PERSISTENT, MOBILE AND TOXIC SUBSTANCES – RISK TO DRINKING WATER IN ENGLAND & WALES (PHASE 2)

Final report

Report for: The Drinking Water Inspectorate

Ref. [DWI 70/2/341]

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Customer:
Drinking Water Inspectorate

Customer reference:
DWI 70/2/341

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ED15803

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12th January 2023

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ACKNOWLEDGEMENTS

We are very grateful to the following people and organisations for supply of data during this project: Luke Holmes and Mark Beeken from the Environment Agency and Thomas Andrejz and colleagues from Natural Resources Wales for supply of environmental monitoring data. Dr Vicky Bell from CEH for making available predicted discharge estimates from the MaRIUS project and the associated flow direction grid. We would also like to thank Stefan Reis (CEH) and colleagues for making available their gridded estimates of population density for the UK.

EXECUTIVE SUMMARY

Substances that are both persistent and environmentally mobile have a greater potential to pass natural barriers like riverbanks and migrate to groundwater. They will remain in surface water rather than be removed from the water phase through partitioning to sediment or organic matter and have a greater propensity to ‘breakthrough’ in standard drinking water treatment. Consequently, substances with these intrinsic properties and especially when considered in combination with toxicity may pose a risk to human health and the environment through contamination of drinking water sources. In recent years there has been an increasing body of work to explore definition of a hazard class relating to persistent, mobile, and toxic substances (PMT), and very persistent (vP) and very mobile (vM) substances, with the aim of protecting natural resources that could be used for drinking water supply.

Defra and the DWI have commissioned this project to understand the potential risk from PMT or vPvM substances to drinking water sources in England and Wales. The findings will be used to develop guidance for water companies on risk assessment and targeted monitoring to ensure drinking water supply is safe.

Substances that meet proposed PMT/vPvM criteria have been studied to investigate their potential risk to drinking water supply. Substances were selected for study based on their relevance to England and Wales and were identified as high priority for further study based on previous research, their properties, tonnage, and potential environmental emissions. They represent a subset of all substances that are likely to meet the proposed criteria for identification as PMT/vPvM.

Evidence on environmental occurrence in raw and treated drinking waters from both UK and international monitoring studies for the substances of interest have been collated. There are frequent detections in surface water and groundwaters in England and Wales for some PMT substances; these include saccharin, amantadine, 2,4,7,9-tetramethyl-5-decy-ne, melamine, 1,4-dioxane A similar pattern is observed in groundwater. There are no monitoring data available for some of the substances of interest in this project. No monitoring data for treated drinking water in England and Wales were found in the published literature for any of the substances studied. This is an evidence gap that should considered a priority in any future work.

Data and intelligence on the nature of use of the group of PMT substances studied in this project have been used to estimate quantities released to the environment and used to derive modelled surface water concentrations. A wide variety of information sources were searched. However very little information is publicly available on the amounts of each substances supplied and used in the UK. Consequently, estimates of use and release derived in this study may have a high degree of uncertainty. Conservative assumptions have been used in the absence of more accurate information.

Removal rates for each substance in both conventional drinking water treatment and advanced treatment processes have been determined. Data on the potential for removal of the compounds of interest during drinking water treatment processes (DWTPs) have been generated. Conventional drinking water treatment processes are moderately effective at removing most of the substances whilst advanced DWTPs are predicted to have a high removal efficiency.

Peer-reviewed toxicological information for each substance has been used to determine a health based guidance value (HBGV). Finally, a tiered risk assessment has been performed to characterise risk to drinking water supply at surface water abstraction points. For those substances identified as a potential risk in lower tier screening assessment, a spatially based risk assessment was then performed for England and Wales.

A tiered risk assessment using conservative assumptions and modelled exposure data suggest that most of the substances studied pose little risk to drinking water supply. Higher tier, spatially based risk assessments were performed for three of the 22 substances identified as having a potential risk to drinking water in the screening level assessment. These substances are 1,4-dioxane, tetrachloroethylene and 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride. All three substances had risk characterisation ratios (RCRs) greater than one at some surface water abstraction sites when negligible degradation in the stream network and only conventional drinking water treatment was assumed. When advanced treatment processes are considered, none of the 22 substances had a risk characterisation greater than one and are considered to pose little risk to human health.

Most monitoring data available for England and Wales were not accurately measured and there are uncertainties associated with concentrations reported. For this reason, we have not used the data to perform any validation of model outputs. Further work to validate the model outputs using fully quantitative monitoring data for substances of interest at drinking water abstraction points would be a very useful next step.

Quantitative monitoring data for those substances with the highest potential risk in both surface water and groundwaters would be a useful additional line of evidence. None of the substances studied have been identified as a very high risk.

1,4-dioxane, tetrachloroethylene and 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride should be considered for including in targeted risk based monitoring. It would be more appropriate to monitor in water for the hydrolysis product of 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride (chlorendic acid), than the substance itself.

Taking a precautionary approach, those substances identified as having a potential risk in the tier 2 assessment with conventional treatment could also be considered for monitoring to obtain quantitative data and better characterise typical environmental levels in English and Welsh water. This includes 2,4,7,9-tetramethyldec-5-yne-4,7-diol, trichloroethylene, melamine, dinoseb, dapsone, amantadine, tricarbonyl(methylcyclopentadienyl) manganese, 2-morpholinoethanol and 2,2'-dimethyl-2,2'-azodipropiononitrile.

Widespread environmental occurrence of melamine is reported. We have combined emissions estimates of melamine and melamine cyanurate, which dissociates to melamine when estimating a total emission to surface water. However, melamine is also identified as a major degradation product (70% of parent) of cyromazine, which has been used as a biocide for the control of fly larvae in animal husbandry, outdoor manure heaps, slurry reservoirs and landfill sites and other breeding sites in animal housing. Potential indirect sources of melamine, such as such as the biocidal uses for animal health and slurry management described here should be explored further to better understand and quantify their potential for release to the environment.

The project has studied 22 substances that meet proposed criteria for identification as PMT/vPvM. However, there are likely to be other substances that meet PMT/vPvM criteria and are relevant to surface water drinking water sources in England and Wales. The list of relevant PMT substances should be reviewed and updated periodically.

1. INTRODUCTION

The World Health Organisation's (WHO) drinking water safety plan principles recommends a risk-based approach to monitoring drinking water quality. This has been adopted in national regulations for England and Wales, whereby water companies and private water suppliers have a legal requirement to provide wholesome drinking water. The definition of wholesomeness requires that the water 'does not contain any substance at a concentration or value which would constitute a potential danger to human health'. A risk assessment and relevant monitoring must be carried out at each treatment works to establish whether there is a significant risk of supplying water that may cause harm to human health.

Substances that are both persistent (P) and mobile (M) have a greater potential to pass natural barriers like riverbanks and migrate to groundwater. Such substances will remain in surface water rather than be removed from the water phase through partitioning to sediment or organic matter. They will also have a greater propensity to 'breakthrough' in standard drinking water treatment because of their physico-chemical properties. Consequently, substances with these intrinsic properties and especially when considered in combination with toxicity (T) may pose a risk to human health and the environment through contamination of drinking water sources.

In recent years there has been an increasing body of work to explore data criteria for the definition of a hazard class relating to persistent, mobile, and toxic substances (PMT), and very persistent (vP) and very mobile (vM) substances, with the aim of protecting natural resources that could be used for drinking water supply (Neumann and Schlieber, 2019; Schulze *et al*., 2019; ECETOC, 2019). The German Environment Agency (UBA) and the Norwegian Technical Institute (NGI) have funded several research projects, published reports (Neumann and Schlieber, 2019) and held workshops to develop criteria for the identification of PMT and vPvM substances under REACH. The most recent workshop on PMT substances was held in March 2021. A useful summary of the outputs of that workshop presenting the current state of knowledge and highlighting key evidence gaps is provided by Hale et al., 2022. A five year research programme, ZeroPM, funded by the European Horizon's Horizon 2020 research and innovation programme commenced in October 2021. The programme aims to develop an evidence based multilevel framework to reduce pollution from persistent and mobile substances.

In Europe, substances that are persistent (P), mobile (M) and toxic (T) or very persistent (vP) and very mobile (vM) have been proposed as an additional hazard class under REACH and the Classification, Labelling and Packaging (CLP) regulations. In 2020 the European Commission published its 'Chemicals Strategy for Sustainability Towards a Toxic-free Environment' (European Commission, 2020) which commits to the introduction of PMT and vPvM as categories of substances of very high concern (SVHC). In September 2022 the European Commission consulted on a draft amendment to the CLP regulations proposing new hazard classes including PMT/vPvM.

In 2018, the Drinking Water Inspectorate (DWI) funded research to begin to understand whether some of the substances identified as potential PMT/vPvM by the UBA and NGI in 2018 might pose a risk to drinking water (DWI, 2020). The study critically reviewed the original list of 58 substances identified as potentially PMT or vPvM, summarised knowledge on the chemicals and their potential to reach water and estimated their concentration in source waters used for public drinking water supply.

The study had several limitations. Estimates of usage were very worst-case with low accuracy, as they were based on the upper bound of REACH tonnage bands. It was not possible to identify areas in England and Wales where concentrations may be higher. Furthermore, occurrence data and knowledge on removal by water treatment processes collated in the study was limited.

The DWI now requires a more refined assessment of the potential risk from PMT or vPvM substances to drinking water sources in England and Wales. Specifically:

- which PMT substances are likely to be present in water used for drinking water supply? What is the range of likely exposure concentrations in raw waters (groundwater and surface water sources)?
- what is the spatial distribution of environmental contamination and what are the risk factors that could be used to indicate potentially high sources/concentrations in a catchment?
- an understanding of the toxicology of the substances of interest
- the likelihood of removal during treatment for drinking water supply
- which substances pose the greatest risk to human health through exposure via drinking water in England and Wales?

This is needed to better understand the implications for human health and potential risk to drinking water sources from PMT substances. In turn, this will support the development of guidance for water companies on risk assessment and targeted monitoring of PMT substances to ensure drinking water supply is safe. It will also be of wider value to inform development of future UK policy on PMT substances as part of the developing Chemicals Strategy.

Evidence on occurrence of PMT substances in raw and treated waters, information on usage in England and Wales, modelled environmental exposure concentrations and knowledge of the toxicology of the listed PMT substances have been collated in this project and are presented in the following chapters.

1.1 REVIEW OF SUBSTANCES FOR FURTHER STUDY IN PHASE 2

Information on use in the UK and environmental fate gathered as part of this project has been used to review and refine the original list of PMT substances identified in phase 1 (DWI, 2020). We have also considered wider research. The following information sources have been considered when reviewing and prioritising the phase one PMT substance list:

- identification of substances as PMT or vPvM according to the UBA commissioned evaluation of all REACH registered substances (Arp & Hale, 2019)
- identification as PMT/vPvM on other lists such as the ChemSec SINLIST.
- potential for environmental release; based on emission likelihood (Arp & Hale, 2019)
- Current environmental monitoring programmes and available occurrence data
- Supply tonnage according to REACH tonnage band
- Potential for UK based point sources as identified through information collected in objective 3 of this project, for example, substances with UK REACH grandfathered registrations (as notified to HSE and published on 30th September 2021).

Removing less relevant substances from the list has allowed the study to focus in more detail on the remaining substances and inclusion of other substances that are believed to be of greater interest. Justification for inclusion or exclusion of a substances in this phase 2 work is documented in Appendix 1. The list of substances for the current project is provided in Table 1.1.

Our final list is not an exhaustive list of substances that meet the PMT/vPvM criteria but does represent a subset of substances that have been prioritised as UK relevant based on available information. At the time of writing, criteria for identification of PMT/vPvM under UK REACH have not been specified and policy development is ongoing in both the UK and EU. We recommended that the list of substances should be reviewed and updated periodically as further data become available or UK policy develops further and if it diverges from the criteria and approach proposed in the EU.

Brief background on these data sources is provided in the following sections.

1.1.1 Identification and assessment of REACH registered substances as PMT/vPvM (UBA)

The German Environment Agency (UBA) and the Norwegian Technical Institute (NGI) have funded several research projects, published reports (e.g., Neumann & Schlieber, 2019), and held workshops to develop criteria for the identification of PMT and vPvM substances under REACH.

As part of the UBA's programme of work, proposed PMT/vPvM criteria (Neumann & Schlieber, 2019) were applied to all REACH registered substances (as of May 2017) to identify PMT/vPvM candidates and priorities for further action (Arp & Hale, 2019). The criteria were applied to 15469 substances using available hazard data. A 'traffic light' system was used to categorise substances and account for uncertainties and variability in data quality when evaluating P, M and T. The authors observed that nearly 40% (3,748) of substances, had insufficient or low-quality persistence (P) data which led to either no conclusion or conflicting outcomes for assessment against P criteria. Full details are described by Arp & Hale (2019) and not repeated here.

Thirty-six percent of substances assessed were concluded to be **not** PMT/vPvM. Only 260 (3%) of REACH registered substances were identified as PMT/vPvM. Of these, 58 substances were PMT, 47 were identified as vPvM and 155 substances were PMT & vPvM (Arp & Hale, 2019).

For context, no conclusion could be drawn for 33% of REACH registered substances and a further 24% were assessed as 'potential PMT/vPvM'. This latter category was largely substances where the available P data was not sufficient to neither conclude not PMT/vPvM nor PMT/vPvM.

The final stage of the assessment carried out by Arp & Hale (2019), assigned substances to a priority category. Several factors were taken into account including uncertainties associated with assessment of substances against the proposed (UBA, 2019) P, M and T criteria, emission likelihood, REACH registered tonnage, environmental occurrence data and whether the substance was already subject to regulatory controls – such as substances that are included on the candidate list of substances of very high concern (SVHC) for inclusion on the authorisation list or identified as a priority hazardous substance under the Water Framework Directive. Substances considered by Arp & Hale (2019) to be the highest priority for follow-up – either to confirm their PMT/vPvM status or to further investigate their presence in drinking water sources were assigned to category 1. One hundred and twenty-two substances were included in this category, of which 39 were reported as also detected in water quality monitoring studies. A further 21 substances were assigned to category 2 – these are PMT/vPvM substances that are already receiving regulatory scrutiny by the European authorities.

Table 1.1 List of PMT substances in scope for phase 2 project.

Substance	CAS	EC number
2,4,7,9-tetramethyldec-5-yne-4,7-diol	126-86-3	204-809-1
1,4-dioxane	123-91-1	204-661-8
trichloroethylene	79-01-6	201-167-4
tetrachloroethylene	127-18-4	204-825-9
melamine -	108-78-1	203-615-4
dinoseb	88-85-7	201-861-7
dapsone	80-08-0	201-248-4
amantadine	768-94-5	212-201-2
hexamethyldisiloxane	107-46-0	203-492-7
tricarbonyl(methylcyclopentadienyl) manganese	12108-13-3	235-166-5
1,3,5-triazine-2,4,6(1H,3H,5H)-trione,compound with 1,3,5-triazine-2,4,6- triamine (1:1) (melamine cyanurate)	37640-57-6	253-575-7
2-phosphonobutane-1,2,4-tricarboxylic acid	37971-36-1	253-733-5
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	115-27-5	204-077-3
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	2226-96-2	218-760-9
4-aminophenol	123-30-8	204-616-2
2-morpholinoethanol	622-40-2	210-734-5
2,2'-azobis[2-methylbutyronitrile]	13472-08-7	236-740-8
1,3-dichlorobenzene	*541-73-1*	*208-792-1*
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	*78-67-1*	*201-132-3*
N-butylbenzenesulphonamide	*3622-84-2*	*222-823-6*
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	*81-07-2*	*201-321-0*
triclosan	*3380-34-5*	*222-182-2*

As part of the current project, we reviewed the phase 1 list of 34 substances (see Appendix 1 for phase 1 list), against the lists of priority lists produced from the assessment process described above and carried out by Arp and Hale, (2019).

Three substances were removed from the phase 1 list because they are no longer identified as PMT or vPvM according to the assessment process carried out by Arp and Hale (2019). The substances are; phenol (CAS 108-95-2); calcium 3-hydroxy-4-[(4-methyl-2- sulphonatophenyl)azo]-2-naphthoate (CAS 5281-04-09) and 2-piperazin-1-ylethylamine (CAS 140-31-8).

Several substances identified as 'category 1 – high priority for further follow-up' by Arp and Hale (2019) were added to the current project' list. Justification for inclusion was based on expert judgement considering hazard data, evidence of environmental occurrence in the UK, high tonnage band and high likelihood of emission.

1.1.2 Likelihood of emission

The 'emission likelihood' of a substance was determined by Arp and Hale (2019) using a simple screening approach using REACH registered tonnage data, nature of release e.g. high release to environment, wide dispersive use, environmental combined with REACH environmental release categories and to determine an emission score (E-score; Schulz et al, 2018). The final 'REACH emission likelihood' was based on the E-score and likelihood of monitoring data (Arp & Hale, 2019). Substances with a low emission likelihood, defined by Arp & Hale (2019) as substances not detected in sources of drinking water and associated with a low E-score were considered as possible candidates for removal from the current project list.

1.1.3 ChemSec SINLIST

Assessment of 344 chemicals identified through the screening process by Arp and Hale (2019) described in Section 0 above were further assessed in work carried out by ChemSec in 2019 (ChemSec, 2019). Following collation of additional data such as physico-chemical properties and environmental monitoring data and discussion with experts from member states, 24 substances were added by ChemSec to their SIN list because of their identification as PMT/vPvM. Criteria for inclusion on the ChemSec SIN list are: (i) fulfilled the proposed PMT/vPvM criteria (ii) showed substantial structural similarity to chemicals already regulated as p/vP and/or T under REACH or the Stockholm convention and (iii) degraded in the environment to substances that fulfil the proposed PMT criteria

Expert judgement was applied to consider whether substances not already identified on the current project list but included on the SIN list because their PMT properties should also be included in the phase 2 project. Carbon tetrachloride, chlorendric anhydride and chloroform were considered for inclusion but only chlorendric anhydride was included on the final list Environmental monitoring data (see Appendix 1)

1.1.4 REACH tonnage

Substances with REACH registrations less than 10 tonnes/annum in the EU were lower priority than substances with much higher tonnage bands and were removed from the list.

1.1.5 Substances already monitored by water companies or under regulatory scrutiny

Following discussion and agreement with the DWI, any substance already monitored by water companies in England and Wales was removed from scope. An objective of the current project is to identify additional substances that pose a risk to drinking water sources that may need to be considered by water companies in their risk based targeted monitoring. Two PFAS were included on the initial list supplied at the start of the project. PFAS are a large group of substances, many of which meet PMT/vPvM criteria and are receiving considerable scrutiny by the scientific community and regulators. PFAS are being considered in separate DWI funded research and were excluded from this project to avoid duplication of effort.

