater for 2010/2011 as 0.23 µg/l, and a 95th percentile value of 0.44 µg/l, and for 2016-2019 a mean of 0.14 µg/l and a 95th percentile value of 0.43 µg/l.

3.3.2. International

A study in French drinking water supply sources (both ground and surface water) detected nonylphenol and/or NPEOs in 24% of the samples at least at trace level (Colin *et al*., 2014). Nonylphenol was found at concentrations between 0.1 and 0.6 µg/l, with the maximum concentration found in a groundwater sample, although the frequency of detection was higher in surface waters. Most contaminated groundwater resources were located in karst or alluvial areas. The study found that there was almost no relationship between nonylphenol and NPEOs concentrations, and hypothesised that this may be due to the higher adsorption of nonylphenol to sediments, meaning that predominantly NPEOs are found in the dissolved phase. Sampling of treated water also detected nonylphenol and NPEOs, although in lower concentrations, which indicates that treatment is effective to some degree in removing these substances; however, it is also possible that chlorinated by-products are formed. An analysis of tap water from four drinking water sources in Spain found nonylphenol up to a maximum daily concentration of 0.126 µg/l (Valcárcel *et al*., 2018).

A study carried out for nonylphenol and NPEOs at 35 Canadian sites between 2014 and 2019 detected higher concentrations in urban and wastewater effluent influenced sites, with a downward temporal trend (Lalonde & Garron, 2021).

3.4. Drinking water treatment

Nonylphenol can be biodegraded by bacteria, fungi and microalgae (Bhandari *et al*., 2021). Removal of nonylphenol through conventional drinking water treatment is only partially effective; in Taiwan, the treatment steps of coagulation/sedimentation and filtration together achieved a 50% reduction in concentration (Chen *et al*., 2013). However, similarly to E2, some more novel techniques are promising in removing nonylphenol from both wastewater and drinking water, including adsorption to activated carbon, membrane bioreactor or nanofiltration, reverse osmosis, advanced oxidation (photocatalytic, chemical, sonochemical, electrochemical), or cell immobilization (Bhandari *et al*., 2021). Werkneh *et al*. (2022) gives an overview over treatment options for different endocrine disrupting compounds.

4. Stakeholder risk perception and information requirements

The below sections present an overview of interview partner's perspectives of the different aspects covered throughout the interviews (conducted May & June 2023).

4.1. Level of concern

Generally, stakeholders feel that Scotland's water quality is high compared to other countries such as England, alleviating major fears about impacts of emerging contaminants. At the same time, there is awareness that this cannot lead to complacency. Concerns over emerging contaminants and especially the substances in question vary a little depending on the stakeholder's area of interest.

In a drinking water context, especially for the public water supplies, respondents expressed confidence in high water quality overall. This seems confirmed by current sampling not picking up high concentrations of the contaminants. Additionally, there is a "safety net" of treatment available, albeit at the current stage of knowledge and technology it would mean financial investments to put this in place. Providers and regulators both expressed the view that in the tightly regulated context of drinking water, it is possible to meet regulatory standards, so the concern centres mainly around doing so efficiently and being able to demonstrate good awareness of where these substances occur in which concentrations. This is especially pertinent from a public awareness perspective, as especially for PFAS concerns have been growing over the past years.

For private water supplies, the case is a little different, as there is generally a lack of awareness of emerging concerns, and risk assessment and management focuses on very immediate health concerns such as lead and pathological contamination. Respondents therefore took the view that this makes private water supplies more vulnerable to pollution by emerging contaminants. Additionally, reactive ability, and possibilities for source control and treatment are much more limited. An added challenge for implementing risk mitigation measures in private water supplies is the limited evidence on health impacts, and thus it is difficult to assess which investment costs can reasonably be asked of those responsible for maintenance of the private supply.

