

Drinking Water Inspectorate (DWI)

**Likelihood of three endocrine disrupting
substances reaching drinking water
DWI 70/2/328 (25853)**

Final Report



Report for

Drinking Water Inspectorate (DWI)
Defra
Marsham Street
London

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Appendix A Risk Maps for England and Wales
 Appendix B Systematic literature review protocol

Glossary

Acronym	Description
BAC	Biologically Activated Carbon
BACS	British Association for Chemical Specialities
BGS	British Geological Survey
BPA	Bisphenol A
CBV	Chemical Benchmark Values
CIP	Chemical Investigation Programme
DW	Drinking Water
DWD	Drinking Water Directive
DWF	Dry Weather Flow
E2	17-Beta-estradiol
EDCs	Endocrine Disrupting Chemicals
EQS	Environmental Quality Standard
FoI	Freedom of Information
GCMS	Gas chromatography-mass spectrometry
GDP	Gross domestic product
HAAs	Haloacetic Acids
HNMs	Halogenated Nitromethane
LCMS	Liquid chromatography-mass spectrometry
LOD	Limit of detection
LOQ	Limit of Quantification
NP	Nonylphenol

NPE	Nonyl Phenol Ethoxylate
ONS	Office of National Statistics
PBIAS	Percent Bias
PE	Population equivalent
PEC	Predicted Environmental Concentrations
PI	Population Intervention
PIT	Population Index Test
PNEC	Predicted No-Effect Concentration
PO	Population Outcome
PRTR	Pollutant Release and Transfer Register
PVC	Polyvinyl chloride
RMSE	Root Mean Squared Error
RQ	Risk Quotient
SOCOPSE	Source Control of Priority Substances in Europe
SPE	Solid phase extraction
SPZ	Source Protection Zone
THMs	Trihalomethanes
TNPP	Tris(4-nonylphenyl, branched and linear) phosphite
TOC	Total organic carbon
WFD	Water Framework Directive
WHO	World Health Organisation
WWTWs	Wastewater treatment works

Executive summary

EDCs are a diverse group of chemicals that have the potential to alter the normal functioning of the hormonal system across a wide range of wildlife and in humans (especially during early development). Their presence in a variety of applications and direct pathways for release to environment also means that EDCs could reach drinking water through typical use of EDC containing products. Continuous domestic release of many of these chemicals (particularly to wastewater systems) gives rise to pseudo-persistence in the environment, and they have frequently been found within the sewerage system and rivers. Peer-reviewed and grey literature verifies the occurrence of 17-Beta-estradiol (E2), Nonyl phenol (NP) and Bisphenol A (BPA) in both surface and groundwater. The rate of incidence of these three EDCs in wide scale surface/groundwater monitoring programmes such as the Chemical Investigation Programme (CIP) and BGS surveys suggests that their occurrence could be expected at low levels in drinking water sources across England and Wales. Limited information is currently available on concentrations of these substances in source/treated water or their removal using advanced drinking water treatment technologies. Thus, understanding the potential risk of compliance to proposed drinking water standards requires consideration. This project aims to close the knowledge gap on quantities of these substances used, their presence in surface and groundwater and the potential scale of the risk for drinking water across England and Wales.

In 2016 the completion of a regulatory fitness evaluation for the Drinking Water Directive¹ (98/83/EC) (DWD) found that the DWD was largely successful in delivering the provision of high-quality drinking water across Europe. Levels of compliance were noted to be high, yet one specific area of attention has been the list of pollutants/parameters that are reported². This list has not been updated since 1998 (the year the DWD was implemented) and does not consider any emerging contaminants. To ensure safe drinking water for all EU citizens, a number of policy options were recently identified by the EC³, including a) Update of the parameters in Annex I according to scientific progress and following recommendations of the WHO Guidelines; b) Updating the list of parameters in the Annex I to longer list C (including all parameters potentially harmful); or c) Reduction of the number of parameters in Annex I to a minimum list, with the same limit values than those specified under the current Annex I of the DWD.

The EC has since proposed to revise the Directive in order to improve the quality of drinking water and update parameters monitored and set over 20 years ago. An outcome of this evaluation is recommendations for three endocrine- disrupting compounds: 17-Beta-estradiol: 0.001 µg/L; Nonyl phenol: 0.3 µg/L; and Bisphenol A: 0.1 µg/L. The proposed standards for these three EDCs are being used as precautionary benchmarks, (close to the environmental quality standard (EQS) for aquatic protection), to indicate possible estrogenic activity in drinking water as they are already known to be found in surface (source) water.

Since the project started, BPA will now (as of October 2020) be added to the DWD with a health-based parametric value of 2.5 µg/l so we have evaluated possible risk of exceedance in relation to both the original (0.1 µg/L) and newly proposed (2.5 µg/L) standards for BPA. The other substances NP and E2 do not have benchmark values specified in the latest version of the DWD but will instead be added to a "watchlist".

The purpose of proposing chemical benchmark values (CBV) is to determine if (pre-treatment) drinking water sources are impacted by treated effluent or other sources known to contain EDCs. If any of the three EDCs are detected above the CBV in surface waters, then a risk may be posed to drinking water supplies and thus the need to revisit the efficacy of treatment or source control. If the three EDCs are not found to exceed the proposed drinking water standards at the source water intake then there is little need to model potential drinking water risk further at a greater level of detail; in this situation, measurements would need to be taken post-treatment in drinking water to confirm that removal in treatment is adequate.

¹ Staff Working Document on the REFIT Evaluation of the Drinking Water Directive 98/83/EC SWD (2016) 428 final.

² highlighted by the 2014 implementation report of the DWD, available at: <http://www.safe2drink.eu/dwd-evaluation/>

³ Study supporting the revision of the EU Drinking Water Directive, Final Impact assessment, November 2017. EC.

This project seeks to identify situations/locations in England and Wales where there is a risk to compliance with proposed DWD standards for NP, BPA and E2 and where additional monitoring may be necessary. The study outcomes will allow Defra and DWI to develop informed and effective policy approaches to manage the risks identified.

The outputs from this project indicate the following conclusions in relation to these three EDCs and key areas within England and Wales where the highest potential risk of exceeding the proposed values in drinking water:

- **For NP the likelihood of exceeding the proposed standard in drinking water supplies appears to be relatively low.** The data available both within the literature but also from the modelling of surface water concentrations indicates that exceedances of the proposed drinking water standard are infrequent apart from in very low flow conditions. Furthermore, NP has not been detected in groundwater monitoring data from the Environment Agency and the chemical properties of the substance indicate that it is unlikely to migrate to groundwater supplies. Restrictions on use are also likely to further reduce environmental concentrations of NP;
- **For E2 there is some evidence to indicate that it does occur in river sources above the benchmark value.** E2 has not been detected in drinking water above the proposed standards, although this is based on limited analytical data. This is consistent with bench scale studies that report high removal of E2 during by water treatment. When undertaking the modelling assessment for treated drinking water derived from surface water (Task 3) we see no exceedances of the 1ng/l proposed DWD standard when using the average/mean concentration estimates. However, in simulated low flow situations, around half of the abstraction points exceed the 1ng/l proposed DWD standard even after applying drinking water treatment, predominantly in the Thames, Anglian and Midlands regions.; and
- **For BPA, of the three EDCs examined in this study, appears to present the highest likelihood of exceeding the original proposed value in drinking water supplies in England and Wales. Whilst considering the proposed standard of 2.5 µg/l and mean concentrations, all the river reaches with abstraction points in England and Wales are at low risk.** In low flow conditions, the majority of the river reaches are at low risk with 38% at medium risk and no reaches identified as at high risk. Highest risk areas for groundwater within England and Wales appear to be in proximity to limestone aquifers of the South east, Anglian and Midland regions which agrees with the results from the surface water modelling of concentrations of BPA at drinking water abstractions points.

Recognising that this study takes a first step to risk assess water bodies used for abstraction, it must be noted that the results presented in this report should be interpreted with care especially those from the surface water modelling. As noted from the systematic literature review, data to corroborate estimates of the three EDCs is sparse and as such there is a high level of uncertainty in the predictions made. Overall, for all the EDCs, there is a paucity of data on occurrence of these substances in drinking water sources in the UK and the effectiveness of drinking water treatment processes. Further monitoring is suggested for all three EDCs.

1. Introduction

1.1 This report

Wood Environment and Infrastructure Solutions UK Limited (hereafter 'Wood') has been contracted by the Drinking Water Inspectorate (DWI) to provide services on:

" The likelihood of three endocrine disrupting chemicals (EDCs) reaching drinking water in England and Wales above the proposed standards under the recast of the Drinking Water Directive (DWD)".

Wood is working in partnership with Brunel University and the Centre for Ecology and Hydrology (CEH), both acting as subcontractors to Wood.

This is the final report for the study, produced following the completion of tasks 1, 2 and 3 of the study. It includes details of the following sections:

- Sections 1 and 2 contain information on the background to the study and an overview of the approach;
- Section 3 covers Task 1 – systematic review of the literature on the three EDCs in drinking water;
- Section 4 reports on Task 2 – mapping the sources and pathways of each of the three EDCs to the aquatic environment;
- Section 5 contains results from Task 3 – estimating the potential risk and likelihood of contamination of each of the three EDCs to both surface water (3a), drinking water and groundwater (3b); and
- Finally, Section 6 presents the overall conclusion of the study.

1.2 Background and policy context for Endocrine Disrupting Chemicals (EDCs) and drinking water

1.2.1 Rationale

EDCs are a diverse group of chemicals that have the potential to alter the normal functioning of the hormonal system across a wide range of wildlife and in humans (especially during early development). Their presence in a variety of applications and direct pathways for release to environment also means that EDCs could reach drinking water through typical use of EDC containing products. Continuous domestic release of many of these chemicals (particularly to wastewater systems) gives rise to pseudo-persistence in the environment, and they have frequently been found within the sewerage system and rivers. Peer-reviewed and grey literature verifies the occurrence of 17-Beta-estradiol (E2), Nonyl phenol (NP) and Bisphenol A (BPA) in both surface and groundwater. The rate of incidence of these three EDCs in wide scale surface/groundwater monitoring programmes such as the Chemical Investigation Programme (CIP) and BGS surveys suggests that their occurrence could be expected at low levels in drinking water sources across England and Wales.

Limited information is currently available on concentrations of these substances in source/treated water or their removal using advanced drinking water treatment technologies. Thus, understanding the potential risk of compliance to proposed drinking water standards requires consideration. This project aims to close the knowledge gap on quantities of these substances used, their presence in surface and groundwater and the potential scale of the risk for drinking water across England and Wales.

1.2.2 Drinking Water Directive draft proposal

In 2016 the completion of a regulatory fitness evaluation for the Drinking Water Directive⁴ (98/83/EC) (DWD) found that the DWD was largely successful in delivering the provision of high-quality drinking water across Europe. Levels of compliance were noted to be high, yet one specific area of attention has been the list of pollutants/parameters that are reported⁵. To ensure safe drinking water for all EU citizens, a number of policy options were recently identified by the EC⁶ including a) Update of the parameters in Annex I according to scientific progress and following recommendations of the WHO Guidelines; b) Updating the list of parameters in the Annex I to longer list C (including all parameters potentially harmful); or c) Reduction of the number of parameters in Annex I to a minimum list, with the same limit values than those specified under the current Annex I of the DWD.

The EC has since proposed to revise the Directive in order to improve the quality of drinking water and update the list of chemical parameters monitored and standards set over 20 years ago. An outcome of this evaluation is the proposed recommendations for three endocrine- disrupting compounds:

- 17-Beta-estradiol (E2): 0.001 µg/L;
- Nonyl phenol (NP)⁷: 0.3 µg/L; and
- Bisphenol A (BPA): 0.1 µg/L

The proposed standards for these three EDCs are being used as precautionary benchmarks, (close to the environmental quality standard (EQS) for aquatic protection), to indicate possible estrogenic activity in drinking water as they are already known to be found in surface (source) water. Note that the draft Directive published in 2018 included a value of 0.01 µg/L for BPA, the Commission clarified that this value should have been 0.1 µg/L which was the benchmark value suggested by WHO. Since the project started, BPA will now be added to the DWD with a health-based parametric value of 2.5 µg/l so we have evaluated possible risk of exceedance in relation to both the original (0.1 µg/L) and newly proposed (2.5 µg/L) standards for BPA. The other substances NP and E2 do not have values specified in the latest version of the Directive but will be added to a "watchlist".

This project therefore aligns with the draft DWD proposal and the introduction of the risk-based approach to water safety. We recognise that this study takes a proactive step to include a risk assessment of water bodies used for abstraction and the potential risk posed to groundwater drinking supplies of these three EDCs. Further consideration of a supply risk assessment and a domestic distribution risk assessment may be necessary if a risk to drinking water at tap is identified. This study forms the basis of the risk assessment for England and Wales, which may then highlight to Defra/ the DWI a need to explore remedial/source control measures as appropriate.

1.2.3 Key issues and challenges that we are proposing to address

The purpose of proposing chemical benchmark values (CBV) is to determine if (pre-treatment) drinking water sources are impacted by treated effluent or other sources known to contain EDCs. If any of the three EDCs are detected above the CBV in surface waters, then a risk may be posed to drinking water supplies and thus

⁴ Staff Working Document on the REFIT Evaluation of the Drinking Water Directive 98/83/EC SWD (2016) 428 final.

⁵ highlighted by the 2014 implementation report of the DWD, available at: <http://www.safe2drink.eu/dwd-evaluation/>

⁶ Study supporting the revision of the EU Drinking Water Directive, Final Impact assessment, November 2017. EC.

⁷ Nonyl phenol (NP) (CAS 25154-52-3) is primarily used as an intermediate in the production of nonylphenol ethoxylates (NPEs), noting that NPEs degrade in the natural environment back to NP. In monitoring studies NP and NPEs are often quoted together within one value on the assumed NP output. Furthermore, NP can exist as a straight chain, but also as a branched form (4-nonyl phenol (branched) CAS 84852-15-3). Under the EU REACH regulation NP + NPEs are subject to a restriction while 4-NP (branched) is an SVHC (and thus managed differently). The EQS Directive refers to NP, NPEs and 4NP (branched) as one group listing. While the proposal for the DWD simply refers to 'NP' without clarification. For the purposes of the current study NP is assumed to mean nonyl phenol (CAS 25154-52-3) and nonylphenol ethoxylates – matching the definitions laid out in Annex XVII of REACH. 4-nonyl phenol (branched) has not been included except where stated.

the need to revisit the efficacy of treatment or source control. If the three EDCs are not found to exceed the proposed drinking water standards at the source water intake then there is little need to model potential drinking water risk further at a greater level of detail; in this situation, measurements would need to be taken post-treatment in drinking water to confirm that removal in treatment is adequate.

This project seeks to identify situations/locations in England and Wales where there is a risk to compliance with DWD standards for NP, BPA and E2 and where additional monitoring may be necessary. The key challenges that must be met for this project include:

- Systematic identification of the most relevant background literature on NP, BPA and E2 in drinking water in the UK;
- Obtaining the most appropriate analytical methods with necessary limits of detection for drinking water quality monitoring;
- Determining key NP, BPA and E2 sources, their pathways, and potential drinking water receptors (including estimating quantities present at each stage);
- Development of predictive precautionary models for estimating concentrations of NP, BPA and E2 in raw water (pre-treatment), upon which further drinking water treatment removal efficiencies can be applied to estimate risk to non-compliance; and
- Determining the scale of risk mapping for NP, BPA and E2 in drinking water that will be useful for targeted monitoring by Defra/DWI and water companies.

2. Approach

2.1 Project aims

The purpose of this project is to investigate the risk of non-compliance of 3 EDCs (NP, BPA and E2) in drinking water across England and Wales, under the proposed drinking water standards issued by the European Commission. This study will present a review and modelling investigation into the potential of 3 EDCs to be present in drinking water (DW) across England and Wales at levels above those set by the revised draft DWD. An assessment will also be made as to the potential high-risk areas. The study outcomes will allow Defra and DWI to develop informed and effective policy approaches to manage any risks identified.

2.2 Overview of methodological approach

To assess the risk posed by each of the three EDCs entering UK drinking water supplies, the study has addressed three discrete tasks which mirror the objectives set out in the original terms of reference:

- **Task 1:** Comprehensive review of all existing peer reviewed and grey literature on sources, occurrence, and concentrations of NP, BPA and E2 already reported in DW. This will also include reports on the efficiency of removal technology to treat the EDCs and analytical methods for quantification;
- **Task 2:** Mapping routes/pathways of NP, BPA and E2 to drinking water, from source (use) to tap and estimate quantities of each EDC present at each stage; and
- **Task 3:** Estimate risks to DW from the EDCs at surface water abstraction sites using an existing exposure model and estimate risk posed to groundwater. A final calculation step is incorporated to estimate the post DW treatment concentration of EDCs in DW across England and Wales.

3. Task 1: Systematic evidence map of the literature on three EDCs in drinking water

Objectives:	Systematic identification of existing data on the presence of the 3 EDCs in drinking water (and drinking water sources), methods of analysis and the removal efficiency of different water treatment processes.
Task Leader:	Dr Alice Baynes, Brunel University

3.1.1 Approach

A systematic evidence map, to identify and evaluate key information from all relevant existing literature has been completed. The aim of this review is to establish the current knowledge base and validate the outcomes of later tasks. The proposed methodology considered the code of practice for systematic review in chemical risk assessment⁸. This approach follows a rigorous, objective and transparent process, avoiding the potential pitfalls of traditional literature reviews (e.g. reviewer and publication bias). The management of this task was supported by the online tool CADIMA⁹ to facilitate the coordination of the project team and guarantee the thorough documentation of the evidence gathering process. The systematic mapping process is based on a method described by James *et al.* (2016)¹⁰ and consists of the following stages:

- Stage 1: Setting the review scope, questions and eligibility criteria;
- Stage 2: Defining the search strategy; and
- Stage 3: Searching and screening the evidence.

Stage 1 - Setting the review scope, questions, and inclusion criteria

Early decisions made during the protocol development stage can have a significant impact on the scope and form of the systematic map. Protocol development is underpinned by imparting a common understanding of the context and motivation for the review. Our initial question formulation followed a similar procedure as that for systematic reviews, i.e. using PI/ECO (population, intervention/exposure, comparator, outcome), PIT (population, index test, target condition) or PO (population, outcome) statements.

For this systematic map, three separate questions and therefore statements have been formulated and agreed by Defra/DWI (Table 3.1). Each of these statements has a different structure. A copy of the full protocol (revised following review by Defra/DWI) can be found in Appendix B.

Table 3.1 Key questions driving the scope of the systematic review

#	Question
1	What is the occurrence of 17 β -estradiol, nonylphenol, bisphenol A in drinking water and sources of drinking water?
2	What methods of chemical analysis are available for these EDCs?
3	How effective is removal by drinking water treatment?

⁸ <http://policyfromscience.com/second-international-expert-workshop-standards-for-systematic-reviews-efficient-use-of-resources/>

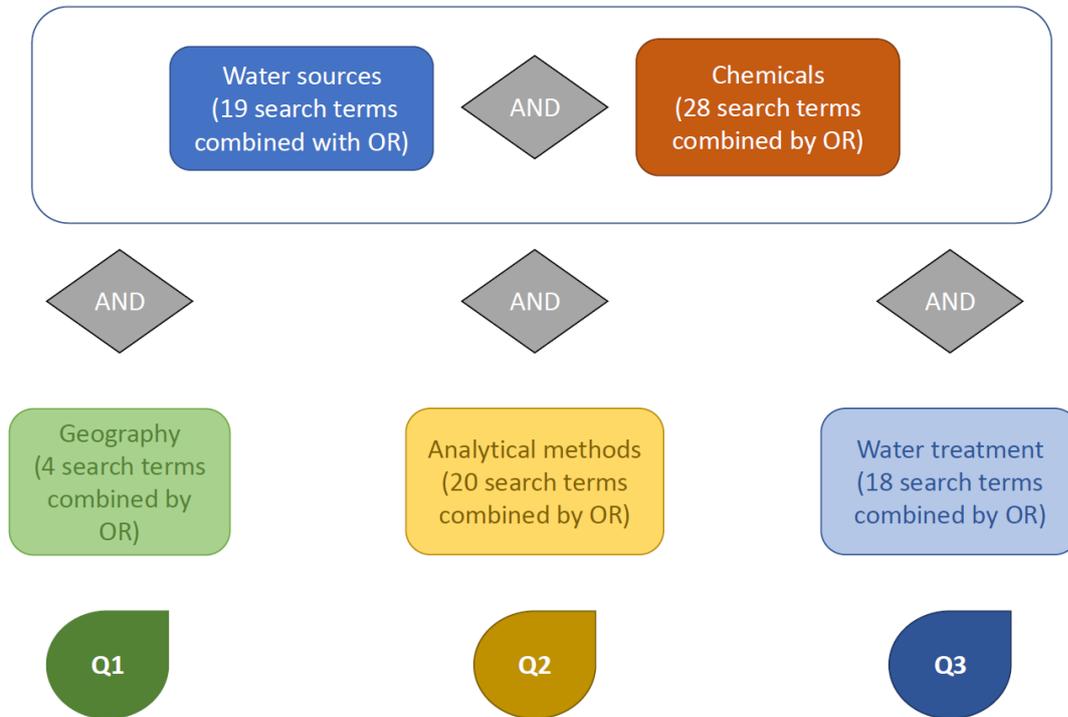
⁹ <https://www.cadima.info>

¹⁰ James *et al.* (2016) *Environ Evid*, 5:7 DOI 10.1186/s13750-016-0059-6

Stage 2 Defining the search strategy

Search algorithms were developed for Web of Science, PubMed and Scopus and revised following review by Defra/DWI as illustrated in Figure 3.1 and described in detail in the protocol (Appendix B).

Figure 3.1 Schematic representation of the literature search strategy for the three review questions



The number of results of each of the pilot searches listing a total of 88 search terms and their combination in the three literature databases (Web of Science, Scopus and Pubmed).

Stage 3 Searching and screening the evidence

Literature searches in all three databases have now been completed. The following table shows the number of hits in each database.

Table 3.2 Number of search results for each literature database and each specific review question

Database	Number of hits
Question 1: What is the occurrence of 17β-estradiol, nonylphenol, bisphenol A in drinking water and sources of drinking water?	
Web of Science	168
Scopus	81
PubMed	2,583
Number of individual records (duplicates identified)	2,694 (138)
Question 2: What methods of chemical analysis are available for these EDCs?	

Web of Science	1,239
Scopus	735
PubMed	2,583
Number of individual records (duplicates identified)	3,264 (1,293)
Question 3: How effective is removal by drinking water treatment?	
Web of Science	1,834
Scopus	942
PubMed	5,348
Number of individual records (duplicates identified)	6,861 (1,263)

Grey literature and industry data search

In addition to the above systematic approach, to answer Question 1, "What is the occurrence of 17 β -estradiol, nonylphenol, bisphenol A in drinking water and sources of drinking water?", Water Industry and Environment Agency chemical analysis data sets which include measurement of the three EDCs in ground waters and surface waters were investigated. These data sets were either specifically made available for this report (Water Company and UKWIR Chemicals Investigation Programme (CIP2) data, Environment Agency FoI request) or freely available online to download (Environment Agency, surface water data).

- Water companies provided chemical analysis data on anonymised raw drinking water sources for NP and BPA to the DWI for inclusion in this report (E2 data were not measured/provided). This data set was provided without surrounding metadata such as the volume of sample, how the sample was treated/extracted or analytical methodology;
- The Environment Agency regularly measures water quality, including chemical contaminants for regulatory compliance and monitoring purposes. Environment Agency's "open water quality archive datasets" (<https://environment.data.gov.uk/water-quality/view/download/new>) for England were accessed and downloaded (4th August 2020). These were interrogated to identify measurements of the three EDCs in river water, groundwater and still waters (pond/lake/reservoir) only, as these could be abstraction sources for drinking water. Measures relating to estuary, seawater, wastewaters, etc. were not included in the analysis. This open access data set was provided without surrounding metadata such as the volume of sample, how the sample was treated/extracted or analytical methodology; and
- A Freedom of Information (FoI) was also made to the Environment Agency to gain additional data from the WIMS Water Quality Database between 2010 and 2020. An access database of GCMS and LCMS Scan samples were provided. As above, these were interrogated to identify any measurements of the three EDCs in river water, groundwater and still waters (pond/lake/reservoir) only. Metadata such as the volume of sample, how the sample was treated or extracted were not provided. Analysis method was classed as either LCMS scan or GCMS scan.

The CIP is the UK water Industry's response to current and emerging legislation on trace substances in the water environment. The CIP has primarily focused on contaminants emanating from wastewater treatment works, however, CIP2 has also measured contaminants at river sites up and downstream of effluent outfalls across England and Wales. E2 and NP, but not BPA, data were included in the 74 substances measured in CIP2.

3.1.2 Results from Task 1, Question 1

Reports of measured concentrations of 17-Beta-estradiol (E2), nonylphenol (NP) and Bisphenol A (BPA) in drinking water, surface waters and sources waters in England and Wales.

The searching protocol retrieved 2838 articles; once duplicates were removed, 2758 articles were screened using the title and the abstract using the chemical name and source water inclusion criteria, 2595 articles were excluded at this stage. For the full text screening, 163 articles were assessed, with 141 excluded (mainly due to geographic location). Twenty-two papers were within the geographic range (England and Wales) and included measurements of E2, BPA and/or NP in surface waters (rivers, reservoirs), ground waters or from drinking water treatment works.

Five articles were excluded from the tables below at the full text screening stage for the following reasons; (Lye *et al.*, 1999) (**2576**) reported target chemicals in estuarine stretches of rivers, which would not normally be considered sources of drinking water extraction, Peck *et al.* (2004) used yeast oestrogen screen (YES) on river water samples (**998**), Thomas *et al.* (2001) used a toxicity identification evaluation (TIE) approach which combined YES and GC-MS that was not sensitive enough to measure compounds in surface waters (**936**), Comber *et al.* (2018) measured sewage effluent concentrations and predicted river water values from dilutions (**1882**), and Williams *et al.* (2012) (**804**) reported results as 'mean oestradiol equivalent' (i.e. a calculation of relative potency when E1, E2 and EE2 are summed together).

Sixteen articles measured target compounds in river water (Table 3.3). Only one publication investigated the target compounds in a reservoir (Table 3.4), another measured BPA in groundwater (Table 3.5) and one measured target compounds in final water from drinking water treatment plants (Table 3.5). Figure 3.2 illustrates the number of experiments (individual studies may survey several study sites) per source of water and analyte.

Figure 3.2 Heat map of the published literature investigating the occurrence of BPA, E2 and nonylphenol and its ethoxylate in drinking water and its sources in England and Wales ([Interactive view](#)).

Chemical name (group)	groundwater	surface - reservoir	surface - river	drinking - waterworks
Bisphenol A	1	1	16	2
Estradiol		1	80	2
Nonylphenol		1	42	2
Nonylphenol ethoxylate		1	11	2

Three articles reported nonylphenol concentrations above the chemical benchmark values (CBV) of 0.3 µg/L, however all these were published before the 2003 NP ban (Table 3.3). Whereas, articles published after the NP phase out and ban reported low ng/l concentrations of NP (Table 3.2). Of the nine articles that measured 17β-estradiol (E2) above their LOD in surface waters, six were above the CBV of 1 ng/L. Most of these studies were conducted downstream of WwTW (Table 3.3 and Table 3.4). Of the seven articles that reported Bisphenol A above their LOD, none were above CBV (2.5 µg/L) in surface water (six articles, Table 3.3) or above the CBV in groundwater (one article, Table 3.4). It is important to note that the only paper that measured target compounds in final water from drinking water treatment plants had a very high limit of detection for BPA (5.1 µg/L, (Fawell *et al.*, 2001) Table 3.5), well above the CBV, which hampers its usability for

this compound. Other authors had much more refined analytical methods with more sensitive LODs (e.g. 0.2 ng/L for BPA (Lopardo, Rydevik and Kasprzyk-Hordern, 2019)).

Table 3.3 Summary data extracted for question 1, concentrations of 17-Beta-estradiol, nonylphenol, Bisphenol A in river surface waters in England and Wales

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
(Blackburn and Waldock, 1995) 1596	Multiple sites on the River Lea, River Aire, River Thames, River Wye, River Ouse	<ul style="list-style-type: none"> Grab samples; Spiked with internal standards; and GC-MS. 	-	<0.2-53 µg/L LOD = 0.03-0.2 µg/L	-	Pre 2003 ban on NP NP above CBV 0.3 µg/L*
(Scullion et al., 1996) 1093	River Rother - South Yorkshire	<ul style="list-style-type: none"> Grab samples (2L); and HPLC LC-MS. 	-	5.6 µg/L LOD = 0.05 µg/L	-	Pre 2003 ban on NP NP above CBV 0.3 µg/L* alkylphenol ethoxylate (nonylphenol ethoxylate (NP9))
(Blackburn, Kirby and Waldock, 1999) 1008	Named rivers across England (Lea, Dee, Mersey, Thames, Exe, Aire)	<ul style="list-style-type: none"> Grab samples; Spiked with internal standards; and GC-MS. 	-	<0.2-30 µg/L LOD 0.1 µg/L	-	Pre 2003 ban on NP NP above CBV 0.3 µg/L*
(Fawell et al., 2001)	River Tame/Trent	<ul style="list-style-type: none"> Sampling method unclear; E2 and NP: GC-MS; and 	Not detected	Not detected	Not detected	BPA LOD above CBV (2.5 µg/L)

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
1845	confluence (Chetwynd Bridge), River Trent (Shardlow), River Derwent (Church Wilne raw water intake), River Severn (Strensham raw water intake).	<ul style="list-style-type: none"> BPA: HPLC. 	LOD = 0.3 ng/L	LOD = 0.4 µg/L	LOD = 5.1 µg/L	
(Xiao, McCalley and McEvoy, 2001) 962	River Thames - Reading	<ul style="list-style-type: none"> Sampling method unclear; E2 spikes; and GC-MS. 	0.5 ng/L LOD = 0.06 ng/L	-	-	

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
(Williams et al., 2003) 1457	River Nene, upstream and downstream of Great Billing STP and River Lea, upstream and downstream of East Hyde STP	<ul style="list-style-type: none"> Grab samples (5L); Spiked with internal standards; and GC-MS. 	<1 ng/L LOD 0.1-0.4 ng/L	-	-	Concentration ranges assessed visually from graphs (figures not reported)
(Liu, Zhou and Wilding, 2004) 2541	Samples from more than one river in East and West Sussex, up and downstream of STP	<ul style="list-style-type: none"> Grab samples; Internal spikes; and GC-MS. 	<LOD-17 ng/L LOD = 3.4 ng/L	<LOD LOD = 0.8 ng/L	<LOD-13 ng/L LOD = 5.3 ng/L	E2 above CBV (1 ng/L) Methods paper - highest value given for all 9 different makes of SPE cartridges used BPA LOD above CBV (2.5 µg/L)
(Matthiessen et al., 2006) 375	Up and downstream of livestock farms across England and Wales	<ul style="list-style-type: none"> Passive samplers (POCIS) deployed; Extracts spiked with internal standards; and LC-MS/MS. 	LOD-0.89 ng/L LOD = 0.15 ng/L	-	-	

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
(Zhang, Hibberd and Zhou, 2008) 450	Up and downstream of Sheffield Park STP, River Ouse, West Sussex	<ul style="list-style-type: none"> Daily grab samples (1L) or Passive samplers (POCIS) deployed; Spiked with internal standards; and GC-M. 	Grab samples 11.8 to ~25 ng/L POCIS ~3-10 ng/L LOD = "from 6 to 487 pg/L"	-	Grab samples 19.5 to ~50 ng/L POCIS ~6-20 ng/L LOD = "from 6 to 487 pg/L"	E2 above CBV (1 ng/L) Some concentrations estimated from graphs. LOD not given for each compound POCIS results did not correlate well with daily grab samples – authors suggest more work needed to improve usability of POCIS.
(Hibberd et al., 2009) 1086	River Medway - Kent	<ul style="list-style-type: none"> Grab samples (2.5L); Internal spikes and recovery data; and GC-MS/MS. 	3.1-21.4 ng/L LOD = 0.28 ng/L	LOD-4.4 ng/L LOD = 0.01 ng/L	69.3 ng/L LOD = 0.49 ng/L	E2 above CBV (1 ng/L)
(Grover, Balaam, et al., 2011) 1725	River Ray and River Ock – Wiltshire and Oxford up and downstream of STP	<ul style="list-style-type: none"> Grab samples (2.5L) or Passive samplers (POCIS) deployed 4 time per year over 3 years; Spiked with internal standards; and LC-MS/MS. 	<1.2–7.6 ng/L LOD = 0.4-1.2 ng/L	-	-	E2 above CBV (1 ng/L)
(Grover, Zhou, et al., 2011) 2683	River Ray and River Ock – Wiltshire and Oxford up and	<ul style="list-style-type: none"> Grab samples (2.5L); E2 spikes; and LC-MS/MS. 	~1-7 ng/L LOD = 1.2 ng/L	-	-	E2 above CBV (1 ng/L) Concentrations estimated from graphs.

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
	downstream of STP					
(Wilkinson et al., 2017) 1929	Hogsmill River (Greater London), source water, Chertsey Bourne River, source water, Blackwater River, source water.	<ul style="list-style-type: none"> Grab samples (0.2L); Spiked with internal standards; and LC-MS/MS. 	-	-	<3.87–1420 ng/L LOD = 1.17 ng/L	
(Lopardo, Rydevik and Kasprzyk-Hordern, 2019) 2131	Upstream and downstream of STP effluent discharge within Wessex water catchment	<ul style="list-style-type: none"> Grab samples (0.1L); Spiked with surrogates; and UHPLC-QTOF. 	-	12.1 ng/L LOD = 0.7 ng/L	14.3 ng/L LOD = 0.2 ng/L	

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
(Petrie <i>et al.</i> , 2019) 2069	South West England (upstream and at least 0.5 km downstream of 4 STPs)	<ul style="list-style-type: none"> • Grab samples; • Spiked with internal standards; and • UPLC-MS/MS. 	-	-	<p>< 0.1-116.9 ng/L</p> <p>LOD = <1 ng/L</p>	

Table 3.4 Summary data extracted for question 1, concentrations of 17-Beta-estradiol, nonylphenol, Bisphenol A in surface reservoirs and ground waters in England and Wales

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
(Fawell <i>et al.</i> , 2001) 1845	Church Wilne raw water storage reservoir	<ul style="list-style-type: none"> • Sampling method unclear; • E2 and NP: GC-MS; and • BPA: HPLC. 	25 ng/L* LOD = 0.3 ng/L	Not detected LOD = 0.4 µg/L	Not detected LOD = 5.1 µg/L	E2 above CBV (1 ng/L) BPA LOD above CBV (2.5 µg/L)
(Manamsa <i>et al.</i> , 2016) 642	Multiple groundwater sites across England and Wales	<ul style="list-style-type: none"> • Grab samples (1L); and • GC-MS (multi-residue GCMS method which is semi-quantitative and screens for N= 800 organic compounds). 	-	-	~ 100 ng/L	

*Fawell *et al.* indicated this concentration of 25 ng/L was a true result, but may have been contamination (Fawell *et al.* 2001).

Table 3.5 Summary data extracted for question 1, concentrations of 17-Beta-estradiol, nonylphenol, Bisphenol A in drinking water treatment works in England and Wales

Reference Article number in appendix (excel)	Location(s)	Analysis approach	Target compounds concentration(s) and limit of detection (LOD)			Comments
			17-Beta-estradiol (E2)	Nonylphenol (NP)	Bisphenol A (BPA)	
(Fawell <i>et al.</i>, 2001) 1845	Church Wilne final water and Strensham final water	<ul style="list-style-type: none"> • Sampling method unclear; • E2 and NP: GC-MS; and • BPA: HPLC. 	Not detected - <0.3 ng/L LOD = 0.3 ng/L	Not detected LOD = 0.4 µg/L	Not detected LOD = 5.1 µg/L	BPA LOD above CBV (2.5 µg/L)

Results from grey literature and industry data search

In addition to the published articles identified via the systematic process, within the grey literature, a UK Water Industry Research Limited study in 1997 investigated E2 concentrations in final water produced by six drinking water treatment works (fed by river water sources), reported all samples as having not detected E2, i.e. E2 concentrations (if present) were below their limit of detection of 0.2 ng/L E2 (UKWIR 1998¹¹).

Data supplied by Water Companies directly to DWI

Anonymised data of analytical chemistry of raw water sources was supplied by water companies to the Drinking Water Inspectorate and supplied for inclusion in this report. Details of methodology for how water samples were taken, prepared or analysed were not supplied with the dataset. For BPA analysis, two water companies supplied data, one supplied 4 results from samples taken in 2009 with limits of quantification ranging from 0.02-1 µg/L, BPA was not detected above the LOQs in any of these four raw water samples. The other water company provided 3440 data points for BPA from raw sources water sampled from July 2009 to June 2019. For this set of raw water BPA analysis, the limit of quantification was 0.01 µg/L, on 130 occasions BPA was reported above the LOQ (3.78% of samples), and on only eight occasions BPA was measured at or above the 2.5 µg/L BPA CBV (overall mean 0.83 ± 2.66 µg/L BPA, maximum 21 µg/L BPA).

In the same water company data set, six water companies provided 13,157 data points for 4-NP from raw water sources samples from 2009 to 2019. Of these companies only two had an LOQ below the CBV level of 0.3 µg/L NP. One company provided a total of 2,356 data points. From 2009-2013 the LOQ was 0.013 µg/L NP, with 415 samples (31.37%) being above this limit (mean 0.059 ± 0.087 µg/L NP, max 1.0 µg/L NP). From 2014-2019 the LOQ was reduced to 0.0072 µg/L NP. However only one sample (0.1%) from this time period was above this new limit (0.013 µg/L NP). In total, from 2009 to 2019 only 9 samples were measured at or above the CBV level of 0.3 µg/L NP (max 1.0 µg/L NP). The other company provided data on 3,102 samples analysed for 4-NP. From 2009-2013 the LOQ was 0.0049 µg/L NP, with 22 samples (1.66%) being above this limit (mean 0.019 ± 0.028 µg/L NP, max 0.12 µg/L NP). From 2014-2019 the LOQ was 0.0072 µg/L NP, with 20 samples (1.51%) being above this limit (mean 0.014 ± 0.007 µg/L NP, max 0.035 µg/L NP). At this second water company, between 2009 to 2019, no samples were measured at or above the CBV level of 0.3 µg/L NP.

Data for NP-all isomers was also supplied by two water companies. One company provided 1025 data points for NP-all isomers from raw sources water sampled from January 2014 to June 2019 with a LOQ of 0.013 µg/L. For this set of raw water NP-all isomers analysis 211 samples (20.6%) were above the LOQ (mean 0.056 ± 0.52 µg/L NP, max 0.43 µg/L NP) with only 1 sample measured at or above 0.3 µg/L. The other water company provided 598 data points from November 2009 to June 2019. However, until 2019 the LOQ was very high, between 1-5 µg/L NP-all isomers. In 2019 LOQ reduced to 0.3 µg/L NP-all isomers. In the 2009 to 2018 data set on five occasions NP-all isomers was reported exactly at the LOQ (i.e. exactly 5 or 1), these seem likely to be data entry errors (i.e. not added the < symbol in the adjacent cell) rather than measured concentrations. In 2019, with the lower LOQ, none of the samples of raw water were reported above 0.3 µg/L.