2. NATURE OF USE AND ESTIMATES OF EMISSIONS

Characterising and quantifying exposure represents a major source of uncertainty in assessing both environmental and human health risk. We have collated publicly available information on each substance to establish the nature of use and estimate quantities used in England and Wales. This information has been used to refine estimates of amounts used previously generated in the phase one project (DWI,2020) and derive a realistic estimate an environmental release per capita per day which could be used as an input for the subsequent exposure modelling to derive concentrations of each substance in rivers and treated drinking water (see Chapter 5). An overview of the steps is illustrated below in Figure 2.1.

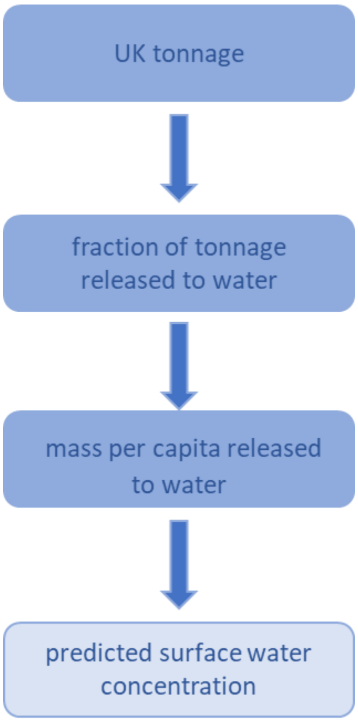

Figure 2.1 Overview of steps to derive a per capita emission estimate

2.1 UK TONNAGE ESTIMATION

A tiered approach to estimating amounts used in the UK was taken and used subsequently in the risk assessment (Chapter 5). **Error! Reference source not found.**.1 presents three tonnage estimates for each substance identified as tiers one to three. The tier one values represent a very worst-case scenario and assumes the upper bound of the reported REACH registration band is used in the UK. It is highly unlikely that this reflects reality but has been used as a very conservative screening level risk assessment (Chapter 5). The tier two estimate is the value estimated in the phase one study (DWI, 2020). This value is the upper bound of the REACH registration tonnage band adjusted to reflect the UK market share (9% of total EU tonnage; DWI 2020). In this project we have sought to refine worst-case estimates generated in phase one to reflect a more realistic estimate of use and release to water.

There is no single, publicly available UK data source providing tonnage information on chemical supply and use in products on the market or apportionment of tonnage across different sectors/uses. A broad range of data sources including both scientific and grey literature were searched between February 2022 and May 2022 to collate information on the nature of use of each substance, estimate amounts used and pathways of environmental release in the UK. Key sources included REACH registration dossiers accessed through the European Chemicals Agency (ECHA) public database; UK customs data accessed through the public UK Trade Info service from HM Customs and Revenue (HMRC); the Eurostat database; the Nordic SPIN database; the US EPA CompTox chemical dashboard and safety data sheets (SDS) published on company websites. The availability of information and the accuracy of data varies considerably between substances and across product types. Further details on each data source are provided in Appendix 2.

Registration of substances under UK REACH has been considered, however there are currently no UK specific tonnage data publicly available. The only information available at the time of writing is the list of substances grandfathered under UK REACH. Using this list, it was possible to determine if the substance is manufactured in the UK or imported into the UK from outside of the EU/EEA, in quantities greater than 1 tonne/annum.

The lack of UK-specific tonnage information for most substances, despite extensive data searching, necessitated alternative approaches to refining phase one (DWI, 2020) estimates of use. The approach varies by substance according to the availability of additional and more accurate information of use and release in the UK.

For some substances it was not possible to refine the previous worst-case tonnage estimate further. In other instances, additional data and intelligence on use enabled these tonnage estimates to be refined. Additional qualitative information on use has been obtained for all substances which adds significantly to the understanding how these substances are used and their potential releases to the environment. Reported uses for each substance are described below in **Error! Reference source not found.**.1

Several substances are used as pharmaceuticals. A different approach has been used for these substances because the REACH reported tonnage will not reflect pharmaceutical use. Instead, publicly available information on treatment rate and number of cases in the UK have been used to estimate amounts used and released.

For triclosan, no tonnage information was available. The REACH registration dossier notes that the substance is not currently manufactured or imported in the EU or UK. Instead, wastewater treatment works (WWTW) effluent monitoring data collected as part of the UKWIR Chemical Investigation Programme phase 2 (CIP) was used to estimate a per capita release per day.

For some substances, such as 4-aminophenol which is used in hair dye, sufficient information on weight fraction inclusion in products and knowledge on consumer behaviour and frequency of use was available to estimate quantities released and refine the previous phase one tonnage estimate.

Some substances have multiple uses. Where possible, the total tonnage has been apportioned between different uses, but for most substances no information was available to allow us to apportion the total tonnage between different uses. In these instances, a conservative assumption has been made and the total tonnage has been applied to the scenario with the largest releases to generate an environmental release estimate for exposure modelling. Further details are provided in Appendix 2.

2.2 FRACTION RELEASED TO WATER

The fraction of the total tonnage released to water at each stage of the life cycle has been estimated for each substance. Refining total tonnage by considering fraction released in this manner allows a further refinement from phase one to generate a conservative but more realistic emission estimate with available data. Where evidence indicated that a life cycle stage was not relevant to the UK, for example if a substance is not manufactured in the UK, no release estimate has been derived for that stage of the life cycle.

For most substances the fraction released has been determined by applying generic release factors to the total UK tonnage. Environmental Release Categories (ERCs) appropriate to the type of substance and nature of use have been used. A summary of relevant ERCs is provided in Appendix 2. These generic release factors are conservative assumptions used for environmental exposure estimation in REACH chemical safety assessments. Where available, Specific Environmental Release Categories (SpERCs) have been used. SpERCs have been developed by industry associations for use in REACH chemical safety assessments, reflect current good practice and report key parameters for environmental emission modelling such as substance use rates. Only peer reviewed SpERCs deemed acceptable for use on chemical safety assessment by ECHA have been used in this project.

For all substances studied, widespread dispersive release to the environment through consumer use and industrial applications is anticipated. A per capita per day release has been estimated by distributing the fraction of total tonnage released throughout Great Britain according to population density.

For some substances, we have identified point sources, for example manufacturing sites, and these have been explicitly considered. Detailed information on locations of manufacturing sites are not included in this report. Information on the location of downstream industrial sites (e.g. formulation) and associated releases are typically not available. Consequently, for substances with emissions that may occur during formulation and/or where industrial uses are identified, we have assumed that population density can provide a reasonable representation of the distribution of industrial sites. The combination of conservative tonnage estimates and emission fractions is expected to provide a degree of conservatism, aimed at generating realistic but precautionary outputs that should result in a higher probability of false positives, as opposed to false negatives.

The amount of quantitative and qualitative information on use varies between substances, but for most substances it has been possible to refine the previous phase one (tier two) release estimates. An overview of UK tonnage and release fractions is provided for each substance below in **Error! Reference source not found.**, with further details of how tonnage estimates have been derived provided in Appendix 2.

Table 2.1 Summary of nature of use and estimates of amounts used and released in the UK

Substance	use	Tier one (tpa)	Tier two (tpa)	Tier three (tpa)	Release estimate (tpa)
2,4,7,9-tetramethyldec-5-yne-4,7-diol	Used in printing inks, polymerization processes and as a wetting agent and defoamer in cleaning products. Information in the REACH registration dossier and the Nordic SPIN database indicate that use in cleaning products is minor (<1%).	10000	900	900	2.3
1,4-dioxane	Used in a wide range of solvents to reduce irritation from other chemicals (Health Canada, 2021) but also occurs as a contaminant in alcohol ethoxylates, used in cosmetics, cleaning (mostly degreasing), and personal care products. It is also used as processing aid.	10000	900	228	228
Trichloroethylene	Trichloroethylene is a volatile organic solvent. It has been used in the vapour degreasing of metal parts and in consumer applications such as typewriter correction fluids, paints removers and strippers, adhesives, and spot removers (PubChem, 2022). Trichloroethylene is a substance of very high concern (SVHC) under REACH. It is on the authorisation list with a sunset date in 2016. This means that non-exempted and non-authorised uses of the substance are now banned in the UK. A single UK application for authorisation is currently under review.	100000	9000	42	0.004
Tetrachloroethylene	Wide range of uses. It is used in heat transfer media, surface cleaning, dry cleaning, and film cleaning. Use to formulate adhesives, sealants and coatings are also cited (PubChem, 2022). The major use, as listed in the Hazardous Substances Data Bank (HSDB) has been as a chemical intermediate for fluorocarbons and as a solvent for dry-cleaning.	1000000	90000	2500	2500
Melamine	Primarily used for melamine-formaldehyde resins, in which the melamine will be chemically bound within a polymer and generally considered unlikely to be released. There is some evidence of the release of residual melamine monomer from such articles, and it is unclear whether degradation of these polymers can lead to the release of melamine. Melamine is also identified as a major degradation product (70% of parent) of cyromazine, an insect growth regulator used as a biocide (product type 18) for the control of fly larvae in animal husbandry, outdoor	1000000	90000	90000	1782

Substance	use	Tier one (tpa)	Tier two (tpa)	Tier three (tpa)	Release estimate (tpa)
	manure heaps, slurry reservoirs and landfill sites and other breeding sites in animal housing. Cyromazine has also previously been used as a plant protection product (insecticide), primarily for tomato crops. As of 1st June 2022, GB or NI no Authorised Biocidal Products containing cyromazine as the active ingredient are listed.				
Dinoseb	Dinoseb, also known as DNBP, is used as a polymerisation control agent (styrene retarder). Research indicates that all dinoseb registered under REACH is manufactured at a single UK site. Historically dinoseb has been used as a pesticide but is not currently approved for use as a pesticide in either the UK or EU.	10000	900	54	2.7
Dapsone	Wide variety of uses; as a resin in articles, as an intermediate in the manufacture of polymers, and as a pharmaceutical indicated for use as an anti-infective for treatment of leprosy, dermatitis herpetiformis and prevention of pneumonia.	10000	900	900	94
Amantadine	Amantadine is primarily used as an active pharmaceutical ingredient. for treatment of Influenza A, Parkinson’s disease, and Herpes zoster.	1000	90	10	10
Hexamethyldisiloxane	Hexamethyldisiloxane (107-46-0) has a variety of uses, mostly in personal care products, automotive cleaning products, pharmaceuticals and cosmetics but also in industrial applications with reported uses as an intermediate and within polymers.	10000	900	900	900
Tricarbonyl(methylcyclopentadienyl) manganese	Used as a fuel additive to improve the octane number in unleaded petrol. The substance has been grandfathered under UK REACH. No evidence of UK manufacture has been identified. We have assumed that formulation into fuels and use of fuels are the main emission pathways.	10000	900	545	0.3
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1)	Also known as melamine cyanurate, it is used as a flame retardant in plastics and coatings primarily in the building industry along with use in greases and lubricants. The compound is also used in the textile industry. The substance is a high molecular weight complex, comprising one to one ratio of molecules of melamine and cyanuric acid, strongly bound in the crystal lattice.	100000	9000	9000	Cyanuric acid: 300 Melamine : 292

Substance	use	Tier one (tpa)	Tier two (tpa)	Tier three (tpa)	Release estimate (tpa)
2-phosphonobutane-1,2,4-tricarboxylic acid	Used in water treatment for its anti-scale properties in industrial uses of reverse osmosis water in industrial cooling or circulatory systems. It is also reported with widespread use in cleaning agents & drinking water treatment processes.	100000	9000	9000	9000
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	Used in resin formation in polymer and plastic products manufacture. Release to the environment is anticipated to occur from industrial use in the production of articles and from thermoplastic manufacture.	1000	90	250	12.5
4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	Used in a wide range of products by down-stream consumers, largely found in finished articles, by professional workers (widespread uses), in formulation or repacking, at industrial sites and in manufacturing. Data reported to the Nordic SPIN database suggests that extraction of crude petroleum and natural gas and manufacture of chemicals and chemical products are the main uses.	10000	900	900	900
4-aminophenol	4-aminophenol is primarily used in hair dye.	100	9	31	31
2-morpholinoethanol	2-morpholinoethanol is used as an intermediate in the manufacture of fine chemicals (small scale production, high purity, high value chemicals) and as an intermediate in pharmaceuticals,	1000	90	90	1.8
2,2'-azobis[2-methylbutyronitrile]	Used as a polymerization initiator.	1000	90	90	6.005
1,3-dichlorobenzene	Used as a chemical intermediate	1000	90	90	1.8
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	Used in polymerization processes. Information from the Nordic SPIN database suggests use in coating and building materials.	10000	900	900	74
N-butylbenzenesulphonamide	N-butylbenzenesulphonamide (BBSA) is used in the production of plastics for the automotive sector.	10000	900	875	467
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin) is primarily used in pharmaceuticals, polymer modifiers, adhesives, cosmetics, and food sweeteners. Its main identified uses appears to be in the cosmetic sector, specifically lip application products.	1000	90	822	822
Triclosan	Historically, triclosan has been used in personal care products.	111.1	10	0	

3. TOXICOLOGY

This chapter describes the approach taken for the collection of toxicological data for each PMT substance. A toxicological evaluation was undertaken to identify the most sensitive point of departure (PoD) for each substance, which was then used to determine a health-based guidance value (HBGV). A health-based guidance value (HBGV) is a science-based recommendation for the maximum oral exposure to a substance that is not expected to result in an appreciable risk to human health. These HBGVs could then be compared to estimated human exposure concentrations to determine if there is a human health risk, as shown in the risk assessment (see Chapter 6), to identify the substances most likely to pose the highest risk to human health via drinking water in England and Wales. The data compilation and final HBGV for each substance was peer reviewed by multiple members of the project team to ensure a robust, reliable, and unbiased data collation and HBGV selection.

3.1 LITERATURE SEARCH

Toxicological data were collated from several sources to determine the hazards each substance may pose to human health. Where available, authoritative reviews were used to ensure that reliable, peer reviewed data have been used. A standard assessment template was populated for each chemical. Completed templates are supplied as an Excel based technical appendix to this report (ED15803_Objective 2 - technical appendix).

Publicly available data from the following international and national bodies were reviewed, using multiple chemical identifiers, including CAS and EC numbers, to ensure a comprehensive search:

- European Chemicals Agency (ECHA)
- Committee on Toxicity (COT)
- European Food Safety Authority (EFSA)
- Organisation for Economic Co-operation and Development (OECD)
- Joint Expert Committee on Food Additives (JECFA)
- World Health Organisation (WHO), including the International Programme on Chemical Safety (IPCS) and Environmental Health Criteria (EHC) Monographs
- Agency for Toxic Substances and Disease Registry (ATSDR)
- US Environmental Protection Agency (EPA)
- National Toxicology Program (NTP)
- Health Canada
- Australian Industrial Chemicals Introduction Scheme (AICIS)

The authoritative bodies were chosen as they are renowned for the compilation of robust toxicological data which would be relevant to this project. In the absence of sufficient data from the above sources to enable us to collect data which would later allow us to carry out a risk assessment for any one of the substances, we widened our search to other authoritative bodies and the scientific literature. This included the European Medicines Agency (EMA) and the Scientific Committee on Consumer Safety (SCCS), as well as bibliographic databases including PubMed and Google Scholar.

3.2 HAZARD DATA

3.2.1.1 Point of Departure (PoD) Identification

Data was collected on the most sensitive hazards associated with each substance for oral exposure. The substances were all assessed as having a threshold of toxicity, and so a dose (a PoD) could be determined below which toxicity did not occur. PoDs used as part of this data collection include No Observed Adverse Effect Levels (NOAELs), Lowest Observed Adverse Effect Levels (LOAELs) and Benchmark Doses (BMDs). The NOAEL is the highest tested dose at which no adverse effects are observed in a toxicity study. If a NOAEL cannot be determined due to effects being seen at even the lowest dose tested, the LOAEL (the lowest dose at which adverse effects are identified) may be determined. The BMD is the tested dose that caused a predetermined change in response for an adverse effect. This change is response is known as the benchmark response (BMR) and is usually a 5% or 10% change in response rate when compared to a control group. The critical study and endpoint for each PoD was collected for each PMT substance.

3.2.1.2 Health-Based Guidance Values (HBGVs)

The most sensitive PoD for each substance was used to identify or derive a HBGV. HBGVs for oral exposure (i.e. through food and drinking water) are the estimated dose that can be ingested by humans over a lifetime without appreciable risk to health. They are designed to be protective to the health of the entire population, including sensitive subpopulations. HBGVs collected for the substances included tolerable/acceptable daily intakes (TDI/ADI), reference doses (RfD), derived no effect levels (DNEL). When deriving a HBGV from a NOAEL or LOAEL, the PoD has uncertainty factors (UFs) applied to account for interspecies differences and intraspecies variabilities. Further UFs may be applied to account for differences in a study including quality and duration. If a published HBGV was not available from authoritative reviews for a substance, a provisional value was determined based on available PoDs. Justification for the derivation is provided in the completed template for each substance where we have taken this approach.

3.2.1.3 Threshold of Toxicological Concern (TTC) approach

In cases where there were insufficient toxicological data available for a substance to derive a HBGV, a Threshold of Toxicological Concern (TTC) approach was taken, following EFSA guidance (EFSA, 2019) on the use of the TTC approach in food safety assessment, which was considered relevant for drinking water. TTC uses the structure of a substance to assess if there is a likely health risk, by using the toxicological data from other structurally similar substances that have extensively published data. Substances that are identified as potential mutagens and/or carcinogens based on their structure have a TTC value of 0.0025 µg/kg bw/day assigned. Other substances are assigned a Cramer class between I-III, based on structural alerts; these Cramer classes have associated TTC values of 30 µg/kg bw/day, 9 µg/kg bw/day and 1.5 µg/kg bw/day assigned, respectively. Exposure to a substance at levels below the TTC value are unlikely to cause adverse effects to human health.

3.2.1.4 Cancer and non-cancer endpoints

For each PMT substance, the human health endpoint selected is considered to be the most sensitive effect, and a HBGV was chosen based on this. However, chemicals which are known to have a carcinogenic effect have both a cancer- and non-cancer endpoint selected. This allowed the risk assessment to consider both effects. It can be noted that, in the case where the non-cancer endpoint has a lower HBGV than the cancer endpoint for a substance, the non-cancer HBGV will be protective of the cancer effect.