From an environmental point of view, concerns are greater as stakeholders consider the totality of Scotland's environment and waters. Once, and if, the substances are found in concentrations that have impact on the environment, there is no "safety net" of treatment to reduce risks. There is a general feeling that the scale of the problem is not well known. This is partly due to lack of information on occurrence in Scotland, and partly due to lack of information about impacts associated with concentrations in specific ecosystems and under different environmental conditions. For example, it is unclear what the effects are of the combined pressures of chemical pollution and climate change and associated conditions, such as increasing drought events and rising water temperatures.

4.2. Availability and use of information

Generally, it was acknowledged that there is lack of information. Monitoring for these substances in Scotland has been limited and data availability are at best indicative. This means that there is a lack of information on where the contaminants occur and in what concentrations, and from where they originate. There is a general wish to increase the information base and different monitoring programmes are being developed and set-up. For the benefit of managing private water supplies, the need for a national assessment of these substances was expressed.

Due to a lack of data, there is uncertainty regarding the toxicology and potential hazard to human health and the wider environmental impacts of the substances. In the absence of this, stakeholders orientate themselves on regulatory standards and guidance, assuming that these reflect the best available science. A more detailed assessment of human health impacts depending on the level and length of exposure on different groups is only being developed, so responses to potential contamination are still unclear.

Stakeholders with an environmental focus point out that substances may well have environmental impacts even if they are unregulated, and that information and knowledge is simply lacking, especially if public attention has not reached them. Several stakeholders acknowledged that public perception and priorities can shape policy and regulation, and this may not always be in tune with scientific findings. So in view of limited available resources, and with priorities shaped by policy, stakeholders have to find ways to balance demands and prioritise where attention and investment is focused. Public awareness and shifting attention underline the need for precautionary approaches to emerging contaminants and the ability to show preparedness in terms of managing potential risks.

The available data is used in conjunction with evidence available from other areas of the world to risk assess Scotland's freshwater environment. This risk assessment then often informs further monitoring, which again feeds into the risk assessment approach, leading to a cycle of an increasing evidence base shaping risk assessment and response, in turn identifying remaining knowledge gaps. Also, decisions on how to manage these substances need to be based on currently available evidence. Stakeholders use it to make recommendations, e.g. on banning substances or restricting usage.

4.3. Knowledge gaps

In addition to the recognised knowledge gaps in relation to currently regulated substances, stakeholders also feel there is a lack of knowledge about which substances to focus on apart from those already under some form of regulation. In the specific case of PFAS, substances included in standards vary within Scotland, but also between the different nations of the UK, and within Europe. There is considerable uncertainty around which substances are most likely to be found, partly due to limited information about import to and use of these contaminants in Scotland. There is also a lack of understanding around which compounds are likely to have the most detrimental impact, and how this level of impact may vary in different contexts. This is complicated by the fact that thousands of PFAS compounds exist, and further substances are being developed, with unknown properties and applications.

Further, often mentioned knowledge gaps is clear understanding of the impacts these contaminants have on the wider environment and human health. Concern regarding the former impacts concentrates on lack of understanding of impacts of different mixtures of chemicals, the so-called cocktail effect. Another concern exists over changing properties and associated impacts with changing conditions, especially climate change-induced conditions such as rising temperatures and droughts, potentially amplifying toxicity.

4.4. Requirements for risk control

In a drinking water context, there is more research required for treatment methods and the effectiveness of treatment under different conditions. While focus lies on drinking water treatment, wastewater treatment is an option for better source control. However, current treatment technologies create concentrated wastes, meaning that there is danger of contamination cycles through reusing of waste products, and further research is needed how to deal with waste and break the cycle.

Several stakeholders mentioned the role of society in reducing risks. Emerging contaminants usually appear in the environment because consumer demand for certain products and product qualities has led to the development and use of these substances. Awareness of environmental impact and responsible behaviour, e.g. around prescription, usage, and disposal of pharmaceuticals, is seen as a way to reduce input into the environment.