No data was supplied for E2 analysis of raw water from the water companies to DWI for this report.

Environment Agency water quality data

Environment Agency open source surface water data for 2019-2020 were download from "open water quality archive datasets" (<https://environment.data.gov.uk/water-quality/view/download/new>), sites classified as Pond/Lake/Reservoir, River/Running Surface and Groundwater were assessed for this report. Additional sites (e.g. saltwater estuaries, etc.) were removed from the analysis, as these were not deemed to be drinking water sources. Of the sites included, NP was recorded on 882 occasions from 204 sampling locations. A range of LOQs were used across the sampling locations (0.04-0.3 µg/L), with the most common being 0.04 µg/L (used for 96% of all the data points recorded as being "below the LOQ"). In total, 3.5% (31) of data points

¹¹ Report Ref. No. 98/TX/01/1

were above the LOQ for their respective location. Of these only 4 samples from 3 sampling locations were recorded at or above the CBV level of 0.3 µg/L (mean 0.42 ± 0.13 µg/L NP, max 0.62 µg/L NP).

E2 was recorded on 101 occasions from 21 sampling locations. In total, 62 of the 101 occasions E2 (61.4%) was recorded above the LOQ of 0.03 ng/L E2 (mean 0.14 ± 0.30 ng/L E2). There were only 2 samples from one sampling location where E2 was recorded at or above the CBV level of 1.0 ng/L E2 (mean 1.85 ± 0.85 ng/L E2, max 2.7 ng/L E2).

There were no records for BPA from sites classified as Pond/Lake/Reservoir, River/Running Surface and Groundwater was available in the Environment Agency open source surface water data for 2019-2020.

Further data was obtained from the Environment Agency via a freedom of information (FoI) request. This contained surface water samples taken as part of regular or pollution event monitoring activities, using GCMS scans or LCMS scans. As with the previous Environment Agency database, only sites classified as Pond/Lake/Reservoir, River/Running Surface and Groundwater were assessed for this report. From the GCMS scan datasets there were 2233 data points which reported BPA from 785 sampling locations. A Limits of Detection (LOD) of 0.01 µg/l BPA was reported for 2025 of the sampling occasions, with the measured concentration of BPA for all these data points being above the LOD. Of these, 91 samples from 70 sampling locations were recorded at or above the CBV level of 2.5 µg/L (mean 9.06 ± 7.61 µg/L BPA, max 43.04 µg/L BPA). It should be noted that 10 data points were excluded from this analysis. These were measurements taken at pollution events that had measured concentrations of BPA much higher than the rest of the data set, in the range of 95-1660 µg/l BPA.

There were no records of E2 or NP in the from GCMS scan of sites classified as Pond/Lake/Reservoir, River/Running Surface and Groundwater in the Environment Agency FoI datasets. None of the three EDCs were identified in LCMS scan in the Environment Agency FoI datasets. Results for Bisphenol S (BPS, CAS no. 80091), but not BPA, were recorded in the LCMS scans, but not reported here.

Chemical Investigation Program 2 (CIP2) data

Chemical Investigation Program 2 (CIP2) raw data was also available for inclusion in this report. The CIP focuses on chemicals emanating from wastewater treatment works (WWTW) effluents, therefore river water samples were taken up-stream (391 sampling locations) and downstream (440 sampling locations) of WWTW effluents, and are not necessarily locations where drink water abstraction occurs. However, these measures are still reported, as they could be indicative of river waters nationally. BPA was not included in the CIP2 chemical analysis suite. Both nonylphenol and E2 were reported in water samples taken downstream of WWTW, only NP was reported in upstream WWTW sites.

Upstream of WWTW, between 2015 to 2019, NP was reported in 13,172 samples from all 391 sampling locations. A range of LOQs were used across the sampling locations (0.01-0.3 µg/L), with the most common being 0.04 µg/L (used for 84% of all the data points recorded as being "below the LOQ"). A total of 29.4% (3,873) of the samples were above the NP LOQ for their respective location. Of these, 197 samples from 77 sampling locations were recorded at or above the CBV level of 0.3 µg/L (mean 0.77 ± 0.87 µg/L NP, max 7.15 µg/L NP).

Downstream of WWTW, between 2015 to 2019, NP was reported in 15,208 samples from all 440 sampling locations. As with the upstream samples, a range of LOQs were used across the sampling locations (0.01-0.3 µg/L), with the most common being 0.04 µg/L (used for 90% of all the data points recorded as being "below the LOQ"). In total, 41.6% (6,329) of the samples reported NP above LOQ for their respective location. From these, 461 samples from 105 sampling locations recorded NP at or above the CBV level of 0.3 µg/L (mean 0.44 ± 0.17 µg/L NP, max 1.91 µg/L NP).

Between 2015 and 2016, E2 was detected on 17 occasions from one sampling location downstream of a WWTW. In total, 7 samples (41.18%) were measured above the E2 LOQ of 0.3 ng/L (mean 0.59 ± 0.98 ng/L E2). Only one sample (4.5 ng/L) was above the CBV level of 1.0 ng/L E2.

3.1.3 Results from Task 1, Question 2

Reports of methods of chemical analysis available for the three EDCs

A wide range of techniques are available to monitor concentrations of the EDCs in all environmental media. The key methods retrieved can be seen in Table 3.3 to Table 3.5 above and From the grey literature. The UKWIR report discussed in Q1, found no detectable E2 in final waters at six water treatment sites using a variety of drinking water technologies (ozone + GAC, GAC, microstraining, coagulation + pH adjustment) (UKWIR 1998). However, in each case the source water intakes were not analysed, so E2 removal rates could not be confirmed for these technologies (UKWIR 1998). Within the same UKWIR study, benchtop scale (5L) investigations using borehole water spiked with 50 ng/L E2 were conducted to investigated E2 removal by a number of drinking water treatment processes. These benchtop studies suggested ozonation, chlorination and PAC provided high levels of E2 removal (96-99%) from spiked borehole water, whereas coagulation and filtration showed less promise (UKWIR 1998). Similar results have been found from other bench scale studies (e.g. Snyder *et al.*, 2007, Westerhoff *et al.*, 2005)

Table 3.6 to Table 3.8 below, along with their LOD. Each has a different limit of quantification/detection depending on the laboratory conducting the analysis and the refinement of the method protocol. There is no one specific method that is used consistently for any of the EDCs but most/many use chromatography.

As E2 is on the Water Framework Directive (WFD) current 'watch list', recent attempts have been made to assess methods for detecting E2 in surface waters across Europe, to determine if Member States have the capacity to detect the proposed sub ng/l EQS levels. In a 2019 JRC workshop, all fifteen Member States involved reported the ability to detect E2 at sub ng/l in surface water, with twelve of the Member States represented reported limit of quantification (LOQ) ≤ 0.4 ng/l (JRC 2019). Of the fifteen Member States represented in the JRC report LC-MS/MS was the most frequently used method (12 out of 15 participants), although GC-MS, GC-MS/MS and LC-TOF-MS methods also produced sub ng/l LOQs (JRC 2019).

The UK Water Industry has significant experience in measuring steroid oestrogens (e.g. estrone, estradiol and ethinyl estradiol), BPA and NP in wastewater effluents and surface waters through their involvement in Chemical Investigation Program (CIP1 and CIP2). Indeed, an UKWIR report on final waters, demonstrates that methods for measuring E2 at sub ng/L have been around for more than two decades in the UK (UKWIR 1998). Raw data provided to DWI from Water companies, the CIP2 and the Environment Agency for this report did not come with associated meta data relating to sampling, extraction and analytical methods. However, it is clear from the data that a range of methods are used with varying sensitivities, resulting in different LOQs from different laboratories (and over time within the same company). The Environment Agency had the most sensitive methods for E2 (LOQ 0.03 ng/L) and BPA (LOD 0.01 $\mu\text{g/L}$) analysis, whereas one of the Water companies, which sent anonymised raw water data, had the most sensitive methods for NP analysis (LOQ 0.0049 $\mu\text{g/L}$). However, it is worth noting that only two out of the six Water companies had sufficiently sensitive analytical methods for NP (i.e. LOQ below the CBV, e.g. 1 $\mu\text{g/l}$). There are clearly some differences in analytical laboratory performance within the sector for NP which were also evident in the CIP2 dataset, although LOQ were generally at or below the CBV (0.01-0.3 $\mu\text{g/l}$ NP). The CIP2 data set also provided strong evidence of methods to detect E2 (LOQ 0.3 ng/l) below the proposed CBV level. Therefore, although UK Drinking Water laboratories do not have a history of routinely measuring these EDCs, there is significant expertise within the water industry (and at UK regulatory laboratories) more widely, which could be adopted to enable monitoring of these compounds in drinking water.

Figure 3.3 Heat map of the analytical methods applied to study occurrence of BPA, E2, nonylphenol and its ethoxylates in drinking water sources ([Interactive view](#))

Method type	Source	Bisphenol A	Nonylphenol	Nonylphenol ethoxylate	Estradiol
GC	drinking - tap	1			
	drinking - distribution	1			
	drinking - waterworks		1	1	1
	surface - reservoir		1	1	2
	surface - river	4	6	2	6
	groundwater	1			
LC	drinking - distribution				2
	drinking - waterworks	1			
	surface - reservoir	1			
	surface - river	4	1	1	5
	groundwater				1

3.1.4 Results from Task 1, Question 3

Reports of 17-Beta-estradiol (E2), nonylphenol (NP) and Bisphenol A (BPA) in drinking water sources before and after drinking water treatments (limited to drinking water treatment processes routinely used in England and Wales, at pilot scale and above).

Within the literature search, drinking water treatment search terms included: ozonation, activated carbon (incl. GAC, PAC), sand filtration, UV radiation, chlorination, disinfection, clarification, advanced oxidation process (e.g. H₂O₂ and UV), coagulation, flocculation and air flotation.

The literature search retrieved 2788 articles. Once duplicates were removed, 1563 articles were screened using the title and the abstract and 1440 articles were excluded at this stage. For the full text screening, 123 articles were assessed for eligibility, with 109 excluded (mainly due to non-eligible water treatment type). Fourteen papers were included in the evidence map.

However, during data extraction, a further nine articles were excluded for various reasons. Sun *et al.* (2008) (**1219**) reported estrogenic activity (via yeast screen) of nonylphenol ozonation by-products rather than specific removal of target compounds. Pereira *et al.* (2011) (**1159**) investigated ozonation by-products of E2 spiked groundwater. Ma *et al.* (2015) (**1477**) used a small bench scale set up to investigate E2 removal in spiked pure water by UV/H₂O₂ treatment process. Li *et al.* (2017) (**546**) used synthetic surface water (RO water with added TOC) spiked with E2 to investigate different carbon sources on the removal efficiency biologically activated carbon (BAC) treatment. High levels of removal were reported (98.9%) prior to adding carbon sources to the BAC, however the limit of detection was 5.8 ng/L, almost six times the E2 CBV (1 ng/L (Z. Li *et al.*, 2017), **546**). Fawell *et al.* (2001) (**1845**) did not specify the drinking water treatment process or give before and after concentrations of target compounds, this article was also identified in question 1.

Three articles seemed to use the same pilot scale set-up fed by tap water in China. These assessed chlorination of target compounds. Li *et al.* (2015) (**332**) investigated chlorination of Bisphenol A spiked (100 µg/L) tap water, the focus was not specifically BPA removal by chlorination but the formation of halogenated compounds and occurrence of brominated BPA. He *et al.* (2016) (**202**) investigated the removal of E2 spiked (25 µg/L) into tap water in a pilot-scale plant via chloramine addition (removal rates of 59.8-96.6% were reported). Trihalomethanes (THMs), haloacetic acids (HAAs), and halogenated nitromethane (HNMs) during the degradation E2 in the pilot system were also reported. Li *et al.* (2017) (**68**) investigated chlorination of E2 spiked (100 µg/L) water, although they reported E2 removal rates of 91.91-99% their main finding related to the formation of trihalomethanes (THMs) and halogenated acetic acids (HAAs) in the system.

A heat map of eligible studies reporting removal efficiencies during water treatment is shown in Figure 3.4.

Figure 3.4 Heat map of eligible studies reporting removal efficiencies of BPA, E2 and nonylphenol by drinking water treatment processes ([Interactive view](#))

	Treatment type				
	clarification	activated carbon	chlorination	disinfection	other
Bisphenol A	1	2	1	1	1
Estradiol		1	2	1	2
Nonylphenol	1	1		1	

Three articles investigated E2 removal at pilot scale or above using real environmental source waters (From the grey literature. The UKWIR report discussed in Q1, found no detectable E2 in final waters at six water

treatment sites using a variety of drinking water technologies (ozone + GAC, GAC, microstraining, coagulation + pH adjustment) (UKWIR 1998). However, in each case the source water intakes were not analysed, so E2 removal rates could not be confirmed for these technologies (UKWIR 1998). Within the same UKWIR study, benchtop scale (5L) investigations using borehole water spiked with 50 ng/L E2 were conducted to investigate E2 removal by a number of drinking water treatment processes. These benchtop studies suggested ozonation, chlorination and PAC provided high levels of E2 removal (96-99%) from spiked borehole water, whereas coagulation and filtration showed less promise (UKWIR 1998). Similar results have been found from other bench scale studies (e.g. Snyder *et al.*, 2007, Westerhoff *et al.*, 2005)

Table 3.6). Kleywegt *et al.* (2011) did not detect any E2 in a large range of drinking water plant influent or effluents in Canada, but the LOD was 2 ng/L (double the proposed CBV for E2). Zhang *et al.* (2016) showed high E2 removal rates (97-99%) in spiked surface water in a pilot plant using multiple treatment steps, however the spike concentration was above environmental levels (~245 ng/L) and they did not report their LOD or LOQ. Azzouz & Ballesteros (2013) investigated E2 removal from raw source waters in Spain and demonstrated good removal rates mainly below the E2 CBV (1 ng/L), these seemed to fluctuate seasonally.

One article was retrieved which demonstrated removal of nonylphenol (NP) from source waters by drinking water treatment processes (Stackelberg *et al.*, 2007) from 0.3 µg/L to below the CBV (0.3 µg/L, Table 3.7) and two articles demonstrated removal of BPA from source waters from hundreds of ng/L to below the BPA CBV (2.5 µg/L, Table 3.8). However, one of these articles reported BPA levels increasing again in the clarifying step (Rahman *et al.*, 2010) (Table 3.8).

From the grey literature. The UKWIR report discussed in Q1, found no detectable E2 in final waters at six water treatment sites using a variety of drinking water technologies (ozone + GAC, GAC, microstraining, coagulation + pH adjustment) (UKWIR 1998). However, in each case the source water intakes were not analysed, so E2 removal rates could not be confirmed for these technologies (UKWIR 1998). Within the same UKWIR study, benchtop scale (5L) investigations using borehole water spiked with 50 ng/L E2 were conducted to investigate E2 removal by a number of drinking water treatment processes. These benchtop studies suggested ozonation, chlorination and PAC provided high levels of E2 removal (96-99%) from spiked borehole water, whereas coagulation and filtration showed less promise (UKWIR 1998). Similar results have been found from other bench scale studies (e.g. Snyder *et al.*, 2007¹², Westerhoff *et al.*, 2005¹³)

¹² Snyder, Shane A.; Wert, Eric C.; Lei, Hongxia (Dawn). 2007 Removal of EDCs and Pharmaceuticals in Drinking and Reuse Treatment Processes .ISBN 10: 1583215557

¹³ <https://pubs.acs.org/doi/10.1021/es0484799>

Table 3.6 Summary data extracted for question 3, removal of 17-Beta-estradiol (E2) from sources waters via drinking water treatment processes

Reference Article number in appendix (excel)	Analysis approach	Source water (type, location)	Drinking water treatment process	Removal efficiency (%)	Comment(s)
(Kleywegt et al., 2011) 619	<ul style="list-style-type: none"> Grab sample (800 mL); and LC. <p>LOD = 2ng/L</p>	Variety of drinking water treatment sites Canada	Variety of drinking water treatments	-	E2 not detected in influent or effluent but LOD above CBV (1 ng/L)
(Azzouz & Ballesteros, 2013) 1873	<ul style="list-style-type: none"> Grab sample (100 ml); and GC-MS. <p>LOD 0.05 ng/L LOQ 0.15 ng/L</p>	Surface water (Spain) Raw water concentration 7.8-32 ng/L	Multi-step process: preoxidation/coagulation, Filtration and chlorination	73.1-95.2%	Concentration in finished water LOQ-1ng/L
(Zhang et al., 2016) 2443	<ul style="list-style-type: none"> Grab sample (40 ml); and SPE-HPLC-MS/MS. 	Surface water (USA) Spiked at 245 ng/L ± 9%	Pilot plant: pre-ozonation-dissolved air flotation-intermediate chlorination-dual media filtration-GAC-UV/H2O2	97-99%	Removal efficiency read from bar graph. LOD and LOQ not reported

Table 3.7 Summary data extracted for question 3, removal of nonylphenol (NP) from sources waters via drinking water treatment processes

Reference Article number in appendix (excel)	Analysis approach	Source water (type, location)	Drinking water treatment process	Removal efficiency (%)	Comment(s)
(Stackelberg et al., 2007) 2254	<ul style="list-style-type: none"> Grab sample (4x1L); and GC-MS. 	River water (USA) Starting concentration 0.100 - 0.342 µg/L	Multi-step process: clarification, disinfection, activated carbon	73% after all treatments	Average concentration in finished water 0.092 µg/l LOD and LOQ not reported

Table 3.8 Summary data extracted for question 3, removal of Bisphenol A (BPA) from sources waters via drinking water treatment processes

Reference Article number in appendix (excel)	Analysis approach	Source water (type, location)	Drinking water treatment process	Removal efficiency (%)	Comment(s)
(Stackelberg et al., 2007) 2254	<ul style="list-style-type: none"> Grab sample (4x1L); and GC-MS. 	River water (USA) Starting concentration 0.045 - 0.108 µg/L	Multi-step process: clarification, disinfection, activated carbon	76% after all treatments (reported steps in excel)	Average concentration in finished water 0.026 µg/l LOD and LOQ not reported
(Rahman et al., 2010) 1842	<ul style="list-style-type: none"> Grab sample (1L); and LC-MS/MS. LOD = 10 ng/L	Starting concentration 400 ng/L	ozonation/H2O2	Not quantifiable	ozonation/H2O2 treatment appears to remove BPA to <LOD but BPA is then measured again in clarifying step
(Kleywegt et al., 2011) 619	<ul style="list-style-type: none"> Grab sample (800 mL); and LC. LOD = 2ng/L	Variety of sources (ground, lake, surface) in Canada	Variety of treatment technologies (GAC or GAC+ UV)	80-99%	Concentration range not detected (below 2ng/L) to 87 ng/l (median 2.1 ng/l)

3.1.5 Summary by chemical

Bisphenol A

The occurrence of BPA in drinking water sources in England and Wales has been primarily investigated in river waters, upstream and downstream of sewage treatment plants. Six of the seven eligible studies retrieved reported concentrations of BPA in river waters in the ng/L range. There was no evidence of the chemical benchmark revised value (CBV) of 2.5 µg/L being exceeded in raw water and only two studies (Table 3.3). The study by Fawell *et al.* (2001) (**1845**) is unfortunately uninformative as it employed an insensitive analytical method. Their limit of detection (LOD) is 5.1 µg/L, twice the CBV. Manamsa *et al.* (2016) (**642**) is the only study that measured BPA in groundwater. It reported concentrations around 0.1 µg/L but this was close to the LOD of the analytical method they employed. Unfortunately, Fawell *et al.* (2001) is the only published study to have investigated the occurrence of BPA in reservoir or in drinking water treatment plants but the insensitive analytical method limits the usefulness of their data.

The non-peer reviewed data (industry/monitoring data) provides a more promising dataset, with LOQ of 0.01 µg/L BPA.

Environment Agency water quality data obtained via FoI reported 4.1% of the river water, groundwater and still water (pond/lake/reservoir) samples in the database, where BPA was detected, were at or above the CBV of 2.5 µg/L (91 samples out of a total of 2233 occasions). Some very high concentrations of BPA (up to 1660 µg/L) were also reported in this Environment Agency dataset linked to specific pollution event/investigations. These occasions were removed from average calculations. It is worth repeating that the Environment Agency and CIP2 data are not necessarily located with drinking water intakes/sources. Rather they are representative of river waters more generally. However, the high concentrations occurring in these pollution events may need to be addressed if co-located with drinking water sources.

One water company also provided a large dataset for BPA analysis, collected on raw drinking water samples between 2009 and 2019. Out of 3440 samples 8 (0.2 %) were at or above the CBV of 2.5 µg/L, with one occasion concentration measured almost ten times the CBV (21 µg/L BPA). However, the mean BPA concentration over the 10 years was 0.83 ± 2.66 µg/L BPA. This and the Environment Agency data suggests BPA concentrations may occasionally fluctuate in source waters quite considerably.

Both gas and liquid chromatography have been applied to the quantification of BPA in surface waters. For gas chromatography, the method described by Hibberd *et al.* (2009) (**1086**) reported a limit of quantification (LOQ) of 1.63 ng/L, well below the CBV of 2.5 µg/L. For liquid chromatography, the methods described by Wilkinson *et al.* (2017) (**1929**) and Lopardo *et al.* (2019) (**2131**) also reported LOQs (3.87 and 0.8 ng/L) well below the CBV, that would ensure the useful application in this context. Although analytical methods were not supplied with the Water companies, Environment Agency or CIP2 datasets, LOQ and LODs were all below the CBV for BPA, suggesting methods are frequently available to measure BPA in drinking water sources in England and Wales.

There is a paucity of data on the effectiveness of drinking water treatment processes to remove contaminants such as BPA. More attention has been given to the occurrence of BPA in distribution systems or the generation of halogenated disinfection by-products. Nonetheless, Stackelberg *et al.* (2007) (**2254**) and Kleywegt *et al.* (2011) (**619**) demonstrated removal efficiencies of BPA of over 75% from source waters from hundreds of ng/L to below one ng/L. However, Rahman *et al.* (2010) (**1842**) reported increasing BPA levels after the clarifying step.

Estradiol

Similarly, the occurrence of E2 has been primarily investigated in river water in England and Wales, often upstream and downstream of sewage works. The values measured in these studies may not be representative of the concentrations at drinking water abstraction points. Whilst earlier studies in the early noughties

tended to report concentrations of E2 below 1 ng/L, more recent investigation report concentrations from the low ng/L range up to 25 ng/L (From the grey literature. The UKWIR report discussed in Q1, found no detectable E2 in final waters at six water treatment sites using a variety of drinking water technologies (ozone + GAC, GAC, microstraining, coagulation + pH adjustment) (UKWIR 1998). However, in each case the source water intakes were not analysed, so E2 removal rates could not be confirmed for these technologies (UKWIR 1998). Within the same UKWIR study, benchtop scale (5L) investigations using borehole water spiked with 50 ng/L E2 were conducted to investigate E2 removal by a number of drinking water treatment processes. These benchtop studies suggested ozonation, chlorination and PAC provided high levels of E2 removal (96-99%) from spiked borehole water, whereas coagulation and filtration showed less promise (UKWIR 1998). Similar results have been found from other bench scale studies (e.g. Snyder *et al.*, 2007, Westerhoff *et al.*, 2005)

Table 3.6). This includes the only peer reviewed study that investigated the presence of E2 in reservoir water, which reported the concentration of 25 ng/L (Fawell *et al.* 2001, **1845**). However, of note, the same study by Fawell also investigated E2 in the raw water of a water treatment plant fed by the reservoir and could not detect E2 (LOD 0.3 ng/L), leading the authors suggest this high value is “probably due to contamination” (Fawell *et al.* 2001, **1845**).

The grey literature and industry data were also considered. E2 was measured in the Environment Agency and CIP2 datasets from river locations. From the Environment Agency 2019-2020 open access data, E2 was detected in 101 samples (LOQ 0.03 ng/L E2), 2% of these were above the CBV of 1 ng/L E2 and these were both reported from one site. From the CIP2 dataset, E2 was only detected at river sites downstream of WWTW effluents (17 occasions, 2015-2016, LOQ 0.3 ng/L E2), one sample was reported at 4.5 ng/L E2, however this was the only one above the CBV (mean 0.59 ± 0.98 ng/L E2).

E2 analysis was not reported in the anonymised Water company data of raw drinking water supplied to the DWI. The only data for E2 analysis in final drinking water from UK locations comes from an UKWIR report where E2 was not detected (LOD 0.2 ng/L E2) in 18 samples of final water (six drinking water treatment works sites, sampled three times in February 1997) (UKWIR 1998). These sites used a variety of drinking water treatments including ozone, GAC, Microstraining, Coagulation and pH adjustment and were primarily fed with river water sources (UKWIR 1998).

Both GC and LC methods have been applied to the quantification of estradiol in drinking water and drinking water sources and the majority report LODs/LOQs below 1 ng/L and would therefore be applicable for monitoring compliance with the proposed revised drinking water parameters. Although analytical methods information were not provided by the Environment Agency or CIP2, it is clear from the data that the analytical methods are sufficiently sensitive to detect sub ng/l E2 concentrations in water samples (LOQs 0.03-0.3 ng/L), below the CBV of 1 ng/L E2.

Again, there is a paucity of data on removal efficiencies during water treatment processes at background concentrations in the peer-reviewed literature. Studies using water spiked at much higher concentrations than those found to occur in sources of drinking water may overestimate removal efficiencies. Azzouz & Ballesteros (2013) (**1873**) did nonetheless report removal efficiencies over 70% (From the grey literature. The UKWIR report discussed in Q1, found no detectable E2 in final waters at six water treatment sites using a variety of drinking water technologies (ozone + GAC, GAC, microstraining, coagulation + pH adjustment) (UKWIR 1998). However, in each case the source water intakes were not analysed, so E2 removal rates could not be confirmed for these technologies (UKWIR 1998). Within the same UKWIR study, benchtop scale (5L) investigations using borehole water spiked with 50 ng/L E2 were conducted to investigate E2 removal by a number of drinking water treatment processes. These benchtop studies suggested ozonation, chlorination and PAC provided high levels of E2 removal (96-99%) from spiked borehole water, whereas coagulation and filtration showed less promise (UKWIR 1998). Similar results have been found from other bench scale studies (e.g. Snyder *et al.*, 2007, Westerhoff *et al.*, 2005)

Table 3.6) from raw water containing 7.8-32 ng/L E2 and the concentrations in the finished water were below 1 ng/L.

In the same 1997 UKWIR study as discussed above, benchtop studies spiking 50 ng/L E2 were conducted to investigate removal by drinking water treatment processes. These benchtop studies showed ozonation, chlorination and PAC provided high levels of E2 removal (96-99%) from spiked borehole water (UKWIR 1998).

Overall, there is little evidence that the proposed CBV of 1 ng/L E2 would be exceeded in the majority of water sources. Drinking water technologies already employed in the industry may be successful in further reducing E2 concentrations below the CBV.

Nonylphenol

As for other analytes, the occurrence of nonylphenol has been investigated in river water in England and Wales. There is a striking difference in reported concentrations over time. In the nineties, concentrations up to 53 µg/L were reported to occur (Table 3.3). Studies published after the year 2000, as the restrictions implemented in 2003 neared, concentrations of nonylphenol in rivers were marked lower occurring in the ng/l much below the proposed revised drinking water parameter of 0.3 µg/L (Table 3.3). Fawell *et al.* (2001) (1845) is again the only peer-reviewed study that measured nonylphenol in UK reservoir and raw intake water. They could not detect nonylphenol in any of those matrices using an analytical method with reported LOD of 0.2 µg/L.

In addition to the peer-reviewed literature, industry and regulatory/monitoring data were also investigated to determine the concentrations of NP in possible drinking water sources. From the Environment Agency open access database, NP was detected in 882 samples from 204 locations between 2019-2020. However, only four samples from three locations were measured at or above the CBV 0.3 µg/L, with a maximum concentration of 0.62 µg/L NP recorded (LOQ 0.04-0.3 µg/L NP). The CIP2 dataset investigated NP concentrations (LOQ 0.01-0.3 µg/L) at river sites upstream and downstream of WWTW effluent outfalls. Between 2015 and 2019, more than 13,000 samples were analysed for NP at upstream sites, with around 1.5% of samples at or above the NP CBV (mean 0.77 µg/L NP). Over the same time period, more than 15,000 samples were analysed for NP from sites downstream of WWTW, with 3% measuring above the CBV (mean 0.44 µg/L). The maximum concentration reported for NP from the CIP2 dataset was at an upstream sampling site (7.15 µg/L NP). Therefore, although as noted in the peer reviewed literature NP concentrations have reduced from those seen in the late 1990s, in some locations' river waters are likely to exceed the proposed CBV for NP. NP is also listed as a priority substance under the Water Framework Directive (WFD, Directive 2013/39/EU) and concentrations above 0.3 µg/L are in breach of WFD Environmental Quality Standards (EQS). Therefore, further national regulations could be required to reduce NP levels surface waters.

Anonymised data from six water companies were provided for NP analysis from drinking water raw waters for this report, only two companies had LOQ below the CBV. However, these two water companies provided more than 5,000 data points between 2009-2019 (LOQ 0.013-0.0049 µg/L), of these only nine samples were above the CBV of 0.3 µg/L NP (maximum concentration reported 1 µg/L).

GC methods have been applied more frequently to monitor nonylphenol concentrations. All the methods employed in eligible studies that did report their LOD, reported LOD/LOQs well below the proposed revised drinking water parameter. The only study that has applied an LC method to measure nonylphenol is the recent study by Lopardo *et al.* (2019) (2131) and they reported a LOQ in the low ng/L range. Analytical methods information were not provided by the Environment Agency, Water companies or CIP2 with their data. However, it is clear from the range of LOQs in these datasets, some water companies have very sensitive methods for NP analysis (LOQ 0.0049 µg/L), whereas others may need to update their methods to meet analytical requirements down to 0.3 µg/L.

The only eligible study that has investigated the removal of nonylphenol by drinking water processes is that by Stackelberg *et al.* (2007) (2254). They reported an overall removal efficiency (after all treatments) of 73% and average concentrations in finished waters of 0.092 µg/l.

4. Task 2: Sources and routes to water

Objectives:	Identification of sources, pathways and routes to water of each of the 3 EDCs and quantify amount used in England and Wales. Explore trend in chemical use, where possible.
Task Leader:	Rob Whiting, Wood

4.1.1 Approach

Task 2 complements the evidence base created by Task 1, to further develop our understanding of fate and transport of E2, NP, and BPA in terms of quantifying the significant sources of these chemicals, their ultimate destination and likelihood of contamination to drinking water. In order to achieve this, we developed a preliminary source-pathway-receptor based approach including a basic flow diagram of the transport of the specific EDCs into the aquatic environment similar to the example seen below (Figure 4.1).

Task 2 began with an assessment for the active use of all three substances and likely application types to help develop the approach for the sources and routes to water. Based on this analysis it was possible to discern the following:

- **Bisphenol A (BPA):** Concerns regarding the health effects of BPA have been growing for some years now. As of June 2011 (2002/72/EC) the use of BPA in infant feeding bottles was banned; and as of 2 January 2020, use of BPA within thermal papers and food packaging was also banned (EU 2016/2235). However, despite specific applications being banned, the use of BPA is growing globally¹⁴, with high demand for use as an intermediate in the manufacture of polymers, particularly polycarbonate and epoxy resin which have key applications in the construction and automotive sectors. While the UK does not manufacture BPA itself, the UK would be a key market for polymer manufacture and use of BPA;
- **17-Beta-estradiol (E2):** E2 is a natural hormone within the female mammalian physiology. Therefore, emissions within the UK will be likely, with key data sets coming from ONS for human populations, and agricultural data-sets covering cows, pigs, and sheep. Data was required for efficacy of wastewater treatment works, attenuation rates in the environment, and likely presence in run-off from agricultural land; and
- **Nonyl-phenol (NP):** In the UK, the use of nonyl phenol (CAS 25154-52-3) and nonyl-phenol ethoxylate were banned for a wide range of uses under Environmental statute 2004 / no.1816¹⁵. This was then later mirrored at European level, as a REACH restriction (Entry 46 of Annex XVII). The REACH regulation goes further to include maximum concentrations for trace residues within textiles which will be effective from February 2021. ¹⁶Additionally, within the UK, phase-out of NP and NPE for some uses may have been even earlier with SEPA¹⁷ noting a voluntary agreement with industry dating from 1976 to avoid use of NP and NPE in detergents. Currently, no REACH registrations for

¹⁴ <https://www.prnewswire.com/news-releases/bisphenol-a--a-global-market-overview-300282092.html>

¹⁵ NP and NPE was restricted above 0.1% w/w in the following uses: industrial and institutional cleaning (unless in closed systems), domestic cleaning, textiles and leather processing (except for processes where no wastewater is generated), emulsifiers in agricultural treatments, metal working (unless in closed systems), manufacture of pulp and paper, cosmetic products, and personal care products. Note use in pesticides or biocides where authorisations were granted before 2003 are not excluded.

¹⁶ concentration of NPE shall not exceed 0.01% by weight of the textile article, noting that second-hand textiles will be exempt

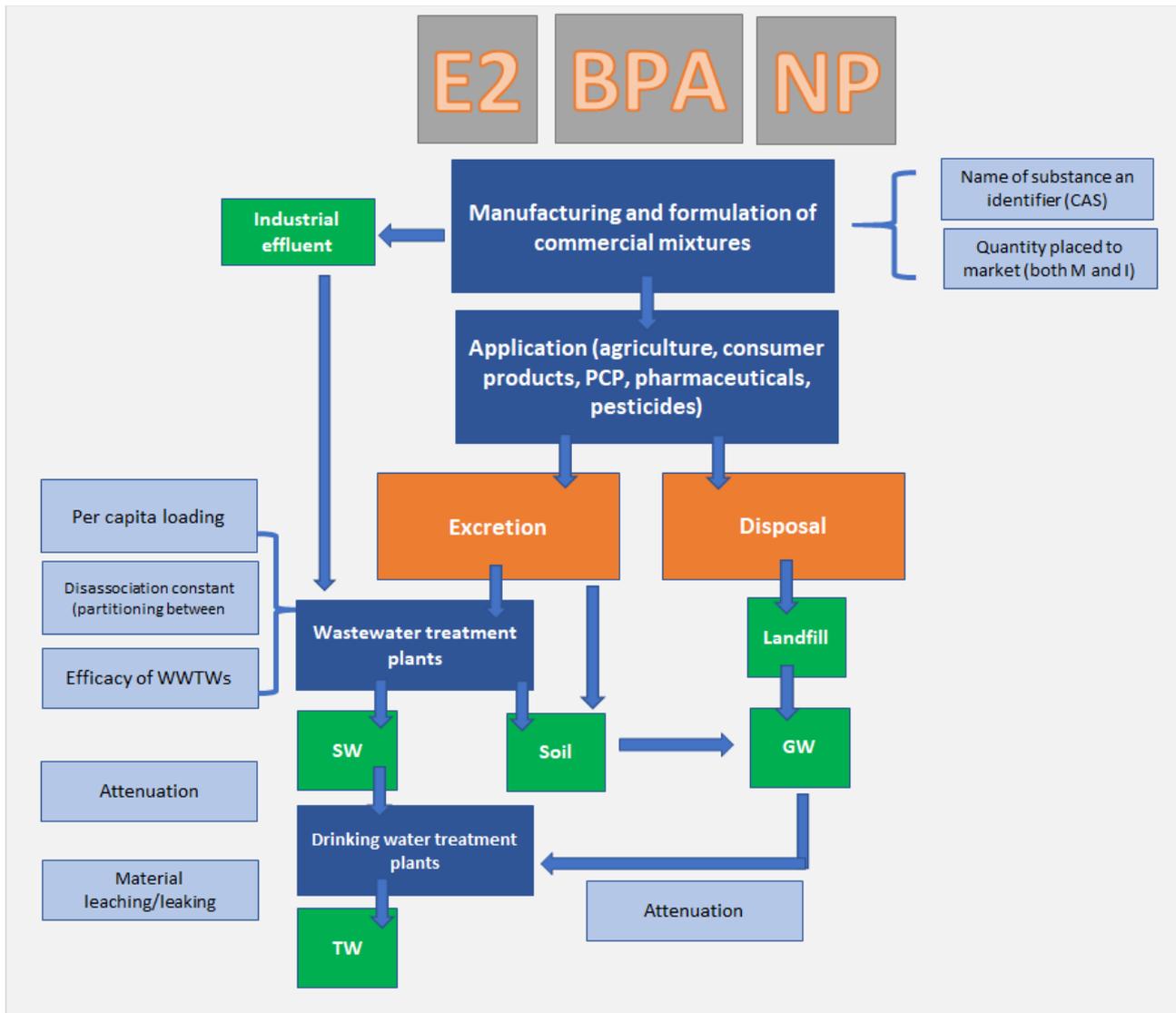
¹⁷ <http://apps.sepa.org.uk/spria/Pages/SubstanceInformation.aspx?pid=154>

NP exist under the ECHA database¹⁸. We therefore expect no current manufacture or use of NP within the UK, and emissions to water will most likely be linked to historic legacy sites of production, landfill, and import of contaminated articles.

This initial assessment to help define our approach for each substance and what data-sets and source reference material would be needed - including the available data from the Task 1. Literature references and UK national statistics were then used to develop a source-flow approach for each substance and emissions to surface water. Data from the chemical investigation programme (CIP) has also been used to help validate the estimates and provide sense-checking to help determine for at least the point source emissions.

¹⁸ Note a clarification, the REACH database of registrations indicates that no registrations for NP (CAS 25154-52-3) exists. However, 4-nonylphenol, branched (CAS 84852-15-3) which is included as a priority substance under the EQS Directive is registered at the 10,000 – 100,000 tonnes per annum bracket for Europe, with six UK manufacturers/importers (Baker Hughes, DuPont, John Hogg Technical Solutions, Lubrizol, Nalco, and SI Group UK).

Figure 4.1 Schematic of sources, pathways and routes of the 3 EDCs to the aquatic environment. TW = tap water, GW = groundwater, SW= surface water.



4.1.2 Results

4.1.3 Bisphenol A

Overview

Bisphenol A is chiefly used as a raw material in the manufacture of other products, primarily polymers including polycarbonate, epoxy resins, phenoplastic resins, and specific polyester products (UBA, 2014)¹⁹. It was also previously used within the polymerisation process (as an inhibitor) for PVC, although this application was voluntarily phased out across the EU in 2003 (EU, 2008)²⁰. Use of BPA within PVC has continued as additive packs for use within soft PVC applications in a more limited fashion (UBA, 2014).