A summary of the critical endpoint, HBGV and key study for each chemical can be found below in Table 3.1. Full details of data collated including references are provided in the substance templates (ED15803_Objective 2 - technical appendix).

Table 3.1: Critical endpoint, associated HBGV and key study for each PMT chemical identified within the scope of this project

Chemical	Critical Endpoints	HBGV	HBGV and Key Study
2,4,7,9-tetramethyldec-5-yne-4,7-diol	Cramer Class III Chemical	1.5 µg/kg bw/day	A HBGV was determined based on chemical structure, taking a TTC approach due to a lack of data (ToxTree, 2022). The TTC approach taken followed a methodology by EFSA (2019).
1,4-dioxane	Renal tubular epithelial and hepatocellular degeneration and necrosis	16 µg/kg bw/day	An oral DNEL was determined by ECHA for renal tubular epithelial and hepatocellular degeneration, based on a study in rats by Kociba, et al. (1974).
	Hepatocellular tumours	96 µg/kg bw/day	A TDI was determined by WHO (2005) for hepatocellular tumours, based on a study in rats by Yamazaki et al. (1994).
Trichloroethylene	Decreased plaque-forming cell response and increased delayed-type hypersensitivity Decreased thymus weight Foetal heart malformations	0.5 µg/kg bw/day	A RfD was determined by US EPA (2011) for decreased plaque-forming cell response and increased delayed-type hypersensitivity in mice, decreased thymus weight in female mice, and foetal heart malformations in rats, based on studies by Peden-Adams et al. (2006), Keil et al. (2009) and Johnson et al. (2003).
	Kidney cancer	0.14 µg/kg bw/day	A HBGV was also determined by US EPA (2011) for kidney cancer, based on a study using route-to-route extrapolation from an inhalation study in humans by Charbotel et al. (2006).
Tetrachloroethylene	Neurotoxicity (acquired dyschromatopsia)	4.7 µg/kg bw/day	A TDI was determined by Health Canada (2015) for neurotoxicity, based on a study in workers by Cavalleri et al. (1994).
	Hepatocellular cancer	5.7 µg/kg bw/day	A HBGV was determined by US EPA (2012) for hepatocellular cancer, based on a study using route-to-route extrapolation from an inhalation study in mice by JISA (1993).
Melamine	Development of urinary bladder stones	200 µg/kg bw/day	A TDI was determined by EFSA (2010) for the development of urinary bladder stones, based on a study in male rats by NTP (1983).

Dinoseb	Increases in haematocrit and decreased extramedullary haematopoiesis of the spleen	0.78 µg/kg bw/day	A HBGV was derived by the project team from a NOAEL reported by OECD (2007) for increases in haematocrit in males and decreased extramedullary haematopoiesis of the spleen in females, based on a study in rats by MHLW (2005).
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	Maternal toxicity	10 µg/kg bw/day	A HBGV was determined by ECHA (2020) for maternal toxicity, based on a study in rats by Anon (2014).
4-aminophenol	Kidney toxicity	100 µg/kg bw/day	A HBGV was derived by the project team from a NOAEL reported by SCCS (2011) for kidney toxicity, based on a study in rats by Centre International de Toxicologie (undated)
Ametryn	Hepatic effects including fatty degeneration of the liver	10 µg/kg/day	A RfD was determined by US EPA (1987) for hepatic effects including fatty degeneration of the liver, based on a study in rats by Ciba-Geigy Corporation (1961).
Dapsone	Carcinogenicity	4.2 µg/kg bw/day	A Maximum Daily Exposure was determined by the European Medicines Agency (2012) for carcinogenicity, based on a study in rats by NTP (1977).
Sulisobenzone	No adverse effects observed at highest tested dose	6250 µg/kg bw/day	A DNEL was determined by ECHA (2021) based on no adverse effects observed at the highest tested dose level in a study in rats by Anon (2018).
2,2'-azobis[2-methylbutyronitrile]	Cramer Class III Chemical	1.5 µg/kg bw/day	A HBGV was determined based on chemical structure, taking a TTC approach due to a lack of data by Health Canada (2016).
Amantadine	Cramer Class III Chemical	1.5 µg/kg bw/day	A HBGV was determined based on chemical structure, taking a TTC approach due to a lack of data (ToxTree, 2022). The TTC approach taken followed a methodology by EFSA (2019).
Hexamethyldisiloxane	Reduced food consumption, reduced body weight gain, reduced liver weight, changes to white cell count and corpuscular parameters.	270 µg/kg bw/day	A DNEL was determined by ECHA (2022) for reduced food consumption, reduced body weight gain, reduced liver weight, changes to white cell count and corpuscular parameters, based on a study in rats by Shin-Etsu (1994).
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	Liver and pancreatic cancer	0.167 µg/kg bw/day	A DMEL was determined by ECHA (2020) for liver and pancreatic cancer, based on a study in rats by NTP (1987).

4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	Liver and spleen weight changes	200 µg/kg bw/day	A DNEL was determined by ECHA (2012) for liver and spleen weight changes, based on a study in rats by Anon (1992).
Tricarbonyl(methylcyclopentadienyl) manganese	Cramer Class III Chemical	1.5 µg/kg bw/day	A HBGV was determined based on chemical structure, taking a TTC approach due to a lack of data (ToxTree, 2022). The TTC approach taken followed a methodology by EFSA (2019).
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1)	Formation of renal crystals	15 µg/kg bw/day	A DNEL was determined by ECHA (2022) for the formation of renal crystals, based on a study in weanling pigs by Stine et al. (2011).
2-morpholinoethanol	Cramer Class III Chemical	1.5 µg/kg bw/day	A HBGV was determined based on chemical structure, taking a TTC approach due to a lack of data (ToxTree, 2022). The TTC approach taken followed a methodology by EFSA (2019).
1,3-dichlorobenzene	Pituitary lesions	20 µg/kg bw/day	An MRL was determined by ATSDR (2006) for pituitary lesions, based on a study in rats by McCauley et al. (1995).
2-phosphonobutane-1,2,4-tricarboxylic acid	No adverse effects observed at highest tested dose	1875 µg/kg bw/day	A HBGV was derived by the project team from a NOAEL reported by OECD (2002) based on no adverse effects observed at the highest tested dose level in a study in rats by Löser et al. (1976).
N-butylbenzenesulphonamide	Liver and kidney toxicity	260 µg/kg bw/day	A DNEL was determined by ECHA (2021) for liver and kidney toxicity, based on a study in rats by Anon (2019).
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	Bladder cancer	3800 µg/kg bw/day	An ADI was determined by COT (2020), EFSA (2018), JECFA (1993) and WHO IPCS (Undated) for bladder cancer, based on a study in rats by the Calorie Control Council (1983).
2,4,4’-trichloro-2’-hydroxy-diphenylether (triclosan)	Histopathological effects in the liver	400 µg/kg bw/day	A HBGV was derived by the project team from a NOAEL reported by OECD (2010) for histopathological effects in the liver of males, based on a study in rats by Anon (undated).

4. ENVIRONMENTAL OCCURRENCE OF PMT SUBSTANCES IN SURFACE WATER AND GROUNDWATER

Environmental occurrence data in both raw and treated waters in England and Wales for the PMT substances in scope for this project have been collated from open access environmental monitoring datasets, scientific and grey literature. Data published in the scientific literature for England and Wales are limited. Consequently, the literature search was extended to a wider geographical scale. An overview of occurrence data in raw and treated waters for each substance is provided in Table 4.1 below and illustrates the evidence gaps for some of the substances of interest.

No monitoring data have been found for the following substances: tricarbonyl(methylcyclopentadienyl) manganese, 2-phosphonobutane-1,2,4-tricarboxylic acid, 4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl 2-morpholinoethanol, 2,2'-azobis[2-methylbutyronitrile], 2,2'-dimethyl-2,2'-azodipropiononitrile (APN), 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride (PE1+) (chlorendric anhydride).

For other substances, available data have been collated and concentrations are summarised in the following sections.

Table 4.1: Summary of available environmental occurrence data reported in English and Welsh ground and surface water and treated drinking water.

Substance	**Environmental occurrence data in English and Welsh waters**			**Environmental occurrence data reported in international waters**	
	EA/NRW Monitoring Data	Scientific literature		Scientific literature	
	Environmental waters	Environmental waters	Treated drinking water	Environmental waters	Treated drinking water
2,4,7,9-tetramethyldec-5-yne-4,7-diol	✓			✓	
1,4-dioxane	✓	✓		✓	✓
Trichloroethylene	✓	✓		✓	
Tetrachloroethylene	✓	✓		✓	
Melamine	✓			✓	
Dinoseb	✓				
Dapsone	✓				
Amantadine	✓			✓	✓
Hexamethyldisiloxane	✓				
Tricarbonyl(methylcyclopentadienyl) manganese					
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6-triamine (1:1)					
2-phosphonobutane-1,2,4-tricarboxylic acid					
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl					
4-aminophenol				✓	✓
2-morpholinoethanol					
2,2'-azobis[2-methylbutyronitrile]					
1,3-dichlorobenzene	✓			✓	
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)					
N-butylbenzenesulphonamide	✓	✓		✓	
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	✓			✓	✓

1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride (PE1+) (chlorendric anhydride)					
Triclosan	✓	✓		✓	

4.1 ENVIRONMENTAL MONITORING DATA IN ENGLAND AND WALES

Publicly available water quality monitoring datasets for England and Wales have been analysed to collate evidence on the presence of the PMT substances within scope for this project. Several datasets have been examined and these are summarised below.

4.1.1 Environment Agency water quality monitoring data, GC-MS, and LC-MS semi-quantitative screen.

The Environment Agency uses targeted screening gas chromatography–mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS) methods to analyse English surface water and groundwater samples for a wide range of substances. The methods are used to collect environmental occurrence data for a broad range of emerging contaminants and the data used as part of the Environment Agency's Prioritisation and Early Warning System for identification of emerging contaminants.

Data on environmental occurrence of the substances of interest in fresh surface waters and groundwater were accessed through the open data portal on gov.uk and downloaded on 13/12/2021. Frequency of detection data was supplied by the Environment Agency in November 2022.

In this chapter monitoring data collected through the Environment Agency's emerging contaminants screening monitoring programme are presented as frequency of detection for each substance monitored. The temporal and spatial sampling frequency varies significantly between substance. Data are reported as a nationally aggregated statistic for each of the most recent five years. Data are reported separately for each analytical method (LC-MS and GC-MS) and surface water (freshwater) and groundwater in Table 4.2 to Table 4.5. These summary statistics were calculated by the Environment Agency and supplied for the purposes of this project.

Data collected are reported by the Environment Agency as a concentration but are semi-quantitative values with a high degree of uncertainty and the numeric concentration values should be treated as indicative only. For completeness we have included these data in Appendix 5.

4.1.2 Environment Agency Water Quality Archive data (WIMS)

The Environment Agency's Water Quality Archive (WIMS) contains fully quantitative water quality measurements. Rivers, lakes, ponds, canals, coastal or estuarine waters and groundwater are sampled. Samples are taken for several purposes including compliance against discharge permits, investigation of pollution incidents and other statutory environmental monitoring requirements for example, Water Framework Directive Regulations.

Data on environmental occurrence of the substances of interest in fresh surface waters and groundwater were accessed through the open data portal on gov.uk and downloaded on 17/12/2021 and 20/12/2021. Samples clearly associated with waste sites, effluent or pollution incidents have been excluded from our data analysis presented below. WIMS sample purpose codes and sampling point descriptors used to identify relevant data are listed in Appendix 3.

CAS numbers are not included as a data field in the Environment Agency's WIMS dataset, making it harder to identify all relevant samples. We have tried to minimise the risk of missing relevant data as far as practicable by searching for different synonyms for each substance. It is possible that some data have not been retrieved because of differences in the spelling or chemical descriptor.

Data are summarised in Table 4.6 and Table 4.7 with relevant search terms used to identify data in WIMS listed as footnotes. Far fewer substances of relevance to this project have reported environmental occurrences in the WIMS water quality archive. This maybe because the data are collected primarily for statutory reporting requirements which typically focus on known environmental contaminants rather than emerging contaminants.

4.1.3 Natural Resources Wales. National non-target screening monitoring data

Data collected as part the national non-target screening campaign in Welsh rivers by Natural Resources Wales (NRW) were interrogated. Surface waters have been sampled at 12 locations across Wales using passive samplers – either Chemcatcher (CC) or silicon rubber (SRM) deployed every two weeks.

The data were compiled in September 2021, from 141 SRM deployed up to February 2021, and 370 CC deployed up to December 2020. Data are reported as presence/absence only here. Data are summarised as presence/absence, as well as detection frequencies where possible, in Table 4.8. Only those substances targeted as part of the analysis are reported.

Table 4.2: Summary of PMT substances detected in English freshwater per annum between 2017 and 2021. Source data: Environment Agency, LCMS water quality semi-quantitative monitoring screen. Supplied Nov 22. (n=total no. of samples)

Compound	CAS	Detection frequency (%)				
		2017	**2018**	**2019**	**2020**	**2021**
		(n=2350)	(n=2295)	(n=2472)	(n=583)	(n=1407)
2,4,7,9-Tetramethyl-5-decyne-4,7-diol	126-86-3	45%	37%	31%	33%	38%
1,4-Dioxane	123-91-1	33%	24%	16%	12%	17%
Trichloroethylene	79-01-6	13%	5%	8%	15%	11%
Tetrachloroethylene	127-18-4	6%	5%	4%	3%	1%
Dinoseb	88-85-7	0	0	0	0	0
Hexamethyldisiloxane	107-46-0	0	0	0	0	0
1,3-dichlorobenzene	541-73-1	4%	2%	2%	1%	0
N-butylbenzenesulphonamide	3622-84-2	0	0	0	0	0
Triclosan	3380-34-5	4%	4%	1%	0	0

Table 4.3: Summary of PMT substances detected in English freshwater per annum between 2017 and 2021. Source data: Environment Agency, GCMS water quality semi-quantitative monitoring screen. Supplied Nov 22. (n=total no. of samples)

Compound	CAS	Detection frequency (%)				
		2017	**2018**	**2019**	**2020**	**2021**
			(n=667)		(n=111)	(n=362)
Melamine	108-78-1			47% (n=386)	31%	30%
Dapsone	80-08-0	1% (n=386)	0	1% (n=393)	1%	0%
Amantadine	768-94-5			54% (n=386)	65%	34%

Compound	**CAS**	**Detection frequency (%)**				
		2017	**2018**	**2019**	**2020**	**2021**
			(n=667)		(n=111)	(n=362)
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	81-07-2	95% (n=43)	96%	90% (n=393)	85%	52%
Triclosan	3380-34-5		84%	66% (n=393)	50%	22%

Table 4.4: Summary of PMT substances detected in English groundwater per annum between 2017 and 2021. Source data: Environment Agency, GCMS water quality semi-quantitative monitoring screen. Accessed Nov 22. (n=total no. of samples)

Compound	**CAS**	**Detection frequency (%)**				
		2017	**2018**	**2019**	**2020**	**2021**
		(n=860)	(n=1027)	(n=976)	(n=170)	(n=47)
2,4,7,9-Tetramethyl-5-decyne-4,7-diol	126-86-3	15%	15%	6%	14%	15%
1,4-Dioxane	123-91-1	8%	3%	2%	1%	4%
Trichloroethylene	79-01-6	15%	5%	10%	8%	9%
Tetrachloroethylene	127-18-4	7%	5%	5%	2%	2%
Dinoseb	88-85-7	0	0	0	0	0
Hexamethyldisiloxane	107-46-0	0	0	0	0	0
1,3-dichlorobenzene	541-73-1	1%	1%	1%	0	0
N-butylbenzenesulphonamide	3622-84-2	0	0	0	0	0
Triclosan	3380-34-5	1%	1%	0	0	0

Table 4.5: Summary of PMT substances detected in English groundwater per annum between 2017 and 2021. Source data: Environment Agency, LCMS water quality semi-quantitative monitoring screen. Accessed Nov 22. (n=total no. of samples)

Compound	CAS	Detection frequency (%)				
		2017	2018	2019	2020	2021
				(n=188)		
Melamine	108-78-1			21%	9% (n=87)	24% (n=21)
Dapsone	80-08-0	1% (n=75)	0 (n=339)	1%	1%(n=87)	0 (n=21)
Amantadine	768-94-5			2%	5% (n=87)	10% (n=21)
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	81-07-2	34% (n=53)	33% (n=339)	24%	23% (n=87)	48% (n=21)
Triclosan	3380-34-5	14% (n=294)	11% (n=75)	9%	6% (n=339)	2% (n=87)

Table 4.6: Summary of PMT substances detected in English fresh surface waters. Source data: Environment Agency Water quality archive (WIMS). Accessed December 2021

Substance	CAS	No. of samples	Date range	% samples above LOD	Min conc. (μg/L)	2nd Percentile (μg/L)	50th Percentile (μg/L)	98th Percentile (μg/L)	Max conc. (μg/L)	St. Dev.
tetrachloroethylene	127-18-4	26,680	2000 - 2021	18%	0.03	0.05	0.05	1.38	7,190	162.4
trichloroethylene	79-01-6	25,845	2000 - 2021	15%	0.01	0.05	0.05	2.00	76	1.4
dinoseb	88-85-7	2,099	2000 - 2016	16%	0.01	0.02	0.02	0.59	70	1.8

Table 4.7: Summary of PMT substances detected in English groundwater. Source data: Environment Agency Water quality archive (WIMS). Accessed December 2021

Substance	CAS	No. of samples	% samples above LOD	Date range	Min conc. (µg/L)	2nd Percentile (µg/L)	50th Percentile (µg/L)	98th Percentile (µg/L)	Max conc. (µg/L)	St. Dev.
tetrachloroethylene	127-18-4	25,782	8%	2000 - 2021	0.03	0.05	0.05	2.02	30,600	272.8
trichloroethylene	79-01-6	25,699	8%	2000 - 2021	0.00	0.05	0.05	1.91	41,500	268.6
dinoseb	88-85-7	19	0	2004 - 2004	0.02	0.02	0.02	0.02	0.02	0.00

Table 4.8: Natural Resources Wales, non-target screening data compiled September 2021.

Substance	Detected	Number of sites	Total detections	Detection frequency (%)
2,4,7,9-tetramethyldec-5-yne-4,7-diol	Y	1	1	0.7
dinoseb	N			
dapsone	N			
amantadine	Y	3	7	1.9
1,3-dichlorobenzene	N			
N-butylbenzene sulphonamide	N			
Triclosan	Y	2	2	1.4

4.2 LITERATURE SEARCH

A comprehensive search of the scientific and grey literature was carried out to compile any further evidence on the occurrence of the PMT substances in the scope of this project in environmental waters and treated drinking waters in England and Wales. In this report, we use the term environmental waters to cover any surface and ground waters sampled and for which detections of the substances of interest are reported. This does not mean that these waterbodies are necessarily associated with abstraction points for drinking water supply.