An observation was also made about the cost of reducing risks, and that it is ultimately up to society to decide the balance between risk reduction and costs of risk control. The uncertainty around impacts of emerging contaminants can be a hindrance to investments that support proactive mitigation. Even when it is possible to estimate the costs of mitigation and adaptation action against the costs incurred from doing nothing, due to long time scales, or not immediately apparent benefits, society may prefer to avoid immediate costs over long-term costs.

4.5. Conclusion

The stakeholder interviews exposed the interwoven nature of regulating and managing emerging contaminant issues. For example, to set regulatory standards for drinking water, it is necessary to understand impact on humans and especially vulnerable groups. To ensure compliance with a statutory standard, awareness is needed of presence and concentration of the substance(s), and effectiveness of treatment methods. To reduce costs of risk control, an understanding is necessary of possible controls, their effectiveness, and their costs. Environmental considerations can mean that source control becomes a favourable option, emphasising the benefit of concerted efforts and a homogenous approach to regulation.

While the interviews discussed three (groups) of compounds, many of the concerns raised and knowledge gaps identified are transferable to emerging contaminants in general, such as a lack of information on sources, occurrence, and environmental and human health impacts. General strategies how to deal with substances that start to become of concern are required.

The management and treatment of drinking water tends to be reactive to statutory requirements, meaning that risk assessment, and underpinning monitoring, will usually start when indications appear that something will be added to the list of regulated substances. The establishment of a drinking water watch list can be seen as a first step towards a more forward-looking strategy, requiring water suppliers to monitor these substances even in the absence of a set standard.

Due to the resulting absence of data and information, risk-based approaches are employed to guide efforts and investment into drinking water surveillance and treatment. This requires an understanding of sources of contaminants, their behaviour in and transfer through different environmental matrices, and within the water supply system. These processes are complex and will be influenced by the specific characteristics of the compound in question, and by the environmental conditions encountered, again varying among supply catchments. Nevertheless, similarities between contaminants (defined by e.g., sources and/or physicochemical characteristics), in combination with catchment characteristics (defined by e.g., soil properties, land management, hydrological behaviour), could support an assessment of general vulnerability of supply sources to types/groups of emerging contaminants.

C. Recommendations

1. Regulation of emerging contaminants in Scotland

Regulation of emerging contaminants is a fast-moving field where new data requires flexible responses. Regulatory theories around 'responsive regulation' and 'smart regulation' (Gunningham, 2023) are widely applied by environmental regulators (EA, 2022; SEPA, 2021) and are reflected in modern environmental compliance regimes (Regulatory Reform (Scotland) Act 2104 and Environmental Regulation (Enforcement Measures) (Scotland) Order 2015; Regulatory Enforcement and Sanctions Act 2008 and Environmental Civil Sanctions (England) Order 2010). High level 'better regulation' principles also apply to all regulators in Scotland and in England including economic regulators and water service providers where they have regulatory functions (DBIS; Government, 2015).

Whilst regulatory discretion is common in environmental regulation, it is less applicable to drinking water regulation, with its focus on technical standards based on public health requirements. Under the Water Industry Act 2002 the DWQR has enforcement powers including enforcement notices (ss 8-19); monitoring and sampling duties on SW are in the Public Water Supplies (Scotland) Regulations SSI 2014/364. Amendments in 2022 introduced the regulatory standards for PFAS, implementing the provisions in the Drinking Water Quality Directive (Recast) (EU 2020) Annex 3 and the Commission Decision on the first watch list (Commission 2022), to which E2 and NP were added.

1.1. Import and use

PFAS are mostly industrial and consumer chemicals and as thus fall under the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) Regulation of the European Union (Regulation (EC) No 1907/2006). Manufacturers and users of chemicals are obliged to register the substances if they exceed 1 tonne per year per company, and companies must identify risks from the substances. Substances posing high risks can be banned. The UK has retained the regulation in national law (UK REACH, SI 2019/758 as amended, SI 2021/904).