¹⁹ UBA, 2014, 'Identification of relevant emission pathways to the environment and quantification of environmental exposure for Bisphenol A', Report 41/2014

²⁰ European Union, 2008, 'European Union Risk Assessment Report for BPA', April 2008 addendum.

The REACH registration database indicates that BPA (CAS 80-05-7) is registered at the 100,000 – 1 million tonnes per annum bracket for Europe, with four UK registrants (out of 65). The EU RAR for BPA (2008) commented that EU production of BPA was ongoing in Germany, the Netherlands, Belgium, and Spain. Production of BPA itself was not identified within the UK, although UK companies will use BPA for the manufacture of polymers and within PVC applications.

Only limited data on UK consumption of BPA was identified, therefore EU data has been used and extrapolated to UK rates of consumption based on GDP.

UBA (2014)²¹ commented that EU production was estimated to be between 1 million and 10 million tonnes per annum based on REACH registrations, which correlates with the EU RAR (2008) estimate of 1.1 million tonnes per annum. This suggests that the current bracket quoted within the REACH registration database (100k -1million tonnes) is likely to be close to or at the 1 million tonne mark per annum for Europe. UBA (2014) study also completed a cross-comparison of EU to global production of BPA, with EU production in 2011 set at 26% (or 1.1 million tonnes) of global production (4.2 million tonnes). Based on GDP, UK consumption rates for BPA in 2011 were estimated to be 220kt or 20% of EU consumption rates. The production of BPA since 2011 has grown strongly, primarily linked to the demand for polycarbonate. Cision (2016)²² estimated global production in 2015 had grown to 7.7 million tonnes, with 8 million tonnes estimated for 2016. The current study assumed that EU production and demand (including the UK) has kept pace with global developments, primarily due to the demand for polycarbonate.

This would see UK consumption rise from 220kt in 2011 to 400kt by 2020, thereafter growth is mapped to forecast GDP growth rates for the UK, which estimates that UK consumption of BPA will reach 500kt by 2025. Table 4.1 provides estimated consumption rates for the UK.

Table 4.1 UK consumption rates of BPA as thousands of tonnes per annum*

Year	2010	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025
UK consumption of BPA (kt)	210	320	330	348	366	385	400	420	440	460	480	500

* Estimates are based on data from UBA 2014, plus the global analysis news article which states demand in BPA has been and continues to increase year on year. Especially for polycarbonate in construction and automotive uses. EU level data has been extrapolated to UK levels using GDP.

Uses

BPA is predominantly used in the manufacture of polycarbonate (75% of all use), a clear tough plastic material which can be used as an alternative to glass. It further has application in paints and lacquers to provide a clear and tough barrier (UBA, 2014). The manufacture of polycarbonate is completed as a closed-loop process with very limited potential for environmental release, while polycarbonate itself is stable and inert. However, polycarbonate will contain unreacted BPA as trace residues (estimated to be around 10mg/kg) which can leach and emit during service life.

The second most significant use is in the manufacture of epoxy resins (17% of all use) which have a range of potential applications, primarily in coatings. Again, the epoxy resin itself is an inert and stable polymer with limited risk of emission. Unreacted BPA will be present as a trace residue (estimated to be around 9 mg/kg), which again can leach from the polymer matrix and emit during service life. The manufacture of epoxy resin will also generate emissions for wastewater treatment works. Based on UBA (2014) this was estimated to be around 1.69 g/tonne of BPA used in Epoxy resin manufacture.

²¹ UBA (2014) 'Identification of relevant pathways to the environment and quantification of environmental exposure for bisphenol A' Report 41/2014.

²² <https://www.prnewswire.com/news-releases/bisphenol-a--a-global-market-overview-300282092.html>

Beyond polycarbonate and epoxy resin, BPA is further used for manufacture of other polymer applications (1% of all use), and as an intermediate in the manufacture of brominated tetrabromobisphenol A (TBBP-A) (<1% of all use). It is also used as a non-polymeric application as an additive pack for soft PVC applications (<1% of all use).

Table 4.2 Full breakdown of BPA uses across all potential applications.

Use	Percentage of total BPA use	Sub-category	Percentage of Total BPA use for category	Potential for release to wastewater
Polycarbonate	75%	Construction	27%	Outdoor application. Potential diffuse emissions, also potential releases to drains (Wastewater)
		Optical media	23%	Primarily for CDs, DVDs etc. Potential for emission very low. No estimate.
		Electronics	21%	Indoor application. Likely to release to indoor air as contaminated dust.
		automotive	12%	Outdoor application. Use is largely external, expect diffuse emissions.
		Domestic appliances	5%	Indoor application. Likely to release to indoor air as contaminated dust.
		PPE	3.5%	Use is primarily for safety glasses, visors etc. possible indoor/outdoor release, but estimates challenging.
		Healthcare	2.5%	Indoor application. Likely to release to indoor air as contaminated dust.
		Bottles (excl. infant bottles)	2.5%	Indoor application. Likely to release to water from washing.
		Other	3.0%	Unknown. – Assume largely indoor contributes to dust.
		Epoxy Resin	17%	Marine
Powder coatings	18%			Indoor application: Primary use is on machinery and metals. Assume release to indoor air as contaminated dust.
electrical	16%			Indoor application. Likely to release to indoor air as contaminated dust.
Civil engineering	15%			Use in this case is internal to cements and concretes. Release unlikely. No estimate.
Can and coil coatings	11%			Indoor application. Likely to release to indoor air as contaminated dust.
Automotive coatings	9%			Outdoor application. Use is largely external, expect diffuse emissions.
composites	5%			Similar to civil engineering, composites are used internally within the composite as a construction material. Assume no release to water.

Use	Percentage of total BPA use	Sub-category	Percentage of Total BPA use for category	Potential for release to wastewater
		adhesives	4%	Similar to civil engineering, adhesives are used internally within the composite as a construction material. Assume no release to water.
		Photocure (film)	2%	Used in specialist applications for specific types of photographic film. Assume no release to water likely.
Other polymers	1%	-	-	-
PVC applications	0.2%	Plasticizers	50%	Manufacturing process – will generate waste liquids, but these will undergo waste water treatment prior to release.
		Anti-oxidant packs	25%	Manufacturing process – will generate waste liquids, but these will undergo waste water treatment prior to release.
		Additive packs	25%	Manufacturing process – will generate waste liquids, but these will undergo waste water treatment prior to release.
Other uses	<7%	-	-	-

Source-flow

Based on the analysis of uses it is possible to further disaggregate the use of BPA and potential release of BPA (primarily as free monomer residues within polymers) to the aquatic environment:

- Manufacturing.** BPA is not manufactured directly in the UK but will be used as a raw material in the production of other materials. The manufacture of polycarbonate is expected to take place within closed-loop systems with very limited potential for environmental release. The manufacture of epoxy resin will generate releases to wastewater treatment works, but no direct release of untreated BPA is expected. Similarly use within PVC manufacturing of soft PVC will generate releases to wastewater treatment works;
- In-use (outdoor applications).** Polymers based on BPA (polycarbonate and epoxy resin) will have outdoor applications. Notably within construction (glazing applications, solar panels, safety shields, front panels for advertising boards etc) and automotive (head lights, sun-roof, windows, grills, body-work, within paints and lacquers used on body work, and moulded fixtures). During use it is possible for polycarbonate and epoxy resins to generate micro-fissures in the surface material from weathering. This promotes and allows leaching of BPA from the polymer to rainwater, which will be emitted either directly to environment as a diffuse emission or drains as a release to wastewater treatment works;
- In-use (indoor applications).** Polymers based on BPA are also used for a range of indoor applications. In these cases, the release of free BPA monomer as residual to the polymer will be to indoor air and through contamination of dust. It possible for skin, clothing, and soft furnishings to be contaminated by BPA (adhered to dust), which then enters the wastewater cycle through washing and laundry. The current approach takes the worst-case scenario and assumes all releases to the indoor environment reach the wastewater system; and
- Wastewater treatment works (WWTWs).** WWTWs act as a point of release to surface water. Based on reviews of the available literature the efficacy of WWTWs against BPA (a hydrocarbon)

are relatively good. Petrie (2019)^{23,24} comments that efficacy of UK WWTWs against BPA ranges from 91 – 99%. The source flow-approach has adopted 95% as the middle of this range.

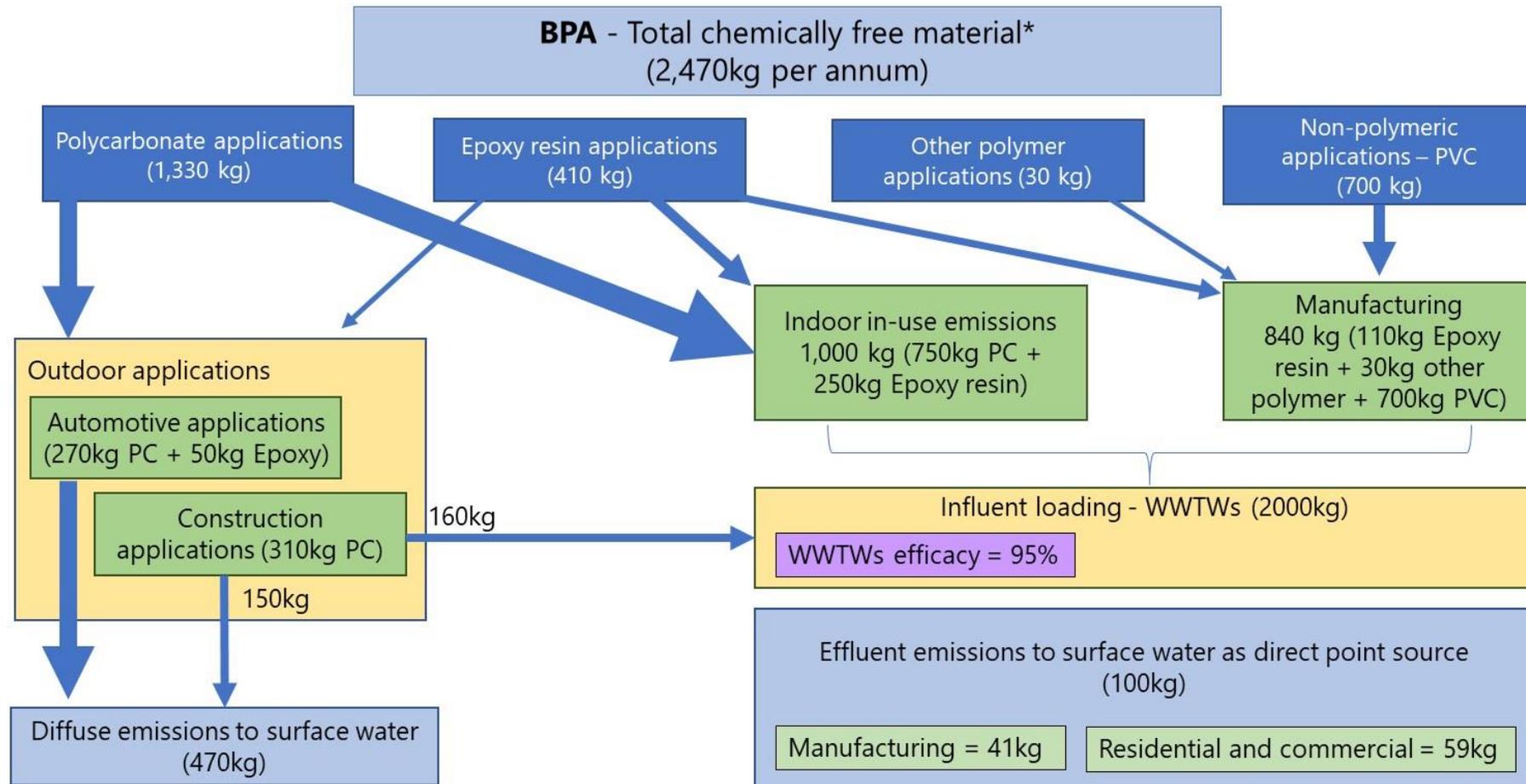
Figure 4.2 provides an indicative source-flow of material for BPA in the UK based on the bullet points above. This maps the flow of “free” BPA as either residuals of unreacted BPA in polymers or BPA used directly in PVC applications. Figure 4.2 indicates an estimate release of 100kg of BPA per annum from WWTWs, which can further be disaggregated as 41kg from manufacturing processes and 59kg from in-use domestic and commercial sources. Furthermore, the source flow also indicates 470kg of BPA released to the aquatic environment largely from automotive uses as a diffuse emission.

²³ Petrie, 2019, ‘Estimation of community-wide exposure to bisphenol A via water fingerprinting’, Environmental International vol 125, pp1-8

²⁴ Petrie et al looked at an extended list of 90 micropollutants (including BPA) from two WWTPs in South-West England with a PE of 105,000 (WWTP A) and 909,000 (WWTP B) respectively. WWTP A had a standard process of screening for grit removal, followed by primary sedimentation, trickling filters, and final sedimentation in humus tanks. WWTP B differed from WWTP A in that it also utilises biological treatment, here, sequential batch reactors (activated sludge) were used.

The approach including the development of 24hr composite samples for both influent and effluent phase, based on hourly sampling (1 litre each) using time paced and volume samplers over the course of 8 days, with samples separated into primary and duplicate batches, stored in cold dark conditions before analysis. Based on this approach 96 composite samples (including duplicates) were generated per day for the eight-day sampling window (768 samples in total). Samples were analysed using a fully validated ultra-high-performance liquid chromatography tandem mass spectrometry methodology using a Waters Acquity UPLC system in Manchester, UK.

Figure 4.2 Source-flow of BPA for UK in 2019 (arrows are weighted to give an indication of scale of contribution)



*BPA is principally used as an intermediate material for the manufacture of polymerised products such as polycarbonate, epoxy resin, polyester, and phenoplast resin. It is also used directly as BPA as an anti-oxidant, stabilizer and plasticizer in specific PVC applications. For polymeric products most of the BPA (>99%) is converted to inert polymer. However a small amount of unreacted BPA remains present within polymer applications as residual material which can be emitted to environment.

Cross-reference checks for wastewater

The estimates presented in Figure 4.2 are based on an aggregation of the different applications, which include emissions over the assumed service life of each application (i.e. Construction applications such as greenhouses have a service life of 10 years. Emission rates increase from years 2-4 as micro-fissures form, and then decrease again from years 5-10 as remaining free residuals decrease and are more difficult to release). The estimates presented for wastewater are an aggregation of approximately 20 different applications (including manufacturing).

Table 4.3 (below) provides a general overview of these emissions against polymer type for the UK. The key message here is that because the vast majority of the BPA (>99%) is converted to polymer, the actual emissions of free unreacted BPA from polymer matrices are comparatively very low against the actual usage rates, and furthermore WWTPs are expected to be highly effective against a hydrocarbon.

Table 4.3 Overview of BPA uses against estimated emissions for 2019

Polymer type	UK consumption rates in kilotonnes	Diffuse emissions to surface water (kg)	Emissions from WWTPs to surface water (kg)	Total surface water emissions (kg)
Polycarbonate	308kt (80% of all BPA use)	420kg	45kg	465kg
Epoxy Resin	66kt	52kg	18kg	70kg
Phenoplast	3kt	-	1.5kg	1.5kg
Polyester	1.2kt	No estimate	No estimate	No estimate
PVC (additive packs non-polymeric use)	0.6kt	-	38kg	38kg
Thermal paper	0.6kt	Neg	Neg	Neg
Other uses	5.6kt	No estimate	No estimate	No estimate

To provide a sense-check it is useful to compare the estimates derived against real world monitoring to assess their validity. On that basis we have used the monitoring completed by Zhang et al (2008)²⁵ on the River Ouse, Sussex as a means of checking release rates. Given the time difference (2008 vs 2019) the sense-check is intended to check for orders of magnitude rather than a close examination to exact release rates.

Zhang et al (2008) completed passive monitoring for BPA in effluent from WWTPs on the River Ouse, with concentrations ranging from 10 ng/l – 48 ng/l. The UK treats and releases approximately 4 trillion litres of effluent per annum (extrapolated from 11 billion per day²⁶). This volume of effluent divided by 100kg of BPA (as estimated from our source-flow approach above) would equate to 25 ng/l. The Petrie (2019) paper quotes UK WWTPs efficacy against BPA as 91-99%. Assuming the lower bound of removal (91%) would increase predicted concentrations in effluent to 47ng/l; while assuming the upper bound (99%) would decrease the predicted concentrations in effluent to 6 ng/l.

Therefore, based on the source-flow diagram in Figure 4.2 and cross-checking against UK monitoring would suggest average BPA releases to surface water from WWTPs of 6-47 ng/l.

²⁵ Zhang et al, 2008, 'Analysis of emerging contaminants in sewage effluent and river water: Comparison between spot and passive sampling', *Analytica Chimica Acta*, Volume 607, Issue 1, 21 January 2008, Pages 37-44

²⁶ Defra, 2002, 'Sewage treatment in the UK', Report detailing the UK implementation of the EC urban wastewater treatment directive.

4.1.4 Beta-estradiol (E2)

Overview

Beta estradiol (E2) is a naturally occurring steroid hormone produced by humans and other mammals (such as livestock) as part of the standard functioning of the hormone system. Small amounts of E2 are excreted within urine and faeces as part of natural processes, but the rates of excretion can vary significantly for a range of factors such as age, race, hormonal status (e.g. pregnant, pre-or-post menopausal), smoking/non-smoking, or as part of natural monthly hormone cycles.

For the human population, all releases of E2 will be to wastewater systems subject to further treatment and management at WWTWs. For livestock (cows, pigs, sheep, and horses) releases will be predominantly as diffuse emissions, primarily as manure/urine excreted to land²⁷.

The physical properties of E2 are also key to its fate and behaviour within wastewater systems and the natural environment. Koh et al²⁸ quotes a log K_{OW} ²⁹ 3.1 for E2 meaning that within wastewater systems significant amounts of E2 will partition into the solid phases. Koh et al further state that microbial biodegradation is a key pathway for the destruction of E2, and final treated sludge is likely to have 'very low concentrations'. Williams et al³⁰ corroborates this position by commenting that terrestrial half-life for E2 is three days, again with microbial biodegradation a key mechanism in the destruction of E2 in the environment.

Manufacture and Uses

Not considered here for E2 as the dominant pathway is from production by humans and other mammals.

Source-flow

The source-flow pathway for E2 needs to consider releases associated with humans (which will be via wastewater treatment processes) and livestock (which will be as diffuse releases directly to soil, followed by environmental attenuation processes taking place in surface water and groundwater).

To calculate the source-flow pathway for humans, data from the office of national statistics (ONS) has been used to quantify total UK population. This is further disaggregated using the work of Green et al (2013)³¹ which comments that 42% of the UK population is female and of an age where sexually mature (this includes post-menopausal women using hormone replacement therapy (HRT)).

Data from Williams et al. (2009) quantifies E2 influent loadings at WWTWs in the UK as 13.8 µg/person/per day. This means it is possible to work out total loadings for E2 at UK WWTWs, based on adjusted population size from Green et al. (2013) and loading factor from Williams et al. (2009).

The function of WWTWs includes both partitioning between liquid phases and solid phases as well as the efficacy of breakdown of E2 with biodegradation as a key pathway. Monitoring of influent and effluent concentrations by Koh et al. (2008) and UK CIP suggests that removal efficacy during wastewater treatment varies between 80-90%. The source flow diagram shown in Figure 4.3 uses the middle value of 85% removal and assumes that the fraction passed into the sludge phase is largely destroyed by biodegradation.

For diffuse input from livestock populations, data has been taken from Defra's UK agricultural holdings statistics (2019), which includes numbers of cows, sheep, and pigs are held in the UK. While data from the national equestrian survey (2019) has been used to quantify horses (total and female fraction). Schoenborn et

²⁷ EQS dossier, 2011, 'beta-estradiol (E2)', EQS dossier developed for the European Commission as part of assessment for EQS development.

²⁸ Koh et al, 2008, 'Treatment and removal strategies for estrogens from wastewater', Environmental Technology, 29:3 pp245-267

²⁹ Octanol/water partition coefficient - The ratio of the concentration of a solute between water and octanol is a well-known property that is commonly used as a measure of hydrophobicity.

³⁰ Williams et al, 2009, 'A national risk assessment for intersex in fish arising from steroid estrogens'. Environmental Toxicology and Chemistry: An International Journal, 28(1), pp.220-230.

³¹ Green et al, 2013, 'Modelling of steroid estrogen contamination in UK and South Australian rivers predicts modest increases in concentrations in the future'. Environmental Science & Technology, 47 (13). 7224-7232

al³² (2015) provides data on loadings to land (primarily from manure) for livestock. Table 4.4 provides an overview of these key values, and humans as a cross-comparison.

Table 4.4 Agricultural loadings of E2 for UK livestock

Livestock	UK female population (2018) (millions)	E2 loading to land (mg/per individual/per year)	Estimated total loading to land (kg)
Cattle	7.03	110	773.30kg
Sheep	14.08	8.4	118.20kg
Pigs	0.50	43	21.50kg
Horses	0.353	110 (assume same as cows)	38.83kg
Total emission			952kg

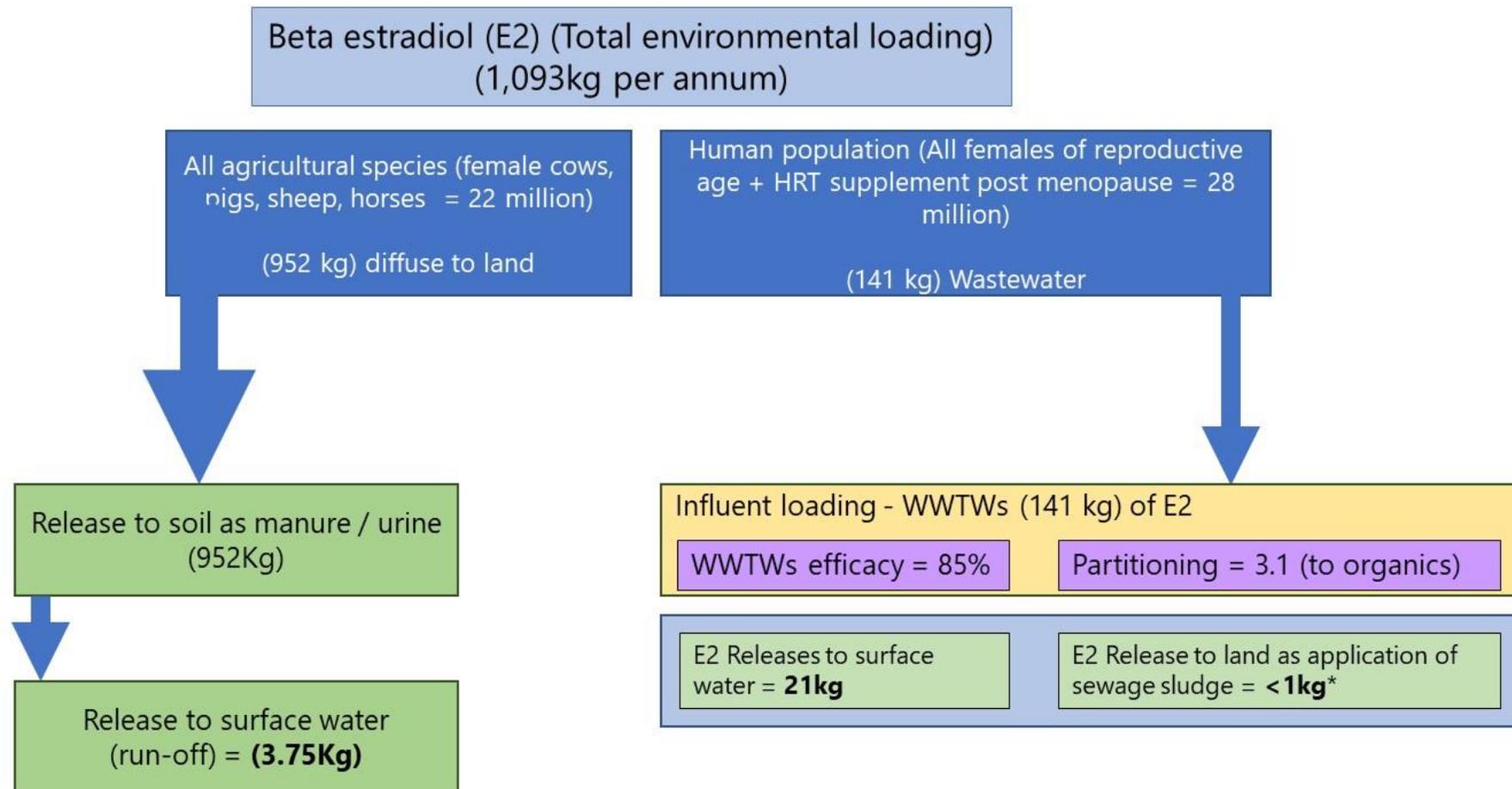
Both Schoenborn et al. (2015) and Williams et al. (2009) comment on the hydrophobic nature of E2 which is likely to remain in the surface layers of soil following release and be subject to biodegradation pathways. Egress to water is however likely in the form of run-off. Williams et al. (2009) estimate that the diffuse emissions of E2 from agricultural processes are likely to make up 15% of total E2 emissions to surface water, with WWTPs the major contributor (85% of all releases). This has been reflected in the source flow pathway in Figure 4.3.

As a further explanation of how the estimates for human emissions have been calculated in Figure 4.3 the following steps were used.

- ONS UK population in 2019 = 66.8 million;
- Green et al (2013) estimates 42% of the population is female and sexually mature (including HRT for post-menopausal) = 66.8 million x 42% = 28 million;
- Williams et al (2009) estimates loadings to WWTPs (influent) is 13.8 µg /per person/per day;
- Influent loading = 28 million x 13.8µg x 365 days = 141,036,000,000 µg of E2 (equivalent to 141 kg);
- Koh et al (2008) estimates WWTP efficacy at between 80-90%, assume medium value of 85%;
- Total quantity of E2 destroyed by WWTPs = 141kg x 0.85 = 120kg; and
- Effluent emission from WWTPs = 141kg – 120kg = 21kg (note that the calculations assume that any partitioning of E2 to sewage sludge is destroyed as part of the overall efficacy of the works).

³² Schoenborn et al (2015) 'estrogenic activity in drainage water: a field study on a swiss cattle pasture', Environmental sciences Europe vol 27.

Figure 4.3 Source-flow of E2 for UK in 2019 (arrows are weighted to give an indication of scale of contribution)



Cross-reference checks for wastewater

To help put the releases from Figure 4.3 into context the release data for WWTWs has been converted into a concentration of treated effluent. This follows the same approach used for BPA where the assumed annual releases of treated effluent from UK WWTWs equates to 4 trillion litres per annum. This would equate to average of 5.25 ng/l of E2 released to surface water from UK WWTWs. Our effluent loading estimate is higher than those reported in the literature and from the UK CIP, which typically range from 0.4 to 1.6 ng/l but we suspect this is due to the high influent loading factor used in our calculations.

The releases from agriculture are more complex as flow is more variable and subject to weather conditions. Williams et al (2009) comments that based on monitoring of field drains E2 concentrations were typically below 1 ng/l (noting that this is the same as the proposed drinking water limit $0.001\mu\text{g/l} = 1 \text{ ng/l}$). Scoenborn et al (2015) concurs with this assessment based on further monitoring studies of field drains, but also adds a word of caution. Based on manure spreading and grazing, concentrations of E2 were at their highest following storm events with increased run-off, where concentrations often exceed 10 ng/l. Furthermore, even a month after manure spreading/grazing elevated concentrations were seen after heavy rain with Scoenborn et al (2015) commenting that persistence in natural soils was considerably longer than laboratory conditions. This could pose an issue where grazing land sits adjacent to rivers, and the potential of run-off to river is increased for E2 during rain events.

4.1.5 Nonyl Phenol

Overview

Nonyl Phenol (NP) (CAS 25154-52-3) is a compound which has only been used as an intermediate in the manufacture of other chemical compounds, primarily Nonyl Phenol Ethoxylate (NPE) (60% of all use), and secondarily within resins and polymers³³. While the UK has manufactured NP in the past (see the next section on uses), all manufacture and use of NP in the UK has now ceased³⁴. Furthermore, the regulatory controls on both NP and NPE (as a precursor to NP) have tightened significantly in the last 20 years, leading to a very significant decline in the overall total use across the UK and Europe.

In conducting the research for this task one further consideration to include is that in many cases NP and NPE are reported together as total combined quantities. Conversely the Environmental Quality Standards Directive (2013/39/EU)³⁵ sets thresholds for only NP (assumed to include the isomers), and the proposed standard for Drinking Water (used in this assessment) refers only to nonylphenol. An approach has been adopted to use data on the combined total of NP and NPE, with further calculations and review for the generation of NP at wastewater treatment works. Further consideration has also been included for diffuse releases of NP primarily as breakdown products of NPE.

Given the significant changes to the regulatory landscape for NP and NPE since the early 1990s, to help capture the full and complete picture for the source-flow of NP within the UK we have adopted the following approach:

- Development of an amended use and source profile for NP and NPE based on all live uses as of 1991. While many of these uses are no longer relevant for the UK (and some never were), it is possible that former manufacture and use provides important clues for legacy issues which may present potential issues for the current picture;

³³ WHO, 2004, 'Integrated risk assessment: Nonylphenol', Report prepared for the ILO International Programme on Chemical Safety

³⁴ Note that based on the REACH registrations the related species 4-nonyl phenol (branched) (CAS 284-325-5) is still manufactured/imported into the UK by six UK based REACH registrants.

³⁵ Entry 24 of the EQSD (2013/39/EU) sets thresholds for Nonyl Phenol (CAS 25154-52-3), commenting that 'nonylphenols' more generally includes CAS 25154-52-3 plus the isomers 4-nonylphenol (CAS 104-40-5) and 4-nonylphenol (branched) (CAS 84852-15-3).

- Use of reported emissions data from the UK Pollutant Release and Transfer Register (PRTR) and England and Wales Pollution Inventory³⁶. The PRTR includes important information of categories of different emitters to surface water and a timeseries from 2007-2017. The pollution inventory further includes important information on below reporting threshold sites (particularly landfills);
- Regulatory review. A review of the regulatory landscape has been completed and cross-compared to the data held by the PRTR and additional literature information sources that predate 2007. This allows some further insight to the emission trends and clues as to potential undocumented sources, especially for the diffuse emissions; and
- Review of the chemical investigation programme monitoring data for NP. This has allowed cross-checking against the source-flow approach. Importantly it has also been used to assess and validate the identified theories for regional variation of concentrations of NP within England and Wales.

Manufacture and Uses

RPA (1999)³⁷ comments that as of 1997 there were four companies within Europe manufacturing NP, with a combined production rate of 77,500 tonnes. SOCOPSE (2009)³⁸ provides an update to this position and comments subsequent to the RPA study a fifth EU manufacturer was identified, however, by 2006 only three manufacturers remained (Sasol in Germany, Polimeri in Italy, and Synteza in Poland). WRc (1997)³⁹ helps complete the picture by commenting that the two remaining manufacturers were Akzo Nobel in Sweden and ICI in the United Kingdom. Both Akzo Nobel and ICI had ceased manufacture of NP by 2006 if not before.

The WRc (1997) report further comments that NP was manufactured at ICI's Teesside plant for the sole purpose of producing NPE. All of the NP manufactured was used on site and not exported to any other location within the UK or external to the UK. While manufacture ceased prior to 2006 it is possible that this location may represent a hotspot risk for legacy groundwater contamination.

No data for production rates of the individual companies has been identified, although the WRc report suggests the plant in Sweden may have been a smaller site. Assuming the Swedish plant produced less than 10,000 tonnes per annum and disaggregating the remainder equally amongst the other four plants would suggest at its peak the ICI plant in Teesside was producing between 15,000 and 20,000 tonnes of NP per annum.

Data on manufacturers of NPE is more limited. The SOCOPSE (2009) study estimated EU production of around 80,000 tonnes of NP and 120,000 tonnes of NPE per annum in 1997. Best estimates based on expert judgement would suggest 6-12 manufacturers of NPE across Europe (assuming 10-20kt per plant), we have identified two within the UK (the previously noted ICI plant in Teesside and a second plant near Southampton which is not named). Based on the tightening regulatory landscape manufacture of NPE within the UK is expected to have now ceased. Note, that based on the PRTR reporting data use of NPE is still ongoing at a small number of sites.

Based on the SOCOPSE (2009) inventory a table of uses has been amended from the SOCOPSE report to assess UK relevance based on data held within the PRTR, the SOCOPSE report itself and regulatory changes implemented in the UK and Europe since 1991. Table 4.5 presents this information.

³⁶ Note that the PRTR applies a reporting threshold for WWTPs of 100,000 population equivalents, with voluntary reporting below this level.

³⁷ RPA, 1999, 'Nonylphenol risk reduction strategy', Report for the UK Department of Environment, Transport and Regions.

³⁸ SOCOPSE, 2009, 'An inventory and assessment of options for reducing emissions: nonylphenol', report part of the Source Control of Priority Substances in Europe.

³⁹ WRc, 1997, 'Proposed EQS for NP in water', report for the Environment Agency.

Table 4.5 Overview of use and source profile for EU with comment on UK relevance (1997)⁴⁰

Nonyl Phenol	Quantities and proportion	UK relevance
Production of NP	73,500 tonnes (EU further imported 5,000 tonnes per annum. Total EU consumption was 78,500 tonnes)	In total five companies manufactured NP across Europe. This includes one site in the UK at Teesside. However, manufacture ceased by 2006 at the latest. Possible relevance for groundwater, but no longer relevant for emissions. Note SOCOPSE (2009) comments wastewater emissions from NP manufacture were already very low initially.
Production of NPE	47,000 tonnes (60%)	Estimate 6 – 12 manufacturers across Europe in 1997. Two of these were in the UK (including the Teesside plant). Manufacture expected to have ceased some time ago. Emissions from manufacture of NPE likely to be less relevant for UK.
Phenol/Formaldehyde resin production	22,500 tonnes (29%)	Unclear if this use ever happened in the UK, but likely. Would expect no current NP use for this application. – possible source for in-use legacy products containing these resins.
TNPP Production	3,900 tonnes (5%)	Same comment as above.
Phenolic oxime production	2,300 tonnes (3%)	Same comment as above.
Epoxy resin manufacture	1,600 tonnes (2%)	Same comment as above
Plastic stabiliser manufacture	785 tonnes (1%)	Same comment as above.
Nonyl Phenol Ethoxylate	Quantities and proportion	UK relevance
Cleaning products	36,000 tonnes (30%)	The UK voluntarily ceased all use of NPE in domestic cleaning products as of 1976, and industrial and institutional products as of 1996. The SOCOPSE report identifies cleaning products, textiles and agrichemicals as the key emitters to environment. Where UK ceased this use many years ago it is unlikely to be relevant source for UK now.
Manufacture of polymers	14,400 tonnes (12%)	Unclear specifically how active the UK were on this source but would have been ongoing. Expect with the negative pressure applied on NP and NPE industry would have transitioned away by now. PRTR identifies one plant manufacturing rubber-based materials still emitting NP to controlled waters. The pollution inventory identifies one further plastics manufacturer with emissions below reporting threshold (1kg).
Use in textile finishing	12,000 tonnes (10%)	Would have been highly relevant for the UK, particularly linked to wool and yarn production. Expect Yorkshire to be important regionally. Possibly also East Anglia, West Country, and parts of Wales. No current use of NPE expected based on regulatory control.
Leather	9,600 tonnes (8%)	Would also be relevant for the UK, however the leather finishing industry has been in decline since the mid-1990s due to competition in Europe

⁴⁰ Note a clarification, 4-nonylphenol, branched (CAS 84852-15-3) is registered at the 10,000 – 100,000 tonnes per annum bracket for Europe, with six UK manufacturers/importers (out of 36 registrants in total) (Baker Hughes, DuPont, John Hogg Technical Solutions, Lubrizol, Nalco, and SI Group UK). Use is defined as an intermediate in the production of polymers, within paints, adhesives, plastics, rubber, and fuel additives.

Nonyl Phenol	Quantities and proportion	UK relevance
		and further aboard, would expect this would have some importance, again East Anglia and West Country likely to be key. No current use of NPE expected based on regulatory control.
Agricultural uses	7,200 tonnes (6%)	Would have had some application in seed treatments, but unclear how prevalent and use should have ceased under regulatory control by 2003.
Paints (surfactant)	6,000 tonnes (5%)	This would have likely been specialist applications based on the surfactant properties of NPE. Unlikely to be widely used by domestic population for residential use. Use would have ceased on or before 2003.
Metallurgy (surfactant)	3,600 tonnes (3%)	This is one of the few remaining permitted uses for NPE, no reported emissions for UK within PRTR. Unclear if it is an issue, but unlikely.
Paper and pulp (process aid)	1,200 tonnes (1%)	This use was banned in 2003, however, based on the PRTR data there is one plant still reporting emissions (legacy contamination?). The pollution inventory further identifies a small number (<5) of additional plants, all below the 1kg per annum reporting threshold. Assume there may be a legacy contamination issue for a small number of sites with ongoing very low emissions to controlled waters.
Other niche uses	30,000 tonnes (25%)	Based on PRTR and pollution inventory data we have identified the following possible industry categories: <ul style="list-style-type: none"> • One oil refinery site; • One pharmaceutical site. (below reporting threshold); • One surface active chemical manufacturer (below reporting threshold); and • Three speciality industrial alcohol manufacturers (all below reporting threshold).

The current approach has also included a review of the changing regulatory landscape for NP and NPE, which includes the following chronology:

- 1976. UK industry voluntarily agrees to withdraw NPE from all domestic cleaning products;
- 1996. The UK industry association for cleaning specialities (BACS) and soap and detergent industry association (SDIA) voluntarily agree to withdraw NPE from all industrial and institutional cleaning applications by no later than 1998;
- 2000. EU sets draft limit for NP in sewage sludge of 50 mg/kg;
- 2002. Use of NPE within plant protection products (EU 2076/2002) bans the use of NPE within all pesticide products for EU (including UK by 2004);
- 2002. UK Chemicals Stakeholder Forum voluntarily agreed to accelerate the removal of NPE as surfactant from a range of products and make available information on use restrictions;
- 2003. Under EU Directive 2003/53/EC the use of NP and NPE was limited to a maximum of 0.1% w/w in:
 - ▶ Co-formulant pesticides and biocides, and agricultural seed treatments;
 - ▶ Domestic cleaning products and personal care products;
 - ▶ Industrial and institutional cleaning products;
 - ▶ Textiles and leather processing;

- ▶ Metal working (unless closed systems); and
- ▶ Manufacture of paper and pulp.
- 2008. Creation of the EQS Directive (2008/105/EC). NP added as one of the 33 priority substances within the EQSD and assigned critical thresholds;
- 2016. REACH restriction (entry 46). NP and NPE not to be placed on the market above 0.1% w/w (incorporates the 2003 EC Directive into REACH);
- 2016. The REACH restriction for NP and NPE was further amended specifically for textile applications to set a lower threshold limit of 0.01% w/w. Importantly this new amendment goes beyond the 2003 ban which covered only manufacture of textiles within the EU. The 2016 ban includes import of treated textiles as well. The ban includes a five-year transition period. This means after 3 February 2021 any imported textiles into the EU must be compliant with the 0.01% w/w threshold. Under the grand-fathering arrangement for Brexit, the same position should apply for the UK; and
- 2018. Draft thresholds for BPA, E2 and NP proposed under the drinking water directive.