To ensure transparency and minimise bias in evidence collation for this objective, the Quick Scoping Review (QSR) methodology was adopted. This involved 3 steps: (i) definition of the primary question, search terms and scope, (ii) carrying out the search and (iii) peer review of the search outcome. Search terms and criteria for inclusion/exclusion of search results are provided in Appendix 4 together with a summary of the QSR outcome.

The bibliographic databases PubMed and Science Direct were accessed and searched in January 2022. The scientific papers on PubMed were searched using the USEPA Abstract Sifter (v6.1), a Microsoft Excel based application that enhances searching capabilities by allowing users to effectively search, triage and track articles of interest (Baker, Knudsen, and Williams, 2017). In Science Direct, only the first 300 search results were reviewed since no relevant hits were being returned after the first 100 titles.

The search included scientific journals published from 2000 onwards, however, due to the limited quantity of relevant data, journals with data sampled pre-2000 but published post-2000 were included in this project.

To ensure a comprehensive search, multiple search identifiers including chemical names, CAS number, EC number and other synonyms were used. Monitoring data for England and Wales was very limited, therefore the search was extended to a broader geographic scale and included the rest of the world.

As illustrated in Table 4.1, no occurrences (inclusive of England and Wales) were reported in the scientific literature data for the following substances; dinoseb, dapsone, hexamethyldisiloxane, tricarbonyl(methylcyclopentadienyl) manganese, 1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1), 2-phosphonobutane-1,2,4-tricarboxylic acid, 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride, 4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl, 2-morpholinoethanol, 2,2'-azobis[2-methylbutyronitrile], and 2,2'-dimethyl-2,2'-azodipropiononitrile (APN).

4.2.1 Data for England and Wales reported in the scientific literature

Data for England and Wales are reported in Table 4.9 below. Due to the limited quantity of occurrence data in the scientific literature, samples clearly associated with waste sites, effluent or pollution incidents have been included in the tables below but are highlighted in bold.

Occurrence data were only reported for eight of the substances of interest in environmental waters in England and Wales. Most detections are in surface waters – primarily rivers. A handful of studies have also reported occurrence data for groundwater.

Substances that have been detected in England and Wales and reported in the scientific literature include 1,4-dioxane, trichloroethylene, tetrachloroethylene, N-butylbenzenesulphonamide and triclosan (Bravo-Linares, Mudge and Loyola-Sepulveda, 2007; Ellis and Rivett, 2007; Kaspryzyk-Hordern, Dinsdale and Guwy, 2008; Kaspryzyk-Hordern, Dinsdale and Guwy, 2009; Lapworth *et al*., 2015; Manamsa *et al.* 2016; Rivett *et al*., 2012; Sabaliunas *et al*., 2003; Stuart *et al*., 2012; Weatherill *et al*., 2014).

There were no reports in the scientific literature of any of the substances of interest in treated drinking water in England and Wales.

Triclosan has been detected in the River Taff and River Ely in Wales. Concentrations reported are less than 1µg/L(Kaspryzyk-Hordern, Dinsdale and Guwy, 2008; (Kaspryzyk-Hordern, Dinsdale and Guwy, 2009). Triclosan is an antibacterial agent commonly used in soaps, antiseptics, antimicrobial detergents, skin care and oral care products (PubChem, 2022g). Triclosan has been reported in other surface water samples from England and Wales (Petrie *et al*., 2016; Sabaliunas *et al*., 2003; Stuart *et al*., 2012). An absence of triclosan was reported in groundwater samples taken from 300 sites across the chalk of England (Lapworth *et al*, 2015).

Concentrations of 70 to 80 µg/L of 1,4-dioxane concentrations of have also been reported in groundwaters of England and Wales as part of a national-scale assessment of micro-organics in 2650 primary and secondary aquifer sites in England and Wales (Manamsa *et al.,* 2016). These data have been collected as part of the Environment Agency's National Monitoring Programme and are likely a sub-set of the data reported in Section 4.1.1.

4.2.2 Occurrence data reported in international sampling studies

Due to the lack of occurrence data present in the literature for the PMT substances of interest in England and Wales, the literature search was extended to include anywhere outside of England and Wales. These data are reported in Table 4.10 below. In contrast to Section 4.1, the limited quantity of occurrence data reported has led to samples clearly associated with waste sites, effluent, or pollution incidents being included in our data analysis presented below. These sites are clearly highlighted in bold. Much of the literature covers the occurrence of 1,4-dioxane, trichloroethylene, 1,3-dichlorobenzene, and triclosan.

The occurrence data presented in the literature for treated water reported the presence of 1,4-dioxane, amantadine, 4-aminophenol and 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin) (Adamson *et al*., 2017; Carrera *et al*., 2019; de Souza *et al*., 2020; de Souza *et al*., 2021; Dsikowitzky *et al*., 2015; Gan *et al*., 2013; Simazaki *et al*., 2015; Stepien *et al*., 2014).

Low levels (less than 1.5 µg/L) of 1,4-dioxane, amantadine and 1,2-benzisothiazol-3(2H)-one1,1-dioxide (saccharin) were reported in drinking water samples from Japan, the USA, Germany, China and Korea (Adamson *et al*., 2017; de Souza *et al*., 2021; Gan *et al*., 2013; Simazaki *et al*., 2015; Stepien *et al*., 2014).

In areas where pollution events have been sampled, concentrations of 1,4-dioxane and 1,3-dichlorobenzene are reported to be typically less than 5 µg/L (Carrera *et al*., 2019; de Souza *et al*., 2020; de Souza *et al*., 2021; Dominguez *et al*., 2018; Dsikowitzky *et al*., 2015; Regnery *et al*., 2011; Santos *et al*., 2018). The exception is 4-aminophenol, where concentrations reported in Brazilian drinking water and surface water are between 1090 ± 0.21 µg/L and 2100 ± 0.5 µg/L. 4-aminophenol is used in personal care products such as hair colourants, and hair conditioners (PubChem, 2022a). The study authors suggest the high levels reported could be a result of pollution from a nearby hairdressing salon (de Souza *et al*., 2020; de Souza *et al*., 2021).

Occurrences of trichloroethylene in groundwaters sampled in Africa and Ukraine have been detected at concentrations less than 1µg/L (Nikolopoulou *et al*., 2022; Sorensen *et al*., 2015). In Italy and Switzerland much higher concentrations of trichlorethylene have been reported (≤ 77.5 µg/L) (Filippini *et al*., 2020; Pollicino *et al*., 2021). The concentration of trichloroethylene reported in the groundwater in Israel is notably higher with concentrations up to 50000 µg/L reported (Gafni et al., 2020). Samples were taken from ten sites with historical trichloroethylene concentrations of more than 50 µg/L. The authors were not aware of any current sources of contamination.

There are numerous reports of the presence of triclosan in water in the wider scientific literature (Balakrishna *et al*., 2017; Bu *et al*., 2013; Dhillon *et al*., 2015; Lopez-Pacheco *et al*., 2019; Milanovic *et al*., 2021; Reichert *et al*., 2019; Xiang *et al*., 2021). A recent review by Malinovic *et al.* (2021) provides a useful summary of reported occurrences of triclosan in international studies sampling surface water, groundwater and drinking water.

Table 4.9: Summary of PMT substances detected in surface water and groundwater sources in England and Wales reported in literature.

Substance	CAS	Media	Sampling Date Range	Conc. Range (µg/L)	Location	Reference
1,4-dioxane	123-91-1	Groundwater	2002 - 2012	≤ 70 - 80	England and Wales	(Manamsa *et al.* 2016)
Trichloroethylene	79-01-6	Surface Water	2001	0.1 - 6	River Tame - Birmingham	(Ellis and Rivett, 2007)
			2011	1 - 40	River Tern - North Shropshire	(Weatherill *et al*., 2014)
		Groundwater	2001	≤ 62	Birmingham	(Ellis and Rivett, 2007)
			1998 - 2008	**0 – 5000**	**Birmingham**[1]	**(Rivett *et al*., 2012)**
			2011	2 – 4.5	North Shropshire	(Weatherill *et al*., 2014)
Tetrachloroethylene	127-18-4	Surface Water	2006	0 – 0.046	River Mersey – Liverpool Bay	(Bravo-Linares, Mudge and Loyola-Sepulveda, 2007)
N-butylbenzenesulphonamide	3622-84-2	Groundwater	2011	0	Chalk of England	(Lapworth *et al*., 2015)
Triclosan	3380-34-5	Groundwater	2011	0	Chalk of England[2]	(Lapworth *et al*., 2015)
		Surface Water	n.d.	0.10 ± 0.0092	South-West England	(Petrie *et al*., 2016)
			1992 – 2009	≤ 2.1	England and Wales	(Stuart *et al*., 2012)
			2000	0.044 – 0.09	Mag Brook, Huddersfield	(Sabaliunas *et al*., 2003)
			2006 - 2007	< 0.005 – 0.095	River Taff – Brecon Beacons	(Kaspryzyk-Hordern, Dinsdale and Guwy, 2008)
				< 0.005 – 0.019	River Taff – Merthyr Tydfil	
				< 0.005 – 0.020	River Taff – Abercynon	
				< 0.005 – 0.015	River Taff – Pontypridd	
				< 0.005 – 0.018	River Taff – Trefforest Estate	

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[1] Data was collected from numerous sites that are located at industrial sites, therefore may be subject to contamination as a result

[2] Data was collected from 300 sites across the chalk of England

Substance	CAS	Media	Sampling Date Range	Conc. Range (µg/L)	Location	Reference
				< 0.005 – 0.011	River Taff – Cardiff Bay	
				< 0.005 – 0.012	River Ely – Llantrisant Forest	
				< 0.005 – 0.024	River Ely – Talbot Green	
				< 0.005 – 0.005	River Ely – Peterson-super-Ely	

Table 4.10: Summary of PMT substances detected in surface water and groundwater sources outside of England and Wales reported in literature.

Substance	CAS	Media	Sampling Date Range	Conc. Range (µg/L)	Location	Reference
2,4,7,9-tetramethyldec-5-yne-4,7-diol	126-86-3	Surface Water	1999	≤ 63.5	Lippe River - Germany	(Dsikowitzky *et al*., 2004)
		Groundwater	2013 - 2014	≤ 0.0006	Zambia - Africa	(Sorensen *et al*., 2015)
1,4-dioxane	123-91-1	Drinking Water	**n.d.**	**0.49 – 0.6**	**USA**[3]	**(de Souza *et al*., 2021)**
			n.d.	**0.034 – 1.68**	**Germany**[4]	**(de Souza *et al*., 2020)**
			2010	**0.36 – 2.05**	**Germany**[5]	**(Dsikowitzky *et al*., 2015)**
			2012 - 2013	0.49 – 0.6	Germany	(Stepien *et al*., 2014)
			2013 – 2015	> 0.35	USA	(Adamson *et al*., 2017)
			2015	**≤ 4.36**	**Spain**[6]	**(Carrera *et al*., 2019)**
		Groundwater	1995 - 1998	0.3 - 16	Japan	(Abe, 1999)
			2009 – 2012	0.12 – 1.63	Oderbruch, Germany	(Stepien *et al*., 2013)
			2014 – 2015	0.15 – 15	Germany	(Karges, Becker and Puttmann, 2018)
			2015	0.29 – 241.09	Spain	(Carrera *et al*., 2017)

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[3] Data collected from a site that was subject to contamination from a hairdressing salon

[4] Data collected from a site that was subject to contamination from a hairdressing salon

[5] Data collected from a site that was subject to contamination from a paper production site

[6] Data collected from a site that was subject to contamination from resin manufacturing plant spills and dioxane contaminated wastewater discharge

Substance	CAS	Media	Sampling Date Range	Conc. Range (µg/L)	Location	Reference
		Surface Water	**n.d.**	**0.11 – 2.2**	**USA[7]**	**(de Souza *et al*., 2021)**
			1995 – 1998	0.3 – 16	Japan	(Abe, 1999)
			2011 – 2012	1.61 – 3.29	Germany	(Stepien *et al*., 2013)
			2018 - 2019	0.21 – 8.31	Huangpu River, China	(Wang *et al*., 2022)
Trichloroethylene	79-01-6	Groundwater	n.d.	≤ 50000	Israel	(Gafni, Siebner and Bernstein, 2020)
			2013	≤ 10	Switzerland	(Filippini *et al*., 2020)
			2013 – 2014	≤ 0.0005	Africa	(Sorensen *et al*., 2015)
			2016	1.0 – 77.5	Italy	(Pollicino *et al*., 2021)
			2018	< 1	Ukraine	(Nikolopoulou *et al*., 2022)
Tetrachloroethylene	127-18-4	Groundwater	2016	1.0 – 77.5	Italy	(Pollicino *et al*., 2021)
		Surface Water	1998 – 2000	0.20 ± 0.47	Scheldt Estuary - Belgium	(Huybrechts *et al*., 2002)
Melamine	108-78-1	Surface Water	2021	6.42 – 11.33	Southern China	(Peng *et al*., 2018)
Amantadine	768-94-5	Drinking Water	2006 - 2010	≤ 0.009	Japan	(Simazaki *et al*., 2015)
		Surface Water	2006 – 2010	0.005 – 0.061	Japan	(Simazaki *et al*., 2015)
			2016	0.11 – 1.79	China	(Lopez-Pacheco *et al*., 2019)
4-aminophenol	123-30-8	Drinking Water	**n.d.**	**1090 ± 0.21**	**Brazil[8]**	**(de Souza *et al*., 2021)**
			n.d.	**2100 ± 0.5**	**Brazil[9]**	**(de Souza *et al*., 2020)**
		Surface Water	**n.d.**	**1670 ± 0.27**	**Brazil[10]**	**(de Souza *et al*., 2021)**
			n.d.	**1300 ± 0.2**	**Brazil[11]**	**(de Souza *et al*., 2020)**
1,3-dichlorobenzene	541-73-1	Groundwater	**n.d.**	**≤ 0.18**	**Spain[12]**	**(Santos *et al*., 2018)**

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[7] Data collected from a site that was subject to contamination from a hairdressing salon

[8] Data collected from a site that was subject to contamination from a hairdressing salon

[9] Data collected from a site that was subject to contamination from a hairdressing salon

[10] Data collected from a site that was subject to contamination from a hairdressing salon

[11] Data collected from a site that was subject to contamination from a hairdressing salon

[12] Data collected from a site that was subject to contamination from Hexachlorocyclohexane (HCH) waste

Substance	CAS	Media	Sampling Date Range	Conc. Range (µg/L)	Location	Reference
			n.d.	**≤ 0.00051**	**Spain[13]**	**(Dominguez *et al*., 2018)**
			2013 – 2014	≤ 0.00013	Africa	(Sorensen *et al*., 2015)
		Surface Water	1998 – 1999	0.05 – 0.9	Greece	(Lekkas *et al*., 2004)
			2001	0.00011 – 0.00034	Mexico	(Owens and Niemeyer, 2006)
N-butylbenzenesulphonamide	3622-84-2	Groundwater	2011	0.1 – 1.28	France	(Lapworth *et al*., 2015)
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	81-07-2	Drinking Water	2011 – 2012	≤ 0.68	China	(Gan *et al*., 2013)
		Groundwater	2011 – 2012	0.052 – 0.063	China	(Gan *et al*., 2013)
			2013	0.0026 – 0.0096	Barbados	(Edwards *et al*., 2019)
		Surface Water	n.d.	0.02 – 3.2	Catalonia	(Arbelaez *et al*., 2015)
			2011 – 2012	≤ 0.34	Hong Kong	(Sang *et al*., 2014)
			2011 – 2012	≤ 0.49	Finland	(Perkola and Sainio, 2014)
			2014	0.00049 – 0.0052	Mediterranean Sea	(Brumovsky *et al*., 2017)

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[13] Data collected from a site that was subject to contamination from a nearby landfill site

4.3 DISCUSSION

In this section we summarise detections in environmental waters in England and Wales as reported in Table 4.2 to Table 4.9 and any additional studies published in the scientific literature.

Data collected as part of the Environment Agency's targeted screen monitoring programme are semi-quantitative and it is appropriate to treat them as presence/absence data only. Consequently we have not commented further on the concentrations reported in Appendix 5 since there is uncertainty associated with these data.

There are very few reports of dapsone, N-butylbenzenesulphonamide and hexamethyldisiloxane in surface water and groundwater samples.

Of the substances of interest in this project, 2,4,7,9-tetramethyldec-5-yne-4,7-diol is reported most frequently in English freshwater and groundwaters. There are also a small number of detections in Wales (0.7%) of surface water samples from monitoring data collected by Natural Resources Wales (NRW) non-target screening. No further reports of this substance in English and Welsh waters have been found in the scientific literature, but occurrence of 2,4,7,9-tetramethyldec-5-yne-4,7-diol have been reported in surface water in Germany (Dsikowitzky *et al*., 2004) and groundwater in Zambia (Sorensen *et al*., 2015).

Substances that have also been sampled for and reported frequently include 1,4-dioxane, trichloroethylene, tetrachloroethylene, triclosan, saccharin, 1,3-dichlorobenzene, melamine, amantadine and dinoseb.

Over the past 5 years, the detection frequency of 1,4-dioxane has gradually decreased from 33% and 8% to 17% and 4% in freshwater and groundwater, respectively. This may be an artefact of sampling, since the total number of samples taken has also decreased. A report by (Manamsa *et al.,* 2016) reports comparable data from a different data range collected as part of the same sampling programme.

There have been several reports of 1,4-dioxane in environmental waters and treated drinking waters in international studies with highest concentrations of 16 µg/L reported in Japanese surface water samples between 1995 and 1998 (Abbe, 1999). Other studies have also reported the presence of 1,4-dioxane in international surface waters, ranging from 1.3µg/L in Germany, up to 241µg/L in Spain (Abbe, 1999; Carrera *et al*., 2017; Karges, Becker and Puttmann, 2018; Stepien *et al*., 2013; Wang *et al*., 2022). Several studies have also reported the presence of 1,4-dioxane in drinking water (de Souza *et al*., 2020; de Souza *et al*., 2021; Dsikowitzky *et al*., 2015; Manamsa *et al.* 2016; Stepien *et al*., 2014). Concentrations are summarised in Table 4.10, with the concentrations up to 4.35 µg/L being reported in samples associated with pollution from resin manufacturing plant spills and dioxane contaminated wastewater discharge (Carrera *et al*., 2019).