Under EU REACH, PFCAs with a carbon chain of nine or more fall under ANNEX XVII, which places restrictions on the manufacture, placing on the market and use of the included substances. PFCAs, their salts and related substances may not be manufactured or placed on the market since February 2023 (Commission Regulation (EU) 2021/1297). It is also prohibited to use or place them on the market as a constituent, mixture, or article if the concentration exceeds a certain threshold, with some exceptions (e.g., for aqueous film forming foams (AFFF) in some circumstances). PFOS and related compounds and PFOA are also regulated under UK REACH.

The information on volume and use of PFAS in the UK is incomplete, due to a number of factors related to registration obligations under EU and UK REACH, e.g., no registration requirement for imports <1 t/y, long lead-times for submitting transitional registrations for low tonnage (<10t/y), and no obligation to register polymers. An initial investigation by HSE (2023) identified 40 PFAS imported to the UK from the EU, and 182 PFAS in the EU REACH database (ECHA, undated). Highest tonnages (1000-15,000 t/y) are reported under UK REACH for polyfluoroalkyl substances comprising hydrofluorocarbons (HFCs), -ethers (HFEs), and -olefins (HFOs), and perfluoroalkenes.

The HSE Analysis of the most appropriate regulatory management options (RMOA) for PFAS identifies a number of measures to reduce the risk from PFAS, including restricting the manufacture, use and placing on the market of PFAS and some products containing PFAS, extending the requirements for UK REACH authorisations, investigating further substances, extending restrictions for some substances under UK REACH, and developing statutory standards for PFAS in England and Wales (HSE, 2023). The RSC also suggests a national inventory of PFAS sources, and the establishment of a national chemicals regulator (RSC, 2023).

Currently, a proposal to restrict PFHxA, its salts and related substances under REACH is being considered by the European Commission, as well as a proposal by ECHA to reduce the use of PFAS in firefighting foams (ECHA, 2023a). Additionally, Germany, Denmark, the Netherlands, Sweden and Norway have proposed restricting a wide range of PFAS (as 'any substance that contains at least one fully fluorinated methyl (CF_3-) or methylene (-CF_2-) carbon atom (without any H/Cl/Br/I attached to it)') (ECHA, 2023b). A decision on the proposal is expected in 2025.

Nonylphenol and Nonylphenol ethoxylates are on Annex XVII of the EU REACH. Nonylphenol and NPEOs may not be placed on the market or used in concentrations equal to or greater than 0.1% by weight for the purpose of: industrial and institutional cleaning (with some exceptions); domestic cleaning; textiles or leather processing unless there is no wastewater released or wastewater is treated; emulsifier in agricultural teat dips; metal working except in controlled systems with recycling of washing liquid; manufacturing of pulp and paper; cosmetic products; other personal care products; co-formulants in pesticides and biocides. These controls on Nonylphenol and NPOEs were already effective before REACH through Directive 2003/53/EC, which was implemented in the UK through The Controls on Nonylphenol and Nonylphenol Ethoxylate Regulations 2004. Since 2021, NPEOs must also not be contained in textile articles if they will likely be washed out during the product's life cycle. This restriction includes textiles imported from outside the EU.