Amec (2013)⁴¹ highlight the potential impact on manufacture and use of NP and NPE at European level from the transition as the regulatory landscape became tighter:

- 1997 – EU consumption of NP 78,500 tonnes; and NPE 120,000 tonnes; and
- 2010 – EU consumption of NP 10,000 -50,000 tonnes; and NPE 32,000 tonnes.

This recognises that post-2010 the landscape has continued to further target reductions in emissions of NP and NPE to water. One issue identified by RAC (2012)⁴² was that while the 2003 ban on NP and NPE targeted EU production, the use of NPE for textiles in particular for other parts of the world continued or even increased in use. The England and Wales Environment Agency commented that they estimated 20% of all NPE emissions to surface water came from imported textiles. In particular it was recognised that NPE residues in clothing are washed out within the first few washes to wastewater treatment plants. The 2016 amendment to the REACH restriction specifically targets this application.

Chokwe et al (2017)⁴³ comments that as recent as October 2017 textiles from outside the EU still contain significant quantities of NPE, and highlights the challenge posed by the very low 0.01% w/w threshold. This may suggest that phase-out of NPE from imported textiles is still ongoing and that the February 2021 deadline is likely to be challenging.

Source-flow

Alongside the work detailed in the preceding sections, the current approach has also assessed the reported emission data to surface water for PRTR. Figure 4.4 provides details for total emission of NP and NPE combined to surface water from 2007-2017.

For all reporting years of the PRTR the emissions are dominated by wastewater treatment works which make up >90% of all emissions. Figure 4.4 also shows a significant decline in the quantity of emissions after 2008 (creation of the EQSD) with a fall from approximately 80 tonnes to 20 tonnes per annum, although in the more recent time-series (2013 onwards) emission rates are estimated to be broadly static in the PRTR.

For the most recent reporting year (2017) the PRTR estimates a release to surface water of NP and NPE (combined) is 14.7 tonnes based on the aggregated total of 143 facilities in the UK. This includes four

⁴¹ Amec, 2013, 'Estimating the abatement costs of hazardous chemicals – a review of the results of six case studies', Report for the European Chemicals Agency.

⁴² RAC, 2012, 'Annex XVII restriction dossier under REACH', rapporteur England and Wales Environment Agency.

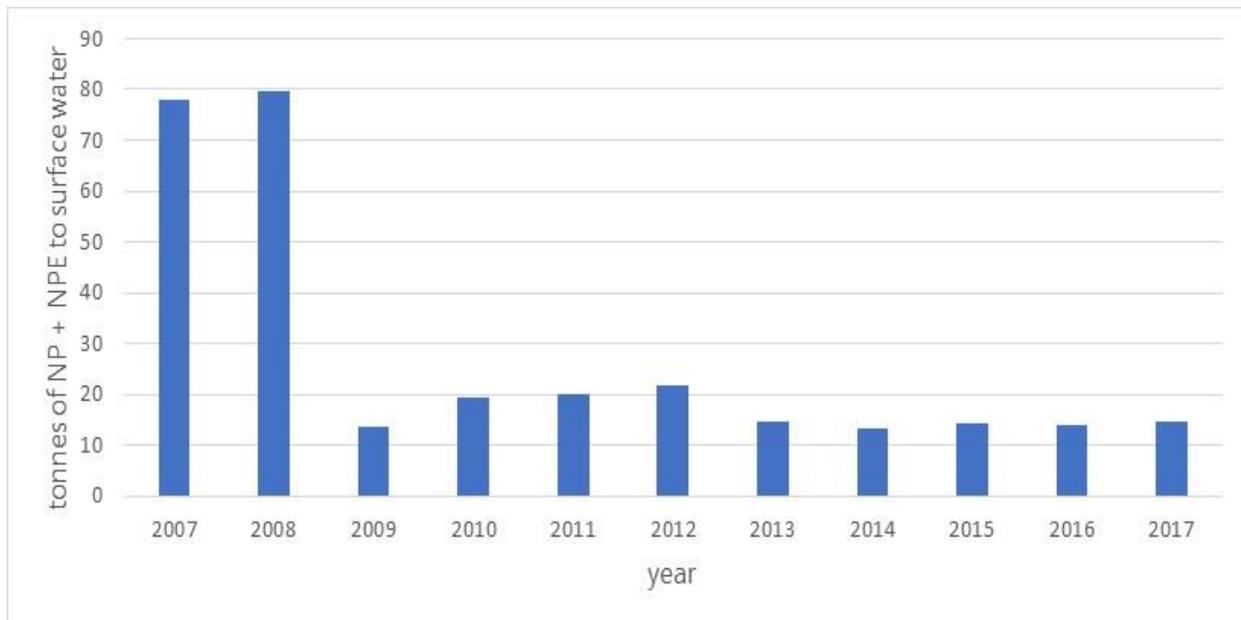
⁴³ Chokwe et al, 2017, 'Distribution, exposure pathways, sources and toxicity of nonylphenol and nonylphenol ethoxylates in the environment', Water SA Vol 43. No4

industrial facilities and 139 wastewater treatment works, with the single largest release coming from Beckton sewage treatment works (1.1 tonnes). However, these estimates conflict with the monitoring data compiled under UK CIP. Based on the CIP data for monitoring of treated effluent at UK WWTPs a UK average concentration of 0.147µg/l NP is derived. Assuming that the UK treats 4 trillion litres of wastewater annually, would estimate total UK arisings of NP released to surface water from UK WWTPs as 590kg.

As part of the requirements of the PRTR reporting facilities are further required to provide information on how their estimates were derived. An analysis of WWTPs within the UK PRTR notes that for nonyl phenol in all cases the estimates are based on calculations rather than monitoring. This might suggest that older emission factors are in use (again reflecting upon the fact that monitoring has shown a steep decline in concentrations over the last twenty years).

Therefore, the authors believe that the PRTR may be a useful reference point in terms of key emission sources, but for the source flow model, it is more appropriate to utilise the data reported by CIP monitoring of WWTPs.

Figure 4.4 Overview of PRTR data (total UK emissions)



Further review for WWTPs has been completed to assess partitioning and efficacy. NP and NPE are both largely hydrophobic⁴⁴ with partitioning to sewage sludge an important pathway for removal of NP and NPE. Bouki et al (2010)⁴⁵ comments on studies to assess the partitioning within urban wastewater conditions, this indicated that about 90% of NP was removed from the water phase into biosolids within the first hour. After equilibration (some NP is emitted from biosolids back into effluent), the concentration of NP in biosolids was still two orders of magnitude greater than in the water phase. The REACH registration dossier for 4-NP (branched) (CAS 84852-15-3) provides log K_d (distribution coefficients) values for both linear NP (CAS 25154-52-3) and the branched form. For NP the log K_d values range from 1.4 to 3.0. These values can be used to aid partitioning. As an example:

Loading at the WWTP (influent) = 1000kg, log k_d of NP is 3.0 = 1000Kg / 3.0 k_d = 333kg in liquid phase and 667kg in biosolids phase.

⁴⁴ Log K_{OW} values for NP and NPE are 4.5 and 4.2 respectively.

⁴⁵ Bouki et al, 2010, 'Adsorption of nonylphenol on activated sludge biomass under aseptic conditions', Clean soil air water

For the liquid phase the efficacy of WWTWs removal rates are assumed to be around 80% (assumed average efficacy based on review of available literature; Table 4.6). Additionally, the breakdown of NPE within WWTWs will also form NP. Estimates for conversion of NPE to NP ranging from 2.5% - 4% of total NPE loading at the inlet to WWTWs⁴⁶.

Table 4.6 Estimated efficacy of wastewater treatment works for NP and NPE

Efficacy of WWTWs against NP/NPE	Reference	Comments
37 – 77%	Birkett, J. Endocrine Disrupters in Wastewater and Sludge Treatment Processes; CRC: Boston, MA, USA, 2003; pp. 35–58.	Based on sampling in USA.
55 – 89%	Gao et al, 2014, Removal of surfactants and nonylphenol ethoxylates from municipal sewage-comparison of an A/O process and biological aerated filters', Chemosphere vol 97 pp130-134	Based on sampling in China.
85-99%	Ho and Watanabe, 2017,' Distribution and Removal of Nonylphenol Ethoxylates and Nonylphenol from Textile Wastewater—A Comparison of a Cotton and a Synthetic Fiber Factory in Vietnam', Water vol 9 pp386	Based on sampling of WWTWs in region densely populated with textile treatment in Vietnam
97-99%	Klecka et al, 2010, 'Occurrence of Nonylphenol Ethoxylates and Their Metabolites in Municipal Wastewater Treatment Plants and Receiving Waters', Water Environment Research Vol. 82, No. 5 (May 2010), pp. 447-454	Based on sampling at three municipal wastewater treatment works.
82 – 93% (NP) 6 – 82% (NPE)	Derco et al, 2017, 'Removal of Alkylphenols from Industrial and Municipal Wastewater', Chem. Biochem. Eng. Q., 31 (2) 173–178 (2017)	Based on sampling at industrial wastewater treatment works in the USA.

For sewage sludge Table 4.6 provides a range of emission factor values for NP within finalised sewage sludge from WWTWs as dry weight. This illustrates again the impact on concentrations from the regulatory control of NP and NPE with a reduction of more than 90% over the space of 10 years. It can be expected that post-1997 with further controls that concentrations would continue to fall at a similarly dramatic rate. The more recent 2012 data from Ankara, Turkey suggests working concentrations of 1-2.5 mg/kg of sludge. For the source-flow diagram we have assumed a working concentration of 1 mg/kg which has been applied to national statistics for sewage sludge disposal.⁴⁷ This would therefore assume 1.9 tonnes of NP is disposed of onto agricultural land annually (assuming a 100% disposal rate to land).

Table 4.7 Emission factor values for NP within sewage sludge

Country	year	NP concentration in sewage sludge as dry weight	Percentage reduction
Germany*	1989	264 mg/kg	
	1997	10 mg/kg	96%
Switzerland*	1984	1010 mg/kg	
	1997	90 mg/kg	91%
Turkey**	2012	1.0 – 2.5 mg/kg	

⁴⁶ Environment Agency, 2013, 'Nonylphenol ethoxylates (NPE) in imported textiles.', Report.

⁴⁷ <http://www.defra.gov.uk/environment/statistics/waste/wrsewage.htm>

United Kingdom*	1991	823 mg/kg	
	1997	82 mg/kg (extrapolated)	91%
	2012	1 mg/kg (assumed to match lower limit of Turkey ref)	98%

*ref Chokwe et al (2017) ** ref Murdocj et al (2015) 'seasonal monitoring of NP compounds in sewage sludge', proceedings of env sci and tech Rhodes, Greece conference.

To help develop the source-flow model shown in Figure 4.5 we have used a series of back-calculations to derive the total NP loading into the system and have further apportioned this based on the known sources, which included use of both the England and Wales pollution inventory and the PRTR. These calculations work as follows:

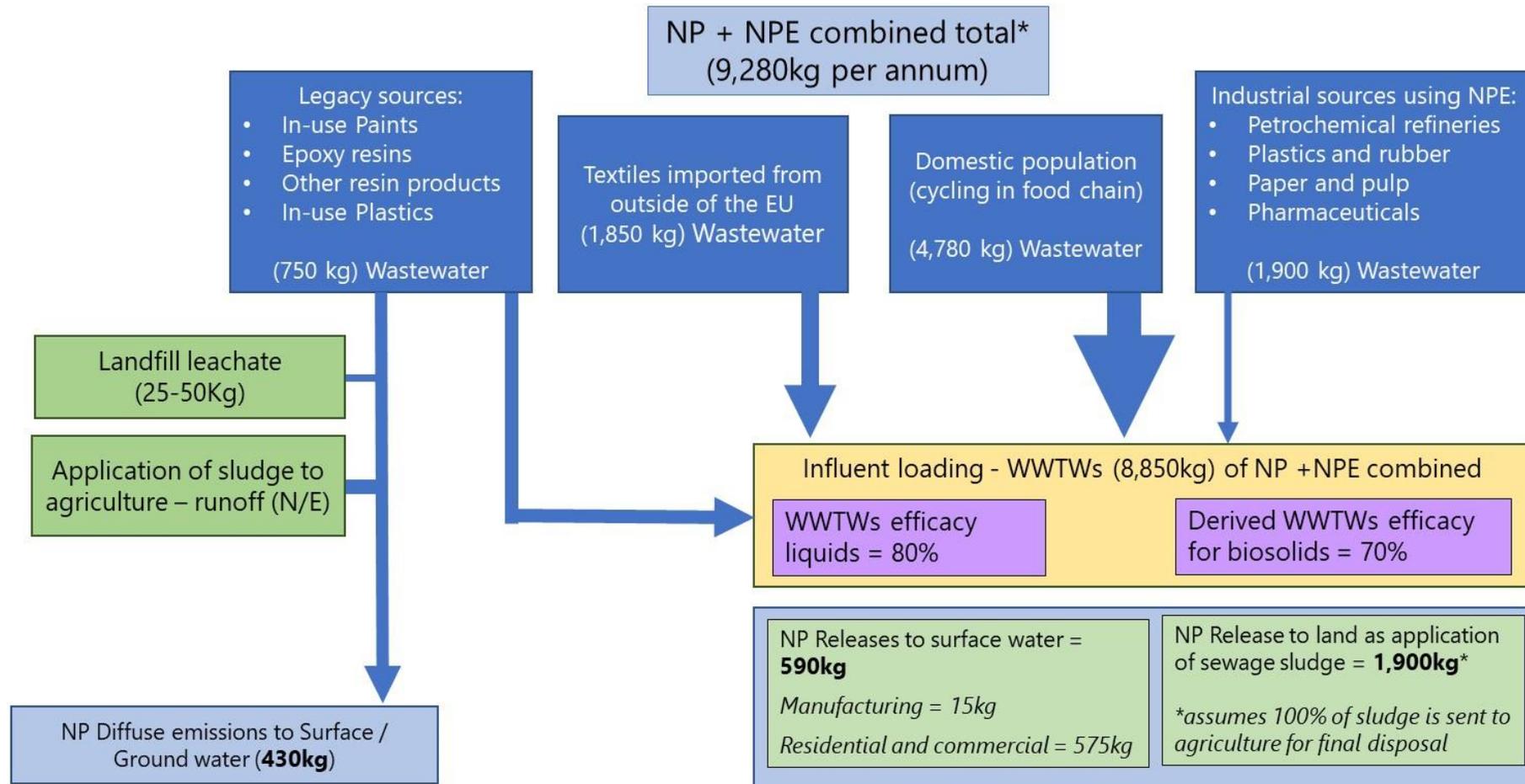
Releases to surface water are assumed to be 590kg based on the derived average concentration from UK CIP data and assumed process rate of 4 trillion litres of wastewater annually. The average efficacy of the works is assumed to be 80% based on the literature values. This means the loading in the liquid phase pre-treatment is 2,950 kg (i.e. $590\text{kg} / 20 * 100$). Based on a maximum log Kd of 3.0, total loading into the WWTPs pre-treatment is 8,850kg (i.e. Based on the log Kd, two thirds of all NP/NPE partitions into the biosolids).

The emission of NP in sewage sludge (which is assumed applied to agricultural land) was derived based on the literature emission factors assuming 1mg/kg and UK sewage sludge generation rates, which equates to 1,900 kg per annum.

Based on derived total input to WWTPs and partitioning (via log Kd). The total loading into biosolids pre-treatment is calculated to be 5,900kg with 1,900kg in the final treated sludge. This gives a derived efficacy of 70% for WWTPs on the biosolids.

The top-level figures have been apportioned in the following way. For industrial sources (top right box in Figure 4.5) data from the pollution inventory of England and Wales has been used including the 80% uplift to account for the efficacy of WWTWs, which provides an estimate of pre-treatment loading of 1,900kg of NP/NPE. Further to this the EA report estimated that 20% of all NP/NPE emissions came from imported textiles. This has been used to derive pre-treatment loadings of 1,850kg per annum. For the legacy sources and diffuse emissions a combination of pollution inventory data (primarily landfill leachate) and literature review has been used to develop an estimate of loadings equivalent to 750kg, this includes in-use resins within pipes and therefore a proportion of these releases actually go to wastewater treatment works as well. The remaining quantity of loadings pre-treatment (4,780kg) is assumed to come from the general population as cycling in the food chain. Figure 4.5 provides the full details of the material flow.

Figure 4.5 Source-flow for Nonyl Phenol



*Nonylphenol (NP) is wholly used as an intermediate in the manufacture of other compounds (including polymers and resins). The most significant use of NP (60% of all use) is in the manufacture of nonylphenol ethoxylates (NPE), which have a range of different applications. Additionally, during wastewater treatment processes and in the natural environment NPE can degrade to form NP. Where these substances are closely linked, data is often presented as the combined amount of NP +NPE. For this flow diagram NP+NPE are presented as the combined amount unless where stated.

The key overall message to understand from Figure 4.5 is that while the majority of commercial use for NPE has ceased, and while the import of treated textiles (assumed to be 20%) is duly noted, a significant proportion (70%) of all combined NP and NPE loadings to WWTWs is unaccounted for. Based on all of the preceding work and narrative, the best conclusion is that the largest fraction of NPE loadings to WWTWs come from cycling of NPE in the food chain, with the final disposal of sewage sludge to agricultural land a key mechanism in that cycling.

Pistocchi et al (2019)⁴⁸ report on a study by the EU's joint research centre to collate a bank of data from across the UK on the 33 priority substances. This includes monitoring and modelled data, as well calculations to interrogate the data held by PRTR to calculate the ratio of point vs diffuse sources. For NP the ratio was 58:42 in favour of point sources. This value has been used to calculate the diffuse releases annually based on the point source releases. Assuming 50kg from landfill leachate and 380kg from other sources. However, also note the caveat that the PRTR data (for the UK at least) looked significantly overstated when compared to the CIP monitoring data. Therefore, the diffuse estimates within Figure 4.5 should be treated with caution and assume a possible over-estimate. As a further comment on possible sources for these diffuse emissions include leachate from landfills (estimate based on England and Wales pollution inventory), runoff from agricultural land for sewage sludge and legacy emissions from polymers and resins.

Cross-reference checks for wastewater

As with the BPA source-flow reporting it is important to conduct some validation checks to help sense-check the estimates provided within the source-flow diagram. The comparison between reporting releases from WWTWs under the PRTR and monitoring data from the second Chemical Investigation Programme (CIP2) at WWTWs shows a very significant disparity. Based on data from Defra, the UK releases 4 trillion litres of wastewater back to surface waters annually, while the CIP2 data for NP provided an average concentration of NP in treated effluent of 0.147 µg/l, leading to an estimated load of 590kg per annum. Conversely the PRTR data estimates an emission of 14,000kg annually aggregated from 134 facilities. One key caveat is that the methodology for deriving emission estimates by facilities in the PRTR suggests that estimates are based on calculations rather than monitoring. This is reason why the current study has given preference to the CIP data.

The secondary issue is that the analysis completed has highlighted the importance of textiles as a source of NP with possible regional differences. In particular Yorkshire, East Anglia, the West Country, and parts of Wales may be important based on links to wool and leather finishing. To test this theory the CIP2 data has been further analysed to assess whether upstream concentrations in those areas are significantly higher than the UK background average.

To further analyse the CIP data, monitoring results for treated effluent and upstream concentrations were used. A mean average was derived and all concentrations for treated effluent and upstream concentrations fifty percent or more above the mean identified. These were then mapped geographically to look at trends in release data. For treated effluent concentrations (at or above fifty percent of the mean value CIP data) two key regions were identified. Firstly, around Greater London with a band stretching west-ward along the Thames valley as far north as Oxford and as far west as Swindon. The second key geography was in the north west spanning the territory around and between Liverpool and Manchester. A limited number of other sites were identified at single locations in East Anglia, Lancashire, and around Nottingham.

For upstream concentrations (at or above fifty of the mean of CIP data) assumed to represent background concentrations, again two key geographies are identified. Firstly, in the territory surrounding and between Liverpool and Manchester, and secondly a band beginning around Bristol and stretching south-west over

⁴⁸ Pistocchi et al (2019) 'River pollution by priority chemical substances under the water framework directive: A provisional pan-European assessment', Science of the total environment 662 pp434-445

Somerset, Dorset and Devon (as far as Exeter). A number of single sites also occur in locations in Durham, parts of Greater London (especially Essex) and around Nottingham.

The analysis of the CIP data against the expected regions dominated by textiles industry shows no or little correlation, which warrants further investigation. One key point is that for the CIP data where this is driven by water company input it is possible some water companies may have provided more sites than others which could skew the geographic trends depending on whether some companies are more active than others.

5. Task 3: Estimation of EDC concentrations and compliance

Objectives:	<p>Identification of areas or catchments at high risk of non-compliance, separately for 17-βestradiol, Nonylphenol and Bisphenol A</p> <p>Calculate likely concentrations and risk of non-compliance of 17-βestradiol, Nonylphenol and Bisphenol A (from estimated source water concentration and removal efficiency of DW treatment)</p>
Task Leader:	CEH and Wood

5.1 Task 3a - Surface water modelling component

Task 3 requires the estimation of likely concentrations of each of the three EDCs in both source and treated water, including consideration of surface and groundwater.

The estimation of surface water concentrations of E2, NP and BPA across England and Wales, is generated using the LF2000-WQX model which has been developed by UKCEH. This model holds data on the hydrology of England and Wales (spatial distribution of flow in catchments) and the location, type, human population, and flow associated with most UK wastewater treatment works (WWTWs) (Williams et al. 2009).

The estimation of EDCs concentration and compliance in drinking water from surface water abstractions has been completed through a series of stages detailed below:

- Data collection and input;
- Prediction of potential environmental concentrations;
- Risk classification based on environmental standards; and
- Prediction of concentration estimates at surface water abstraction points.

5.2 Approach

5.2.1 Data collection and input

To model estimates of E2, NP and BPA, data is required to quantify concentrations of these in WwTW influent or final effluent. Thus, estimated concentrations for WWTWs across England and Wales have been based, as far as possible, on measured data from the Chemical Investigations Programme Phase II (CIP2) database and on findings from Tasks 1 and 2. Within CIP2, a total of 74 substances were sampled across over 600 WwTWs between 2015 and 2020.

As an initial step, measured data from the CIP2 database has been investigated. This database, provided by Wood, contains measured data for a variety of substances in wastewaters (final effluent) and freshwater locations upstream and downstream of selected sewage treatment works. The CIP2 database provides information about sampling locations, concentrations and dates and it contains data relevant to individual sampling events as well as summary statistics (number of samples, mean, standard deviation, minimum and maximum value) for each sampled location. However, the CIP2 data provided did not contain any flow measurements at any of the sampling points for any of the concentration measurements. Thus, chemical

loads could not be estimated, instead surrogate data had to be used to estimate a possible relationship between WwTWs properties and chemical concentrations.

The information required to characterise each WwTW, such as population served, dry weather flow (average daily flow to a WwTWs during a period without rain) or type of treatment applied, has been extracted from LF2000-WQX.

All the available measured data for E2, NP and BPA from the CIP2 dataset has been extracted and further analysed. As the CIP2 data does not cover all WwTW across England and Wales, the data has been investigated to establish possible correlations between final effluent concentrations and WwTW characteristics. For chemicals which mainly enter sewage treatment works via human use or consumption, in fact, a correlation between the WwTW effluent flow and the final effluent load may be expected. However, in the absence of measured flows, concentrations could only be correlated with WwTWs characteristics.

Pearson correlation coefficient has been used to analyse the relationship between final effluent concentrations and the ratio between population served (PE) and dry weather flow (DWF). This coefficient is a widely use correlation statistic that measures the linear relation between two variables. For the purpose of this study, all the statistical analysis has been undertaken in R (v. 3.6.3). In particular, the function *cor.test()*, specifying Pearson as correlation method, has been used and the results are expressed using two variables: correlation coefficient *r* and *p-value*. The correlation coefficient *r* indicates the intensity of correlation and can vary between 1 and -1, where 1 is positive linear correlation, 0 is no correlation and -1 is negative linear correlation. The *p-value* shows the statistical significance of the test, where values lower than 0.05 is considered statistically significant for the purposes of this report.

5.2.2 Results

The data available within the CIP2 database for E2, NP and BPA is characterised in Table 5.1, the database contains sampling at the WwTW final effluent (Effluent) as well as in-stream river measurements upstream and downstream of the WwTW final effluent discharge point into the river. For effluent data, only those sites that could be matched with a WwTW included within the LF2000-WQX database have been retained.

For E2, a total of 61 different effluent locations with measured data available have been identified. Of these, 10 locations have been discarded: 4 did not have locations within the CIP2 dataset, and 6 could not be cross-referenced with the LF2000-WQX database.

For NP, a total of 436 different effluent locations for which measured data is available within CIP2 have been identified. Of these, 20 locations have been discarded as they could not be cross-referenced with the LF2000-WQX database.

Table 5.1 Number of in-stream and effluent locations in which Beta estradiol (E2), Nonylphenol (NP) and Bisphenol A (BPA) samples have been taken. Minimum and maximum number of samples across all locations included in the analysis are indicated in parenthesis.

	Upstream	Effluent	Downstream
Nonylphenol (NP)	381 (1-40)	416 (13-36)	434 (18-44)
Beta estradiol (E2)	1 (17)	51 (1-26)	1 (17)
Bisphenol A (BPA)	0	0	0

The availability of CIP2 data across the considered chemicals is extremely disparate. For NP, data is available for final effluent (Figure 5.1) as well as in-stream river water (Figure 5.2). For E2, only 51 WwTWs were sampled at the final effluent (Figure 5.1) while in-stream river data are available in just two locations (upstream and downstream the same WwTW) (Figure 5.2). For BPA, no measured data is available within the

CIP2 data provided. Measurements for BPA were included within CIP1 but not included in CIP2 due to low measured levels in final effluents compared to PNEC values and lack of regulatory driver in the near future. The project team did not have access to the raw CIP1 data during the course of this analysis.

The spatial coverage, for both NP and E2, is adequate and, generally, equally distributed in England. However, the data obtained does not cover Wales.

Figure 5.1 Effluent locations of Beta estradiol (E2) and Nonylphenol (NP) samples.

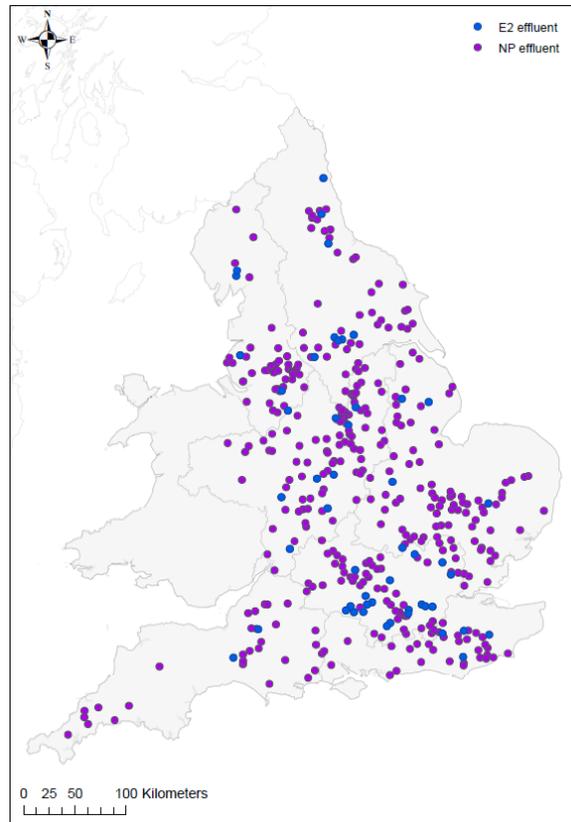
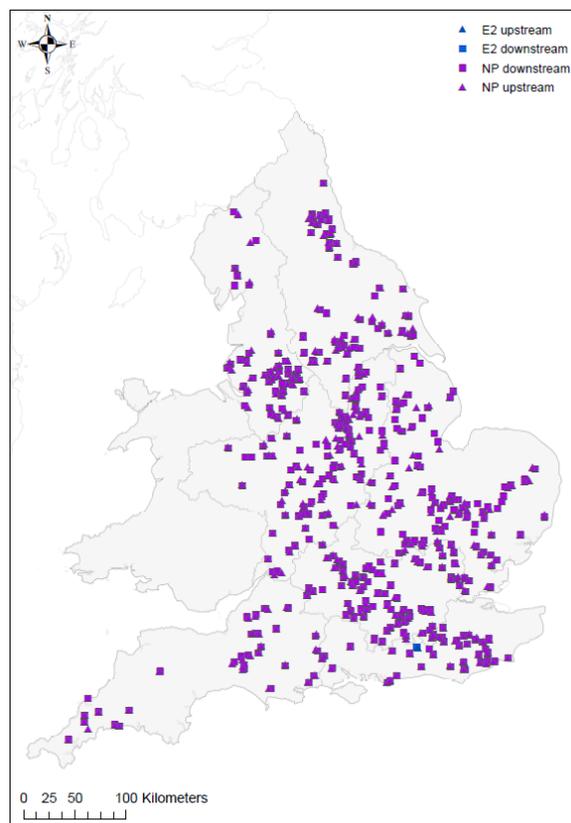


Figure 5.2 In-stream locations of Beta estradiol (E2) and Nonylphenol (NP) samples.



In the absence of CIP2 data for BPA, possible correlations have only been investigated for E2 and NP using the final effluent data only. The in-stream data will be used to corroborate the model results.

To account for the disparity in the sampling frequency at each location, the mean values per location have been considered: these values are provided by the CIP2 database in the statistics section. Specifically, the attribute "Mean_halfFV" has been considered: this represents the mean of all sampling concentrations, with concentrations below detection limit set to half of the detection limit.

To capture general trends across England, correlation between the EDCs concentrations and the ratio of WwTWs' served population (PE) and dry weather flow (DWF) have been computed for all available locations. Then, the analysis was undertaken at regional levels (EA regions) to highlight possible regional trends. Finally, differences between types of treatment have been also considered, dividing WwTW's treatment types as primary, activated sludge and biological filter.

Results are here presented for all WwTWs in England, since further division by regions has not resulted in increased correlation.

For NP, no significant correlation has been found between the chemical concentration and the ratio PE/DWF (Table 5.2 and Figure 5.3) in England. Further division based on WwTW treatment type does not improve correlation. The lack of correlation results from the complexities of the WwTW systems and their differences in terms of disparities not only in terms of treatment and treatment performance but also possible overloads and differences in site management. Further differences can stem from the fact that NP in WwTWs is the result of the degradation of NP ethoxylates which are used in industrial processes and also in domestic detergent (Soares *et al.*, 2008).

Despite a significantly lower number of measured data for E2, a similar search for correlation have been undertaken. In England, no significant correlation has been identified, either considering all data available or grouping WwTWs by treatment type (Table 5.2 and Figure 5.4). This result is unexpected as domestic sources are the main source, however the reduced amount of data could explain the absence of correlation. Furthermore, several of the WwTWs included have high proportion of industrial waste (DWF/PE > 300 l/cap/day).

Table 5.2 Pearson correlation coefficient and p-value for Nonylphenol (NP) and Beta estradiol (E2), considering wastewater treatment works (WwTWs) divided by treatment types in England.

WwTW type	Nonylphenol (NP)		Beta estradiol (E2)	
	r	p-value	r	p-value
All treatment types (England)	0.039	0.42	0.078	0.59
Activated sludge (England)	0.16	0.066	-0.066	0.74
Biological filter (England)	0.0031	0.96	0.22	0.31

Figure 5.3 Comparison between Nonylphenol (NP) measured effluent concentrations and the ratio between population served (PE) and dry weather flow (DWF) for wastewater treatment works in England.

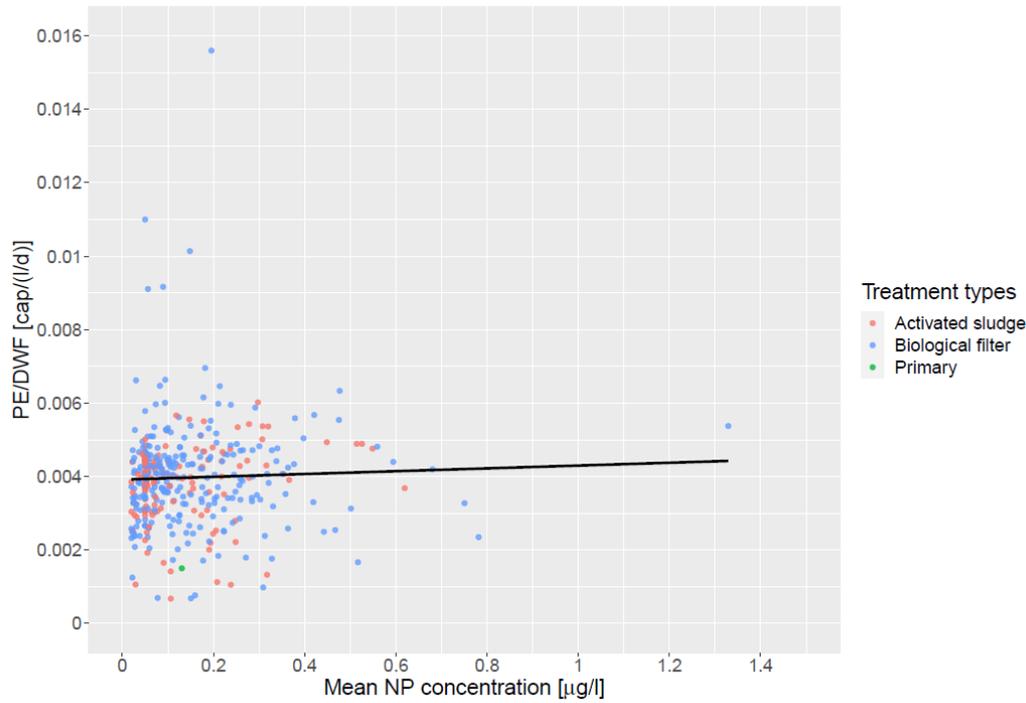
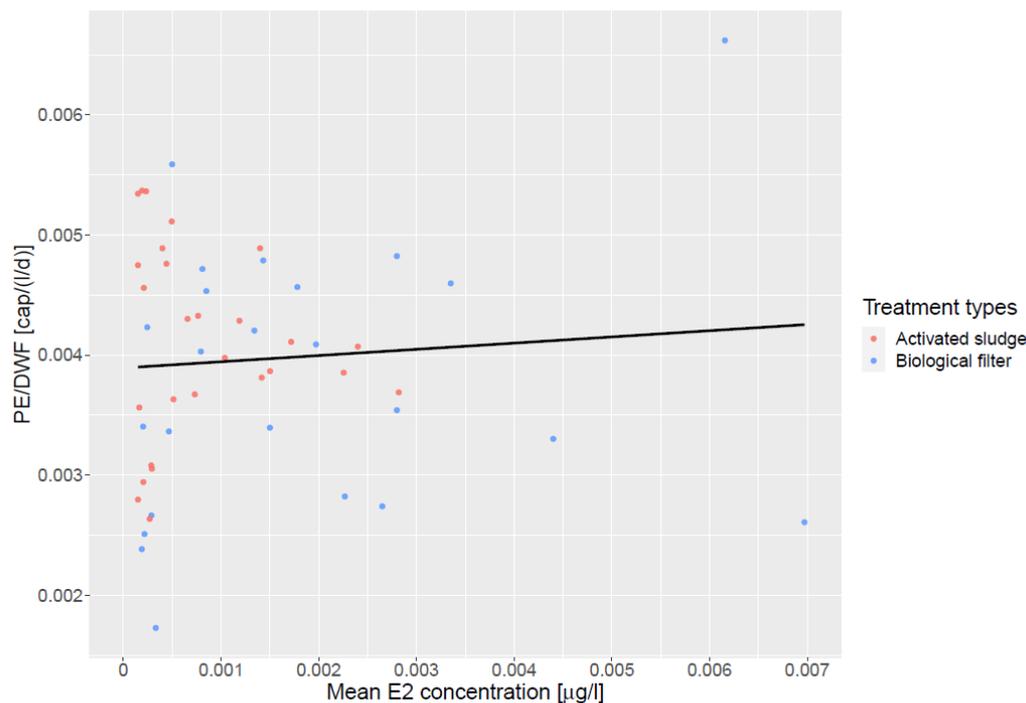


Figure 5.4 Comparison between Beta estradiol (E2) measured effluent concentrations and the ratio between population served (PE) and dry weather flow (DWF) for wastewater treatment works in England.



In the absence of consistent correlation evidence between chemicals concentration in the final effluent and WwTW characteristics, a general method for predicting effluent concentration for individual WwTWs across England was not feasible based on the CIP2 data provided. Thus, in an attempt to maximise the use of measured data, the concentration range in final effluent for all WwTWs available have been calculated.

Concentrations ranges and some additional statistics (mean, median and standard deviation) in final effluent data presented in Table 5.3.

Table 5.3 Measured Concentration ranges and statistics (mean, median and standard deviation) in final effluent of Beta estradiol (E2) and Nonylphenol (NP) across all wastewater treatment works final effluent.

	Beta estradiol (E2)	Nonylphenol (NP)
Minimum (µg/l)	0.00015	0.02
Maximum (µg/l)	0.014	1.3
Mean (µg/l)	0.0016	0.15
Median (µg/l)	0.00077	0.096
Standard deviation (µg/l)	0.0023	0.14

For each EDC studied, results from the literature search undertaken within Task 1 and Task 2 have also been used to characterise the influent load and the removal rates occurring during WwTWs treatment. This characterisation of influent load will be also used as input for the LF2000-WQX model.

5.3 Prediction of potential environmental concentrations

5.3.1 Approach

The surface water quality model, LF2000-WQX, has been selected to derive potential concentrations of E2, NP, and BPA in stream waters across England and Wales. The LF2000-WQX model can estimate the release of chemicals via WwTWs using two methods:

- **Characterisation of the final effluent:** this method relies on the availability of measured data at the final effluent. Concentration in the final effluent for each WwTW is defined by means of a distribution; and
- **Characterisation of the influent:** this method provides a simple representation of removal processes occurring within WwTWs. Influent loads are user-defined by means of a per capita consumption rate, treatment removal rates are also user-defined. The model, in this case, estimates the final effluent concentration for each WwTW from the WwTW characteristic held in the in-built database.

Within the LF2000-WQX model, in-stream removal can be included by means of a first order decay rate. Each substances can be either degradable or conservative. Degradation processes are affected by several factors

such as water temperature and HpH^{49} . Within LF2000-WQX, the variation of the degradation rate with the water temperature can be accounted for.

To maximise the use of measured data (CIP2 data) and available literature (outputs from Tasks 1 and 2), the two WWTW characterisation methods have been used for each chemical. This approach will also provide an insight into which method is most appropriate whilst evaluating the results against in-stream measured data.