Frequent detections of both trichloroethylene and tetrachloroethylene have been reported in English surface and groundwaters in both the Environment Agency's targeted scan monitoring programme and the fully quantitative monitoring data as reported through the water quality archive WIMS. Over 25,000 surface water samples were collected and analysed for trichloroethylene between 2000 and 2016 as part of routine water quality monitoring, yielding detections above the limit of detection (LOD) in 15% of samples. Over that sampling period, surface water concentrations ranged between the LOD (0.01µg/L) up to a maximum of 70µg/l, with a 50th percentile concentration of 0.02µg/L.

In English groundwater samples, 8% of samples are above the LOD and concentrations of trichloroethylene are typically less than 0.1µg/L. In the wider scientific literature high concentrations of trichloroethylene, up to 5000µg/L, have been reported in groundwater in the Birmingham area. The authors of the monitoring study note that the Birmingham area has history of significant metal and engineering industry which may have contributed to the reported concentrations in the area (Rivett *et al*., 2007).

Typical concentrations of tetrachloroethylene reported in English groundwaters range from less than the LOD to 2µg/L and in surface water from 0.03µg/L to 1.40µg/L. Similar levels have been reported in a separate study Bravo-Linares, Mudge and Loyola-Sepulveda, 2007) in samples taken from the River Mersey (Liverpool Bay), with a maximum reported concentration of 0.045µg/L.

Triclosan has been screened for in surface water as part of the Environment Agency's targeted monitoring programme since 2007, and in groundwater from 2009. In the last 5 years, triclosan has been detected from 0-54% of samples in surface water and 0-14% of groundwater samples. Presence of triclosan has been reported in the 2021 compilation of Natural Resources Wales non-target screening monitoring data, at a detection frequency of 1.4%. The presence of triclosan has also been extensively reported in the wider scientific literature.

In surface waters in England and Wales, detections of triclosan have been reported in multiple studies, up to a maximum concentration of 2.1µg/L (Petrie *et al*., 2016; Sabaliunas *et al*., 2003; Stuart *et al*., 2012). In contrast, concentrations of triclosan below the LOD (0.01µg/L) was reported in the groundwater from 300 sites of the Chalk of England sampled during 2011 (Lapworth *et al*., 2015). There are numerous reports of the presence of triclosan in water in the wider scientific literature (Balakrishna *et al*., 2017; Bu *et al*., 2013; Dhillon *et al*., 2015; Lopez-Pacheco *et al*., 2019; Milanovic *et al*., 2021; Reichert *et al*., 2019; Xiang *et al*., 2021). A recent review by Malinovic *et al.* (2021) provides a useful summary of reported occurrences of triclosan in international studies sampling surface water, groundwater and drinking water.

Saccharin has also been sampled for as part of the Environment Agency's targeted monitoring screening and its presence is reported in surface water and groundwater samples taken between 2014 and 2021. It is very frequently detected, with occurrences reported at a frequency of up to 96% in freshwater and up to 48% in groundwater. Saccharin is used as an artificial sweetener and its presence in environmental waters is likely to be associated with excretion by humans following consumption in food and drink.

1,3-dichlorobenzene has only been present in 0-4% and 0-1% of surface water and groundwater samples respectively in the past 5 years (2017-2021). It has not been sampled for as part of the Environment Agency's fully quantitative monitoring programmes and has only very limited mention in the wider scientific literature. 1,3-dichlorobenzene was screened for in Welsh rivers as part of Natural Resources Wales (NRW) non-target screening campaign, however an absence was reported.

Melamine was added to the Environment Agency's targeted screen in 2019, so the number of detections for this substance are not directly comparable with substances such as 1,4-dioxane that have been monitored over a much longer period. Melamine has been reported in up to 47% and 24% of surface and groundwater samples respectively. Melamine has not been sampled as part of the Environment Agency's fully quantitative water quality monitoring programme and there are no reports of its presence in English environmental waters or drinking water in the wider scientific literature. In international monitoring studies, the presence of melamine in concentrations from 6 to 11µg/L in surface water samples collected in Southern China has been reported (Peng *et al*., 2018).

Amantadine, a commonly used pharmaceutical has been monitored since 2019 as part of the Environment Agency's targeted scan monitoring programme. The occurrence of amantadine has been reported more frequently in surface water (34-65%) than groundwater (2-10%). Amantadine has not been sampled for as part of the Environment Agency's fully quantitative monitoring programmes and there are no reports of its presence in English environmental waters or drinking water in the wider scientific literature. Amantadine has been detected at a 1.9% frequency in Welsh rivers as part of the Natural Resources Wales (NRW) non-target screening campaign. Internationally, the presence of amantadine has been reported in Japanese drinking water and surface water (≤ 0.009µg/L and ≤ 0.061µg/L) as well as in surface water samples collected in China (≤ 1.785µg/L) (Lopez-Pacheco *et al*., 2019; Simazaki *et al*., 2015) and European surface water and groundwater samples (Schulze *et al*., 2019).

Dinoseb has been sampled from 2008 as part of the Environment Agency's targeted monitoring screen, however it has not been widely detected, with no occurrences reported in English surface or groundwaters. Dinoseb has been sampled for as part of the Environment Agency's fully quantitative monitoring data as reported through the water quality archive WIMS in sampling between 2000 and 2020. However, detections are infrequent, with only 16% of detections above the LOD in 2099 surface water samples and no detections above the LOD in 19 groundwater samples. Dinoseb was screened for in Welsh rivers by Natural Resources Wales (NRW) as part of a national non-target screening campaign, however an absence was reported. There are no reported detections of dinoseb in reported in the wider scientific literature.

5. SURFACE WATER EXPOSURE MODELLING & REMOVAL THROUGH DRINKING WATER TREATMENT

5.1 ESTIMATION OF CONCENTRATIONS IN RIVERS AND TREATED DRINKING WATER

Concentrations in raw water for the 22 PMT substances were predicted using previously developed algorithms described by Whelan et al. (2007). Exposure of humans to the PMT chemicals of interest via drinking water was predicted from the predicted riverine exposures after allowing for removal in typical drinking water treatment trains (see Bevan et al., 2012; Crump et al., 2013).

Geospatial data describing locations of drinking water abstraction points were supplied by the DWI and have been used to identify locations in England and Wales where predicted exposure concentrations may be high enough to pose a potential risk to human health via drinking water in England and Wales.

Publicly available information has been used to estimate an environmental release per capita per day for each substance. This has been used as an input for the estimation of concentrations in rivers and treated drinking water. For all substances studied, widespread release is anticipated through consumer and industrial applications.

Information on the nature of use of the 22 substances of interest indicated that emissions to surface water were the most relevant. None of the substances studied were applied directly to soil, for example through use as a plant protection product. Consequently, groundwater concentrations were not modelled in this study to focus project resource on the most relevant pathways. However, the risk to groundwater from PMT substances should be explored further in any future research. Occurrence data collated through objective one indicates the presence of PMT substances in groundwater in England.

5.1.1 Common assumptions applied in exposure estimation

All tiers of assessment assume that the primary route of emission to surface waters is via wastewater discharge. All wastewater is assumed to be treated by at least secondary wastewater treatment and assumes negligible biodegradation during treatment. In all cases, per capita use was calculated from assumed tonnage using a population of 67.22 million for the UK. A value of 150 L cap^{-1} d^{-1} was assumed for domestic water use. This value is low compared to many wastewater treatment plant (WWTP) inflow rates, which also receive trade effluent and urban runoff. This means that predicted concentrations will be conservative.

5.1.2 Removal of chemicals in WWTPs

Removal in WWTPs was calculated using SimpleTreat v4 (Struijs, 2014). Physicochemical properties used as input parameters are provided for each substance on the respective substance factsheet. SimpleTreat v4 specifically accounts for the potential of substances to dissociate. It is considered to be superior to other models, such as the wastewater treatment plant (WWTP) model embedded in EpiWIN (e.g. Clark et al., 1995; Wang et al., 2007) and earlier versions of SimpleTreat (Struijs, 1996) because it explicitly describes chemical dissociation and the different behaviours of the dissociated species (e.g. ionised and neutral). Biodegradation data was collated from publicly available REACH registration dossiers for each substance and is provided on individual substance factsheets. All substances were not readily biodegradable. Degradation was assumed to be negligible during treatment, and the removal fractions in the WWTP calculated are, thus, the combined result of predicted sorption to sludge and volatilisation.

For some chemicals zero removal in WWTPs is predicted. This is likely to be conservative because a small fraction of all chemical substances will be removed in the pore water of wet sewage sludge.

5.2 REMOVAL THROUGH DRINKING WATER TREATMENT

The intrinsic substance properties that lead to persistence in the environment and mobility in the aquatic environment may lead to a breakthrough of PMT substances in drinking water treatment facilities (Rüdel et al., 2020). Some PMT substances may require advanced treatment technology to be removed. Advanced treatment is employed at many works in the UK where source waters are impacted by micropollutants, and the ability of these processes to remove the PMT substances studied in this project has been examined.

The removal of the 22 identified PMTs by different drinking water treatment processes (DWTP) was estimated using the physicochemical properties of the substances (Table A6. 1, Appendix 6) and the best current scientific and technical understanding of the chemical mechanisms as well as the efficacy of various treatment processes employed across the UK. This stage of the modelling was based on application of a 3D-QSPR model used for estimating the effectiveness for micropollutant removal with ozone- and chlorine-based treatment methods (Lei and Snyder, 2007).

5.2.1 Treatment Scenarios Considered

Two treatment scenarios have been considered for surface water. The first was ‘conventional treatment’ (CON) consisting of coagulation/flocculation/filtration and chlorination. The second was ‘advanced treatment’ (ADV) consisting of coagulation-flocculation/filtration, ozonation, activated carbon and chlorination. Two treatments for ground water, sand filtration plus disinfection (FILT) and ultrafiltration by membrane plus disinfection (MEM) were also considered although, as noted above concentrations in groundwater have not been estimated. For each scenario, removal rate ranges have been generated (Table 5.1) The disinfection applied was assumed to be chlorine for all cases.

The DWTPs investigated are listed below with a description of each process (Parsons and Jefferson, 2006) and the removal calculations described.

1. **Coagulation** is the process of adding chemical reagents (iron or aluminium salts) in a mixing tank to destabilise colloidal particles and allow them to agglomerate or flocculate with other suspended particles to form larger, more readily settled particles.

2. **Activated carbon** is a broad-scale adsorbent of dissolved substances. Dissolved, colloidal and particulate substances are attracted and attached to the surface of the carbon particles. It is used to remove taste and odour causing compounds as well as toxic organic chemicals. Precipitation and other chemical reactions also occur on the carbon surface. A variety of carbon adsorbers can be designed, including batch and continuous flow units. The adsorption capacity of the carbon is eventually exhausted. The carbon is regenerated by heating the carbon, which burns and volatilises the substances accumulated on it. The activated carbon can take the form of granules (granular activated carbon – GAC) or powder (powdered activated carbon – PAC).

3. **Ozone (O_3)** is a more powerful oxidising agent than chlorine and a very effective biocide. Ozone reacts with most organic matter by attacking it directly or through the formation of hydroxyl radicals (•OH) formed by the depletion of ozone.

4. **Chlorine (Cl_2)** is by far the most common oxidant used in water treatment. Primarily used as a disinfectant but also for iron and manganese removal its efficacy is pH and dose dependent.

5. A **semi-permeable membrane** is a thin layer of material containing holes, or pores, which allows the flow of water but retains the suspended, colloidal and dissolved species within the flow (depending on the size of the holes). The separation is based on the physical characteristics of the pollutants to be removed such as their size, diffusivity or affinity for specific contaminants. The larger pore size of microfiltration and ultrafiltration membranes compared to nanofiltration, and reverse osmosis membranes means they are generally used to remove larger pollutants such as turbidity, pathogens and particles.

5.2.2 Removal calculations for each drinking water treatment process (DWTP)

5.2.2.1 Removal via coagulation-flocculation/filtration

In general coagulation-flocculation/filtration will only remove charged colloidal species from water (Parsons and Jefferson 2006). Species that are negatively charged (anionic) at pH 7 are more amenable to removal. We would expect no removal of small uncharged molecules during coagulation and limited removal (25%) of small, charged molecules. Any substances sorbed to particulate matter are likely to be removed during these processes. Most of the substances of interest have zero charge according to data collected from Chemspider. Only dinoseb, has a small negative charge. This is not considered sufficient to expect removal by coagulation.

5.2.2.2 Removal via activated carbon

Activated carbon has been included in the advanced treatment scheme as it is common that a surface water treatment works will have barriers such as PAC or GAC for e.g. pesticide, taste and odour compound removal. Each substances was put into one of the following categories based on the log of the n-octanol/water coefficient (log Kow) and the charge at pH 7 (Drewes et al. 2007):

1. log Kow > 4 (pH 7); uncharged
2. log Kow = 0–4 (pH 7); uncharged
3. log Kow < 0 (pH 7); uncharged
4. log Kow = 0–1.5 (pH 7); protonated base
5. log Kow < 0 (pH 7); protonated base
6. log Kow = 0–2.5 (pH 7); deprotonated acid
7. log Kow < 0 (pH 7); deprotonated acid

The removal for each category was as follows:

1. greater than 90% removal
2. 90-50% removal
3. 50-25% removal
4. 90-50% removal
5. 50-25% removal
6. 50-25% removal
7. less than 25% removal

The log Kow values fall mainly into category 2 with five substances in category 3 and a further three substances in category 1 indicating good to excellent removal for most of these substances by PAC/GAC.

5.2.2.3 Removal via chlorination and ozonation

Quantitative structure-property relationship (QSPR) models developed and validated by Lei and Snyder (2007) were used to predict percent reactivity with ozone and free chlorine (HOCl/OCl-) for the PMT substances. The method is described below.

2D to 3D conversion

The mol files of the 23 metabolites selected for study were converted from two dimensional (2D) representations to three-dimensional (3D) ones, using LigPrep software (via Maestro Schrödinger Release 2022-01. Schrödinger Inc., New York, USA). LigPrep uses an energy minimizational approach to calculating 3D structures from 2D structures. Assumptions used for this conversion included an assumed pH of 7 (±2) which sets the ionisation of the metabolite to that most likely in a water treatment scenario. Ionisation of a compound affects the metabolites charge and, hence, reactivity especially with respect to electrophilic reactants such as ozone and chlorine. Additionally, ionisation has a significant effect on other properties of compounds such as sorption to solids (including activated carbon) and volatilisation.

Substance property estimation

Substance properties were estimated using QikProp (via Maestro). QikProp makes its property predictions based on the 3D structure calculated using LigPrep. While many molecular properties were estimated, of key interest with respect to the predicted reactivity with ozone and chlorine were:

(i) the number of reactive functional groups that were unstable and subject to nucleophilic attack (#rtvFG),

(ii) the number of likely reaction pathways via electrophilic pathways (#metab),

(iii) the pi (C-H) component (PISA) of the total solvent accessible surface area (SASA) of the metabolite,

(iv) the weakly polar component (WPSA) of the SASA,

(v) the predicted octanol/water partition coefficient (QP log Kow), and

(vi) the calculated ionisation potential.

Estimation of reactivity

A quantitative structure property relationship (QSPR) approach was used as a screening tool to estimate the reactivity of each of the PMTs. The approach used was based on work by Lei and Snyder (2007). The correlations developed utilized 55 biologically-active compounds as a training set for both ozone and chlorine. The correlations were validated on an independent set of biologically-active compounds. The correlation for percent ozone removal utilised was developed by Lei and Snyder (2007). Specifically, the correlation for percent removal via ozonation was:

$$\%\ \text{ozone removal} = 67.3 + 0.0506 \bullet \text{PISA} + 5.20 \bullet \#\text{metab} - 4.34 \bullet \#\text{rtvFG} - 0.114 \bullet \text{WPSA}$$

The calculated % ozone removal was used to assign a removal rate to each substance. The independent parameters in the model were PISA, the pi (carbon and attached hydrogen) component of SASA (total solvent accessible surface area) in square angstroms, using a probe with 1.4 angstrom radius); WPSA, the weakly polar component of SASA; #metab, the number of metabolites amenable to electrophilic attack; and #rtvFG, the number of unstable functional groups susceptible to nucleophilic attack. Each of these parameters was determined using QikProp software (Schrodinger, New York, NY, USA).

The QSPR model for percent removal during chlorination (percent chlorine removal) was developed by Lei and Synder (2007) in the same manner as the QSPR for percent ozone removal. The resulting QSPR was:

$$\%\ \text{chlorine removal} = 106.8 + 0.791 \bullet (\%\ \text{ozone removal}) + 7.89 \bullet \#\text{rtvFG} + 4.80 \bullet \text{QP log Kow} + 0.175 \bullet \text{FISA} - 15.0 \bullet \text{IP}$$

The calculated percent chlorine removal was used to assign a removal rate for each substance. The independent parameters used were FISA (hydrophilic component of SASA, SASA on N, O, and H on heteroatoms; QP log Kow (predicted octanol/water partition coefficient); #rtvFG (# or reactive functional groups); IP (PM3 calculated ionisation potential), and % ozone reactivity (calculated as described above).

It was possible to calculate the removal by ozone/chlorine using QikProp for 17 of the 22 substances of interest. The approach to the other five compounds is detailed below:

1. Amantadine – Literature data (Simazaki et al., 2015) was available to support removal by conventional and advanced processes and this was used to estimate removal by chlorine (conventional) and ozone (advanced). The modelled data showed 80% removal by GAC alone. The literature data stated GAC+ozone combined gave an average removal of 79% so no further removal by ozone has been assumed.

2. Tricarbonyl (methylcyclopentadienyl) manganese – No literature data was available for this PMT. From looking at the structure (Figure 1) an assumption was made that the tricarbonyl manganese part (B) dissociates from the methylcyclopentadienyl part (A). Removal of methylcyclopentadienyl was assessed only. Data was not available for tricarbonyl manganese.
3. 1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1) – According to the REACH registered dossier (ECHA, 2022), under environmental conditions and at predicted concentrations in the aqueous environment, the substance is expected to dissociate into the two components melamine and cyanuric acid. Therefore read-across from data for melamine and cyanuric acid are justified. the substances has therefore been treated as two separate components which have been assessed separately. Note that the REACH data is not peer reviewed and we have used it at face value.
4. 2-phosphonobutane-1,2,4-tricarboxylic acid – literature data was available for removal by ozonation (Xu et al., 2019).
5. 4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl – no literature data was available for this substance.