1.2. Environmental quality standards and wastewater management

Any activity liable to cause pollution to the water environment is licensed by SEPA under the Water Environment (Controlled Activities) (Scotland) Regulations 2011 SSI 2011/208 (CAR). SEPA authorisations under CAR provide a broad framework for control, both in terms of licensing emissions and processes and for environmental quality standards. Indicative main pollutants are described under schedule 1, including substances with 'carcinogenic or mutagenic properties or properties which may affect steroidogenic, thyroid, reproduction or other endocrine-related functions in or via the aquatic environment'. Hazardous substances under schedule 2 include 'substances or groups of substances which are toxic, persistent and liable to bio-accumulate' as well as 'substances or groups of substances which are entering, or liable to enter groundwater'. SEPA must inter alia 'assess the risk to the water environment…' and 'apply the requirements of the legislation referred to in Part 1 of Schedule 4' (Reg 15). Schedule 4 includes both the Water Framework Directive 2000/60/EC and the Priority Substances Directive 2013/39/EU (PSD). Under Annex I of the PSD 2013, nonylphenol is a Priority Hazardous Substance, and Perfluorooctane sulfonic acid and its derivatives (PFOS) were added to Annex I in 2013. The PSD 2013 introduced the watch list substances for control in the environment, issued by the Commission in 2015 and including E2. Member states were expected to implement this by 2018, and Scotland did so under the provisions of the UK Withdrawal from the EU (Continuity) (Scotland) Act 2021.

The detailed provision for SEPA's implementation of chemical standards is in Directions issued by Ministers (Scottish Government 2014; Scottish Government 2015a). These are binding on SEPA, and establish Environmental Quality Standards for listed substances (as established in the PSD and also the WFD and the Groundwater Directive). The Standards Directions also provide for 'Certain Other Pollutants' for which standards are set under EU law, for 'Dangerous Substances', previously controlled under the Dangerous Substances Directives, and for 'Specific Pollutants' identified by Member States (in the UK, through UKTAG). The Water Environment (River Basin Management Planning: Further Provision) (Scotland) Regulations 2013 SSI 2103/323, as amended provide for specific measures against pollution and implement the PSD 2013, including PFOS and the 'watch list' substances (2015, SSI 2015/211, R 19B).

Current guidance by SEPA (SEPA, 2020) include environmental quality standards for substances added to Annex I in PSD 2013, but do not include E2 or any other watch list substances. However, R19B only required monitoring for 12 months and provided an exception where SEPA has sufficient data. Some data is available from 2016 and 2019 on estradiol concentrations from SEPA's watch list monitoring through the 'Pharmaceuticals in the Water Environment' (SEPA) online database. SEPA is currently implementing the inclusion of a range of PFAS substances in their monitoring (personal communication).

Treatment of wastewater is managed under the Urban Waste Water Treatment Directive (1991/271/EEC) and the Urban Waste Water Treatment (Scotland) Regulations 1994 SI 1994/2842. Reg 5 requires secondary or 'appropriate treatment', and 'more stringent treatment' for sensitive areas. Water quality requirements for wastewater discharges are set in Schedule 3 for biochemical oxygen demand and chemical oxygen demand, and for total phosphorus and total nitrogen for sensitive areas. Wastewater treatment plants (WWTPs) are licenced by SEPA under CAR. Scottish Water must monitor, sample and report to SEPA on the discharges from WWTPs. Discharges of treated wastewater should enable receiving waters to meet the applicable environmental quality standards as described above.

1.3. Slurry, sludge and biosolids

The regulation and management of biosolids is complex, with rules for its treatment under the wastewater licensing system, and potentially (if treated at another location) the waste management licensing system or the pollution prevention and control regime. The Sludge Directive 1986/278/EEC is intended to enable sludge to be used on agricultural land 'in such a way as to prevent harmful effects on soil, vegetation, animals and man' (Art 1). While not specifying treatment methods, it sets limit values for a set of heavy metals both in the sludge and on land, which should be tested before application. It is implemented in the UK by the Sludge (Use in Agriculture) Regulations 1989/1263.

Sludge for application to agricultural land should be treated in accordance with the Sludge Matrix and there are several sets of guidance and codes of practice, including (as best practice) the Biosolids Assurance Scheme. However, most sampling of biosolids has a focus on pathogens and heavy metals, although a range of substances have been found in sludge and biosolids intended for use on agricultural land (JHI, 2018; Stutt *et al*., 2019).

Application of slurry to land is also regulated under CAR through the General Binding Rules (Schedule 3).

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