As no significant correlation has been identified across England or across regions, the effluent data within the CIP2 database has been used to determine an effluent concentration applicable to all WWTWs. For each chemical, a uniform distribution has been defined and characterised by:

- Minimum concentration: derived from the CIP2 dataset as the minimum value of the mean effluent concentration for each WWTW location available; and
- Maximum concentration: derived from the CIP2 dataset as the maximum value of the mean effluent concentration for each WWTW location available.

The characterisation of the influent parameters, as well as the degradability characteristics of each EDC, have been provided by Task 1 and 2. These Tasks have additionally highlighted the importance of diffuse emissions for both NP and BPA: this information have been added to the model considering a constant in-stream minimum background concentration (obtained from the literature review) in some of the scenarios investigated. No background concentration have been, instead, considered for E2, since, for this chemical, the point emissions from WWTWs are dominant over diffuse emissions.

With the above information, the model set-ups have been prepared and the model run to predict in-stream concentrations of E2, NP and BPA across England and Wales. Its results have been, then, validated using in-stream CIP2 data. It is important to note that due to no or limited data availability in the CIP2 dataset provided, the validation has been mainly undertaken for NP.

5.3.2 Results

Each EDC has been modelled using different scenarios based on the WWTW characterisation methods presented in Section 5.3.1. The parameters for each scenario implemented for E2, NP and BPA are presented in Table 5.4, Table 5.5 and Table 5.6, respectively. A brief description of all scenarios is provided below:

- E2 – Scenario 1: characterisation of the influent load, based on per capita inputs (Williams et al., 2009);
- E2 – Scenario 2: characterisation of the effluent concentration;
- NP/BPA - Scenario 1: characterisation of the influent load assuming an in-stream background concentration;
- NP/BPA - Scenario 2: characterisation of the influent load assuming no in-stream background concentration ($C_B=0$);
- NP/BPA - Scenario 3: characterisation of the effluent concentration assuming an in-stream background concentration; and
- NP/BPA - Scenario 4: characterisation of the effluent concentration assuming no in-stream background concentration ($C_B=0$).

⁴⁹ Jürgens, M.D., Holthaus, K.I.E., Johnson, A.C., Smith, J.J.L., Hetheridge, M. and Williams, R.J. (2002), The potential for estradiol and ethinylestradiol degradation in english rivers. *Environmental Toxicology and Chemistry*, 21, pp. 480-488. doi:10.1002/etc.5620210302

Table 5.4 Beta estradiol (E2) parameter values used as input for LF2000-WQX simulations.

Parameter description	E2 – Scenario 1	E2 – Scenario 2
In-stream degradation rate (/d)	0.3 ⁽²⁾	0.3 ⁽²⁾
Change of degradation rate with temperature	1.075 ⁽²⁾	1.075 ⁽²⁾
In-stream background concentration (µg/l)	0 ⁽²⁾	0 ⁽²⁾
Effluent Concentration (µg/l)		
- Minimum; and		0.00015 ⁽¹⁾
- Maximum.		0.014 ⁽¹⁾
Mean influent load (µg/person/d)	13.8 (2) ⁽²⁾	
% Removal in sewage treatments:		
- Primary;	0 ⁽²⁾	
- Secondary biological treatment;	83 (11.8) ⁽²⁾	
- Secondary activated sludge; and	83 (11.8) ⁽²⁾	
- Tertiary.	83 (11.8) ⁽²⁾	

⁽¹⁾ Data generated from CIP2 dataset⁽²⁾ Williams et al. 2009

Table 5.5 Nonylphenol (NP) parameter values used as input for LF2000-WQX simulations.

Parameter description	NP – Scenario 1	NP – Scenario 2	NP – Scenario 3	NP – Scenario 4
In-stream degradation rate (/d)	Conservative chemical	Conservative chemical	Conservative chemical	Conservative chemical
Change of degradation rate with temperature				
In-stream background concentration (µg/l)	0.11 ⁽²⁾	0 ⁽²⁾	0.11 ⁽²⁾	0 ⁽²⁾
Effluent Concentration (µg/l)				
- Minimum; and			0.02 ⁽¹⁾	0.02 ⁽¹⁾
- Maximum.			1.3 ⁽¹⁾	1.3 ⁽¹⁾
Mean influent load (µg/person/d)	119.45 (23.9) ⁽²⁾	119.45 (23.9) ⁽²⁾		
% Removal in sewage treatments:				
- Primary;	0 ⁽²⁾	0 ⁽²⁾		
- Secondary biological treatment;	90 (9) ⁽²⁾	90 (9) ⁽²⁾		
- Secondary activated sludge; and	90 (9) ⁽²⁾	90 (9) ⁽²⁾		
- Tertiary.	90 (9) ⁽²⁾	90 (9) ⁽²⁾		

⁽¹⁾ Data generated from CIP2 dataset⁽²⁾ Data gathered from Task 1 and 2

Table 5.6 Bisphenol A (BPA) parameter values used as input for LF2000-WQX simulations.

Parameter description	BPA – Scenario 1	BPA – Scenario 2	BPA – Scenario 3	BPA – Scenario 4
In-stream degradation rate (/d)	Conservative chemical	Conservative chemical	Conservative chemical	Conservative chemical
Change of degradation rate with temperature				
In-stream background concentration (µg/l)	0.02 ⁽²⁾	0 ⁽²⁾	0.02 ⁽²⁾	0 ⁽²⁾
Effluent Concentration (µg/l)				
- Minimum			0.01 ⁽²⁾	0.01 ⁽²⁾
- Maximum			1.9 ⁽²⁾	1.9 ⁽²⁾
Mean influent load (µg/person/d)	80.82 (16.2) ⁽²⁾	80.82 (16.2) ⁽²⁾		
% Removal in sewage treatments:				
- Primary	0 ⁽²⁾	0 ⁽²⁾		
- Secondary biological treatment	95 (9.5) ⁽²⁾	95 (9.5) ⁽²⁾		
- Secondary activated sludge	95 (9.5) ⁽²⁾	95 (9.5) ⁽²⁾		
- Tertiary	95 (9.5) ⁽²⁾	95 (9.5) ⁽²⁾		

⁽²⁾ Data gathered from Task 1 and 2

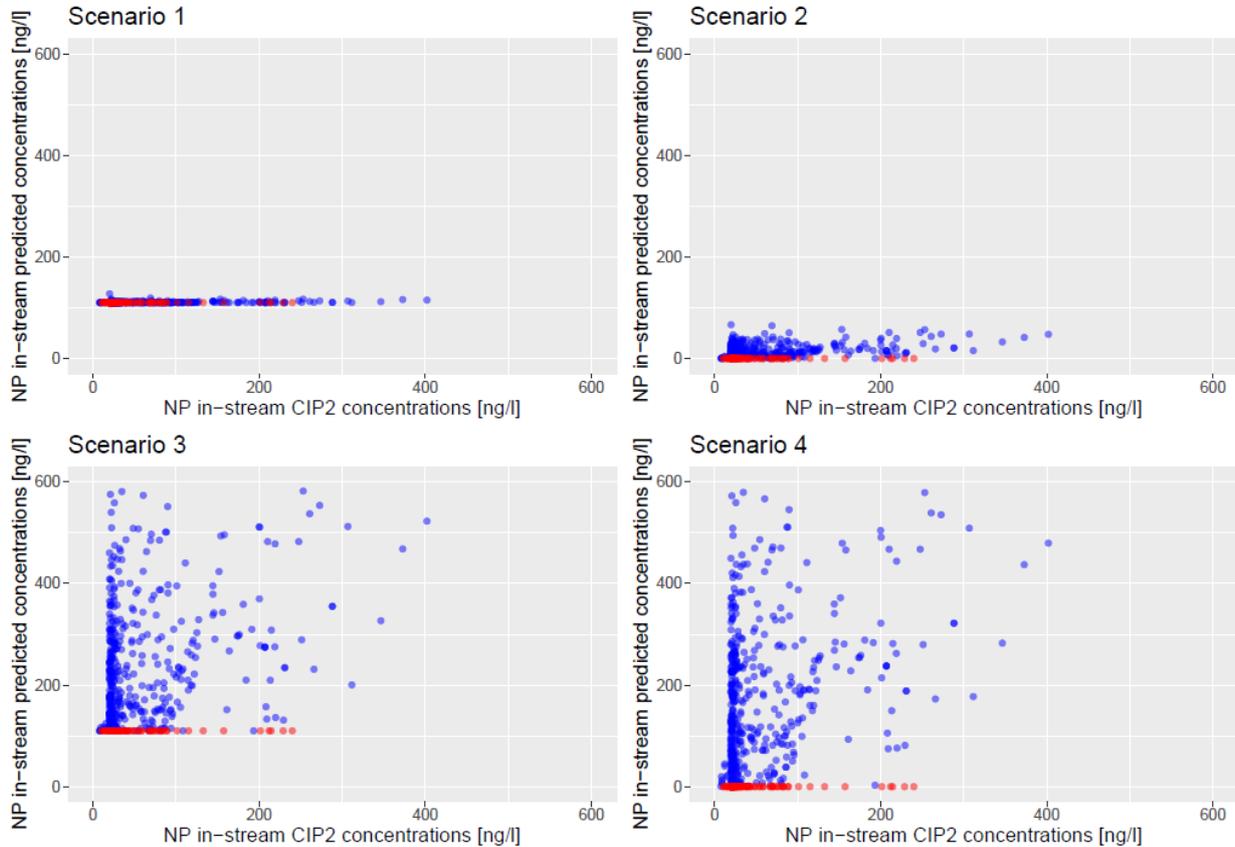
Using the scenarios described above, in-stream concentrations for E2, NP and BPA have been predicted using the river network representation described by Williams et al. (2009). It is important to note that the model does not consider all WwTWs within a catchment. In this original work, a set of filters has been applied to ascertain that only an appropriate number of WwTW were included in the simulation. The first filter was applied at the hydrometric area level: the catchments were ranked in descending order, and only those that accounted for 95% of the total hydrometric area were retained. A second filter based on relative WwTW size within a catchment was applied: all remaining WwTW were ranked in DWF descending order, and those contributing to 95% of the total dry weather flow discharged to the estuary selected for inclusion in the model.

For validation purposes, the predicted concentration estimates have been compared to available measured concentration held within the CIP2 database. This exercise could only be carried out for NP due to lack of in-stream measurement for BPA or insufficient data for E2 (Table 5.4).

A Python script (using package GeoPandas 0.6.1) have been used to associate each CIP2 monitoring site, with relevant data, to the nearest modelled reach in the LF2000-WQX network. As the latter is a reduced river network, the distance between monitoring sites and full river network have also been estimated. Only those monitoring sites for which both distances were equal have been retained. The other sites have been discarded as it was assumed that the monitoring site was likely to be located on a river reach omitted from the LF2000-WQX river network representation.

For all in-stream locations, where the monitoring site is above the most upstream WwTW included in the LF2000-WQX simulation, the predicted concentration is set to the in-stream background concentration. Thus, a flat line (red dots in Figure 5.5) can be observed where predicted concentration are set to 0 ng/l for Scenarios 2 (characterisation of influent load, $C_B=0$) and 4 (characterisation of effluent concentration, $C_B=0$ ng/l) (Table 5.5). In contrast, for Scenarios 1 (characterisation of influent load, $C_B=110$ ng/l) and 3 (characterisation of effluent concentration, $C_B=110$ ng/l) (Table 5.5) the minimum predicted in-stream concentration is 110 ng/l. To prevent skewness in the validation results, those locations above the most upstream WwTW have been discarded.

Figure 5.5 Comparison between observed and predicted in-stream concentrations for Nonylphenol (NP) under the four modelling Scenario (Table 5.5). Red dots indicate monitoring sites above the most upstream sewage treatment plant included in the LF2000-WQX simulation.



A total of 453 CIP2 site locations (and correspondent in-stream predicted concentrations) have been selected for the validation of the NP simulation. For each selected CIP2 site, the observed mean measured concentration have been compared to the predicted mean concentration of the associated stretch.

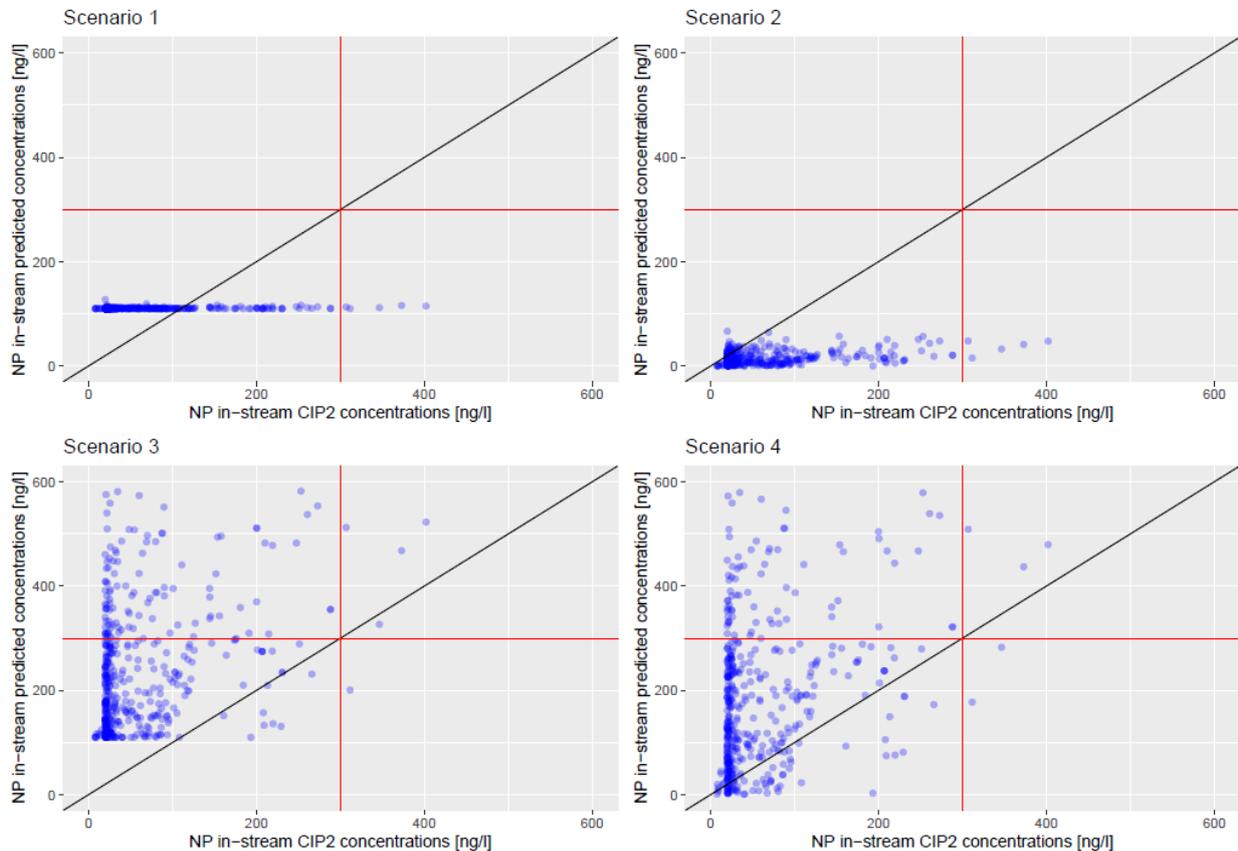
Figure 5.6 presents the comparison of predicted NP in-stream mean concentrations in England under the four modelling scenarios (Table 5.5) with mean measured concentration.

Predicted concentrations from NP-Scenario 1 (characterisation of influent load, $C_B=110$ ng/l) and 3 (characterisation of effluent concentration, $C_B=110$ ng/l) indicate that the background concentration selected within Task 1 and 2 for NP is over-estimated. This is particularly visible whilst applying Scenario 1, where most river reaches have values approximately equal to the background concentration.

Results from NP-Scenario 2 (characterisation of influent load, $C_B=0$ ng/l) indicate that the model tends to under-estimate measured in-stream concentrations. The under-estimation of observed values most likely stems from high uncertainty in mean influent load estimates published in the literature. These per capita estimates are often derived from market data or production volumes which are often associated with significant uncertainty.

For NP, the best performing scenario whilst compared to CIP2 measured data is NP-Scenario 4 (characterisation of effluent concentration, $C_B=0$ ng/l). This scenario, despite overestimating actual concentrations, gives more conservative outputs than the other scenarios. Similarly to the preliminary results for the Thames region, the analysis of the final results have indicated that the use of the CIP2 data to characterise final effluent concentrations is more suitable to predict NP in-stream concentrations.

Figure 5.6 Comparison between observed (from CIP2) and predicted (from LF2000-WQX) in-stream concentrations for Nonylphenol (NP) under the four modelling Scenario (Table 5.5). The black line is the 1:1 line, while red lines indicates NP environmental standard (300 ng/l).



It is important to note that whilst considering NP-Scenario 4 (characterisation of effluent concentration, $C_B=0$ ng/l) in the Thames region (Figure 5.7), predicted concentrations just slightly overestimate measured concentrations from CIP2. This result suggests that this scenario better describes areas with high population density, while in less populated area the overestimation increases.

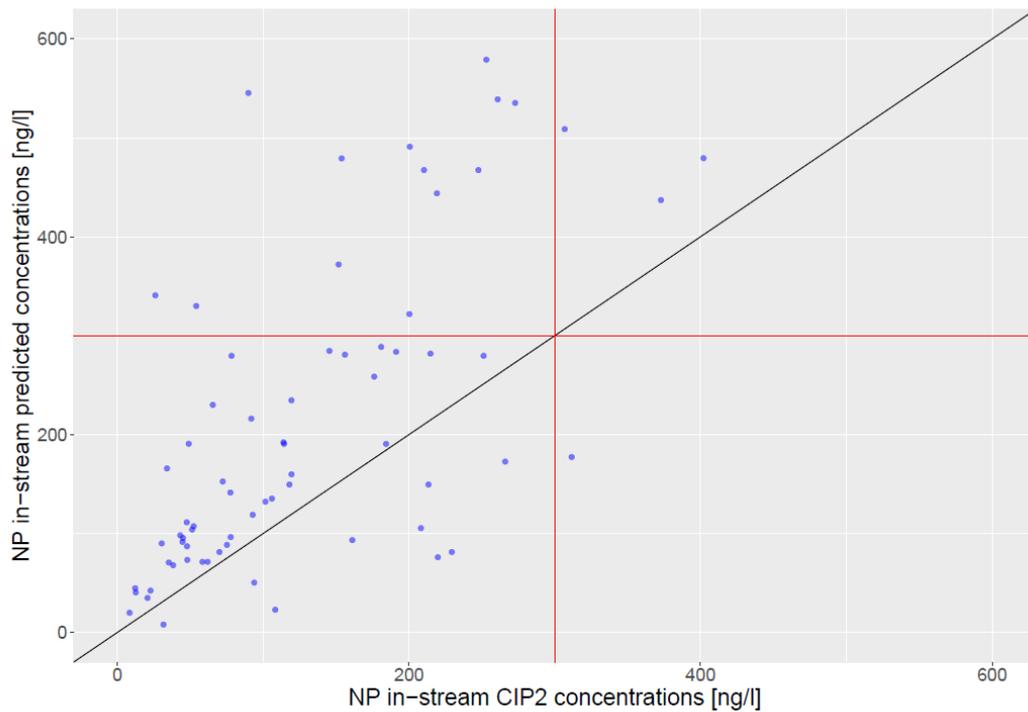
A possible cause of overestimation is the choice of minimum and maximum values describing the uniform distribution. These values are derived from the CIP2 dataset as the minimum and maximum values of the mean effluent concentration for all WwTW location available (Figure 5.8). The highest concentration in the CIP2 dataset (1300 ng/l), and thus maximum value in the distribution, is considerably higher than the second highest concentration (780 ng/l). This is probably the reason why predicted effluent (and consequently in-stream) concentrations are overestimated in many cases. It is also important to note that measured in-stream concentrations are strongly correlated to the flow regime. It is therefore important to acknowledge that for some location the range of measurements might not cover the flow range occurring at the sampled location. Furthermore, there is disparity in the calibration standards used across the various laboratories dealing with the various samples analysed in the CIP2 dataset⁵⁰. The project team had no access to the metadata during

⁵⁰ NP & CAS numbers & calibration standards

- In the 2013 EQSD nonylphenol is listed as a priority substance in the Annex I/Annex X table with the CAS number 25154-52-3. The footnote to the table states nonylphenol (CAS 25154-52-3) includes "isomers 4-nonylphenol (CAS 104-40-5) and 4-nonylphenol (branched) (CAS 84852-15-3)". However, the EQS in Annex II/Annex I is defined solely for CAS 84852-15-3, i.e. the 4-nonylphenol (branched) version only.
- The CIP2 Technical Specification follows the 2013 EQSD in stating nonylphenol (CAS 25154-52-3) is the substance of interest but then goes onto state that the calibration standards to use should be CAS 84852-15-3.

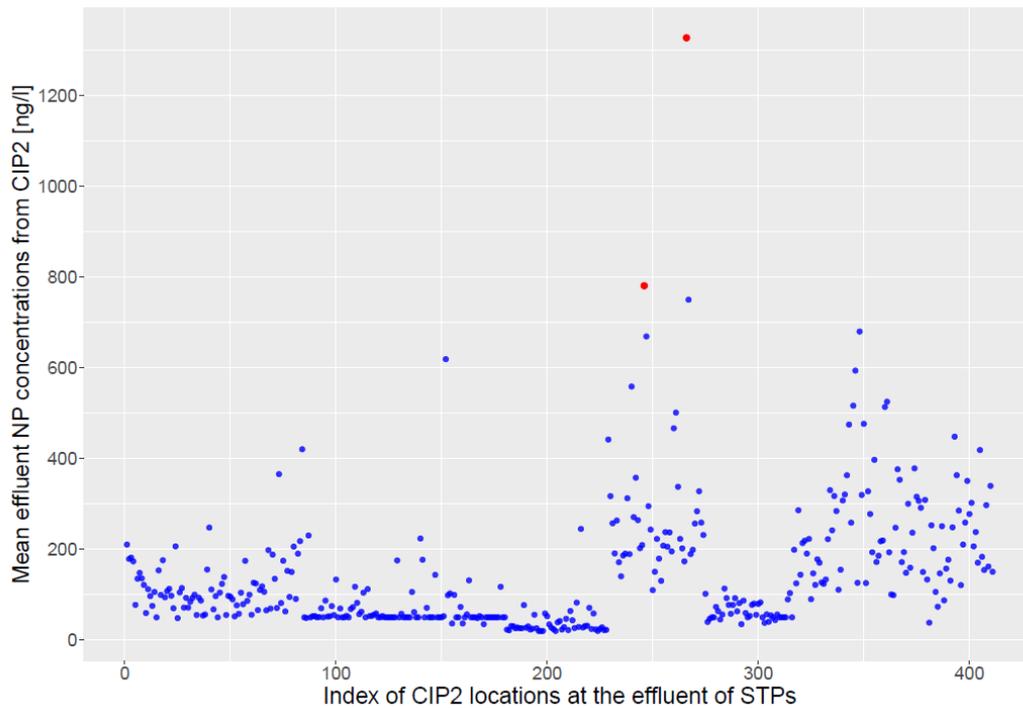
the course of the project, thus, these distinctions could not be made and therefore it is unknown whether this will be an additional source.

Figure 5.7 Comparison between observed (from CIP2) and predicted (from LF2000-WQX) in-stream concentrations for Nonylphenol (NP) under Scenario 4 (characterisation of effluent concentration, $C_B=0$ ng/l; Table 5.5) for the Thames region. The black line is the 1:1 line, while the red lines indicates NP environmental standard (300 ng/l).



- The nonylphenol type on which the EQS is based changed from the 2008 EQSD to the 2013 EQSD. In the 2008 EQSD the 0.3 µg/L river EQS was defined by the 4-nonylphenol linear version (CAS 104-40-5). While the 2013 EQSD 0.3 µg/L EQS was defined by the 4-nonylphenol branched version (CAS 84852-15-3).

Figure 5.8 Mean measured effluent concentrations for Nonylphenol (NP) in ng/l. The red dots indicates the highest and the second highest mean NP concentrations.



To validate the visual outputs of the validation procedure, the root mean squared error (RMSE) and the percent bias (PBIAS) have been computed for the 4 NP-Scenarios (Table 5.5). The RMSE is the square root of the variance of the residuals and it indicates how close the observations are to the model’s predicted values. An RMSE = 0 indicates a perfect fit, and as RMSE value increases the goodness of fit decreases. The computation has been carried out using the R function *rmse()* (package Metrics). The PBIAS measures the average tendency of the predicted values to over- or under-estimate the observations. The optimal value for PBIAS is 0, with positive values indicating over-estimations and negative value indicating under-estimation. The computation has been carried out using the R function *pbias()* (package hydroGOF).

Table 5.7 Percent bias (PBIAS) and root mean squared error (RMSE) between measured (from CIP2) and predicted (from LF2000-WQX) Nonylphenol (NP) concentrations for all scenarios (Table 5.5).

	PBIAS (%)	RMSE (ng/l)
NP-Scenario 1 (characterisation of influent load, $C_B=110$ ng/l)	88.9	113
NP-Scenario 2 (characterisation of influent load, $C_B= 0$ ng/l)	-70.2	108
NP-Scenario 3 (characterisation of effluent concentration, $C_B=110$ ng/l)	292.9	210
NP-Scenario 4 (characterisation of effluent concentration, $C_B=0$ ng/l)	230.6	180

Whilst comparing RMSE and PBIAS outputs (Table 5.7), NP-Scenario 2 (characterisation of influent load, $C_B= 0$ ng/l) is the best performing scenario, followed by NP-Scenario 1 (characterisation of influent load, $C_B= 110$ ng/l). However, predicted concentrations in NP-Scenario 2 (characterisation of influent load, $C_B= 0$ ng/l)



largely underestimate observed values (PBIAS = -70.2%), while NP-Scenario 1 (characterisation of influent load, $C_B = 110$ ng/l) gives an unrealistic representation of concentrations, having large part of the values equal to the background concentration. Therefore, NP-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l) has been considered for further analysis, despite its RMSE value being high.

In the absence of sufficient measured data for both E2 and BPA, the distribution of mean concentrations with modelled reach length across England and Wales for each scenario has been derived for comparison with the relevant environmental standards.

For E2 (Figure 5.9), the two scenarios present similar in-stream concentrations, with approximately 60% of modelled river length expected to be at or below 1 ng/l. Since the result could not be validated, both scenarios have been considered in the following risk analysis and to derive predicted in-stream concentrations at drinking water abstraction points.

BPA-Scenario 3 (characterization of effluent concentration, $C_B = 20$ ng/l) and 4 (characterisation of effluent concentration, $C_B = 0$ ng/l) result in predicted concentrations higher than those generated using BPA-Scenario 1 (characterisation of influent load, $C_B = 20$ ng/l) and 2 (characterisation of influent load, $C_B = 0$ ng/l) (note the different scale of the horizontal axis in Figure 5.10). In line with results from the validation of NP predicted concentrations, BPA-Scenario 1 (characterisation of influent load, $C_B = 20$ ng/l) and 3 (characterizations of effluent concentration, $C_B = 20$ ng/l) indicate that the selected background concentration is over-estimated, since most river reaches have concentrations approximately similar to the background value (BPA-Scenario 1, especially). There is almost a factor 20 between the predicted concentrations in these scenarios. Since no further validation is possible, BPA-Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l) and BPA-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l) have been considered to undertake the risk analysis and to derive predicted in-stream concentrations at drinking water abstraction points.

Figure 5.9 Beta estradiol (E2) in-stream predicted concentrations [ng/l]. The red line indicates E2 environmental standard (1 ng/l). E2-Scenario 1 is based on characterisation of influent load, and E2-Scenario 2 on characterisation of effluent load.

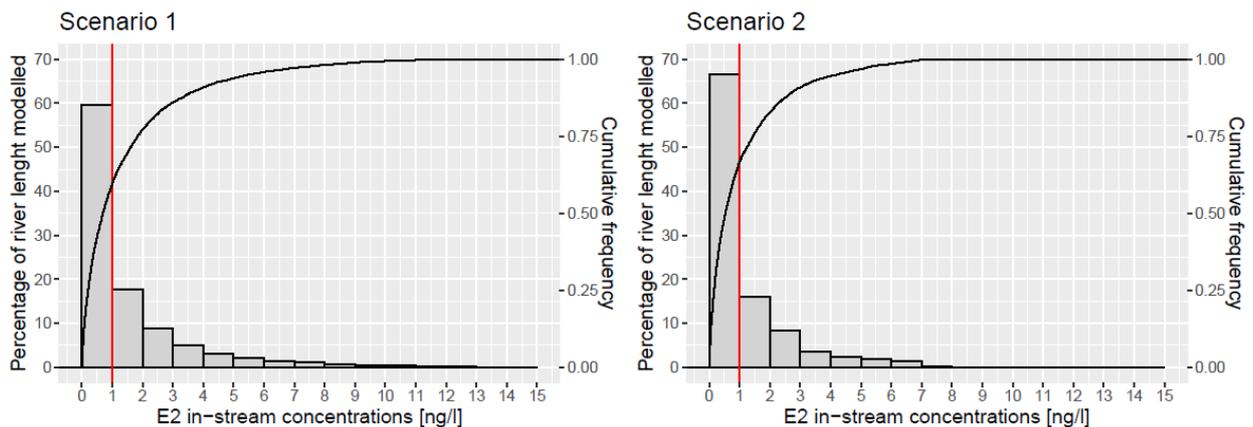
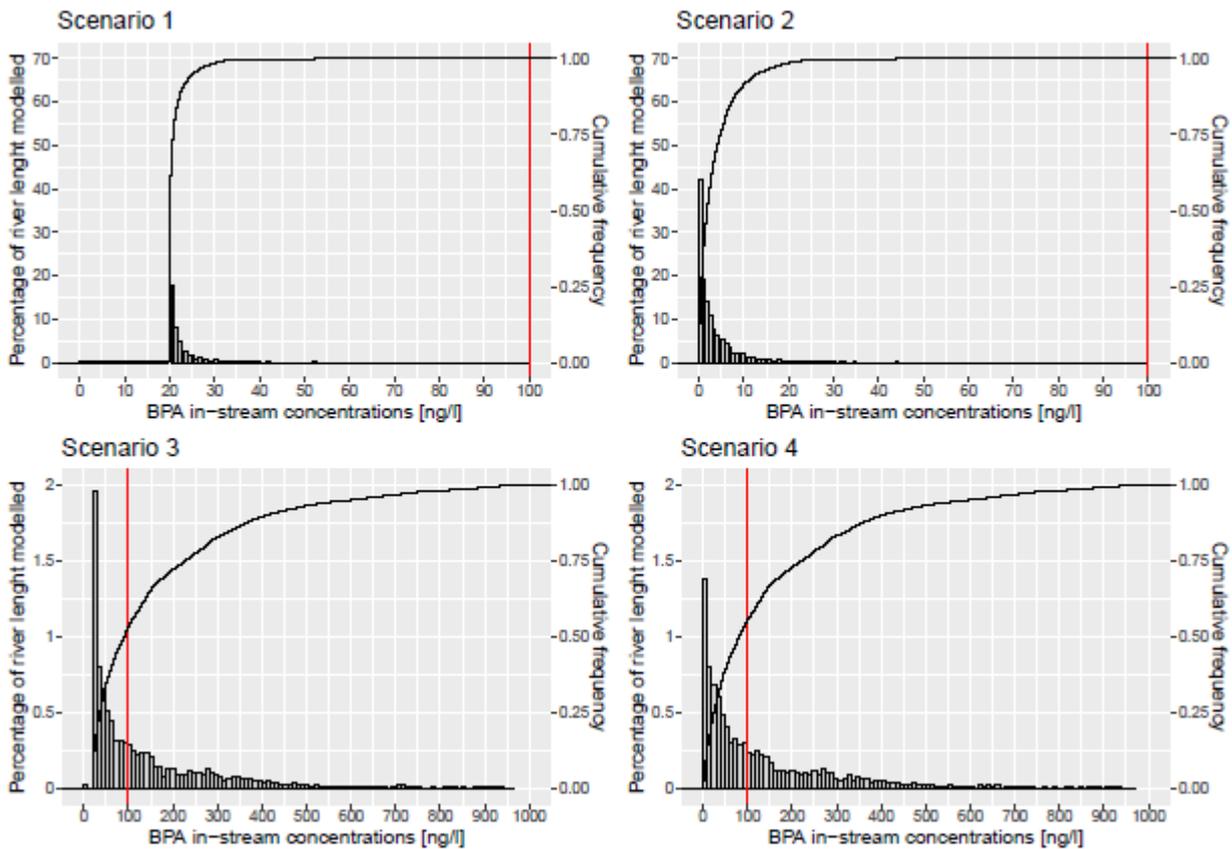


Figure 5.10 Bisphenol A (BPA) in-stream predicted concentrations [ng/l] under all scenarios (Table 5.6). The red line indicates BPA environmental standard (100 ng/l).



5.4 Risk classification based on environmental standards

5.4.1 Approach

The use of a spatially distributed model such as LF2000-WQX allows for assessing the spatial extent of the potential environmental risk arising from the three considered EDCs. Risk levels have been defined using the risk quotient approach. The risk quotient (RQ) is the ratio between the predicted environmental concentrations (PEC) and the predicted no effect concentration (PNEC):

$$RQ = \frac{PEC}{PNEC}$$

For the purposes of this project, as the goal is to assess risk of EDC in drinking water, the PNEC values used correspond to the drinking water standards based on the WHO recommendations. In December 2019, the EU agreed to revise the drinking water directive with the possibility of revising the BPA standard. Thus, this possible new environmental standard for BPA has also been included in this study to ensure completeness. The PNEC values used to assess risk from the three EDC, under consideration in this study, are:

- E2: 1 ng/l;
- NP: 300 ng/l; and
- BPA: 2500 ng/l (current proposed standard), 100 ng/l (previously proposed standard).

The risk quotient has then been used to derive risk categories, as follows:

- Low risk: $RQ < 0.1$;
- Medium risk: $0.1 < RQ < 1$; and
- High risk: $RQ > 1$.

For each EDC, the temporal variability of the risk has been captured by using LF2000-WQX predicted mean concentrations and 90th percentile concentrations, for each retained scenario and suitable PNEC(s) values. The risk assessment derived using mean concentrations is based on long term mean flows and is referred to as a "best case scenario", whereas the use of the 90th percentile concentrations characterizes low flow conditions and is referred to as a "worst case scenario".

5.4.2 Results

The risk assessment analysis has been undertaken using predicted mean concentrations and 90th percentile concentrations on a selection of scenarios for each EDCs:

- NP: only NP-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l; Table 5.5) has been used, with $PNEC_{NP} = 300$ ng/l;
- E2: E2-Scenarios 1 (characterisation of influent load) and 2 (characterisation of effluent concentration) (Table 5.4) have been used, with $PNEC_{E2} = 1$ ng/l; and
- BPA: BPA- Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l) and 4 (characterisation of effluent concentration, $C_B = 0$ ng/l) (Table 5.6) have been used, with $PNEC_{BPA} = 100$ ng/l and $PNEC_{BPA} = 2500$ ng/l.

To represent the spatial variability of the risk, a map has been produced for each EDC and each scenario retained for the risk assessment. As an example, the risk maps of NP under average flow conditions (based on mean concentrations) and low flow conditions (based on 90th percentile concentrations) are presented in Figure 5.11 and Figure 5.12. All remaining maps generated are provided in Appendix A.

Table 5.8 and Table 5.9 summarize percentages of modelled river reaches at low, medium and high risk based on mean concentrations (average flow conditions) and on 90th percentile concentrations (low flow conditions).

Figure 5.11 Risk map for Nonylphenol (NP) using NP-Scenario 4 (characterization of effluent concentration, $C_B = 0$ ng/l; Table 5.5) based on mean concentrations (average flow conditions).

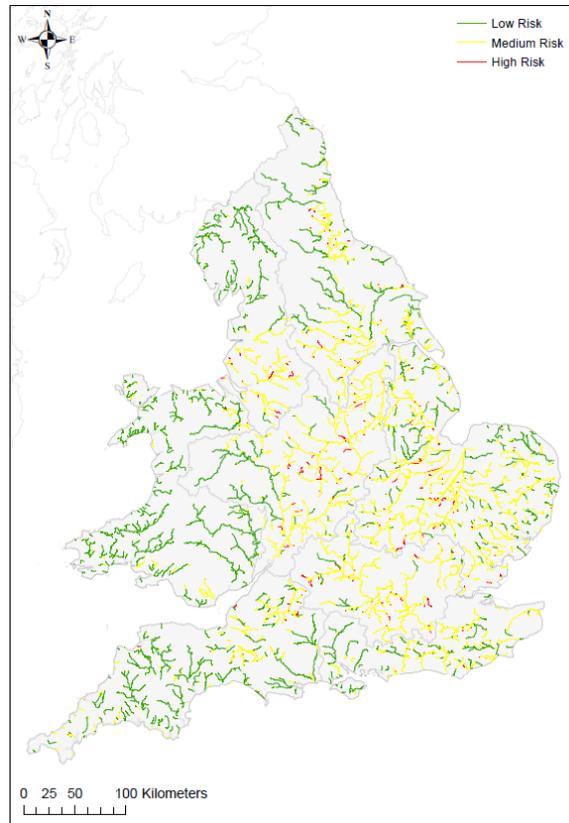


Figure 5.12 Risk map for Nonylphenol (NP) using NP-Scenario 4 (characterization of effluent concentration, $C_B = 0$ ng/l; Table 5.5) based on 90th percentile concentrations (low flow conditions).

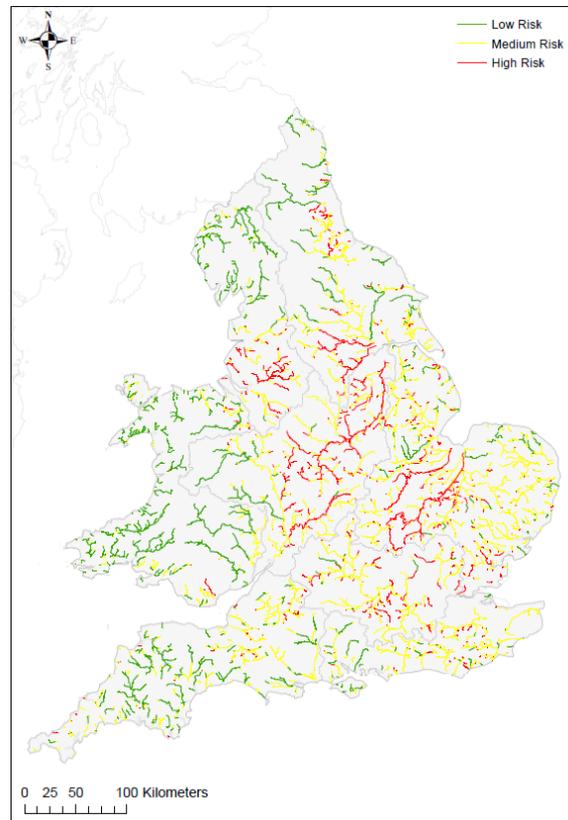


Table 5.8 Percentage of modelled river length at low, medium and high risk based on mean concentrations (average flow conditions) for Beta estradiol (E2), Nonylphenol (NP) and Bisphenol A (BPA).