Where no literature data or modelled data was available, zero removal was assumed for the water treatment process being considered.

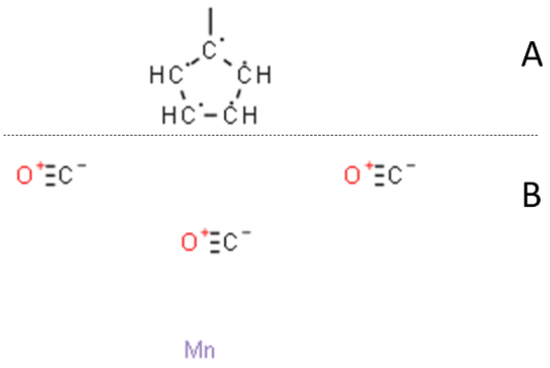


Figure 5.1: Dissociation of Tricarbonyl (methylcyclopentadienyl) manganese (picture from Chemspider [ChemSpider | Search and share chemistry])

5.2.2.4 Removal via Ultrafiltration (UF)

The removal of the substances by UF membranes has been assessed based on their hydrophobicity following work by Yoon et al., (2007). These authors carried out a study on 27 endocrine disrupting chemicals and personal care products with molecular weights in the region of 200 to 600 g/mol and the log Kow values from -2.1-4.77. The 27 substances were put through nanofiltration (NF) and ultrafiltration (UF) membranes. Only UF will be considered in this study. The UF membrane used by Yoon et al., (2007), was a thin film composites with sulfonated polyethersulfone coated with an ultrathin polyimide and had a molecular weight cut-off (MWCO) of 8000 (±1000) Da. Yoon et al.,(2007), reported that that retention for the hydrophobic membranes was influenced by hydrophobic interaction (adsorption). They concluded that compounds having a Log Kow of greater than 2.8 exhibited typically less than 40% recovery whereas compounds with Log Kow less than 2.8 showed higher recovery (greater than 75%).

In our work we have assumed that a substance with Log Kow less than three will not be adsorbed or removed by UF membranes while substances with Log Kow greater than three will be removed in the range 25 to 60%. It is acknowledged that the removals reported in this study are indicative. There are many different UF membrane materials with different configurations and different MWCO values to those reported in this study. The presence of organic matter in the water will also influence the absorption capacity of the membrane.

5.2.3 Overall removal for each treatment scenario

For each treatment scenario, the removal by each process was considered along the treatment train. For example, in a conventional scenario (CON), if coagulation was considered to remove 25% of the compound, the resulting concentration at 75% of the original amount would then be considered for removal via chlorination which could be considered to remove 50% giving a final value of 37.5% of the original concentration. The removal ranges determined for the compounds by each scenario are listed in Table 5.1. Note that where no information was available for chlorine or ozone and/or removal by coagulation was not expected a value of zero has been assigned to assume the worst case.

Table 5.1: Removal percentages of PMT substances by different water treatment scenarios

Substance	Removal (%)			
	CON	ADV	FILT	MEM
2,4,7,9-tetramethyldec-5-yne-4,7-diol	95	100	95	96
1,4-dioxane	15	90	15	15
Trichloroethylene	48	95	48	48
Tetrachloroethylene	48	97	48	61
Melamine	74	95	74	74
Dinoseb	88	100	88	91
Dapsone	81	99	81	81
Amantadine	83	97	83	83
Hexamethyldisiloxane	99	100	99	99
Tricarbonyl(methylcyclopentadienyl) manganese[a]				
Methyl cyclopentane[b]	49	99	49	62
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1)[a]				
Cyanuric acid[b]	40	94	40	40
Melamine[b]	74	95	74	74
2-phosphonobutane-1,2,4-tricarboxylic acid	0	49	0	0
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	78	99	78	86
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	0	50	0	0
4-aminophenol	81	99	81	81
2-morpholinoethanol	62	97	62	62
2,2'-azobis[2-methylbutyronitrile]	95	100	95	97
1,3-dichlorobenzene	45	98	45	59
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	71	98	71	71
N-butylbenzenesulphonamide	44	97	44	44
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	99	100	99	99
triclosan	49	99	49	69

CON – Conventional treatment, ADV – Advanced treatment, FILT - sand filtration plus disinfection, MEM - treatment by ultrafiltration membrane plus disinfection.

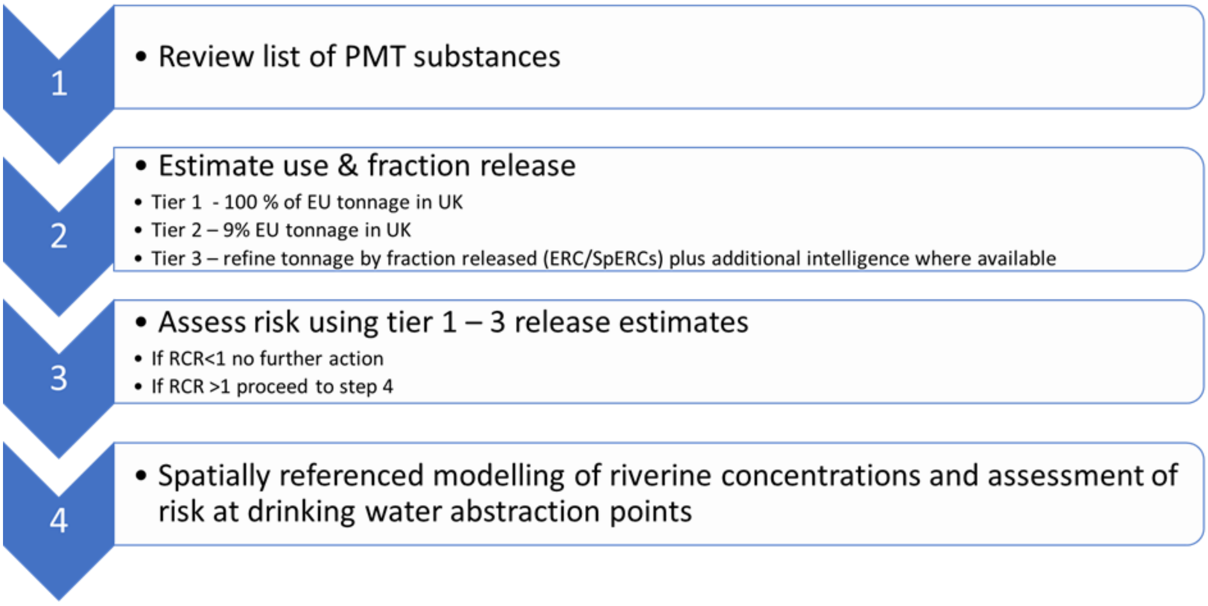
[a] *- Considered as dissociated compounds*

[b] *– dissociated compounds of [a] immediately above*

6. RISK ASSESSMENT

A tiered risk assessment was conducted for each substance to identify those that may pose a risk to human health through drinking water. This comprised up to four tiers of assessment moving from a simple, very conservative first tier of assessment through to a more refined spatially referenced assessment of risk (tier 4) for those substances identified as being of potential risk in lower tier assessment. This is represented by stages three and four in the diagram below (Figure 6.1). In the tier one risk assessment, a highly conservative assumption of environmental release was used, assuming the upper bound of the REACH tonnage band was used in the UK. Estimates of use and environmental release were refined through successive tiers. The tier two risk assessment used tonnage estimates from phase one work (DWI, 2020) whereby an assumption of 9% of the upper bound REACH tonnage band is released to the environment, considered to be a worst case scenario. The tier three risk assessment used refined estimates of tonnage and fraction released using additional intelligence gathered in this project (as described in Chapter 2). Only those substances identified as potential risk in tier three were taken forwards for tier four assessment which involved a spatially referenced modelling of river concentrations and assessment of risk at drinking water abstraction points in England and Wales.

Risks characterisation ratios (RCRs) with and without advanced treatment have been determined and are presented separately, acknowledging that not all treatment works have advanced treatment. An overview of the methodology is illustrated in Figure 6.1. Removal rates in WWTWs and through DWTPs are summarised in Table 6.1 together with the health based guidance values (HBGVs) used for risk assessment.



- Review list of PMT substances

- Estimate use & fraction release
  - Tier 1 - 100 % of EU tonnage in UK
  - Tier 2 – 9% EU tonnage in UK
  - Tier 3 – refine tonnage by fraction released (ERC/SpERCs) plus additional intelligence where available

- Assess risk using tier 1 – 3 release estimates
  - If RCR<1 no further action
  - If RCR >1 proceed to step 4

- Spatially referenced modelling of riverine concentrations and assessment of risk at drinking water abstraction points

Figure 6.1: Overview of tiered risk assessment

Table 6.1: Removal rates in WWTP, conventional water treatment and advanced water treatment for the 22 PMT substances. HBGVs are indicated as either cancer (C) or non-cancer (NC).

Compound	Removal Rate in WWTP (%)	Removal Rate Conventional WTW (%)	Removal Rate Advanced WTW (%)	HBGV (µg/kg/d)
2,4,7,9-tetramethyldec-5-yne-4,7-diol	7.99	94.60	99.76	1.50 (NC)
1,4-dioxane	0.67	15.39	89.62	16.00 (C)
Trichloroethylene	91.96	47.71	94.99	0.14 (C)
Tetrachloroethylene	94.13	47.69	97.17	4.70 (NC)
Melamine	0.00	73.72	95.12	200.00 (NC)
Dinoseb	52.27	87.56	99.95	0.78 (NC)
Dapsone	0.60	80.83	99.35	4.20 (C)
Amantadine	41.03	83.00	96.60	1.50 (NC)
Hexamethyldisiloxane	77.77	99.00	99.98	270.00 (NC)
Tricarbonyl(methylcyclopentadienyl) manganese	0.00	49.33	99.04	1.50 (NC)
Cyanuric Acid	0.00	40.17	94.13	1500.00 (NC)
2-phosphonobutane-1,2,4-tricarboxylic acid	0.28	0.00	49.00	1875.00 (NC)
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	59.77	77.97	99.16	0.17 (C)
4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	0.03	0.00	50.00	200.00 (NC)
4-aminophenol	0.41	80.98	99.20	100.00 (NC)
2-morpholinoethanol	0.37	61.94	97.28	1.50 (NC)
2,2'-azobis[2-methylbutyronitrile]	1.68	95.08	99.87	1.50 (NC)
1,3-dichlorobenzene	82.12	45.29	97.87	20.00 (NC)
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	0.18	71.33	98.21	10.00 (NC)
N-butylbenzenesulphonamide	2.05	43.78	97.29	260.00 (NC)
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	0.09	99.00	99.83	3800.00 (C)
Triclosan	51.97	48.96	98.99	400.00 (NC)

6.1 RISK ASSESSMENT TIERS 1-3

The scenarios for the first three tiers are as follows

Tier 1A: 100% of EU tonnage is assumed to be used in the UK. Removal in WWTPs estimated via SimpleTreat 4.0. **No dilution** in receiving water. **No removal** in drinking water treatment. This is essentially assuming people drink treated WWTP effluent and is, thus, highly conservative.

Tier 1B: 100% of EU tonnage is assumed to be used in the UK. Removal in WWTPs estimated via SimpleTreat 4.0. **No dilution** in receiving water. **Removal** in drinking water treatment via **conventional** (standard) treatment technologies only. This is essentially assuming undiluted WWTP effluent has been treated at the drinking water treatment plant.

Tier 1C: 100% of EU tonnage is assumed to be used in the UK. Removal in WWTPs estimated via SimpleTreat 4.0. **No dilution** in receiving water. **Removal** in drinking water treatment via **advanced** treatment technologies. This is essentially assuming undiluted WWTP effluent has been treated at the drinking water treatment plant.

Tier 2A: 9% of EU tonnage is assumed to be used in the UK. Removal in WWTPs estimated via SimpleTreat 4.0. No dilution in receiving water. No removal in drinking water treatment. This is essentially assuming people drink treated WWTP effluent and is, again, highly conservative.

Tier 2B: 9% of EU tonnage is assumed to be used in the UK. **Removal in WWTPs** estimated via SimpleTreat 4.0. **No dilution** in receiving water. Removal in drinking water treatment via **conventional** (standard) treatment technologies only. This is essentially assuming undiluted WWTP effluent has been treated at the drinking water treatment plant.

Tier 2C: 9% of EU tonnage is assumed to be used in the UK. **Removal in WWTPs** estimated via SimpleTreat 4.0. **No dilution** in receiving water. Removal in drinking water treatment via **advanced** treatment technologies. This is essentially assuming undiluted WWTP effluent has been treated at the drinking water treatment plant.

Tier 3A: A **more refined UK estimate of tonnage** (see Chapter 2). **Removal in WWTPs** estimated via SimpleTreat 4.0. **No dilution** in receiving water. **No removal** in drinking water treatment. This is essentially assuming people drink treated WWTP effluent and is, again, highly conservative, although the tonnage is more realistic.

Tier 3B: A **more refined UK estimate of tonnage** (see Chapter 2). **Removal in WWTPs** estimated via SimpleTreat 4.0. **No dilution** in receiving water. **Removal** in drinking water treatment via **conventional** (standard) treatment technologies only. This is essentially assuming undiluted WWTP effluent has been treated at the drinking water treatment plant.

Tier 3C: A **more refined UK estimate of tonnage** (see Chapter 2). **Removal in WWTPs** estimated via SimpleTreat 4.0. **No dilution** in receiving water. **Removal** in drinking water treatment via **advanced** treatment technologies. This is essentially assuming undiluted WWTP effluent has been treated at the drinking water treatment plant.

6.2 CALCULATION OF RISK CHARACTERISATION RATIOS

In all the tiers described above, no dilution in the receiving water body was assumed. This conservative assumption means that substances can be screened out from the risk assessment process if risk characterisation ratios (*RCR*s) are less than 1 at this stage. The *RCR* is defined as

$$RCR = \frac{C.I.M^{-1}}{HBGV} \tag{1}$$

where *C* is the concentration of chemical consumed in drinking water (μg L^{-1}), *I* is the daily drinking water intake for the individual being assessed (L cap^{-1} d^{-1}), *M* is the body mass of the individual being assessed and HBGV is the health based guidance value (μg kg^{-1} d^{-1}) which is derived from the toxicology assessments (Chapter 3). Values of *I* for infants, children and adults were assumed to be 0.75, 1 and 2 L cap^{-1} d^{-1}, respectively, and values of M for infants, children and adults were assumed to be 5, 10 and 60 kg, respectively. The concentration of chemical, *C*, is derived from

$$C = \frac{T.\delta}{P_{UK}.w}.(1 - r_{WWTP}).(1 - r_{WTW}) \tag{2}$$

where *T* is the annual tonnage assumed for the UK, P_{UK} is the population of the UK, *w* is the water use per capita (150 L d^{-1}), r_{WWTP} is the removal rate in secondary sewage treatment, r_{WTW} is the removal rate in drinking water treatment and δ is a factor to convert tonnes a^{-1} to μg d^{-1}.

Two sets of *RCR* were generated for each chemical in each scenario: (i) *RCR* assuming 100% of exposure to the chemical arises from the consumption of drinking water (Equation 1) and (ii) RCR_T if only 20% of exposure to the chemical arises from the consumption of drinking water. In this case, the total exposure including additional exposure from unknown sources can be calculated as

$$RCR_T = \frac{C.I.M^{-1}}{0.2 * TDI} \tag{3}$$

This assumption is somewhat conservative and whilst it is a more precautionary evaluation of risk, it is less relevant to the central question considered in this report: Do PMT chemicals in drinking water pose a risk to human health?

As noted previously the substance 1,3,5-triazine-2,4,6(1H,3H,5H)-trione, with 1,3,5-triazine-2,4,6-triamine (1:1) is essentially a 50:50 mix of melamine and cyanuric acid. Therefore, 50% of the estimated tonnage in each assessment was added to the melamine tonnage and the remaining 50% was evaluated as cyanuric acid. The HBGV values assumed for melamine and cyanuric acid, were for the individual substances and were 200 and 1500 μg kg^{-1} d^{-1} respectively.

6.3 TIER 4: SPATIALLY-REFERENCED MODELLING OF RIVERINE CONCENTRATIONS

A spatially-referenced model of riverine exposure was constructed for Great Britain. The model operates on a grid for the whole of Great Britain, at a resolution of 1km, similar to that described by Keller et al. (2007) and Whelan et al. (2012) but with updated data on river flow and population density.

For all substances surface water exposure was assumed to occur via the “down the drain” pathways from both industrial and domestic sources. Concentrations were predicted from population density, based on a *per capita* use rate and removal in wastewater treatment combined with dilution and in-stream degradation based on gridded water balance model predictions.

For surface water exposure, we employed algorithms described by Whelan et al. (2012). Chemical load is routed through a flow direction network derived from a digital elevation model, discounting for instream degradation processes, biodegradation, photodegradation or hydrolysis, if applicable, which are assumed to take place according to first order kinetics. For the substances considered in this project, very high persistence was assumed (i.e. a DT_{50} of 10,000 hours) which results in negligible in-stream losses for the velocities and travel distances typically encountered in British rivers. Steady state chemical emissions in each cell were calculated from population density and an assumed *per capita* chemical consumption (U, g cap^{-1} day^{-1}), discounted by the fraction of chemical removed during sewage treatment and adjusted by the fraction of the population served by secondary sewage treatment. Removal of chemical from the wastewater stream during wastewater treatment was predicted using SimpleTreat 4.0, as described for Tiers 1-3.

Concentrations in each 1 km grid cell were calculated from cumulative loads using discharge estimates derived by a cumulative routing of runoff (discharge per unit area of contributing catchment) through the grid using flow direction vectors derived from a digital elevation model (DEM).

We used model estimates of monthly discharge between 1960 and 2015 for a 1 km grid of Great Britain to derive a mean flow and a 95% exceedance flow (Q_{95}) for each grid cell (see Figure 6.2). The model estimates were produced using the CEH Grid-to-Grid (G2G) model for the MaRIUS (Managing the Risks, Impacts and Uncertainties of drought and water Scarcity) project using gridded rainfall data (CEH- Gridded Estimates of Areal Rainfall) and MORECS (Met Office Rainfall and Evaporation Calculation System) evapotranspiration estimates (Bell et al., 2018 but see also Bell et al., 2009). These data were processed using library routines in the NetCDF4 Python package to derive mean flow and Q_{95} grids. Flow directions at a 1km scale were obtained directly from Dr Vicky Bell at CEH. These data were derived using the method of Paz et al. (2006) as applied by Davies and Bell (2009) from the hydrologically corrected 50m integrated-hydrological-digital-terrain-model (IHDTM: Morris and Flavin, 1990; 1994). Flow directions use the D8 method (Jenson and Domingue, 1988), which has eight drainage directions (East = 1, South East = 2, South = 4, South West = 8, West = 16, North West = 32, North = 64, North East = 128). Population density estimates (Figure 6.3) were derived from the UK Gridded Population 2011, based on the 2011 Census and Land Cover Map 2015 (Reis et al., 2011).