	Environmental standard (ng/l)	Low Risk (%)	Medium Risk (%)	High Risk (%)
NP-Scenario 4	300	42.4	50.1	7.5
E2-Scenario 1	1	22.5	42.4	35.1
E2-Scenario 2	1	24.8	46.0	29.2
BPA-Scenario 2	100	92.8	7.2	0.0
	2500	100.0	0.0	0.0
BPA-Scenario 4	100	20.7	38.9	40.4
	2500	80.0	20.0	0.0

Table 5.9 Percentage of modelled river length at low, medium and high risk based on 90th percentile concentrations (low flow conditions) for Beta estradiol (E2), Nonylphenol (NP) and Bisphenol A (BPA).

	Environmental standard (ng/l)	Low Risk (%)	Medium Risk (%)	High Risk (%)
NP-Scenario 4	300	27.9	48.4	23.7
E2-Scenario 1	1	13.1	33.5	53.4
E2-Scenario 2	1	15.7	36.2	48.1
BPA-Scenario 2	100	74.7	25.3	0.0
	2500	100.0	0.0	0.0
BPA-Scenario 4	100	11.6	31.8	56.6
	2500	62.1	37.9	0.0

For NP-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l; Table 5.5), whilst considering average flow conditions (mean concentrations), 42.4% of river reaches are at low risk, 50.1% are at medium risk and 7.5% are at high risk. The river reaches at medium risk for NP in drinking water are mostly in the Southern, Thames, Anglian and Midlands regions and the southern parts of North-West and North-East.

For E2-Scenarios 1 (characterisation of influent load) and 2 (characterisation of effluent concentration), whilst considering mean concentrations, the areas at low risk are those with the highest annual rainfall namely Wales, South-West and North-West regions. The areas at high risk are mostly located in highly densely populated areas such as the Midlands, the Thames and the Anglian region. These results are in agreement with previous outputs from Williams et al. (2009).

For BPA, two different environmental standards have been compared with BPA-Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l) and 4 (characterisation of effluent concentration, $C_B = 0$ ng/l). Whilst considering environmental standard equal to 100 ng/l and mean concentrations, BPA-Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l) there are no river reaches at high risk. BPA-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l), with its higher predicted concentrations, has a higher percentage of river reaches at high risk (56.6%), located in the center and eastern parts of England. Whilst considering environmental standard equal to 2500 ng/l and mean concentrations, all the river reaches in England and Wales are at low risk under BPA-Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l). Considering BPA-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l) and low flow conditions, the majority of the river reaches are at low risk with 38% of river reaches at medium risk and no reaches identified as at high risk.

As it would be expected, for all EDCs under all scenarios, risk is higher and more spread in low flow conditions than in average flow conditions.

It is important to note that the proportion of reaches in each risk category is directly related with the classification chosen. Admittedly, the present risk classification was purposefully designed to be conservative with all stretches where PEC is greater than PNEC being classified as high risk. As the main output of this task is the predicted concentrations, future users will be able to redefine the risk categories to fit appropriately the target end point selected. Future users must also take into account the level of uncertainty associated with predicting NP and BPA which is inherent to the risk maps derived from these predictions.

5.5 Concentration estimates at surface water abstraction points

5.5.1 Approach

To characterise the concentrations of E2, NP and BPA at drinking water abstraction points across England and Wales, abstraction points have been associated with the closest river stretch for which LF2000-WQX predicted concentrations were available.

A database of all abstractions sites was available from the LowFlows2000 software package (Wallingford HydroSolutions Ltd) from which the surface water abstraction were extracted. Using a Python script (package GeoPandas 0.6.1), these sites were overlaid on the LF2000-WQX river reach map of EDC concentrations and each abstraction site was automatically allocated the EDC values of the river reach in which it was nearest to. As the modelled reaches are a reduced representation of the full river network available within LF2000-WQX, the same approach was adopted as in Section 5.3.2 to ensure the abstraction sites were correctly matched. Similar to the procedure set in the selection of CIP sites for the validation exercise (Section 5.3.2), all abstraction sites beyond the modelled network were not included in the analysis.

5.5.2 Results

Within the LowFlows2000 database, a total of 829 drinking water abstraction points were present. Of these, only 144 abstraction points have been associated with LF2000-WQX modelled reaches. Amongst the discarded points, 670 abstraction points have been discarded as they could not be associated with the LF2000-WQX network (as a result of the reduced river network modelled in LF2000-WQX, Section 5.3.2). Another 15 have been discarded since located above the most upstream WwTW included in the LF2000-WQX simulation.

For each EDC, a table containing predicted concentrations from all scenarios implemented in this task (Section 5.3.2) have been generated. However, for the purposes of this analysis, only those scenarios included in the risk analysis (Section 5.4.2) are reported. Since E2-Scenario 1 (characterisation of influent load) and 2 (characterisation of effluent concentration) have similar results in both the validation and the risk analysis, only E2-Scenario 1, as worst case scenario between the two, has been presented here.

It is important to note that all the analysed concentrations are representative of raw water concentrations prior to any treatments that will later occur within drinking water treatment plants.

For NP, only NP-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l) have been considered. Based on predicted mean concentrations, only 2 drinking water abstraction points (1 in the Midlands and 1 in the Thames) have a predicted concentration greater than the standard of 300 ng/l. However, under low flow conditions (90th percentile concentration), there are 11 abstraction points (in Anglian, Midlands and Thames regions) for which the predicted concentration is greater than the standard (Figure 5.13 and Table 5.10).

Figure 5.13 Nonylphenol (NP) concentrations at drinking water abstraction points in England and Wales (Scenario 4, Table 5.5). The red line indicates NP environmental standard (300 ng/l).

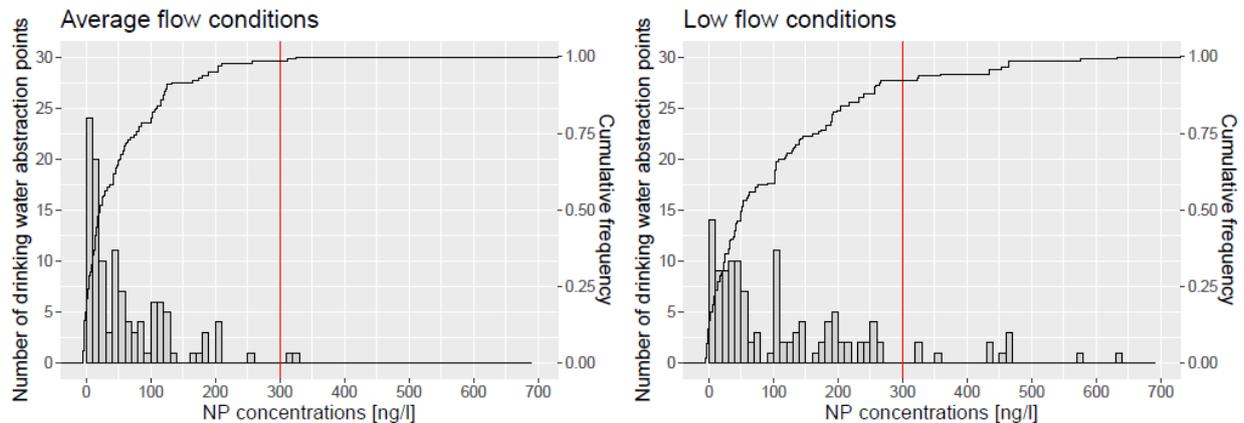


Table 5.10 Number of drinking water abstraction points above and below Nonylphenol (NP) environmental standard (300 ng/l).

	Average flow conditions		Low flow conditions	
	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard
Anglian	0	23	5	18
Midlands	1	19	5	15
North-East	0	20	0	20
North-West	0	6	0	6
Southern	0	11	0	11
South-West	0	19	0	19
Thames	1	21	1	20
Wales	0	23	0	23

For E2, 33 abstraction points (located mainly in the Thames, Anglian and Midlands regions) are associated with predicted mean concentrations greater than the 1 ng/l standard. In contrast, during low flow periods (90th percentile concentration), predicted concentrations are higher, with 60 abstraction points over the standard around England and Wales (Figure 5.14 and Table 5.11).

Figure 5.14 Beta estradiol (E2) concentrations at drinking water abstraction points in England and Wales (Scenario 1, Table 5.4). The red line indicates E2 environmental standard (1 ng/l).

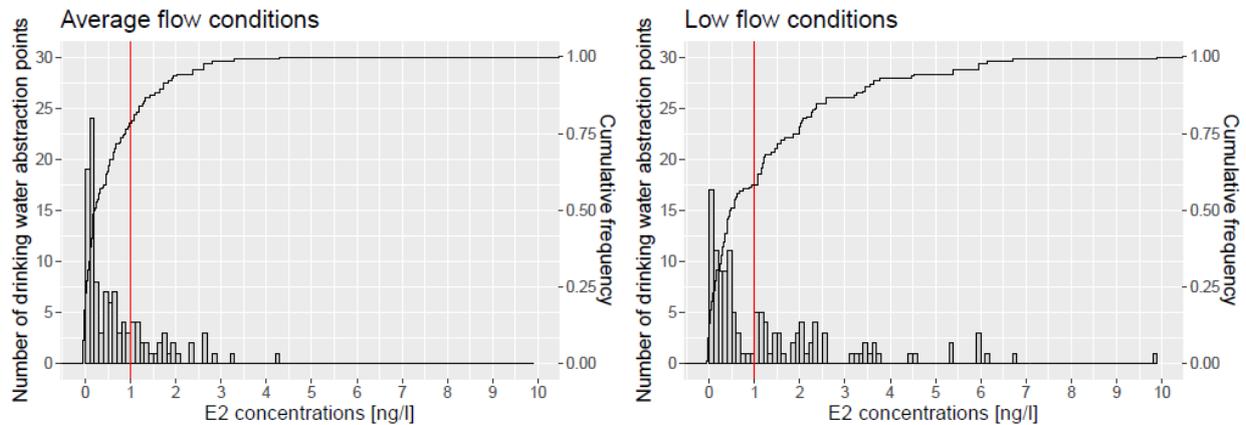


Table 5.11 Number of drinking water abstraction points above and below Beta estradiol (E2) environmental standard (1 ng/l).

	Average flow conditions		Low flow conditions	
	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard
Anglian	7	16	14	9
Midlands	7	13	15	5
North-East	2	18	3	17
North-West	1	5	1	5
Southern	0	11	4	7
South-West	0	19	3	16
Thames	15	7	19	3
Wales	1	22	1	22

For BPA (Figure 5.15), under the previous recommended standard ($PNEC_{BPA} = 100$ ng/l), only 1 abstraction point (in the Thames region) has predicted mean concentrations greater than the standard for BPA-Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l). For BPA-Scenario 4 (characterisation of effluent concentration, $C_B = 0$ ng/l), this number increases to 112 around England and Wales. Whilst considering low flow condition (90th percentile concentrations), 19 abstraction points (BPA-Scenario 2) and 123 abstraction points (BPA-Scenario 4) have concentrations over the environmental standard (Table 5.12).

Whilst applying the newly recommended standard ($PNEC_{BPA} = 2500$ ng/l), in both BPA-Scenario 2 and 4 under average and low flow conditions, no abstraction points are associated with river reaches where the predicted mean concentrations is greater than 2500 ng/l (Table 5.13).

Figure 5.15 Bisphenol A (BPA) concentrations at drinking water abstraction points in England and Wales (Scenario 2 and 4, Table 5.6). The red line indicates BPA environmental standard (100 ng/l).

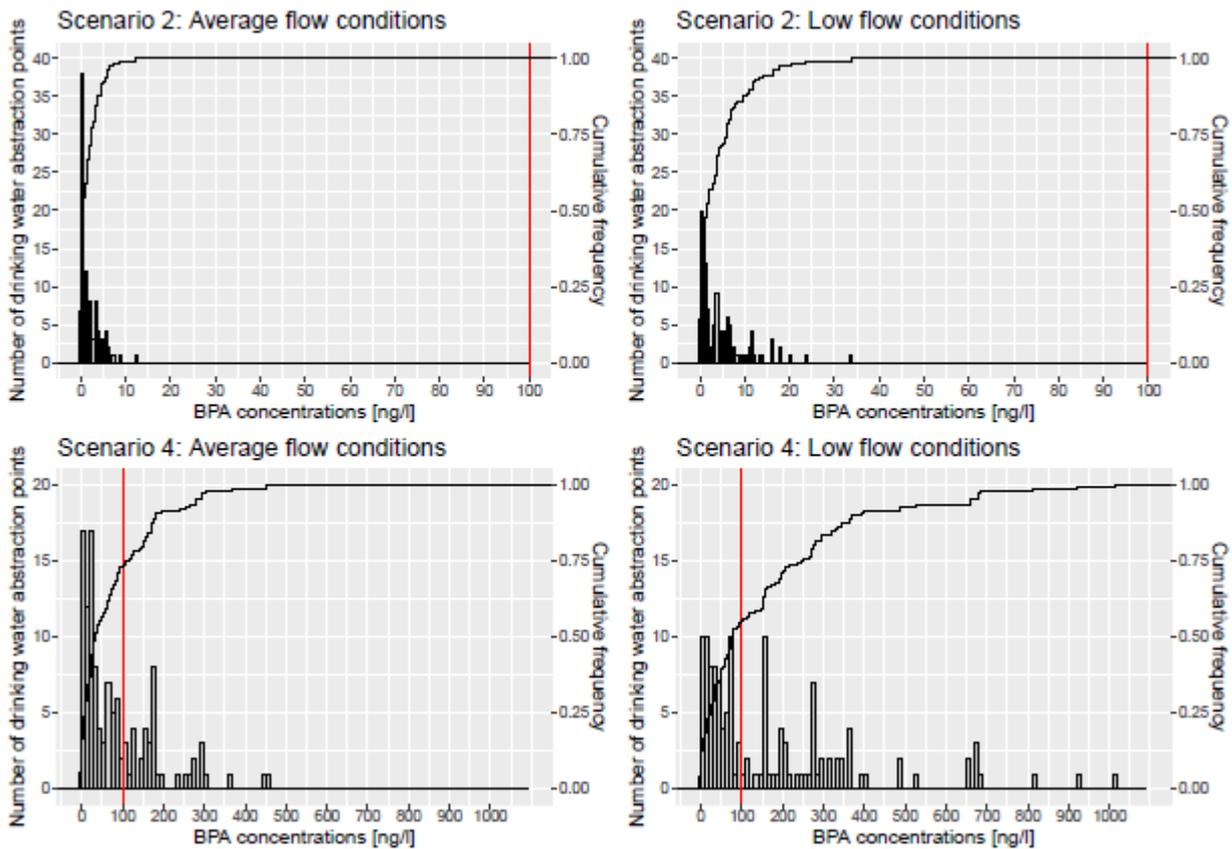


Table 5.12 Number of drinking water abstraction points above and below Bisphenol A (BPA) environmental standard (100 ng/l).

	Average flow conditions		Low flow conditions		
	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	
BPA-Scenario 2	Anglian	0	23	0	23
	Midlands	0	20	0	20
	North-East	0	20	0	20
	North-West	0	6	0	6
	Southern	0	11	0	11
	South-West	0	19	0	19

		Average flow conditions		Low flow conditions	
		Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard
	Thames	0	22	0	22
	Wales	0	23	0	23
BPA-Scenario 4	Anglian	9	14	14	9
	Midlands	7	13	15	5
	North-East	3	17	5	15
	North-West	1	5	1	5
	Southern	0	11	4	7
	South-West	0	19	6	13
	Thames	17	5	19	3
	Wales	1	21	1	21

Table 5.13 Number of drinking water abstraction points above and below Bisphenol A (BPA) environmental standard (2500 ng/l).

		Average flow conditions		Low flow conditions	
		Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard
BPA-Scenario 2	Anglian	0	23	0	23
	Midlands	0	20	0	20
	North-East	0	20	0	20
	North-West	0	6	0	6
	Southern	0	11	0	11
	South-West	0	19	0	19
	Thames	0	22	0	22
	Wales	0	23	0	23
BPA-Scenario 4	Anglian	0	23	0	23

	Average flow conditions		Low flow conditions	
	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard	Number of drinking water abstraction points <u>over</u> the environmental standard	Number of drinking water abstraction points <u>below</u> the environmental standard
Midlands	0	20	0	20
North-East	0	20	0	20
North-West	0	6	0	6
Southern	0	11	0	11
South-West	0	19	0	19
Thames	0	22	0	22
Wales	0	23	0	23

Whilst analyzing the potential environmental risk arising from the three considered EDCs at average flow condition, 57.6% (NP-Scenario 4), 77.5% (E2-Scenario 1) and 20% (BPA-Scenario 4, environmental standard = 2500 ng/l) of river reaches have been characterised as at medium or high risk. However, it is interesting to note that just 1.4% (NP-Scenario 4), 23% (E2-Scenario 1) and 0% (BPA-Scenario 4, environmental standard = 2500 ng/l) of the drinking water abstraction points have concentrations over the environmental limits, indicating that drinking water abstraction points are largely not located in river reaches at risk.

5.6 Remarks on surface water concentrations

Predicted concentrations of E2, NP and BPA have been derived for river reaches across England and Wales. For E2, the characterisation of influent loads across England and Wales were readily available, and CIP2 was used to characterize concentration in final effluent. Both scenarios considered for E2 yield similar predicted concentrations at drinking water abstraction points.

For NP, the scenarios considered produced significantly different risk maps, with admittedly a relatively high level of uncertainty in the results. An attempt was made to characterize the influent load, however due to significant contribution from industrial processes, no significant correlation was established between WWTWs characteristics and measured concentrations. Several scenarios have been applied and compared with the in-stream measured data available within CIP2. For three of the four simulated scenarios, the predicted concentrations are higher than the measured concentrations. Whilst using these results, the level of uncertainty driving the input data must not be ignored.

For BPA, there was no measured data available within CIP2, therefore although predicted estimates of in-stream concentrations were produced, these have not been validated.

5.7 Calculating post-drinking water treatment concentrations using abstraction point data

5.7.1 Approach

The final step of this sub-task draws on the predicted raw water concentrations derived from Task 3a and applies an additional removal step for each of the EDCs to estimate possible concentrations in tap water after drinking water treatment. In turn, these concentrations are then related back to the proposed DWD standards outlined in the introduction to examine the risk of non-compliance for each of the EDCs.

To calculate the rate of non-compliance at drinking water abstraction points across England and Wales, a percentage removal factor was applied to the predicted/modelled concentrations at all 144 surface water abstraction points based on removal efficiencies for drinking water treatment obtained for each of the EDCs in previous tasks. Removal factors were applied to both the mean concentrations estimates but also the upper 90th percentile estimates from the model to give a mean/average flow and worst case (low flow/dry summer) scenario. The great advantage of this approach is that a quantitative estimate of the likely compliance of potable supply from surface waters in England and Wales is available, within a framework that also encompasses the potential application of future surface water (low flow) scenarios.

Final potable water concentrations are then compared to the proposed DWD standards for these chemicals and the extent of potential non-compliance is reported and discussed below.

5.8 Results

5.8.1 Estradiol

When using the modelled predictions of E2 at all 144 abstraction points across England and Wales and applying a subsequent drinking water treatment removal step (assuming 83% removal efficiency) we see no exceedances of the 1ng/l proposed DWD standard when using the average/mean concentration estimates.

In a very conservative scenario using a low flow situation and the 90th percentile concentration estimates from both model simulation scenarios (Task 3), we see between 49 and 60 abstraction point exceedances of the 1ng/l proposed DWD standard after drinking water treatment, predominantly in the Thames, Anglian and Midlands regions.

5.8.2 BPA

Again, like E2, BPA in drinking water sources in England and Wales has been primarily investigated in river waters, upstream and downstream of sewage treatment plants. Six studies retrieved in Task 1 reported concentrations of BPA in river waters in the ng/L range, occasionally exceeding the proposed 0.01 µg/l DWD standard. Manamsa *et al.* (2016) is the only study that measured BPA in groundwater and reported concentrations around 0.1 µg/L.

For BPA we assumed a removal efficiency of 95% during drinking water treatment based on information gained during the previous tasks. This removal estimate applies to sewage treatment so removal rates may be even higher during drinking water treatment processes. Having applied this percentage removal factor to estimates of BPA at all abstraction points, none of the resulting 'tap water' concentrations exceed the newly proposed DWD standard of 2.5µg/l. However, when comparing the post-treatment 'tap water' concentrations from both modelling scenarios (See Task 3) to the previously proposed DWD standard of 0.01 µg/l we see between 13 and 123 abstraction point exceedances (Table 5.7). The exceedances in Scenario 2 (90th % ile worst-case scenario) and Scenario 4 (average/mean) largely occur in the Midlands and Anglian catchment regions.

Table 5.14 Number of exceedances over proposed DWD standard based on estimated surface water concentrations (from both model scenarios 2 and 4) and a subsequent removal step assuming 95% removal efficiency

	BPA Scenario 2 Average flow conditions	BPA Scenario 2 Low flow conditions	BPA Scenario 4 Average flow conditions	BPA Scenario 4 Low flow conditions
Number of points >0.01 µg/l BPA	0	19	13	123
Number of points >2.5µg/l BPA	0	0	0	0

5.8.3 NP

The conclusions drawn from Task 1 of this study indicated that there is little evidence that a revised drinking water standard for nonylphenol of 0.3 µg/L would be exceeded in the UK. This can be largely attributed to the ban implemented after 2003, when concentrations of nonylphenol in rivers were markedly lower occurring in the ng/l range, well below the proposed revised drinking water parameter.

A similar picture is seen in the results of this task when using the modelled predictions of NP at all 144 abstraction points across England and Wales and applying a subsequent drinking water treatment removal step (assuming 90% removal efficiency). There are no exceedances of the 0.3 µg/L proposed DWD standard when using the mean concentration estimates (from both modelled scenarios). However, when using the more conservative model scenario 4 and the 90th % ile (low flow) concentrations we have 12 abstraction point instances where the 0.3 µg/L proposed DWD standard is exceeded, even after applying a subsequent drinking water treatment step. Two of these exceedances are in the Thames region, five in the Midlands and a further five in the Anglian region.

5.8.4 Conclusions on predicted post drinking water treatment concentrations

From the results presented above we see the following key conclusions regarding the likelihood of breaching a proposed benchmark value in drinking water derived from surface water abstraction points across England and Wales:

- There is a very low likelihood of drinking water exceeding the proposed benchmark value for NP and we would also expect use to be reducing further in coming years due to the ban on use of this substance;
- For E2, both the literature and conservative modelling suggest that it could exceed the benchmark value in drinking water during low flow situations ; and
- BPA is the EDC that has the highest likelihood of exceeding the proposed benchmark standard in UK drinking water. Using the proposed DWD standard of 2.5µg/l, the risk of exceedances in drinking water will be negligible but high removal treatment efficiency will need to be maintained across England and Wales.

5.9 Task 3b - Groundwater Modelling Component

5.9.1 Introduction

This section sets out a risk assessment to estimate the relative risk of EDCs reaching a groundwater drinking water supply. In general, risks of EDCs contaminating a groundwater supply are low because:

- EDCs are poorly mobile in soils and groundwater due to their high retardation (affinity for the solid phase) and relatively rapid rate of degradation, which means that they move slowly relative to groundwater and degrade at a rate that is fast compared to their rate of movement. Most groundwater arriving at a drinking water supply is relatively old (several years, or decades), which means that it is unlikely to contain EDCs as they will degrade before reaching the supply;
- There are limited numbers of sources, which means that they are unlikely to be present at elevated concentrations in most catchments; and
- Source concentrations, for most of those sources identified, are relatively low. Where the source concentration is high then it can overwhelm the attenuation capacity of soils and aquifers but in the case of EDCs, low input concentrations are unlikely to do this. A relatively low source concentration and a rapid rate of degradation mean that concentrations fall rapidly in the direction of flow and fall below drinking water standards within a short distance.

As a result, for most groundwater supplies, the risks are likely to be tolerable. However, in some catchments, a proportion of the water arrives rapidly via fissures, particularly as a result of intense rain events. This rapid movement can transport contaminants and micro-organisms that would not normally be found in groundwater and risks of finding EDCs will be higher in these catchments. Rapid flow in fissures is mainly a feature of soluble aquifers (limestones). In England and Wales these include the following Principal Aquifers:

- The Chalk of Southeast England, East Anglian, Lincolnshire and East Yorkshire;
- The Lincolnshire Limestone;
- Carboniferous Limestone mainly found in the Pennines, South Wales and the Mendips; and
- The Corallian Limestone in the North Yorkshire Moors.

Of the three EDCs under consideration, BPA is the most soluble and, based on its physico-chemical properties, the most mobile in groundwater. It is also the only EDC found in groundwater in the EA's WFD groundwater monitoring dataset. As a result, the assessment of risks to drinking water focusses on BPA rather than E2 or NP.

5.9.2 Sources of EDCs to groundwater

For EDCs to enter groundwater there must be a hazard or primary source and a means of that entering groundwater (a pathway). The primary sources are described in more detail in Task 2 but potential secondary sources include:

- Application of waste materials to land (materials to land M2L);
- Drainage to soakaways including road drainage;
- Sewage: permitted discharges to ground from sewage treatment works and septic tanks and leaking sewers;

- Leakage of landfill leachate into groundwater, particularly older dilute-and-disperse landfills which have no engineered liner to minimise leakage rates; and
- Losing stretches of surface watercourses.

5.9.3 Secondary Source concentrations

There is limited information on secondary source concentrations and a comprehensive evaluation is beyond the scope of this project. Indicative concentrations for a number of potential sources are provided in Table 5.15 where data could be found. For land spreading (materials to land or M2L) a source concentration was not found. This will depend on the mass of EDCs in the material, its leachability from that material and on water / infiltration availability and rate of movement through the material and is, therefore, inherently variable. Data for E2 in landfill and surface water was also not found.

In general, source term concentrations are less than or similar to concentrations (less than 10 times) of the proposed drinking water standards for surface water and runoff for E2 and NP. BPA concentrations in surface water are also similar to the proposed DWS. NP concentrations in landfill leachate are lower than the proposed DWS. These data suggest that runoff is unlikely to be a significant source of EDCs and that most surface water is also unlikely to be a source to groundwater. Landfill is also an unlikely source of NP given the low concentrations in the literature.

Table 5.15 Source concentrations of EDCs

Substance	Units	Proposed WHO / EC Drinking Water Standard	M2L	Runoff	Sewage	Landfill	Surface water
17-Beta-estradiol (E2)	µg/l	0.001	No data	0.0017 A	0.0017-0.0112 A	No data	No data
Nonyl phenol (NP)	µg/l	0.3	No data	1.3 A	5.0 -27.0 A	0.05-0.07 B	0.0003-37.3 D
Bisphenol A (BPA)	µg/l	0.01 (now 2.5)	No data	1.2 A	1.1 -4.5 A	0.07-228 B 17 C	0.04 B 0.001 -92 D

A Comber et al. 2014 (average concentrations)

B Asakura et al. 2004

C Magnusson et al. 2017

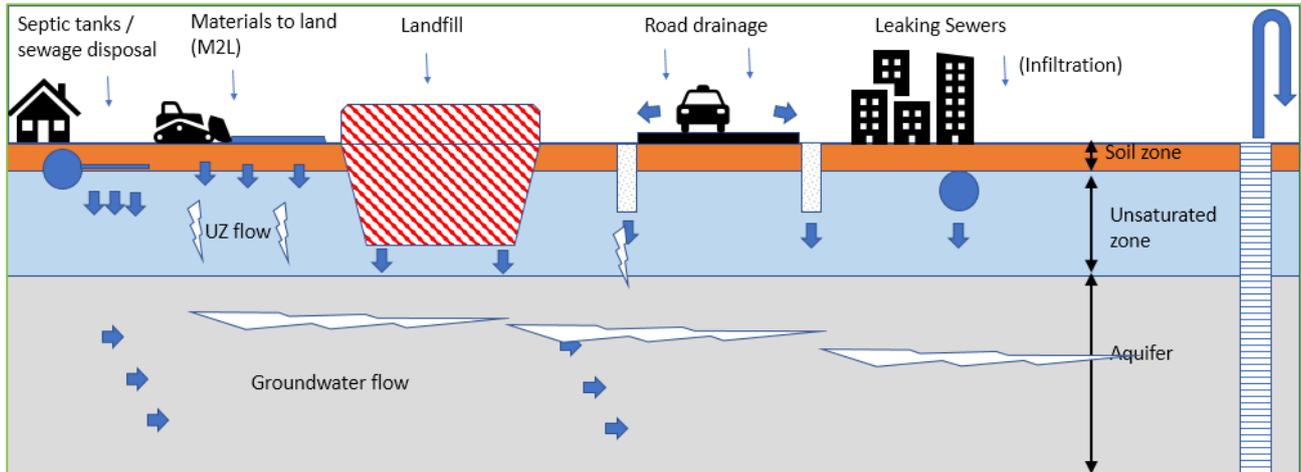
D Careghini et al 2015

5.9.4 EDCs behaviour in the subsurface

Conceptual Model

Figure 5.16 provides a high-level conceptual model of sources and pathways to groundwater supplies.

Figure 5.16 Conceptual model for EDCs to groundwater supplies



Physico-chemical Properties

Table 5.16 sets out the physico-chemical properties of EDCs that are relevant to their fate in groundwater. These are:

- Solubility in water;
- The liquid to solid partition coefficient, K_d . Organic compounds sorb to the organic carbon within in solid materials and therefore have a liquid to organic carbon coefficient, K_{oc} and K_d is then K_{oc} multiplied by the fraction of organic carbon, f_{oc} . The f_{oc} varies, it is highest in soils, where it may be more than 5% and is low in bedrock aquifers, typically well below 1%. Substances with a high K_d will migrate slowly due to their affinity for the solid phase; and
- The degradation half-life, $t_{1/2}$. EDCs undergo biologically mediated degradation in the subsurface. The rate of degradation is often expressed as the degradation half-life or the time for concentrations to decrease by 50%.

Table 5.16 EDCs properties relevant to their transport in the subsurface

Substance	CAS	Solubility (mg/l)	Log K_{oc} (l/kg)	Degradation half life, $t_{1/2}$ (days)
17-Beta-estradiol (E2)	50-28-2	13 E	~3.0	<7 (soil aerobic) E 24 (soil anaerobic) E
Nonyl phenol (NP)	104-40-5	6000 A	3.4-5.6 A	1-13 (soils aerobic) 15-20 (soils anaerobic)
Bisphenol A (BPA)	80-05-7	120,000-300,000 A	2.5-4.5 A	3-37.5 A (soils aerobic conditions) 340 (groundwater)

A Careghini et al. (2015)

E Ying & Kookana (2005)

The properties of the three EDCs vary and this means the risk of them migrating to drinking water supplies varies. BPA presents a higher risk to groundwater than NP and E2 due to its higher solubility and longer degradation half life. As previously mentioned, BPA was also the only EDC detected in groundwater in the EA's WFD groundwater monitoring.

There is some evidence (e.g. Ying and Kookana, 2005, Careghini et al. 2015, Scherr 2009) that EDCs either do not degrade, or degrade slowly under anaerobic conditions. However, anaerobic conditions are rare in principal aquifers.

5.9.5 EDCs in groundwater in the UK

Information Available

An assessment of EDCs in groundwater has been undertaken using Environment Agency (EA) monitoring data. Environment Agency monitoring data on EDCs in groundwater was provided for the period January 2010 to November 2019.

The data were provided by EA region and include the region, a sample date, a national grid reference and a concentration but, with few exceptions, do not identify the monitoring point or aquifer. Only data for BPA have been reported and it is assumed that E2 and NP were not identified in groundwater, despite being tested for. The data include comprises collected by the EA from their observation network and from some water company public water supplies. It also contains data provided by some water companies for public water supplies. The limit of detections for BPA was 0.01 µg/l. The frequency of analysis is also variable but in recent years most location are sampled once every three years.

Data was provided for 592 locations. The number of results per location was variable, a number of locations returned multiple results (up to 15) but over half of the locations only returned a single value. The number of analyses undertaken was not provided so it is not possible to determine the frequency at which BPA was detected, however, most locations will have been sampled on several occasions, so the data suggest that BPA occurrence was sporadic in most cases.

The analysis was by GC-MS or LC-MS Screen. Concentrations were estimated by the EA based on the size of the peak on the scan rather than quantified by comparison to a standard of known concentration and are therefore semi-quantitative. For the purposes of this assessment, concentrations have been assumed to be correct for the purposes of assessment, however the results were qualified by the EA as follows:

- The scans only provide positive results. Therefore, where a chemical was not detected there is no record of that chemical in the scan result;
- Over time, there have been changes to list of substances that the scans can detect. So the absence of records for a substance does not necessarily mean it was not present – it could be that it was not yet possible to test for it at that time;
- If a substance has been analysed one year using GCMS and in subsequent years by LCMS then the later results are likely to be more precise; and
- The data is stored in text files, many of which have been manually entered, therefore the data can contain transcription errors and interpretation of individual data results must be treated with caution.

5.9.6 Assessment of Results

Overall

The EA monitoring did not identify the presence of E2 or NP in groundwater. It is assumed that this means that they were not present in groundwater. The results are, therefore, only for BPA.

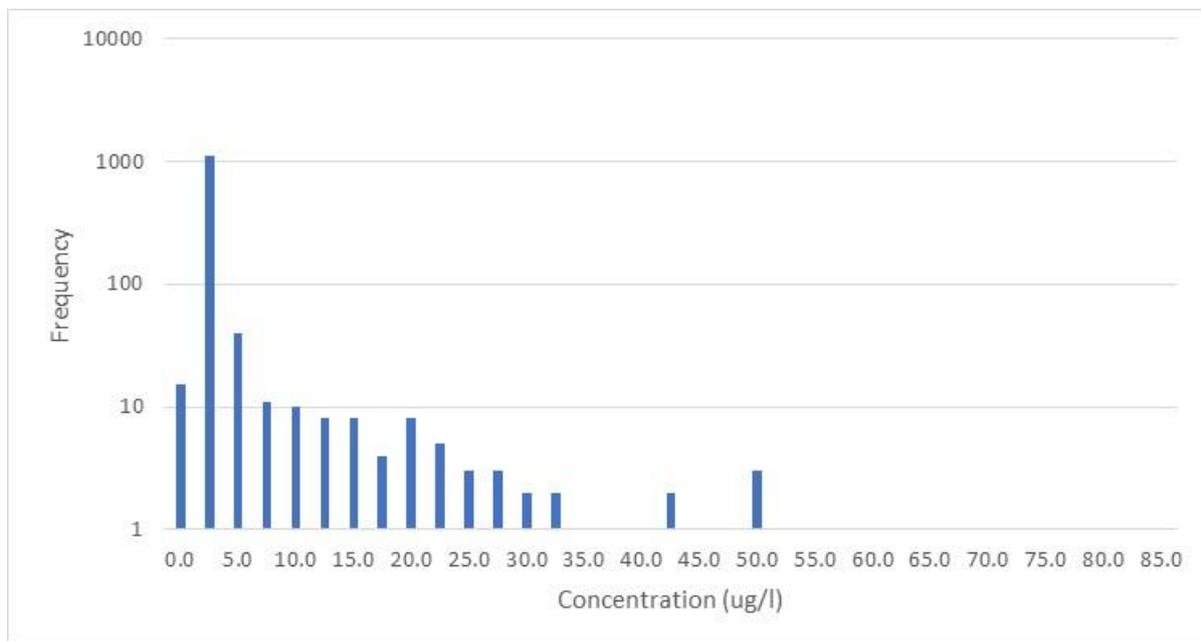
A range of concentrations of BPA were found. Summary statistics are provided in Table 5.17 and a histogram provided as Figure 5.17 (note logarithmic concentration scale). A small number of results were reported as

<0.5 µg/l, which suggests that BPA was identified but could not be quantified. For the summary statistics these 'less than' results have been set to zero. Most (>90%) results for BPA in groundwater were below 2.5 µg/l indicating that BPA where found was generally at low concentrations. There are a small number of high values in the dataset that are potentially outliers and may indicate error in the sampling, analysis or data transcription.

Table 5.17 Summary statistics for groundwater

Substances	Units	No. of results	min	5th percentile	median	mean	95th percentile	max
BPA	µg/l	1253	<0.5	0.03	0.124	1.79	8.00	100

Figure 5.17 Distribution of BPA concentrations in UK groundwater



Spatial Distribution

The spatial distribution of results is shown on Figure 5.18 where it is compared to outcrop aquifer type. It should be noted that as aquifer type is not listed in the dataset, the relationship between aquifer and results cannot be confirmed. In some locations, more than one aquifer is present (e.g. in the east of England the Crag overlies the Chalk). Furthermore, some samples may be superficial deposits overlying confined aquifers. Where more than one result was available, then the highest value is shown on Figure 5.18.

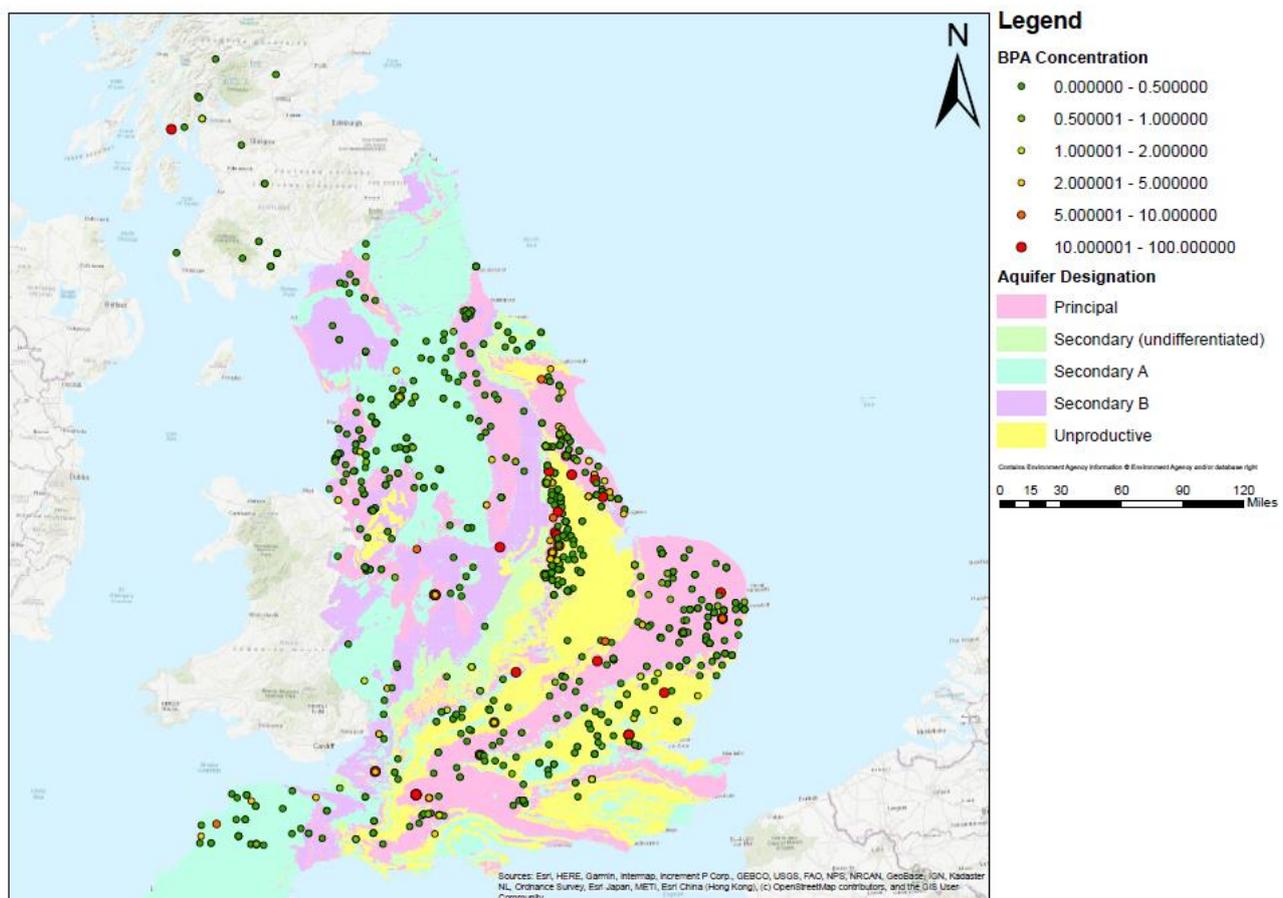
This analysis shows:

- BPA distribution is widespread across England. However, there are gaps in the data spatially, notable in Northeast England and along the south coast, which could mean that there were no detects of BPA in these areas, or that there is no data for these regions. Data are also sparse in the Midlands;

- There are a large number of results over unproductive strata, notably in the south around the Thames Estuary. These are likely to be results for superficial deposits such as River Terrace Gravels;
- Results above 2.5 µg/l were largely found in the south and east of England over the Lincolnshire Limestone and Chalk/Crag aquifer outcrops;
- Only the Lincolnshire Limestone and Lincolnshire Chalk show multiple locations with results over 2.5 µg/l close to each other; and
- Over the Chalk/Crag of East Anglia and Chalk / Lower Greensand in Hampshire there are a number of results >2.5 µg/l but adjacent samples are below this value.

The spatial distribution does not clearly identify a correlation between the distribution of the higher concentrations of BPA and aquifer type but there is an association between higher results and the Lincolnshire Limestone and Chalk.

Figure 5.18 Distribution of BPA in groundwater compared to aquifer type



Temporal

The number of detects per month in the entire dataset is summarised in Table 5.18 along with average concentrations. This shows more samples and higher monthly average concentrations in October and November although average concentrations were also elevated in January. This seasonal increase in the number of detects in groundwater could be linked to the timing of surface activities or to the onset of winter

recharge, or both. The start of recharge may create a “first flush” of contaminants that have accumulated within soils over the summer leading to higher concentrations in groundwater, which are diluted in groundwater over winter by further recharge or degrade within a short space of time. This seasonal variation could also be linked to seasonal surface activities such as landspreading in late summer / early autumn following harvesting of crops.

Table 5.18 Number of BPA results by month

Month	No. of results by month	Average Concentration of results in month (µg/L)
January	65	3.39
February	46	1.50
March	51	1.51
April	61	0.89
May	51	1.14
June	67	2.24
July	75	2.35
August	67	2.94
September	90	2.20
October	150	2.89
November	122	4.18
December	60	1.67

A number of locations had more than one detection of BPA over time and these have been examined to determine whether there are trends in the data. To evaluate the data, locations with more than four results where more than two of those results were above 0.25 µg/l have been plotted (Figure 5.19 to Figure 5.21) and their spatial distribution is shown on Figure 5.22. The value of 0.25 µg/L is 10% of the draft DWS and was used to separate out those locations with higher results. Using a higher screening value screened out too many locations to provide a meaningful data set and use of a lower screening value included a larger number of locations that made evaluation difficult.

Data have been divided into: Lincolnshire Limestone, Chalk and Crag and other strata to aid legibility. The data from these is noisy in that many locations show variable results ranging over orders of magnitude even in samples taken on the same day.

The time-series results show no overall trend in concentrations, neither do most individual locations show obvious trends. At most locations there is a large variation in concentration over time. Only a small number of locations have consistently elevated concentrations

Figure 5.19 BPA Time-series data for locations in the Lincolnshire Limestone with multiple high (>2.5 µg/L) concentrations

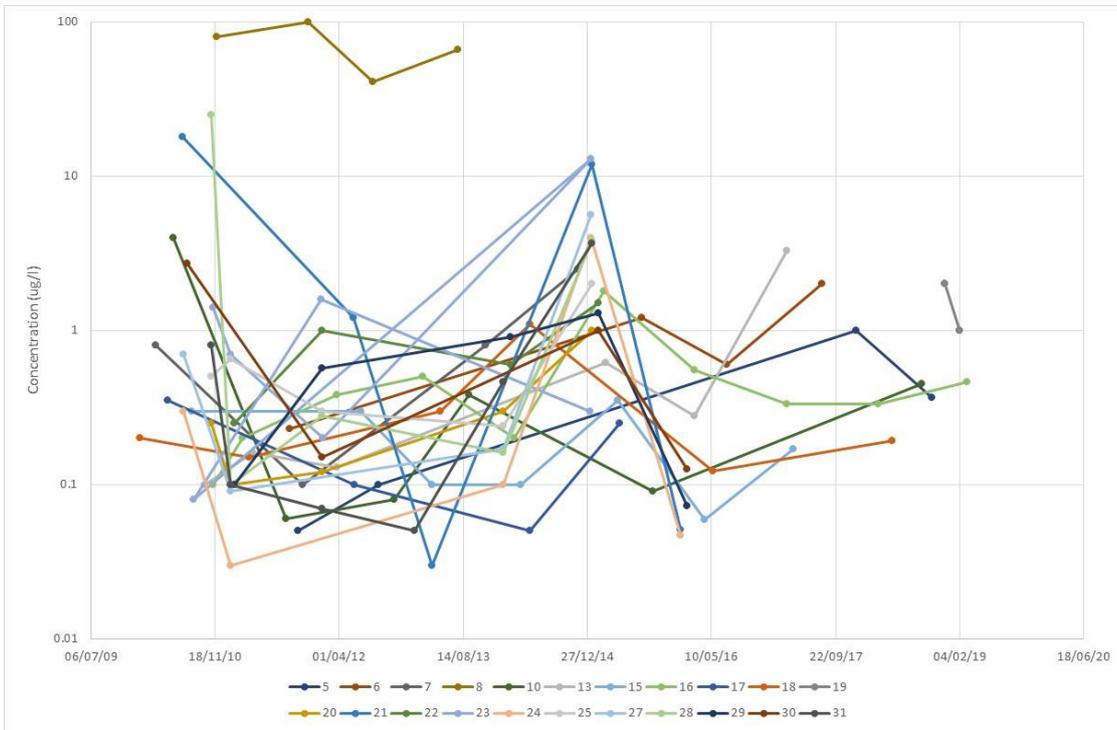


Figure 5.20 BPA Time-series data for locations in the Chalk and Crag with multiple high (>2.5 µg/L) concentrations

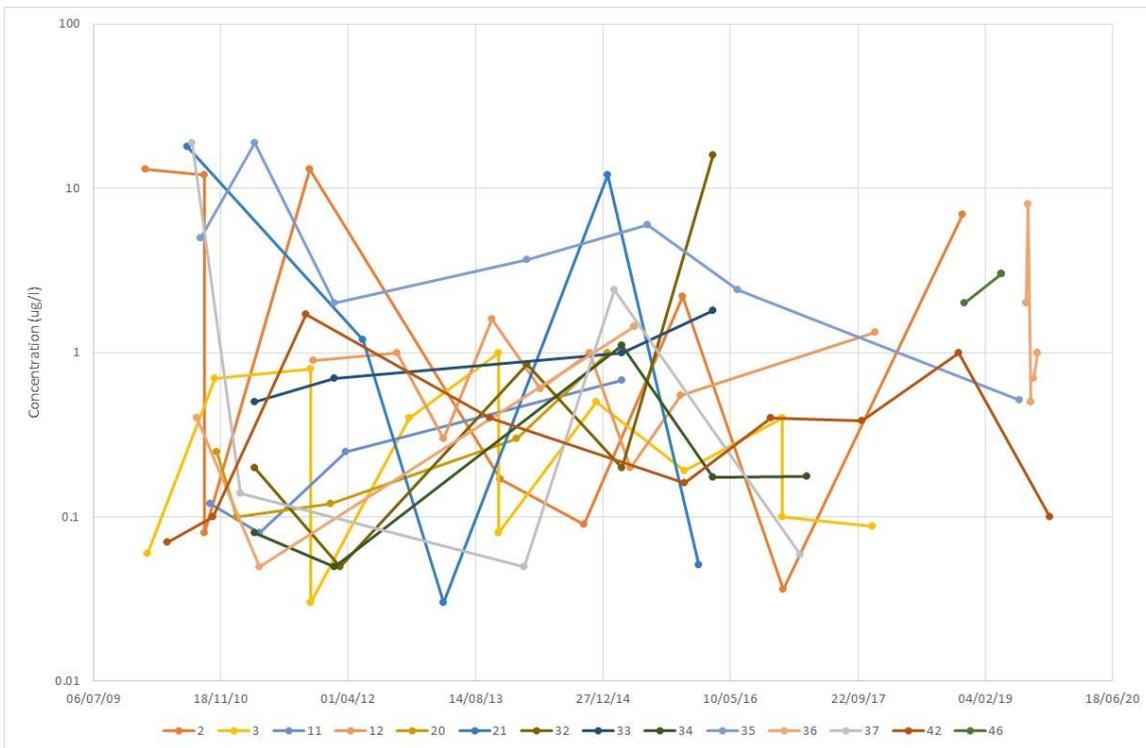


Figure 5.21 BPA Time-series data for locations in the Other Strata with multiple high (>2.5 µg/L) concentrations

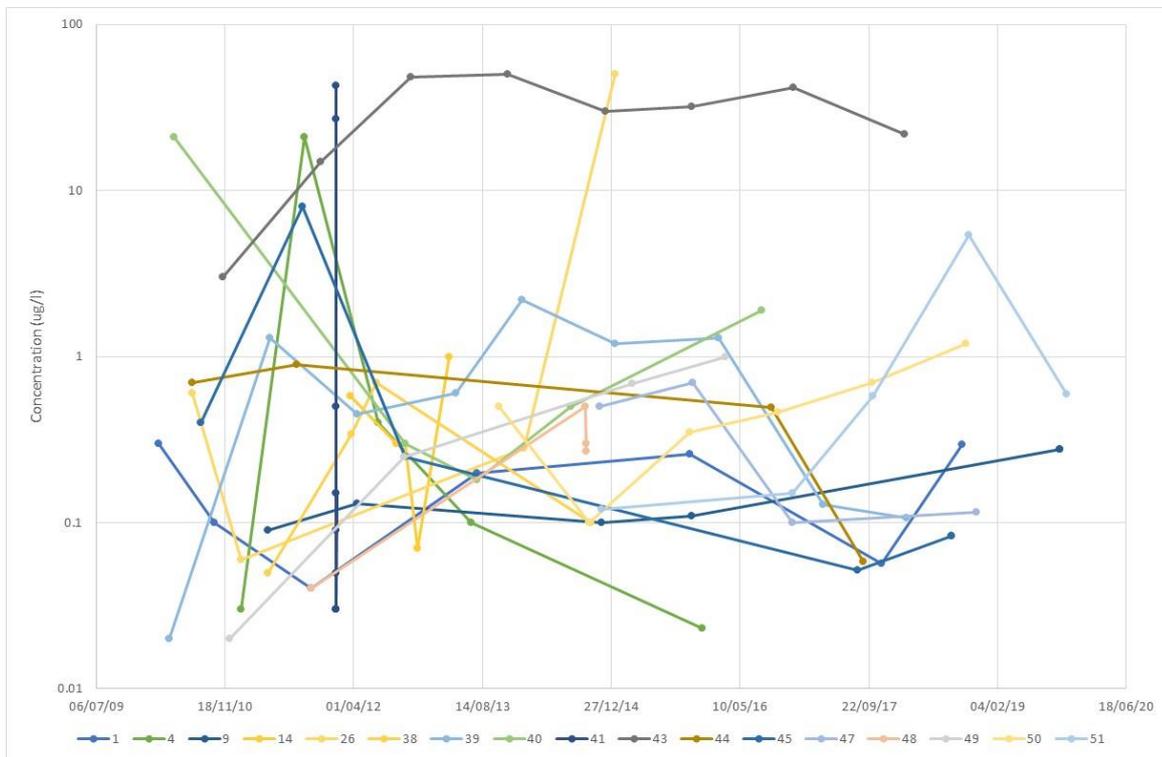
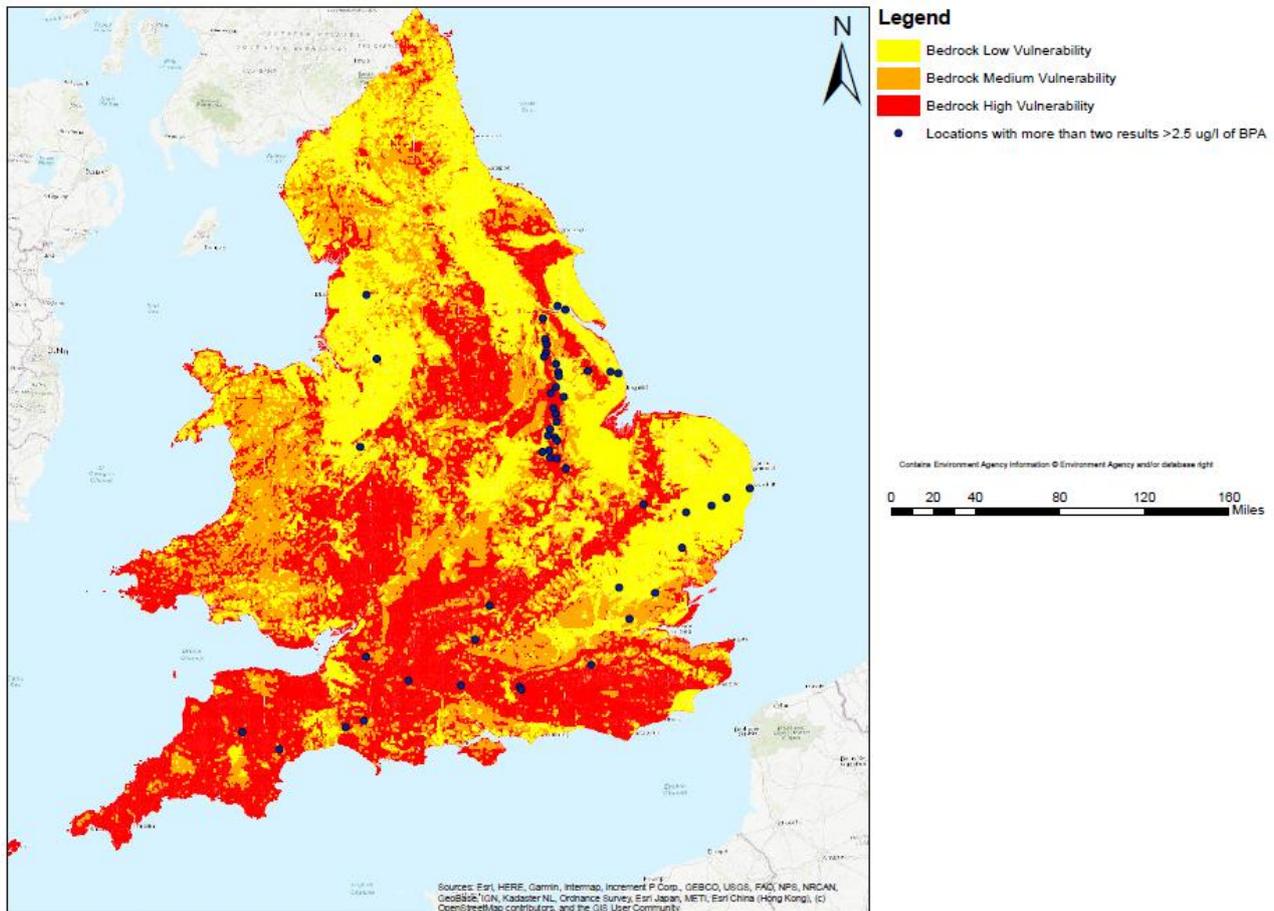


Figure 5.22 Locations with more than two results >2.5 µg/L of BPA



The spatial distribution of the sites with multiple detects above 0.25µg/l shows:

- The locations are predominantly in eastern and southern England;
- The majority of these sites are nominally in the Lincolnshire Limestone and Chalk/Crag. There are also a number of locations in the Lower Greensand aquifer; and
- Most locations are in rural settings away from major roads and urban areas.

These results suggest that:

- The source of the more elevated concentrations of BPA occurs largely in rural settings i.e. is not urban, with the possible exception of major road drainage. Of the identified sources, this indicates M2L or landfill are possible but the widespread occurrence, rural location and outcrop geology suggests that landfill is unlikely;
- Of the principal aquifers, the Lincolnshire Limestone has the most exceedances and the highest density of results;
- There are relatively few locations in the Chalk/Crag when compared to their extent (i.e. there is a low density of occurrence); and
- There are only two results for the Sherwood Sandstone aquifer, which has a large areal extent but there are five locations over the Lower Greensand outcrop. This aquifer has a relatively limited outcrop area compared to the Chalk or Sherwood Sandstone.

The spatial distribution indicates that the Lincolnshire Limestone has the highest number of results and the highest density of results, suggesting that it has characteristics that make it vulnerable to contamination by BPA. The characteristics of this aquifer that may help to explain this are:

- **Rapid recharge** via fissures through thin soils over unconfined bedrock aquifer;
- **Rapid groundwater flow** in solution enhanced fissures (Karst); and
- **Limited dilution** in the saturated zone due to the relatively thin nature of the aquifer.

Rapid flow will limit the time available for degradation of BPA. The Chalk shares some of these characteristics, i.e. it has undergone Karst development in some areas and there are large areas where it has little or no superficial cover such as the North and South Downs. However, over large parts of its outcrop, particularly in East Anglia it is covered by superficial deposits. Karst development is variable across the Chalk. Two features of the Chalk that may reduce its vulnerability to contamination by BPA even where at outcrop are:

- Most recharge is by plug flow through the matrix, this is a slow process in which recharge (and any contaminants contained within it) move slowly downwards through the unsaturated zone at rates of around 1 m per year). This mechanism can be bypassed by storm events and by recharge through Karst features; and
- The Chalk is that it is a dual porosity aquifer in which the movement of contaminants is attenuated by diffusional exchange between mobile fissure water and slow moving or immobile matrix porewater. As a result, contaminant migration can be slow.

Most of the locations on the Chalk are in areas where there is superficial cover and limited Karst development.

The Lower Greensand may meet two of the conditions of the Lincolnshire Limestone in that it can be relatively thin and may have thin overlying soils. The Hythe Formation within the Lower Greensand shows fissure flow characteristics that may allow rapid contaminant movement. However, this aquifer does not contain soluble material and therefore does not undergo solution weathering.

The near-absence of locations in the Sherwood Sandstone suggests that this aquifer is at low risk from BPA.

The findings of this assessment, combined with the understanding of the physico-chemical properties of the EDCs have been used to inform the understanding of the likely fate of EDCs in groundwater and from that the risks to groundwater. However, from the results presented here, it is apparent that in general terms the **likelihood of BPA reaching groundwater at elevated concentrations is low**. The **exception** is in the **Lincolnshire Limestone**.

5.10 Fate of EDCs

The literature review found that most EDCs undergo relatively rapid transformation (degradation) under aerobic conditions compared to well-known persistent contaminants in which they breakdown to smaller and less harmful substances. Degradation rate and partition coefficients (Kd or Koc) are the key variable in understanding the fate of EDCs in the subsurface environment.

Most well-known groundwater contaminants have relatively slow degradation and low Kd such that they move rapidly and degrade slowly allowing them to migrate over distance. In contrast, the EDCs have relatively high Kd and degrade relatively quickly which means that they would not be expected to be widespread in groundwater. From the understanding of their properties, for EDCs to be found in groundwater at a drinking water supply then one or more of the following conditions is required:

- A source of EDCs in the catchment in which concentrations are significantly higher than proposed drinking water standards;
- Aerobic pathway:
 - ▶ Rapid movement from the source to supply; and
 - ▶ Limited attenuation or dilution along the pathway.
- Anaerobic pathway:
 - ▶ Persistent anaerobic conditions along the pathway. Anaerobic conditions will generally be limited to organic rich and waterlogged soils and to groundwater in organic rich low transmissivity confined aquifers. They may also occur where contaminant loading is sufficiently high to overwhelm the attenuation capacity of soils and aquifers.

5.10.1 Soil pathway

The literature review found that degradation rates in soils were fast (5 to 15 days). Simple calculations assuming plug flow through the soil zone suggest that EDCs spread at the surface and subject to leaching by infiltrating rainfall resulting in plug flow are unlikely to be transported beyond the soil zone into aquifers.

Note plug flow is the steady downward movement of water within the wetted part of the soil profile as opposed to rapid movement via macro features (bypass flow). In the context of this study, plug flow is predictable, slow and steady and can be modelled. Flow in macro features varies depending on soil type, time of year and rainfall intensity and is inherently unpredictable and cannot be modelled at the national scale.

Plug flow is likely to be the dominant mechanism for the downward movement of infiltration containing contaminants at most locations for most of the year but there will be situations and locations where bypass flow is the dominant mechanism.

An additional consideration is the timing of downward movement. For a source at the ground surface (mainly M2L) then the timing of application should be controlled to prevent excessive leaching

5.10.2 Unsaturated zone pathway

The degradation rate beneath the soil zone is likely to be much lower than in the soil zone because:

- There are fewer micro-organisms compared to soils which are biologically active;
- The supply of dissolved oxygen can be more limited whereas in soils atmospheric oxygen is readily-available; and
- Fewer nutrients.

As a result, degradation rates are likely to be much lower than in the soil zone. There is limited information on degradation rates in the unsaturated zone and aquifers and it is possible that they are slow. From experience with other contaminants, degradation rates can also vary depending on REDOX conditions, most organic compounds degrade rapidly in aerobic conditions but slowly or not at all in anaerobic conditions. However, information on EDCs was not found. This remains an uncertainty but for the purpose of this assessment, degradation is assumed to take place under a range of conditions.

Similar plug flow calculations to the soil zone but with lower degradation rates indicate that EDCs are unlikely to reach the water table at concentrations of concern where the unsaturated zone is reasonably (e.g. more than 2 m) thick.

Example calculations are provided in Table 5.17, based on the following assumptions:

- Rainfall recharge of 250 mm/yr (typically value for lowland England);
- Effective porosity of 20%;
- Bulk density of 1.8 Mg/m³;
- Leakage rate from an engineered landfill of 50 mm/yr;
- Fraction of organic carbon (foc) of 0.01 (1%) used to calculate a value of K_d (where K_d=K_{oc}.foc);
- Dispersion of 0.1; and
- Contaminant properties for BPA: K_{oc} of 316 (Log k_{oc} of 2.5) and degradation half life of 340 days (Table 3.2).

Table 5.19 Unsaturated zone pathway concentrations

Source	UZ thickness (D)	Unretarded TOT (plug flow) (years)	EDC concentration in source (µg/l)	Retarded TOT (plugflow) (years)	Cuz (no degradation) (µg/l)	Cuz (degradation)
Engineered landfill	3	10.8	228	318	228	<0.001
Unlined landfill	3	2.16	228	64	228	<0.001
M2L	5	100	100	2946	100	<0.001

The results show that retarded plug flow travel times are long and **concentrations at the water table are below detection limits when degradation is taken into account**. It is therefore likely that EDCs found in aquifers do not pass through the soil zone or move via plug flow through the unsaturated zone within infiltration but instead bypass these zones or are subject to hydraulic loading from concentrated runoff such that transit times are quick (hours or days). Alternatively, if EDCs do not degrade in anaerobic conditions, then transport could occur along a pathway where conditions are anaerobic. Such conditions may exist beneath and downgradient of unlined landfills. The analysis suggests that in areas of thick unsaturated zones and / or where the unsaturated zone is composed of granular material that prevents bypass flow then the risk that EDCs will migrate to the water table is very low.

5.10.3 Aquifer pathway

The length of time it will take for an EDCs to travel to the point of abstraction is important because they degrade over time, such that long travel times maximise the opportunity for attenuation. **Travel times in most aquifers are long reflecting the slow movement of groundwater, under these conditions EDCs are unlikely to reach drinking water supplies at concentrations of concern**. There are a number of situations in which this slow movement can be bypassed (after Morris, Undated)), which include:

- Aquifers where flow is via well-developed fracture systems, or possibly gravels where flow is intergranular but permeability and groundwater velocities are high. This includes fracture flow aquifers such as karstic limestones (including some parts of the Chalk) where flow along major fissure systems can be rapid;

- There is interaction with nearby surface water for example shallow boreholes adjacent to rivers where the formation is acting mainly as a filter;
- Where the supply is effectively 'surface water temporarily underground' (term from Morris, undated), which includes springs, wells and boreholes in karstic limestone areas;
- Drains and some catchpit systems drawing from shallow-circulation spring systems; and
- Where the location, design, construction or operation of the supply permits water of recent origin to 'short-circuit' and mix with the main flow system for example where runoff enters via abandoned wells or shafts, or by overland flow to a spring, or ingress down a borehole annulus from defective casing or inadequate sanitary seal. This also includes screen designs for borehole that permit mixing of contaminated water from an upper level, either an overlying superficial aquifer or a separate shallow flow system with deeper groundwater.

Such water supplies are vulnerable to other forms of contamination, notably by micro-organisms / pathogens. As a result of concerns related to migration of cryptosporidium, use of many of the more vulnerable water supplies with rapid runoff has been discontinued by water companies, including a number of sources in the carboniferous limestone.

5.11 Risk to groundwater from BPA

The understanding of the environmental fate of BPA and the data from the EA monitoring have been used to assess risks to drinking water supplies. The **main risk elements** identified by the analysis, which are:

- A source of BPA is required, which is related to land use in a catchment. The analysis of groundwater monitoring data suggests a link to rural land use;
- The source concentration must be high enough to result in detectable concentrations in groundwater and potentially generate concentrations in excess of proposed DWS at the water supply;
- A rapid pathway into groundwater, which requires either hydraulic loading and / or direct pathways into groundwater via fractures or fissures in the unsaturated zone and/ or a thin unsaturated zone otherwise BPA will degrade before it reaches groundwater;
- Rapid flow within an aquifer, which requires fissure or fracture flow or highly permeable intergranular aquifers, otherwise BPA will degrade before it reaches the water supply; and
- Limited dilution within the aquifer.

For there to be a risk the BPA must be present in the catchment to a drinking water supply. Source Protection Zones (SPZs) are divided into 3 zones an inner zone that represents a 50 day travel time, an outer zone that represents a 400 day travel time and the total capture zone. The risks from EDCs will be higher in the inner zone and lower in the TCZ as increased travel time allows for attenuation. However, in aquifers with rapid flow pathways, these can bypass these zones and therefore the risk is across the TCZ.

Most of these factors are included within the EA's Groundwater Vulnerability map (EA, 2017) and, therefore, this has been used as the primary basis for assessing risk.

5.11.1 Sources

Sources of EDCs were set out in Table 5.15. Concentrations of EDCs in some of these sources (sewage, runoff, surface water) are insufficiently high to explain the occurrence in groundwater, i.e. the source concentrations are similar or lower than those found in groundwater, before allowance for attenuation or

dilution along the pathway. In addition, these sources are associated with urban areas and the EA data indicates few occurrences in urban areas. On that basis, these sources are not considered further. The remaining sources are therefore: M2L and landfill. Only BPA is considered. For landfill, it is likely that the source needs to an unengineered landfill, as engineered liners reduce rates of leakage to low values, which means that the flux of contaminants from engineered landfills is low. In addition, engineered landfills over Principal Aquifers are rare due to planning constraints on their location.

5.11.2 Unsaturated zone pathway

Risks are likely to be highest where the unsaturated zone is thin and where recharge bypasses the soil zone either through discharge features such as soakaways or via fissures. The analysis of EA data suggests that sources are largely in rural areas and therefore that discharge features, which are concentrated in urban areas, are not likely to be important. Discharges to ground are also largely for low concentration sources that are incapable of explaining the concentrations observed in groundwater, on this basis, it has been assumed that natural bypass mechanisms are the main pathway. Recharge is likely to be rapid in areas where the following conditions are met:

- Aquifer is at outcrop over most of all of the catchment, i.e. no overlying bedrock;
- Soils are thin and permeable (high leaching potential);
- Superficial deposits are thin and permeable or absent (not mapped) over most of the catchment;
- Most rainfall recharges to the aquifer rather than running off; and
- Aquifer recharge or aquifer flow is known to be fissure / fracture dominated e.g. through solution features such as sink holes.

5.11.3 Aquifer pathway

For EDCs to reach a receptor the saturated aquifer pathway is likely to have to meet some or all of the following conditions:

- Short time of travel from point of entry to water supply, possibly including bypass flow mechanisms that operate under certain conditions;
- Limited dilution, which could be due to a relatively thin aquifer.

5.11.4 Risk Assessment

The assessment of risk has been undertaken using the EA's groundwater vulnerability approach because this identifies the main risk elements of the pathway from the surface to groundwater, namely:

- Dilution potential: how much water is available for dilution;
- Proportion of effective rainfall that forms recharge (how much infiltrates);
- Soil leaching properties;
- Superficial deposit extent, thickness and permeability. The extent determines whether these deposits play a significant role, thickness and permeability govern travel times to underlying aquifers; and
- Unsaturated zone flow mechanisms in terms of whether fracture flow is important, i.e. whether there are fast pathways through unsaturated aquifers to the water table, or not.

The scoring system used by the EA’s groundwater vulnerability mapping is set out in Table 5.20. The score consists of an index score multiplied by a weighting factor. The greater the score, the lower the risk of a pollutant affecting the aquifer. The weighting factor reflects how an attribute affects the vulnerability of an aquifer. Weighting factors have a score between 0 and 3 as follows:

- 0 – layer does not contribute;
- 1 is a minor process;
- 2 is a significant process; and
- 3 is a dominant process.

The index score is related to the evidence that a layer attribute will affect pollutant loading and are:

- 2 = good evidence;
- 1 = some evidence; and
- 0 = no evidence.

Table 5.20 Groundwater Vulnerability Scoring

Characteristic	Attribute	Index Score	Weighting Factor		
			Superficial aquifer	Bedrock aquifer	
Dilution	Available water	<300 mm/yr	0	1	1
		300-550 mm/yr	1		
		>550 mm/yr	2		
Recharge	Infiltration (baseflow index)	>70%	0	1	1
		40-70%	1		
		<40%	2		
Soil	Leaching Class	High 1	0	2	2
		High 2	0		
		High 3	0		
		Intermediate 1	1		
		Intermediate 2	1		
		Low	2		
Superficial Deposits	Extent / patchiness	<90%	0	0	3
		>90%	2		
	Thickness	<3 m	0	0	2
		3-10 m	1		



Characteristic	Attribute	Index Score	Weighting Factor	
	>10 m	2		
	Recharge potential	High	0	0 1
		Medium	1	
		Low	2	
Unsaturated zone	Flow mechanism (fracture, mixed, intergranular)	Fractures (well connected)	0	0 2
		Fractures (poorly connected)	2	
		Mixed	1	
		Intergranular	2	

The combination of weighting and index score is assigned a vulnerability according to Table 5.21.

Table 5.21 Groundwater vulnerability Classification

Vulnerability Classification	Superficial aquifer	Bedrock aquifer
Low	>5	>10
Medium	3-6	7-10
High	<3	<7

Situations with high vulnerability are a combination of most of the following:

- Low infiltration;
- High recharge;
- Permeable soils (High leaching potential);
- Limited presence of superficial deposits (deposits are thin and / or patchy);
- Permeable superficial deposits (high leaching potential); and
- Rapid movement through the unsaturated zone.

These characteristics are also those that are likely to lead to high risk from BPA when combined with a source. On this basis, high groundwater vulnerability and the presence of a source leads to higher risk from BPA.

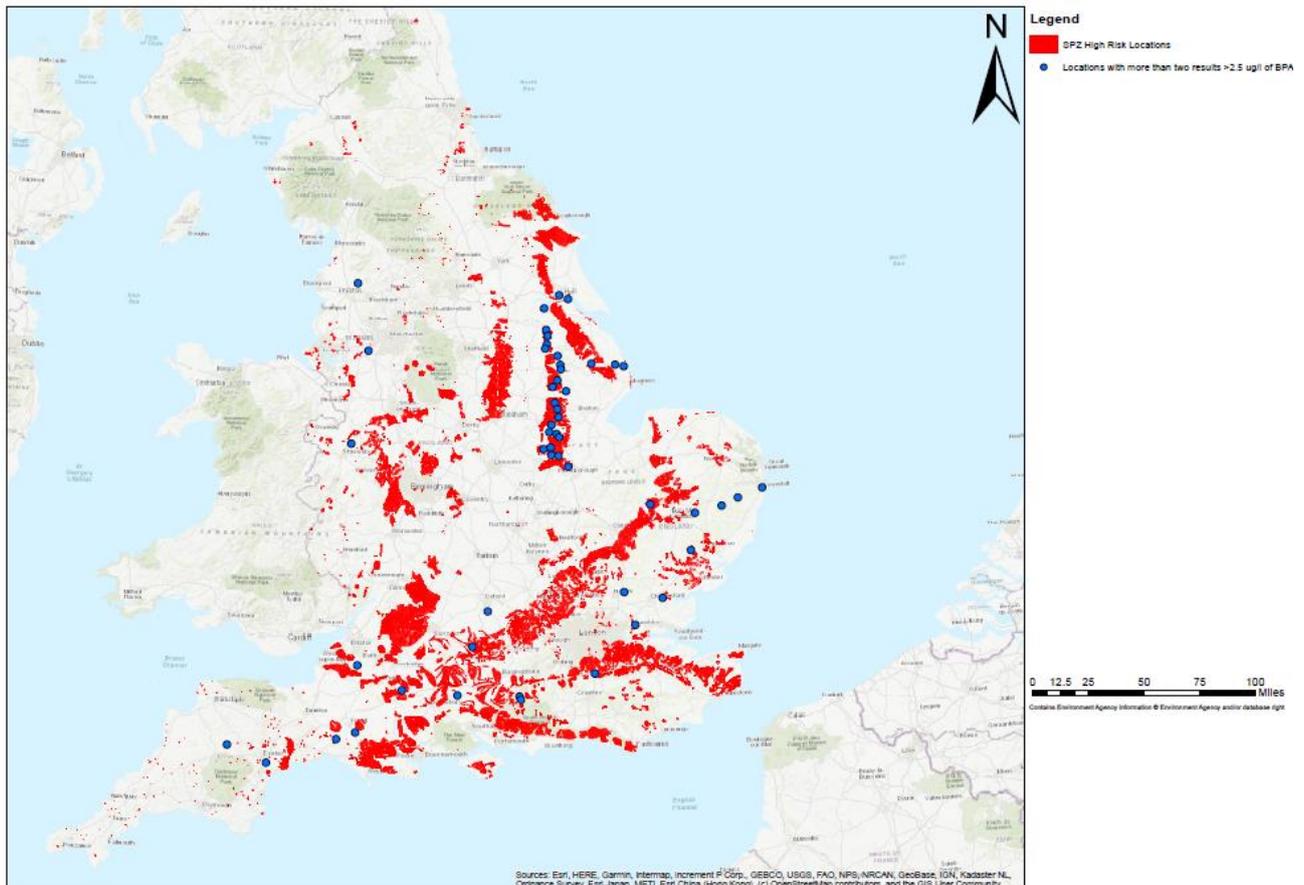
Groundwater vulnerability scoring does not take into account the presence of soluble rocks, however, the presence of such rocks is shown on maps through the use of a stippled layer that indicates areas of higher risk. The presence of soluble rock was taken from information held by the British Geological Survey. Areas where soluble rocks are present are likely to be high risk. The soluble rocks layer is visible on Defra’s magicmap (<https://magic.defra.gov.uk/magicmap.aspx>) but was not available for the figures presented here.



The maps in magicmap also indicate areas where local information or knowledge of the EA indicates higher risk from fast pathways, this mainly applies to areas of soluble rock.

For there to be a risk to drinking water supplies, in addition to vulnerability, the activity must take place within a source protection zone (SPZ). Figure 5.23 shows areas of high vulnerability that lie within a SPZ.

Figure 5.23 Areas of high bedrock groundwater vulnerability within a SPZ and locations where BPA exceedances are reported



5.11.5 Results

Figure 5.23 shows SPZs in areas of high groundwater vulnerability where there are also soluble rocks. The maps show that drinking water supplies that take water from the main limestone aquifers of England and Wales (Chalk, Oolite, Carboniferous Limestone) have a high risk where they are at outcrop. Based on the assessment of the EA data, the Lincolnshire Limestone (part of the Oolite principal aquifer) is particularly at risk, which is likely to be due to limited dilution.

The risk from land use has not been included because a definite link to a particular land use cannot be made from the data. Based on the relatively high occurrence of BPA in the Lincolnshire Limestone, there appears to be a link to arable farming, suggesting that the source is (or was) Materials to Land.

5.11.6 Conclusion

In general, risks of the three EDCs contaminating a groundwater supply are low because:

- EDCs are poorly mobile in soils and groundwater due to their high retardation (affinity for the solid phase) and relatively rapid rate of degradation, which means that they move slowly relative to infiltration and groundwater and degrade at a rate that is fast compared to their rate of movement. Of the three EDCs under consideration, BPA is the more mobile as it has the highest solubility and a relatively lower partition coefficient than the other two EDCs;
- There are limited numbers of sources, which means that they are unlikely to be present at elevated concentrations in most catchments; and
- Source concentrations, for most of those sources identified, are relatively low. Where the source concentration is high then it can overwhelm the attenuation capacity of soils and aquifers but in the case of EDCs, low concentrations are unlikely to do this. A relatively low source concentration and a rapid rate of degradation mean that concentrations fall rapidly in the direction of flow and fall below drinking water standards within a short distance.

Groundwater monitoring across England has identified the **widespread but sporadic presence of BPA at low concentrations** but only a small number of locations show repeated higher concentrations. E2 and NP were not found in groundwater. However, analysis was by GC-MS or LC-MS scan so the results should be treated with caution. **The absence of E2 and NP is consistent with their lower mobility** compared to BPA may also reflect differences in the use of the different EDCs.