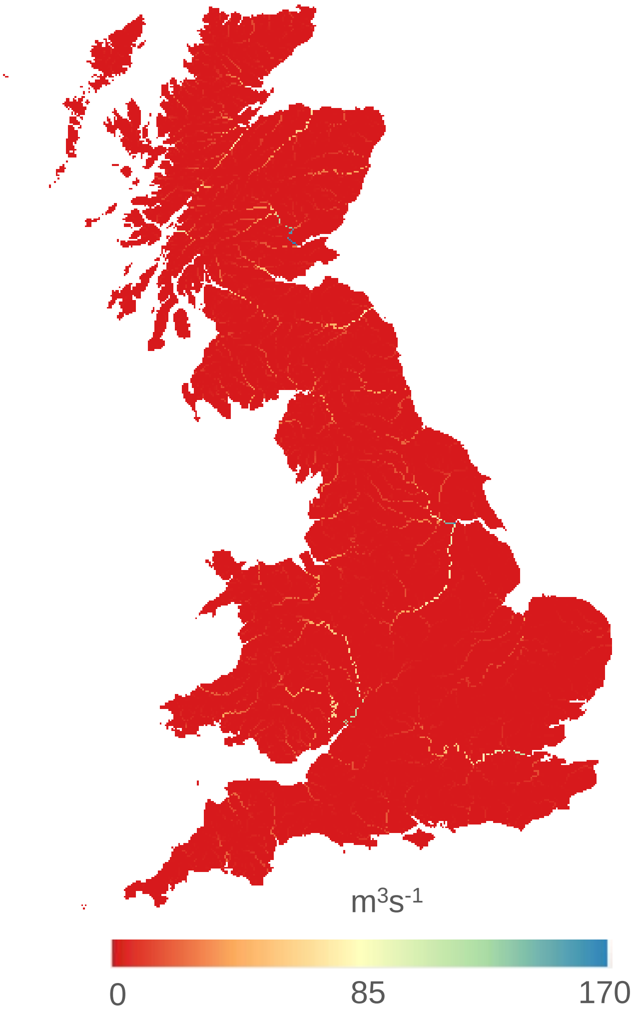


Figure 6.2 Mean flow for Great Britain in a 1 km grid estimated by the G2G model using gridded rainfall data and MORECS evapotranspiration estimates (Bell et al., 2018).

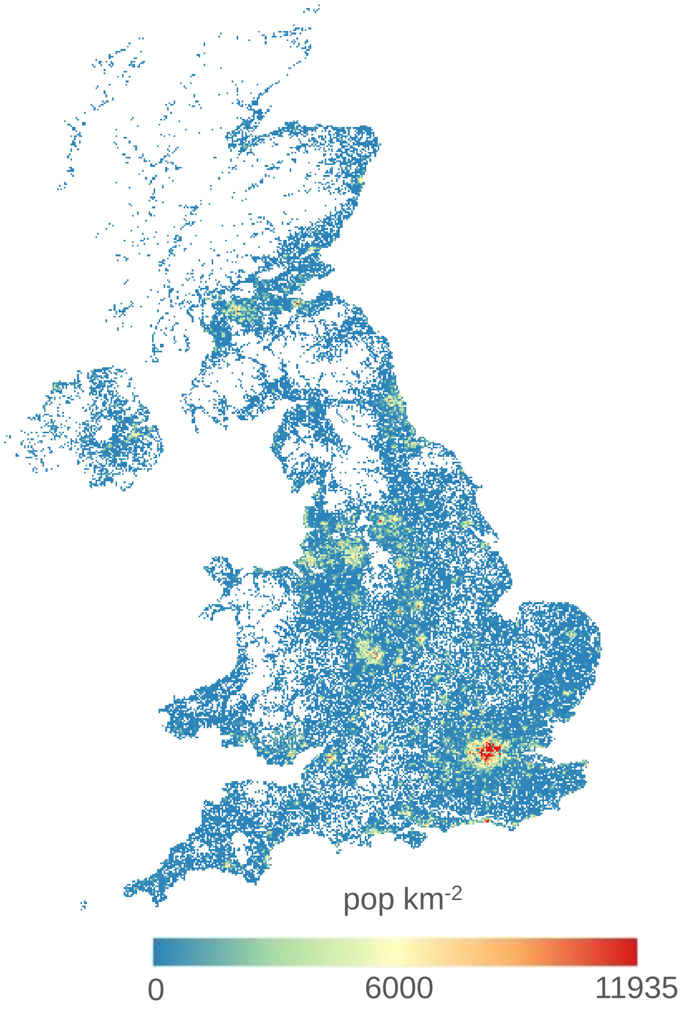


Figure 6.3 Gridded population density estimates based on the 2011 Census and the Land Cover Map 2015 (Reis et al., 2011).

These data were trimmed to a consistent grid (Great Britain - not including Northern Ireland) and imported into the model with a consistent spatial reference system.

In principle, loads can be discounted for degradation, assuming first order kinetics with travel time, calculated as the quotient of the stream path length and a nominal water velocity, allowing for stream channel sinuosity. However, this played a negligible role for the PMT substances considered in this report. Loads are described using:

$$L_x = L_0 . e^{-k.\tau} \qquad (4)$$

where L_x is the chemical load at a particular point in the river, L_0 is the load at a distance x m upstream along the flow path, k is the first-order degradation rate constant for the chemical of interest and τ is the travel time (h) calculated as:

$$\tau = \frac{x}{v} . c \qquad (5)$$

where *x* is the distance along the channel (m), *c* is a factor to convert from seconds to hours (2.78×10^{-4}) and *v* is water velocity ($m\ s^{-1}$). For cell to cell transfer in the horizontal and vertical directions x was calculated as

$$x = z.s \tag{6}$$

and for diagonal transfers x was calculated from Pythagoras theorem as

$$x = \sqrt{2.z^2}.s \tag{7}$$

where z is the cell width (1000 m) and *s* is river sinuosity, defined as the ratio of river length to down-valley length (Leopold and Wolman, 1957). This varies substantially depending on geomorphological setting with reports ranging from ca 1 (nearly straight) to >3 (Stolum, 1996; Stolum, 1998) with averages for natural channels of about 2 (e.g. Frascati and Lanzoni, 2009). Here, we assumed that all rivers have a sinuosity of 3 to account for the fact that valley lengths are also longer than the straight line lengths between grid cells used for flow routing in the model.

Water velocity was calculated from discharge using the empirical equation derived by Round et al. (1998):

$$v = 10^a.{Q_m}^b.\left(\frac{Q}{Q_m}\right)^c \tag{8}$$

where *Q* is the river discharge ($m^3\ s^{-1}$), Q_m is the mean river discharge for the reach in question ($m^3\ s^{-1}$) and *a*, *b* and *c* are empirical parameters reported to be -0.583, 0.283 and 0.495, respectively.

6.4 CONCENTRATION ESTIMATES AT DRINKING WATER ABSTRACTION POINTS

The locations for drinking water abstraction points were supplied by the DWI. After the removal of groundwater abstraction points, duplicate locations and duplicates within grid cells, there were 296 cells containing either a surface water or mixed water abstraction point. Note that the abstraction point in the Scilly Isles was also removed from this list. The locations of these abstraction points are shown in Figure 6.4.

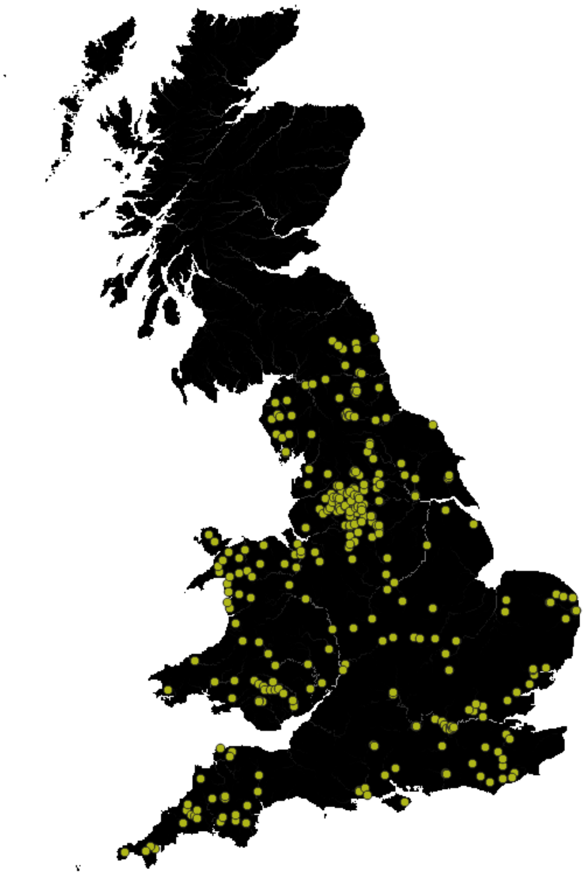


Figure 6.4 Location of surface water abstraction points for drinking water in England and Wales (Data supplied by DWI).

Predicted concentration in raw (untreated) drinking water was assumed to be the concentration predicted for the 1 x 1 km grid square within which the abstraction point was located. These concentrations were then reduced in accordance with the estimated removal rates in different drinking water treatment trains (conventional or advanced, as described above) to generate a distribution of concentrations in treated drinking water, and associated RCRs, under mean flow and Q_{95} conditions.

6.4.1 Accounting for additional emissions at industrial sites

For some substances high emissions may arise from specific industrial locations such as refineries, chemical manufacturing and formulating facilities. The following substances are suspected to have substantial potential emissions from such sites:

- 2,4,7,9-tetramethyldec-5-yne-4,7-diol	1 site identified
- Trichloroethylene	1 site identified
- Dinoseb	1 site identified
- Tricarbonyl(methylcyclopentadienyl) manganese	7 sites identified (oil refineries)

For Tricarbonyl(methylcyclopentadienyl) manganese, all sites are located at coastal or estuarine sites, so these point source emissions will not affect surface water abstractions for drinking water.

The other sites are also downstream of surface water abstraction points (see Figure 6.5) and consequently point source emissions from these sites are also unlikely to influence exposure to humans via drinking water.

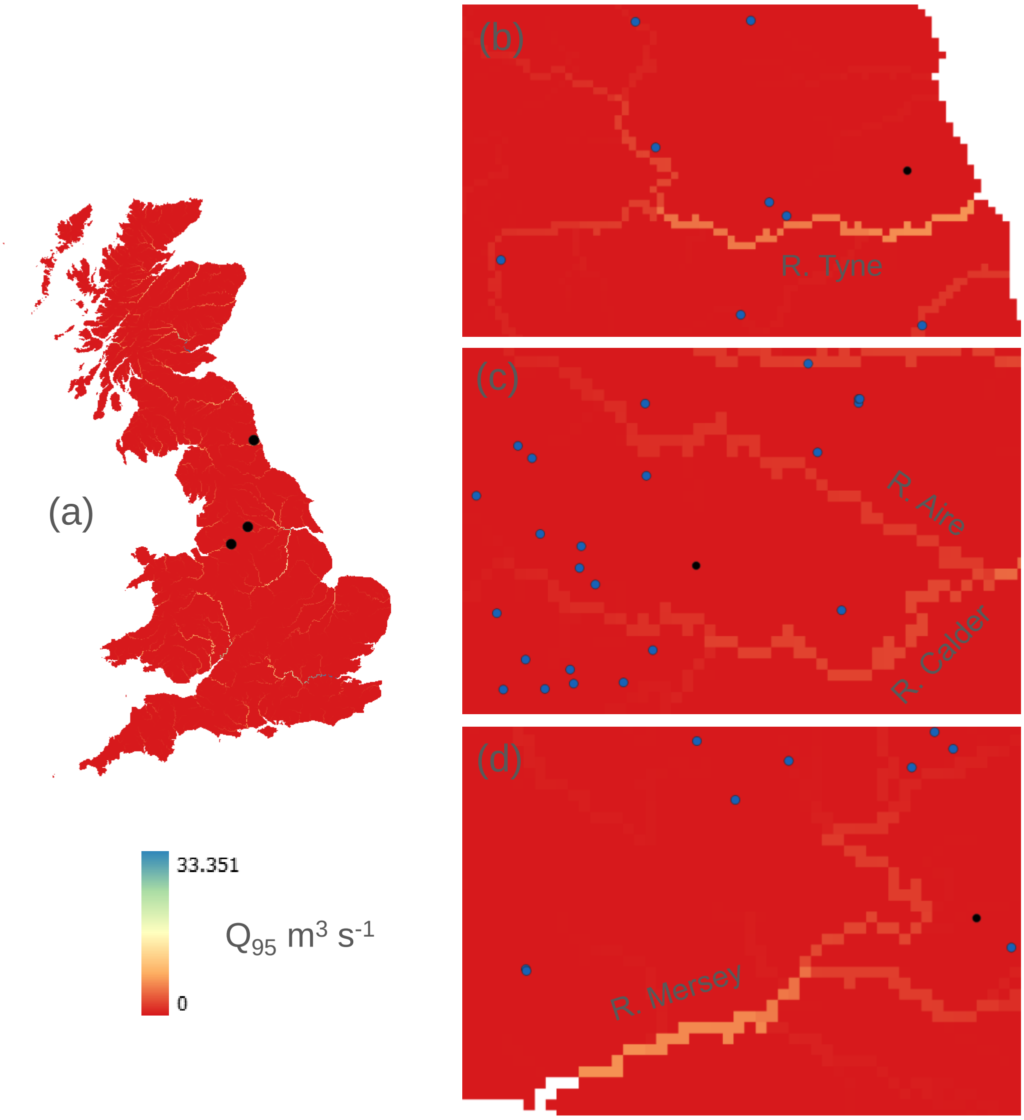


Figure 6.5 (a) Location of known manufacturing sites with potential industrial emissions superimposed on a map of Great Britain showing Q95. Panels (b), (c) and (d) show surface water abstraction points for drinking water (blue dots, data supplied by DWI) and the location of these manufacturing sites (black dots). In all cases, there are no drinking water abstraction points downstream of these sites.

6.5 RESULTS

6.5.1 Tiers 1-3

Predicted drinking water concentrations and RCRs for each chemical in each emission scenario considered in Tiers 1-3 are shown in **Error! Reference source not found.** to **Error! Reference source not found.**. Where relevant HBGVs for both cancer and non-cancer endpoints have been derived, the lowest HBGV was used for the risk assessment and is assumed to be protective for both cancer and non-cancer endpoints. In all cases, the results for the scenario representing an infant (M=5 kg; I=0.75 L d^{-1}) was considered as this is the most conservative for risk assessment. In all cases, removal in WWTPs was considered but **no dilution** in the receiving water body was assumed. In these scenarios, drinking water was assumed to be the only intake route for the chemical. Chemical removal in drinking water treatment was assumed to be zero for Scenario A, the rate predicted for conventional treatment for Scenario B and the rate predicted for advanced treatment for Scenario C.

For Tier 1 (100% of EU tonnage assumed to be used in the UK), most chemicals have RCRs greater than one 1 for scenarios A and B but only seven chemicals have an RCR greater than one for Scenario C (advanced treatment). This suggests that, for most chemicals, advanced treatment would be sufficient to reduce human health risks to acceptable levels even given the most extremely conservative assumptions.

When further refinement of tonnage was employed (tiers 2 and 3), the number of substances with an RCR exceeding one decreased. When assuming the most realistic estimates of emission derived in this project (tier 3) and conventional drinking water treatment provision (Scenario B) no substances were predicted to have a RCR exceeding one. Very high margins of safety (>10) were predicted when advanced DWTP were assumed (Scenario C). This suggests that no dilution is required for an acceptable risk assessment for drinking water consumption by infants, provided that conventional treatment trains are in place. Even in the absence of any water treatment, potential risks (RCR>1) were only identified for tetrachloroethylene and 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride.

Table 6.2 Predicted drinking water concentrations (Conc.) in µg L-1 and RCRs for each chemical in Tier 1. Note RCRs are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR<1. RCRs calculated assuming exposure only via drinking water. RCR values shown as 0.00 indicate values < 0.001.

	No DW Treatment Tier 1A		**Conventional Tier 1B**		**Advanced Tier 1C**	
Compound	**Conc.**	**RCR**	**Conc.**	**RCR**	**Conc.**	**RCR**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	2500.1	**250.01**	134.9	**13.49**	6.0	0.60
1,4-dioxane	2699.0	**25.30**	2283.6	**21.41**	280.1	**2.63**
Trichloroethylene	2184.6	**2340.65**	1142.3	**1223.85**	109.5	**117.33**
Tetrachloroethylene	15949.8	**509.04**	8343.4	**266.28**	451.1	**14.40**
Melamine	285303.2	**213.98**	74990.9	**56.24**	13923.7	**10.44**
Dinoseb	1296.9	**249.41**	161.4	**31.03**	0.6	0.12
Dapsone	2700.9	**96.46**	517.6	**18.49**	17.7	0.63
Amantadine	160.2	**16.02**	27.2	**2.72**	5.4	0.54
Hexamethyldisiloxane	604.0	0.34	6.0	0.00	0.1	0.00
Tricarbonyl(methylcyclopentadienyl) manganese	2717.2	**271.72**	1376.8	**137.68**	26.1	**2.61**
Cyanuric Acid	13585.9	**1.36**	8129.0	0.81	797.5	0.08
2-phosphonobutane-1,2,4-tricarboxylic acid	27095.7	**2.17**	27095.7	**2.17**	13818.8	**1.11**
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	109.3	**98.18**	24.1	**21.63**	0.9	0.82
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	2716.4	**2.04**	2716.4	**2.04**	1358.2	**1.02**
4-aminophenol	27.1	0.04	5.1	0.01	0.2	0.00
2-morpholinoethanol	270.7	**27.07**	103.0	**10.30**	7.4	0.74
2,2'-azobis[2-methylbutyronitrile]	267.2	**26.72**	13.1	**1.31**	0.3	0.03
1,3-dichlorobenzene	48.6	0.36	26.6	0.20	1.0	0.01
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	2712.3	**40.68**	777.6	**11.66**	48.6	0.73
N-butylbenzenesulphonamide	2661.5	**1.54**	1496.3	0.86	72.1	0.04
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	271.5	0.01	2.7	0.00	0.5	0.00
Triclosan	14.5	0.01	7.4	0.00	0.1	0.00

Table 6.3 Predicted drinking water concentrations](*C*) in $\mu g\ L^{-1}$ and RCRs for each chemical in **Tier 2**. Note RCRs are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR<1. RCRs calculated assuming exposure only via drinking water. Concentrations shown as 0.0 indicate values <0.01 $\mu g\ L^{-1}$ RCR values shown as 0.00 indicate values < 0.001.