As a result, **for most groundwater supplies in England and Wales, the likelihood of BPA exceeding the proposed standard (2.5 µg/L) is likely to be tolerable and the likelihood of E2 and NP exceeding the benchmark values is negligible.** However, in some catchments, a proportion of the water arrives rapidly via fissures, particularly as a result of intense rain events and in these catchments there is a **higher risk that BPA will reach drinking water supplies** at concentration of concern. This rapid movement can transport contaminants that would not normally be found in groundwater and risks of finding EDCs will be higher in these catchments. Rapid flow in fissures is mainly a feature of soluble aquifers (limestones). In England and Wales these include the following Principal Aquifers:

- The Chalk of Southeast England, East Anglian, Lincolnshire and East Yorkshire;
- The Lincolnshire Limestone;
- Carboniferous Limestone mainly found in the Pennines, South Wales and the Mendips; and
- The Corallian Limestone in the North Yorkshire Moors.

6. Overall conclusions

The purpose of this project was to investigate the risk of non-compliance of 3 EDCs (NP, BPA and E2) in drinking water across England and Wales, under the newly proposed drinking water standards. Since the project started, the proposed limit value for BPA is under consideration again and may now be revised to 2.5µg/l (from 0.01µg/l), so possible risk of exceedance has been evaluated in relation to both the original proposed limit and newly proposed standards for BPA. E2 and NP are likely only to appear in a watchlist.

Our outputs from each of the proceeding tasks indicate the following conclusions in relation to these three EDCs and key areas within England and Wales where the highest potential risk of exceeding the proposed values in drinking water:

- **For NP the likelihood of exceeding the proposed standard in drinking water supplies appears to be relatively low.** The data available both within the literature but also from the modelling of surface water concentrations indicates that exceedances of the proposed drinking water standard are infrequent apart from in very low flow conditions. Furthermore, NP has not been detected in groundwater monitoring data from the Environment Agency and the chemical properties of the substance indicate that it is unlikely to migrate to groundwater supplies. Restrictions on use are also likely to further reduce environmental concentrations of NP.;
- **For E2 there is some evidence to indicate that it does occur in river sources above the benchmark value .** The limited data that are available for drinking water have not detected E2 in drinking water. This is consistent with bench scale studies that report high removal of E2 during by water treatment . When undertaking the modelling assessment for treated drinking water derived from surface water (Task 3) we see no exceedances of the 1ng/l proposed DWD standard when using the average/mean concentration estimates, however, in a low flow situations, we see almost 50% of abstraction points exceeding the 1ng/l proposed DWD standard even after applying drinking water treatment, predominantly in the Thames, Anglian and Midlands regions; and
- **For BPA, of the three EDCs examined in this study, appears to present the highest likelihood of exceeding the original proposed value in drinking water supplies in England and Wales.** Highest risk areas for groundwater within England and Wales appear to be in proximity to limestone aquifers of the South east, Anglian and Midland regions which agrees with the results from the surface water modelling of concentrations of BPA at drinking water abstractions points. Whilst considering the proposed standard of 2.5 µg/l and mean river concentrations, all the river reaches with abstraction points in England and Wales are at low risk. In low flow conditions, the majority of the river reaches are at low risk with 38% at medium risk and no reaches identified as at high risk.

Recognising that this study takes a first step to risk assess water bodies used for abstraction, it must be noted that the results presented in this report should be interpreted with care especially those from the surface water modelling. As noted from the conclusions of Task 1, data to corroborate estimates of the three EDCs is sparse and as such there is a high level of uncertainty in the predictions made. Overall, for all the EDCs, there is a paucity of data on occurrence of these substances in drinking water sources in the UK and the effectiveness of drinking water treatment processes. Further monitoring is suggested for all three EDCs.

Key sources of all three EDCs need to be better defined to improve estimates of the level of non-compliance of NP, BPA and E2 in drinking water across England and Wales, under the proposed drinking water standards.

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Task 1 Q1 references

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Appendix A

Risk Maps for England and Wales

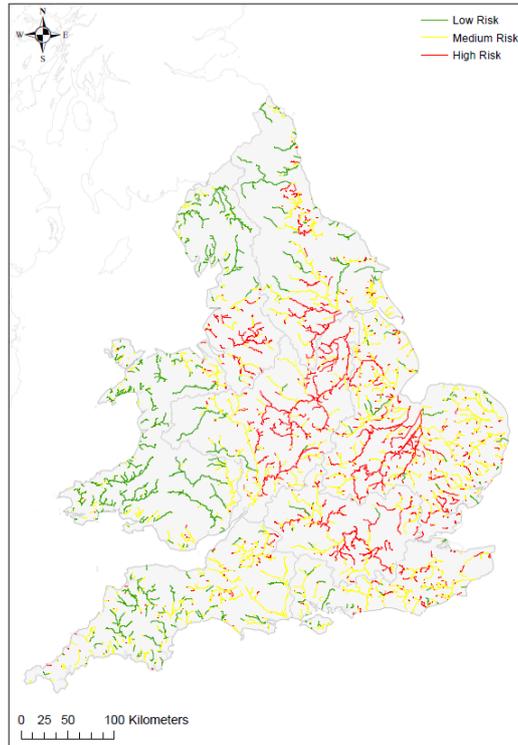


Figure A.1 Risk map for Beta estradiol (E2) using E2-Scenario 1 (characterisation of influent load, Table 5.4) based on mean concentrations (average flow conditions).

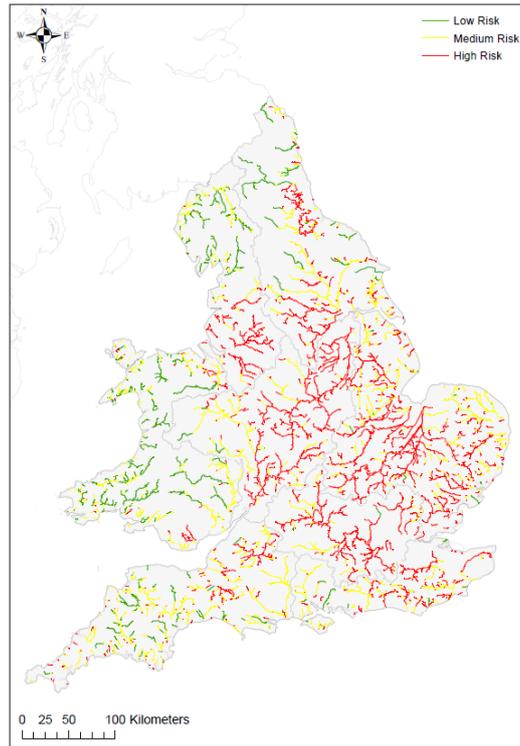


Figure A.2 Risk map for Beta estradiol (E2) using E2-Scenario 1 (characterisation of influent load, Table 5.4) based on 90th percentile concentrations (low flow conditions).

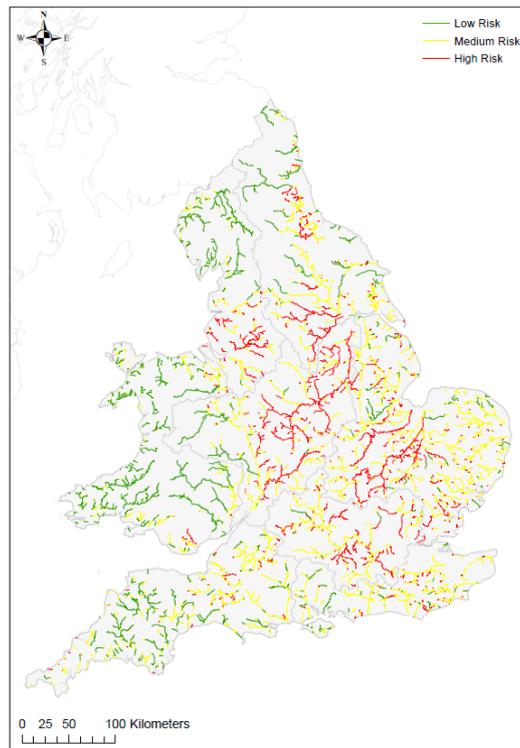


Figure A.3 Risk map for Beta estradiol (E2) using E2-Scenario 2 (characterisation of effluent concentration, Table 5.4) based on mean concentrations (average flow conditions).

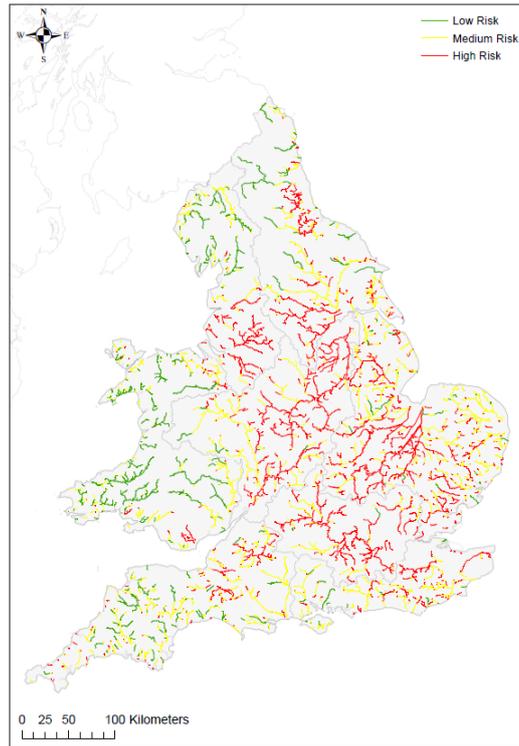


Figure A.4 Risk map for Beta estradiol (E2) using E2-Scenario 2 (characterisation of effluent concentration, Table 5.4) based on 90th percentile concentrations (low flow conditions).

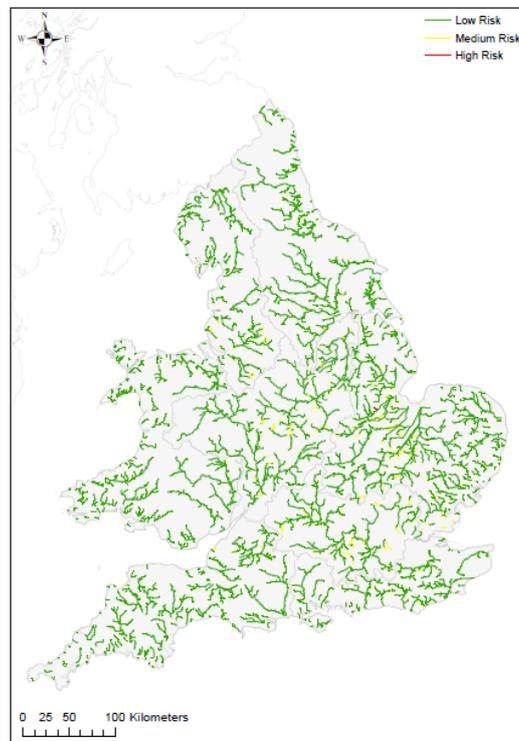


Figure A.5 Risk map for Bisphenol A (BPA) using BPA- Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l, Table 5.6) based on mean concentrations (average flow conditions). The environmental standard of 100 ng/l has been considered.

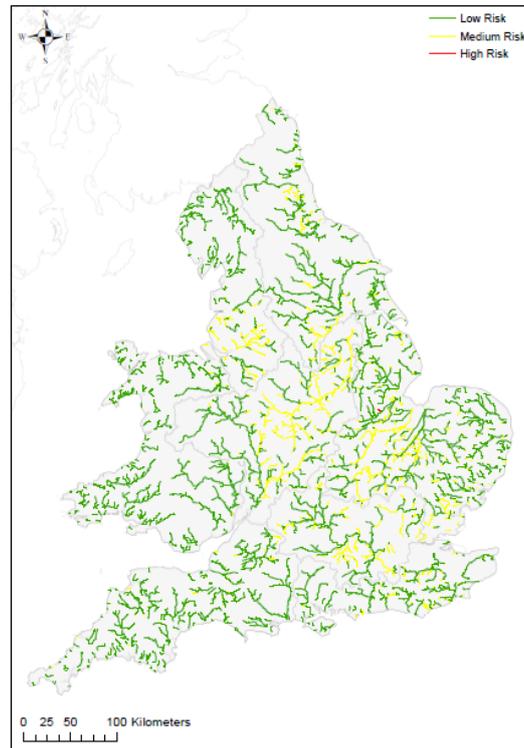


Figure A.6 Risk map for Bisphenol A (BPA) using BPA- Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l, Table 5.6) based on 90th percentile concentrations (low flow conditions). The environmental standard of 100 ng/l has been considered.



Figure A.7 Risk map for Bisphenol A (BPA) using BPA- Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l, Table 5.6) based on mean concentrations (average flow conditions). The environmental standard of 2500 ng/l has been considered.

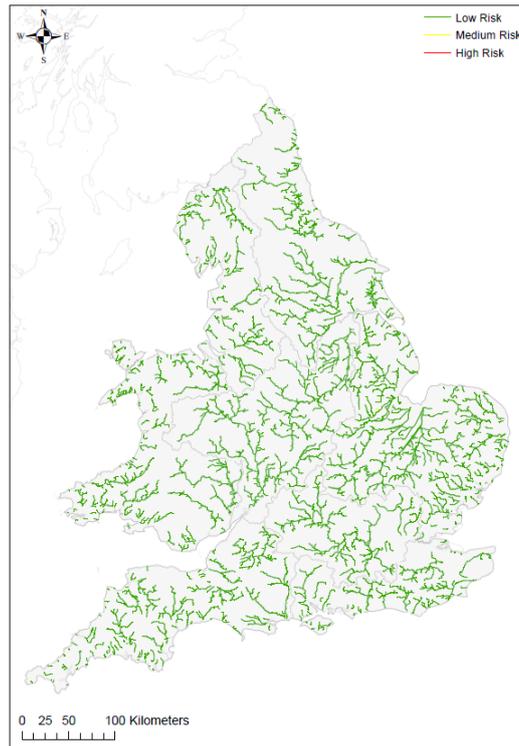


Figure A.8 Risk map for Bisphenol A (BPA) using BPA- Scenario 2 (characterisation of influent load, $C_B = 0$ ng/l, Table 5.6) based on 90th percentile concentrations (low flow conditions). The environmental standard of 2500 ng/l has been considered.

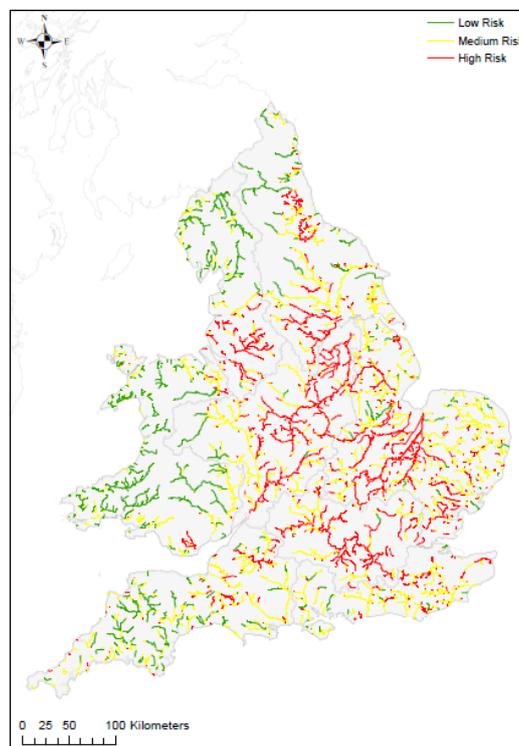


Figure A.9 Risk map for Bisphenol A (BPA) using BPA-Scenario 4, characterisation of effluent load, $C_B = 0$ ng/l, Table 5.6) based on mean concentrations (average flow conditions). The environmental standard of 100 ng/l has been considered.

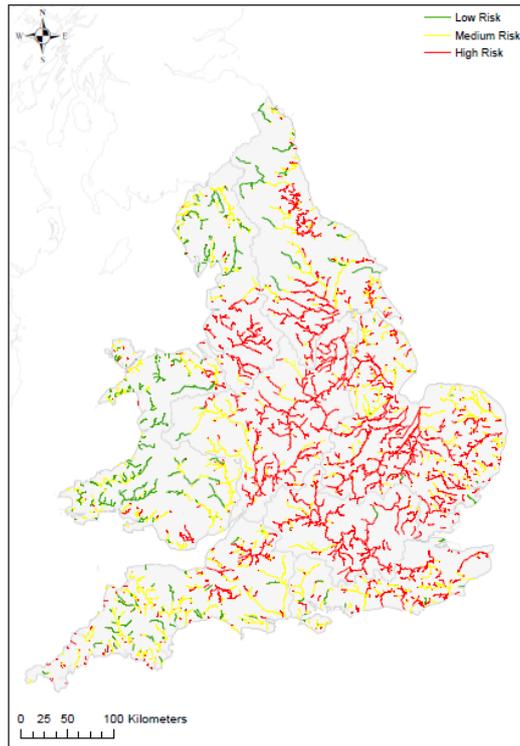


Figure A.10 Risk map for Bisphenol A (BPA) using BPA-Scenario 4, characterisation of effluent load, $C_B = 0$ ng/l, Table 5.6) based on 90th percentile concentrations (low flow conditions). The environmental standard of 100 ng/l has been considered.

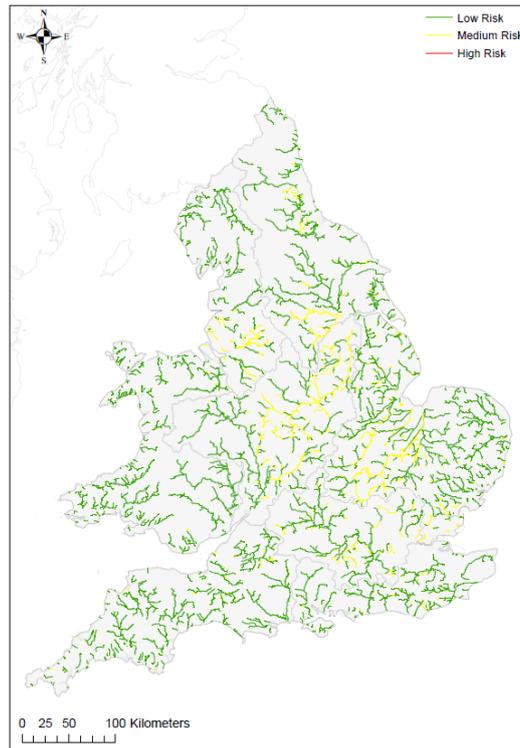


Figure A.11 Risk map for Bisphenol A (BPA) using BPA-Scenario 4, characterisation of effluent load, $C_B = 0$ ng/l, Table 5.6) based on mean concentrations (average flow conditions). The environmental standard of 2500 ng/l has been considered.

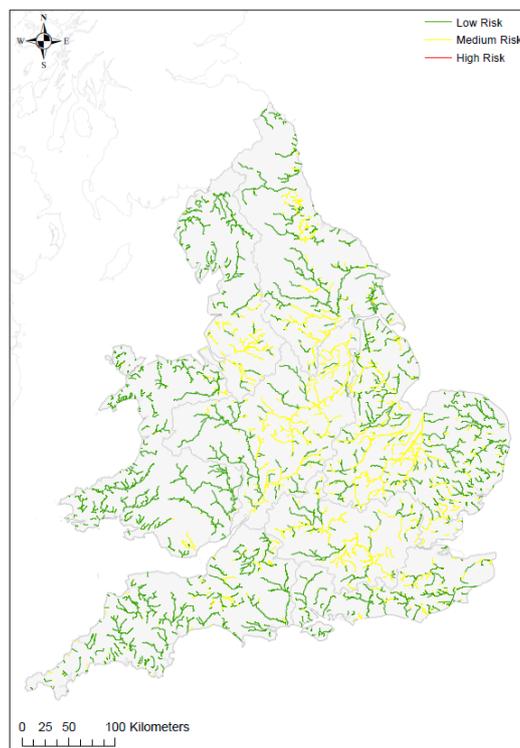


Figure A.12 Risk map for Bisphenol A (BPA) using BPA-Scenario 4, characterisation of effluent load, $C_B = 0$ ng/l, Table 5.6) based on 90th percentile concentrations (low flow conditions). The environmental standard of 2500 ng/l has been considered.

Appendix B Systematic literature review protocol



Protocol for a systematic evidence map of occurrence of 17 β -estradiol, bisphenol A and nonylphenol in drinking water in the United Kingdom

Registration:

Final protocol uploaded to Zenodo and attributed the following digital object identifier,

Authors:

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Authors' contributions

Wood Plc in collaboration with Brunel University London and the Centre for Ecology and Hydrology (CEH) submitted a tender that met the technical specifications of the invitation to tender developed by Department for Food and Rural Affairs (Defra) and the Drinking Water Inspectorate (DWI). This protocol was drafted collaboratively by OVM and AB with the input of JMcP. AB contributed her specialist expertise in ecotoxicology and endocrine disruption in wildlife. JMcP contributed her expert knowledge on information systems and literature databases. OVM contributed her knowledge of water management, endocrine disruption and good practice of systematic review methods.

Funding and sources of support

The time spent on this project by Olwenn V Martin, Alice Baynes, Joanne McPhie and Liz Nicol is funded by Defra.

Role of the funder:

The protocol for this systematic evidence map was developed in response to an invitation to tender (Invitation To Tender reference: itt_5538 (25853), Project DWI 70/2/328) and Defra and DWI reviewed all documents at all stages.

Competing interests

The authors have no competing interests to declare.

Introduction

Regulatory rationale

Endocrine disruptors (EDCs) are a diverse group of chemicals, both naturally occurring and synthetic, that have the potential to alter the normal functioning of the hormonal system across a wide range of wildlife species as well as in humans (especially during early development). Continuous domestic release of many of these chemicals (particularly to wastewater systems) gives rise pseudo-persistence in the environment, and they have frequently been found within the sewerage system and rivers. Peer-reviewed and grey literature verifies the occurrence of 17- β -estradiol (E2), Nonyl phenol (NP) and Bisphenol A (BPA) in both surface and groundwater. The rate of incidence of these three EDCs in wide scale surface/groundwater monitoring programmes such as the Chemical Investigation Programme (CIP) and BGS surveys suggests that their occurrence could be expected at low levels in drinking water sources across England and Wales.

Drinking Water Directive draft proposal

In 2016 the completion of a regulatory fitness evaluation for the Drinking Water Directive (98/83/EC) (DWD) found that the DWD was largely successful in delivering the provision of high-quality drinking water across Europe. Levels of compliance were noted to be high, yet one specific area of attention has been the list of pollutants/parameters that are reported. This list has not been updated since 1998 (the year of the DWD was implemented) and does not consider any emerging contaminants.

The EC has since proposed to revise the Directive in order to improve the quality of drinking water and update parameters monitored and set over 20 years ago. An outcome of this evaluation is the adoption of WHO recommendations for three endocrine- disrupting compounds: 17- β -estradiol: 0.001 $\mu\text{g/L}$; Nonyl phenol: 0.3 $\mu\text{g/L}$; and Bisphenol A: 0.1 $\mu\text{g/L}$. The proposed standards for these three EDCs are being used as precautionary benchmarks, close to the environmental quality standard (EQS) for aquatic protection, to indicate possible estrogenic activity in drinking water as they are already known to be found in surface (source) water.

Thus, understanding the potential risk of non-compliance to proposed drinking water standards requires consideration. This project aims to close the knowledge gap their presence in surface and groundwater and the potential scale of the risk for drinking water across England and Wales.

Aim and objectives

The overarching aim of the project therefore aligns with the draft DWD proposal and the introduction of the risk-based approach to water safety by including an initial non-compliance risk assessment of water bodies used for abstraction posed by the presence of these three EDCs.

Within this context, the aim of this systematic evidence map is to identify the most relevant background literature pertaining to the occurrence of these three compounds in drinking water and sources of drinking water in England and Wales with a specific objective to inform subsequent modelling exercises.

Methods

This protocol has been drafted with specific regards to the PRISMA-P (Preferred Reporting Items for Systematic review and Meta-Analysis Protocols) 2015 checklist⁵¹ and is giving due consideration to the Code of Practice for the Conduct of Systematic Reviews in Toxicology and Environmental Health Research (COSTER)⁵².

Eligibility criteria

Early decisions made during protocol development have significant impact on the scope and form of the systematic map. Protocol development is underpinned by imparting a common understanding of the context and motivation for the review. Well-formulated statements have a critical impact on other components of the review – including the literature search strategy, data extraction, synthesis and presentation of findings.

Question formulation follows a similar procedure as that for systematic reviews, i.e. using PI/ECO (population, intervention/exposure, comparator, outcome), PIT (population, index test, target condition) or PO (population, outcome) statements.

For this systematic map, three separate questions and therefore statements have been formulated and agreed by Defra/DWI. Each of these statements has a different structure.

The first question is related to the occurrence of the compounds of interest in drinking water and sources of drinking water, in which case the population (drinking water, sources of drinking water) must be specified, as well as the outcome (concentrations). The corresponding PO statement is illustrated in Table 1.

Table 22. PO statement related to the occurrence of 17 β -estradiol (E2), nonylphenol (NP) and bisphenol A in drinking water

Q1. What is the occurrence of 17 β -estradiol, nonylphenol, bisphenol A in drinking water and sources of drinking water?	
Population	Ground and surface waters, drinking water at the tap in England and Wales
Outcome	Concentrations of E2, NP, BPA, their precursors and/or conjugates

This PO statement is operationalised as inclusion and exclusion criteria as described in Table 25.

The second question is related to the chemical analysis methods available to detect and measure these compounds, in which case the population (E2, NP, BPA) must be specified, as well as the index test (chemical analysis) and the target condition (detection and measurements of the compounds of interest). The corresponding PIT statement is illustrated in Table 38.

⁵¹ Shamseer L, Moher D, Clarke M, Ghersi D, Liberati A, Petticrew M et al. (2015) Preferred reporting items for systematic review and meta-analysis protocols (PRISMA-P) 2015: elaboration and explanation *BMJ* ; 349 :g7647

⁵² Whaley et al. "A Code of Practice for Conduct of Systematic Reviews in Toxicology and Environmental Health Research (COSTER)" Under development

Table 38. PIT statement related to the analytical chemistry methods available to measure the occurrence of 17β-estradiol (E2), nonylphenol (NP) and bisphenol A in drinking water

What methods of chemical analysis are available for these E2, NP and BPA in drinking water and sources of drinking water?	
Population	Concentrations of E2, NP, BPA, their precursors and/or conjugates
Index Test	Chemical analysis
Target Condition	Quantification of low levels of E2, NP, BPA, their precursors and conjugates in surface, ground and drinking water samples

This PIT statement is operationalised as inclusion and exclusion criteria as described in Table 41.

The final question is related to the performance or efficiency of existing drinking water treatment technologies at removing the compounds of interest, in which case the population (drinking water, sources of drinking water) must be specified, as well as the outcome (concentrations). The corresponding PO statement is illustrated in Table 39.

Table 39. PICO statement related to the removal efficiency of 17β-estradiol (E2), nonylphenol (NP) and bisphenol A by various drinking water treatment technologies

How efficiently are E2, NP and BPA removed by drinking water treatment?	
Population	Sources of drinking water
Intervention	Drinking water treatment technologies
Comparator	Concentrations of E2, BPA or NP prior to treatment
Outcome	Removal efficiencies of E2, NP, BPA, their precursors and/or conjugates

This PICO statement is operationalised as inclusion and exclusion criteria as described in

Table 42.

Table 25. Q1 eligibility criteria

		Inclusion criteria	Exclusion criteria
Population	Ground and surface waters, drinking water at the tap in England and Wales	<ul style="list-style-type: none"> • Groundwater, surface water (both rivers and reservoirs) • Drinking water samples (both as final treated effluent and at the tap?) • Sampled in England and Wales 	<ul style="list-style-type: none"> • Wastewaters, Effluents discharged in drinking water sources. • Water samples sourced outside England and Wales.
Outcome	Concentrations of E2, NP, BPA, their precursors and/or conjugates	<ul style="list-style-type: none"> • E2, BPA and their conjugates • NP and nonylphenol ethoxylates 	Proxy measures such as estrogenicity using <i>in vitro</i> or <i>in vivo</i> bioassays

Table 41. Q2 eligibility criteria

		Inclusion criteria	Exclusion criteria
Population	Concentrations of E2, NP, BPA, their precursors and/or conjugates	E2, BPA and their conjugates NP and nonylphenol ethoxylates	Proxy measures such as estrogenicity using <i>in vitro</i> or <i>in vivo</i> bioassays
Index Test	Chemical analysis	Gas and liquid chromatography Quantification methods	Outdated and/or insensitive methods (thin layer chromatography), methods whose sole aim is the identification of molecule.
Target Condition	Quantification of low levels of E2, NP, BPA, their precursors and conjugates in surface, ground and drinking water samples	<ul style="list-style-type: none"> • Methods that have been demonstrated to be applicable to natural or drinking water samples. • Methods sensitive enough to be able to detect compounds of interest at the range they are typically measured 	Methods applied in different matrices (e.g. biological samples, sewage effluent) where different sample preparation steps may be necessary.

Table 42. Q3 eligibility criteria

		Inclusion criteria	Exclusion criteria
Population	Sources of drinking water	Sources of drinking water or treated water at all stages of drinking water treatment up to the tap.	Wastewater influent and effluent at all stages of wastewater treatment.
Intervention	Drinking water treatment technologies	Water treatment technologies commonly applied in the UK (e.g. granulated activated carbon filtration, ...)	Novel methods not yet commonly applied at large scale. Methods common in contexts other than the UK (e.g. desalination)
Comparator	Concentrations of E2, BPA or NP prior to treatment	E2, BPA and their conjugates NP and nonylphenol ethoxylates	Proxy measures such as estrogenicity using <i>in vitro</i> or <i>in vivo</i> bioassays
Outcome	Removal efficiencies of E2, NP, BPA, their precursors and/or conjugates	Removal efficiency or sufficient data allowing te estimation of removal efficiencies, i.e. concentrations before after treatment taking into account typical retention times.	Concentrations before after treatment measured during temporally disconnected instances.

Information sources

Searches for peer-reviewed articles will be conducted in the following bibliographic databases:

- Web of Science Core Collection
- MEDLINE
- Scopus
- Full text databases e.g. CINAHL Plus and ScienceDirect
- The British Library service Zetoc to search for conference papers via resources

Further, in order to identify ongoing research, we will examine conference papers via resources like the British Library service [Zetoc](http://zetoc.jisc.ac.uk/) (<http://zetoc.jisc.ac.uk/>).

To identify grey literature not listed in databases, manual searches will be carried out using topic focused search engines such as **Environar**. Additional searches will be carried out in open access bibliographical databases such as [OpenGrey](http://www.opengrey.eu/) (<http://www.opengrey.eu/>) which searches grey literature across Europe by interrogating open access items in institutional repositories.

Manual searches of the bibliography and citations of eligible studies will be carried out.

Finally, this can be complemented by targeted manual searches of open repositories on the website of British institutions such as Defra, EA, DWI, UKWIR, and UK Water Companies.

Language capabilities within the project team include German, and French in addition to English. For studies in languages not covered by the project team and for which no English version can be located, the full text will be interrogated through the use of online tools such as Google Translate.

Search strategy

Constructing search strategies for complex review questions can be challenging and has led to the use of multi-stranded strategies instead of a single combination of key elements, e.g. such as PI or IT. An initial series of five groups of search terms targeting either water sources, chemicals, the geographical context of interest, analytical methods or water treatment technologies elements has been developed to be run sequentially and then combined using the Boolean operators ‘AND’ and ‘OR’⁵³. The combination of these five lists of search terms corresponding to each of the three review questions is illustrated in *Figure 24* below.

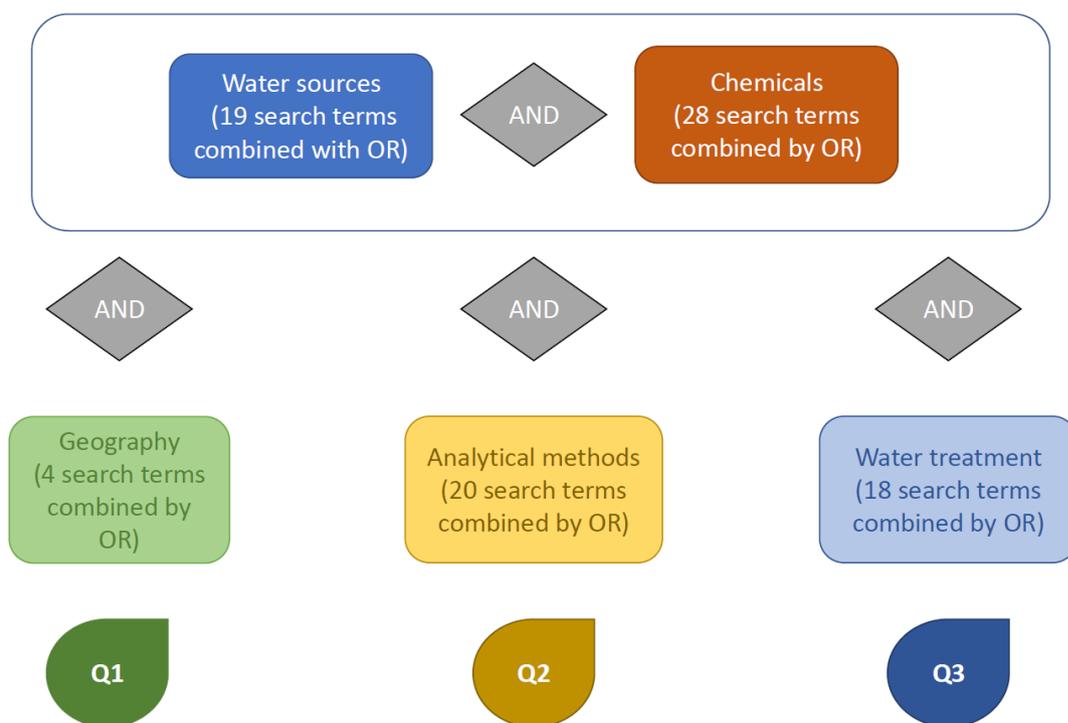


Figure 24. Schematic representation of the literature search strategy for the three review questions

A time limit of 20 years (published in 1999 or after) was agreed to insure the current relevance of the literature retrieved.

The result of pilot searches listing a total of 88 search terms and their combination in the three literature databases Web of Science, Scopus and Pubmed can be found in Appendix A.

The quality of the revised literature search strategy will be assessed by testing for its ability to retrieve pre-identified key papers and by using the EFSA critical appraisal tool (CAT) for systematic/extensive literature searches⁵⁴. The CAT focuses on both the search strategy; and the completeness of the information sources used.

⁵³ EFSA (2017). EFSA supporting publications 2017:EN-1207. 48 pp. doi:10.2903/sp.efsa.2017.EN-1207

⁵⁴ EFSA (2015) EFSA supporting publication 2015:EN-836. 65 pp. Appendix D.

Data management

Literature and all systematic review processes will be managed and coordinated with the support of the freely available online tool CADIMA established in a close collaboration between the Julius Kühn-Institut and the Collaboration for Environmental Evidence

(<https://www.cadima.info/index.php/area/evidenceSynthesisDatabase>).

Relevance screening

The list of eligibility criteria will be applied to the merged reference lists for each question with at least 10% or 200 records duplication (i.e. by two people working independently), whichever is the largest, and in two stages. In the first stage, only titles and abstracts will be checked for relevance to the study question. Clearly irrelevant studies will be excluded. The full text of the resulting list of included references after title/abstract screening will then be retrieved and examined for inclusion. The reason for exclusion of studies after assessment of the full text will be recorded.

Multiple reports of the same research (e.g. multiple publications, conference abstracts etc.) will not be excluded but instead the methodological information from each of the reports shall be collated as part of the data extraction process as one unit of evidence.

The CADIMA online tool facilitates the process of consistency check by identifying disagreement between the two evaluators. Disputes will be arbitrated and resolved by a third party, the project manager and most senior ecotoxicology expert. For quality control purposes, the percentage agreement between the two independent evaluators and kappa statistic will be reported.

The inter-rater reliability (level of agreement between two or more assessors) of clearly formulated inclusion and exclusion criteria will be also piloted and eligibility criteria shall be clarified and amended accordingly, if necessary.

Data extraction

Although this systematic evidence map has been organised around three central questions, and as such requires three separate statements and corresponding eligibility criteria, a non-negligible proportion of articles can be reasonably expected to meet the criteria for more than one question. Further, all studies measuring concentrations of the compounds of interest in drinking water sources or following drinking water treatment will include some description of the analytical method used. There is therefore an opportunity, in addition to collating data about suitable analytical method development, to collect data about the methods that have been used in studies of interest. This is advantageous due to the difficulties related to systematic review or evidence mapping of development of methods and the requirements to define equivocal concepts such as novelty. It was therefore decided to design one data extraction suitable for all three questions. Two questions, the first about the geographical scope and the other about whether water treatment technologies were investigated, guide the selection of parameters for which data will be extracted from individual references (i.e. superfluous parameters are shaded in grey).

One reference may report more than one experiment at more than one study site or have measured more than one of the substances of interest. Another important step prior to data extraction is therefore to define the unit of evidence, i.e. the unit that will require filling one row of the data extraction template. It is suggested that one unit of evidence will consist of one chemical per site, i.e. if several experiments have been carried out at the same site for the same chemical, summary statistics for all successive experiments will be extracted.

As all eligible records, regardless of the question they aim to answer, will report information about sampling and analytical method performance, the critical appraisal of methods is central to this exercise and forms part of the data extraction and coding itself. There is therefore an overlap between data extraction and risk-of-bias. Furthermore, the latter step is not automatically required in systematic evidence mapping. In this specific instance, it was found that this would duplicate data extraction and risk-of-bias was therefore not included. Concerns about the design or conduct of studies related to aspects other than analytical methods will be noted in the corresponding comment column. An initial data extraction template has been created comprising of elements relevant for different types of studies, e.g.:

- Meta-data (e.g. authors, date, journal name or report number),
- Information about the chemical (e.g. name, CAS number),
- Information about sampling, including:
 - Type of water source,
 - Location of sampling site,
 - Coordinates (if reported),
 - Information about the sampling method, volume, storage and preparation,
- Details of the chemical measurement method including;
 - The type of method and method name,
 - Whether a standard operating procedure exists (SOP),
 - The use of internal standards,
 - Sensitivity (limit of detection and/or limit of quantification),
 - Any reported information relevant to specificity,
- Information about water treatment type and performance.

The resulting data extraction template, included as Appendix B, will be piloted by extracting data from representative articles by all evaluators in parallel duplicates.

Data analysis

A description of the volume and characteristics of the evidence base collated in the previous step, such as the state-of knowledge on current levels of the chemicals of interest in British drinking water sources, availability of analytical methods, and performance of water treatment will be summarised narratively and if data permits visually and presented using the capabilities of the data visualisation software Tableau. An in-depth qualitative analysis will also be carried out by combining results by chemical of interest.