	No DW Treatment		**Conventional**		**Advanced**	
	Tier 2A		**Tier 2B**		**Tier 2C**	
Compound	**Conc.**	**RCR**	**Conc.**	**RCR**	**Conc.**	**RCR**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	225.0	**22.50**	12.1	**1.21**	0.5	0.05
1,4-dioxane	242.9	**2.28**	205.5	**1.93**	25.2	0.24
Trichloroethylene	196.6	**210.66**	102.8	**110.15**	9.9	**10.56**
Tetrachloroethylene	1435.5	**45.81**	750.9	**23.97**	40.6	**1.30**
Melamine	25677.3	**19.26**	6749.2	**5.06**	1253.1	0.94
Dinoseb	116.7	**22.45**	14.5	**2.79**	0.1	0.01
Dapsone	243.1	**8.68**	46.6	**1.66**	1.6	0.06
Amantadine	14.4	**1.44**	2.5	0.25	0.5	0.05
Hexamethyldisiloxane	54.4	0.03	0.5	0.00	0.0	0.00
Tricarbonyl(methylcyclopentadienyl) manganese	244.5	**24.45**	123.9	**12.39**	2.3	0.23
Cyanuric Acid	1222.7	0.12	731.6	0.07	71.8	0.01
2-phosphonobutane-1,2,4-tricarboxylic acid	2438.6	0.20	2438.6	0.20	1243.7	0.10
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	9.8	**8.84**	2.2	**1.95**	0.1	0.07
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	244.5	0.18	244.5	0.18	122.2	0.09
4-aminophenol	2.4	0.00	0.5	0.00	0.0	0.00
2-morpholinoethanol	24.4	**2.44**	9.3	0.93	0.7	0.07
2,2'-azobis[2-methylbutyronitrile]	24.0	**2.40**	1.2	0.12	0.0	0.00
1,3-dichlorobenzene	4.4	0.03	2.4	0.02	0.1	0.00
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	244.1	**3.66**	70.0	**1.05**	4.4	0.07
N-butylbenzenesulphonamide	239.5	0.14	134.7	0.08	6.5	0.00
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	24.4	0.00	0.2	0.00	0.0	0.00
Triclosan	1.3	0.00	0.7	0.00	0.0	0.00

Table 6.4 Predicted drinking water concentrations (*C*) in μg L^{-1} and RCRs for each chemical in **Tier 3**. Note RCRs are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR<1. RCRs calculated assuming exposure only via drinking water. Concentrations shown as 0.0 indicate values <0.01 μg L^{-1} RCR values shown as 0.00 indicate values < 0.001.

	No DW Treatment Tier 3A		**Conventional Tier 3B**		**Advanced Tier 3C**	
Compound	**C**	**RCR**	**C**	**RCR**	**C**	**RCR**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	0.6	0.06	0.0	0.00	0.0	0.00
1,4-dioxane	61.5	0.58	52.1	0.49	1.6	0.06
Trichloroethylene	0.0	0.00	0.0	0.00	0.0	0.00
Tetrachloroethylene	39.9	**1.27**	20.9	0.67	5.7	0.04
Melamine	484.2	0.36	127.3	0.10	50.6	0.02
Dinoseb	0.4	0.07	0.0	0.01	0.0	0.00
Dapsone	25.4	0.91	4.9	0.17	0.2	0.01
Amantadine	1.6	0.16	0.3	0.03	0.0	0.01
Hexamethyldisiloxane	54.4	0.03	0.5	0.00	0.0	0.00
Tricarbonyl(methylcyclopentadienyl) manganese	0.0	0.00	0.0	0.00	0.0	0.00
Cyanuric Acid	81.5	0.01	48.8	0.00	0.1	0.00
2-phosphonobutane-1,2,4-tricarboxylic acid	2438.6	0.20	2438.6	0.20	27.0	0.10
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	1.4	**1.23**	0.3	0.27	0.0	0.01
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	244.5	0.18	244.5	0.18	2.5	0.09
4-aminophenol	8.4	0.01	1.6	0.00	0.0	0.00
2-morpholinoethanol	0.5	0.05	0.2	0.02	0.0	0.00
2,2'-azobis[2-methylbutyronitrile]	1.6	0.16	0.1	0.01	0.0	0.00
1,3-dichlorobenzene	0.1	0.00	0.0	0.00	0.0	0.00
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	20.1	0.30	5.8	0.09	0.1	0.01
N-butylbenzenesulphonamide	124.3	0.07	69.9	0.04	0.1	0.00
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	223.2	0.01	2.2	0.00	0.0	0.00
Triclosan	0.0	0.00	0.0	0.00	0.0	0.00

When the more conservative assumption that only 20% of chemical intake arises from the consumption of drinking water (again, assuming no riverine dilution), RCRs increase. These RCR_T values are shown in **Error! Reference source not found.** to **Error! Reference source not found.**. In this case, even in Tier 3 (**Error! Reference source not found.**), three chemicals have RCR_T are greater than one for conventional water treatment (Tier 3B), although all chemicals have RCR_T less than one for the advanced treatment scenario. This suggests that none of the chemicals considered pose a risk to human health providing advanced treatment is in place.

Under conventional water treatment, this screening assessment identified **three** chemicals of potential concern, which were considered for inclusion in Tier 4:

(i) 1,4-dioxane;
(ii) tetrachloroethylene;
(iii) 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride

All other chemicals were not considered further in the tier 4 risk assessment because no risk was identified in the highly conservative lower tiers of assessment.

The highest RCRs were generated for tetrachloroethylene. These high RCR values were driven by tetrachloroethylene' s moderate toxicity (HBGV: 4.7 ug/kg/d) and moderate tonnage (2500tpa) Some monitoring data in the UK are available (e.g. 26,680 samples in England and Wales: Table 4.6) which suggest that tetrachloroethylene has frequently been detected (18% of samples) above LOD. The 98th percentile concentration was 1.38 µg/L which is an order of magnitude lower than the concentration predicted in treated wastewater effluent for tier 3 tonnage. .

Tetrachloroethylene was selected to illustrate the tier 4 spatial assessment. However, the relative pattern of exposure will be similar for all substances. Predictions of spatial patterns of riverine concentrations for the other two chemicals with RCR_T values greater than one in tier 3B (20% of total exposure from drinking water) were also generated and are shown in Appendix 6.

Table 6.5 Predicted drinking water concentrations (*C*) in $\mu g\ L^{-1}$ and RCR_T for each chemical in **Tier 1**. Note RCR_T values are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR_T <1. RCR_T calculated assuming exposure via drinking water represents 20% of total exposure. RCR_T values shown as 0.00 indicate values < 0.001.

	No DW Treatment Tier 1A		**Conventional Tier 1B**		**Advanced Tier 1C**	
Compound	**Conc.**	**RCR**	**Conc.**	**RCR**	**Conc.**	**RCR**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	2500.1	**1250**	134.9	**67.45**	6.0	**2.99**
1,4-dioxane	2699.0	**127**	2283.6	**107.04**	280.1	**13.13**
Trichloroethylene	2184.6	**11703**	1142.3	**6119.27**	109.5	**586.67**
Tetrachloroethylene	15949.8	**2545**	8343.4	**1331.39**	451.1	**71.99**
Melamine	285303.2	**1070**	74990.9	**281.22**	13923.7	**52.21**
Dinoseb	1296.9	**1247**	161.4	**155.15**	0.6	0.62
Dapsone	2700.9	**482**	517.6	**92.44**	17.7	**3.16**
Amantadine	160.2	**80**	27.2	**13.62**	5.4	**2.72**
Hexamethyldisiloxane	604.0	**2**	6.0	0.02	0.1	0.00
Tricarbonyl(methylcyclopentadienyl) manganese	2717.2	**1359**	1376.8	**688.40**	26.1	**13.03**
Cyanuric Acid	13585.9	**7**	8129.0	**4.06**	797.5	0.40
2-phosphonobutane-1,2,4-tricarboxylic acid	27095.7	**11**	27095.7	**10.84**	13818.8	**5.53**
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	109.3	**491**	24.1	**108.17**	0.9	**4.11**
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	2716.4	**10.19**	2716.4	**10.19**	1358.2	**5.09**
4-aminophenol	27.1	0.20	5.1	0.04	0.2	0.00
2-morpholinoethanol	270.7	**135.36**	103.0	**51.51**	7.4	**3.68**
2,2'-azobis[2-methylbutyronitrile]	267.2	**133.58**	13.1	**6.57**	0.3	0.17
1,3-dichlorobenzene	48.6	**1.82**	26.6	1.00	1.0	0.04
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	2712.3	**203.42**	777.6	**58.32**	48.6	**3.64**
N-butylbenzenesulphonamide	2661.5	**7.68**	1496.3	**4.32**	72.1	0.21
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	271.5	0.05	2.7	0.00	0.5	0.00
Triclosan	14.5	0.03	7.4	0.01	0.1	0.00

Table 6.6 Predicted drinking water concentrations (*Conc.*) in $\mu g\ L^{-1}$ and RCR_T for each chemical in **Tier 2**. Note RCR_T values are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR_T <1. RCR_T calculated assuming exposure via drinking water represents 20% of total exposure. Concentrations shown as 0.0 indicate values <0.01 $\mu g\ L^{-1}$. RCR_T values shown as 0.00 indicate values < 0.001.

	No DW Treatment		**Conventional**		**Advanced**	
	Tier 2A		**Tier 2B**		**Tier 2C**	
Compound	**Conc.**	**RCR**	**Conc.**	**RCR**	**Conc.**	**RCR**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	225.0	**112.50**	12.1	**6.07**	0.5	0.27
1,4-dioxane	242.9	**11.39**	205.5	**9.63**	25.2	**1.18**
Trichloroethylene	196.6	**1053.29**	102.8	**550.73**	9.9	**52.80**
Tetrachloroethylene	1435.5	**229.07**	750.9	**119.83**	40.6	**6.48**
Melamine	25677.3	**96.29**	6749.2	**25.31**	1253.1	**4.70**
Dinoseb	116.7	**112.23**	14.5	**13.96**	0.1	0.06
Dapsone	243.1	**43.41**	46.6	**8.32**	1.6	0.28
Amantadine	14.4	**7.21**	2.5	**1.23**	0.5	0.25
Hexamethyldisiloxane	54.4	0.15	0.5	0.00	0.0	0.00
Tricarbonyl(methylcyclopentadienyl) manganese	244.5	**122.27**	123.9	**61.96**	2.3	**1.17**
Cyanuric Acid	1222.7	0.61	731.6	0.37	71.8	0.04
2-phosphonobutane-1,2,4-tricarbohxylic acid	2438.6	0.98	2438.6	0.98	1243.7	0.50
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	9.8	**44.18**	2.2	**9.73**	0.1	0.37
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	244.5	0.92	244.5	0.92	122.2	0.46
4-aminophenol	2.4	0.02	0.5	0.00	0.0	0.00
2-morpholinoethanol	24.4	**12.18**	9.3	**4.64**	0.7	0.33
2,2'-azobis[2-methylbutyronitrile]]	24.0	**12.02**	1.2	0.59	0.0	0.02
1,3-dichlorobenzene	4.4	0.16	2.4	0.09	0.1	0.00
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	244.1	**18.31**	70.0	**5.25**	4.4	0.33
N-butylbenzenesulphonamide	239.5	0.69	134.7	0.39	6.5	0.02
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	24.4	0.00	0.2	0.00	0.0	0.00
Triclosan	1.3	0.00	0.7	0.00	0.0	0.00

Table 6.7 Predicted drinking water concentrations (*Conc.*) in μg L^{-1} and RCR_T for each chemical in **Tier 3**. Note RCR_T values are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR_T <1. RCR_T calculated assuming exposure via drinking water represents 20% of total exposure. Concentrations shown as 0.0 indicate values <0.01 μg L^{-1}. RCR_T values shown as 0.00 indicate values < 0.001.

	No DW Treatment Tier 3A		**Conventional Tier 3B**		**Advanced Tier 3C**	
Compound	**C**	**RCR**	**C**	**RCR**	**C**	**RCR**
2,4,7,9-tetramethyldec-5-yne-4,7-diol	0.6	0.29	0.0	0.02	0.0	0.00
1,4-dioxane	61.5	**2.88**	52.1	**2.44**	1.6	0.30
Trichloroethylene	0.0	0.00	0.0	0.00	0.0	0.00
Tetrachloroethylene	39.9	**6.36**	20.9	**3.33**	5.7	0.18
Melamine	484.2	**1.82**	127.3	0.48	50.6	0.09
Dinoseb	0.4	0.34	0.0	0.04	0.0	0.00
Dapsone	25.4	**4.53**	4.9	0.87	0.2	0.03
Amantadine	1.6	0.80	0.3	0.14	0.0	0.03
Hexamethyldisiloxane	54.4	0.15	0.5	0.00	0.0	0.00
Tricarbonyl(methylcyclopentadienyl) manganese	0.0	0.00	0.0	0.00	0.0	0.00
Cyanuric Acid	81.5	0.04	48.8	0.02	0.1	0.00
2-phosphonobutane-1,2,4-tricarboxylic acid	2438.6	0.98	2438.6	0.98	27.0	0.50
1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride	1.4	**6.14**	0.3	**1.35**	0.0	0.05
4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl	244.5	0.92	244.5	0.92	2.5	0.46
4-aminophenol	8.4	0.06	1.6	0.01	0.0	0.00
2-morpholinoethanol	0.5	0.24	0.2	0.09	0.0	0.01
2,2'-azobis[2-methylbutyronitrile]	1.6	0.80	0.1	0.04	0.0	0.00
1,3-dichlorobenzene	0.1	0.00	0.0	0.00	0.0	0.00
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	20.1	**1.51**	5.8	0.43	0.1	0.03
N-butylbenzenesulphonamide	124.3	0.36	69.9	0.20	0.1	0.01
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	223.2	0.04	2.2	0.00	0.0	0.00
Triclosan	0.0	0.00	0.0	0.00	0.0	0.00

6.5.2 Tier 4 assessment results

The predicted spatial pattern of surface water exposure for all the substances investigated in this report are very similar because they are calculated using the same exposure assumption and data sets (population density, topographically-derived flow routing and river discharge). Only one example; tetrachloroethylene is shown here for illustrative purpose. This compound was selected because it has the highest predicted RCR_T value at tier 3B, has several different wide dispersive uses and has a relatively large body of environmental occurrence data in English rivers. Predicted tier 4 riverine concentrations of tetrachloroethylene are shown in **Error! Reference source not found.** for mean flow (a) and Q_{95} conditions (b).

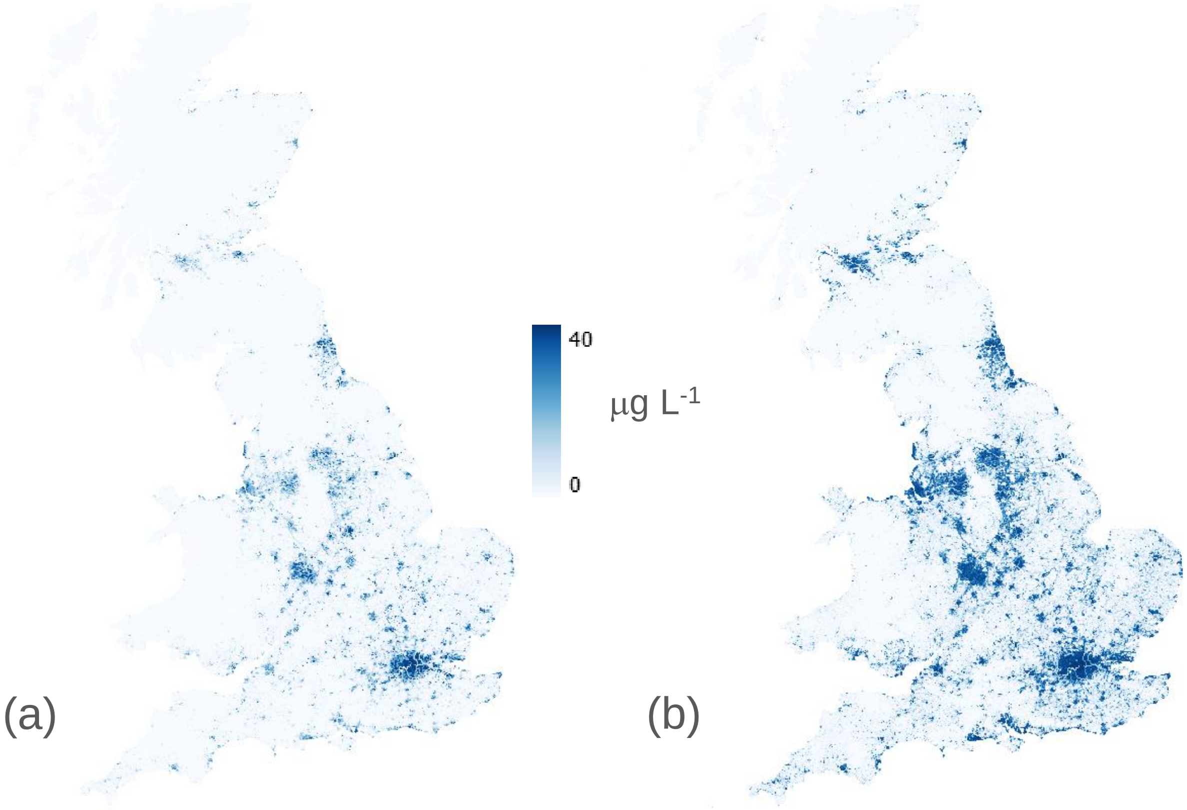


Figure 6.6 Predicted spatial patterns of the concentration of tetrachloroethylene in river water for Great Britain under (a) mean flow and (b) Q_{95} conditions.

Clearly, some cells have predicted riverine concentrations of tetrachloroethylene up to 39 μg L^{-1} under Q_{95} conditions, which is close to the concentration calculated for WWTP effluent – suggesting little dilution at low flow: see Table 6.7. Highest concentrations are, principally, predicted in densely populated areas including Greater London, the West Midlands, the Mersey basin (Manchester and Liverpool), West Yorkshire, the Northeast of England and the Central belt of Scotland.

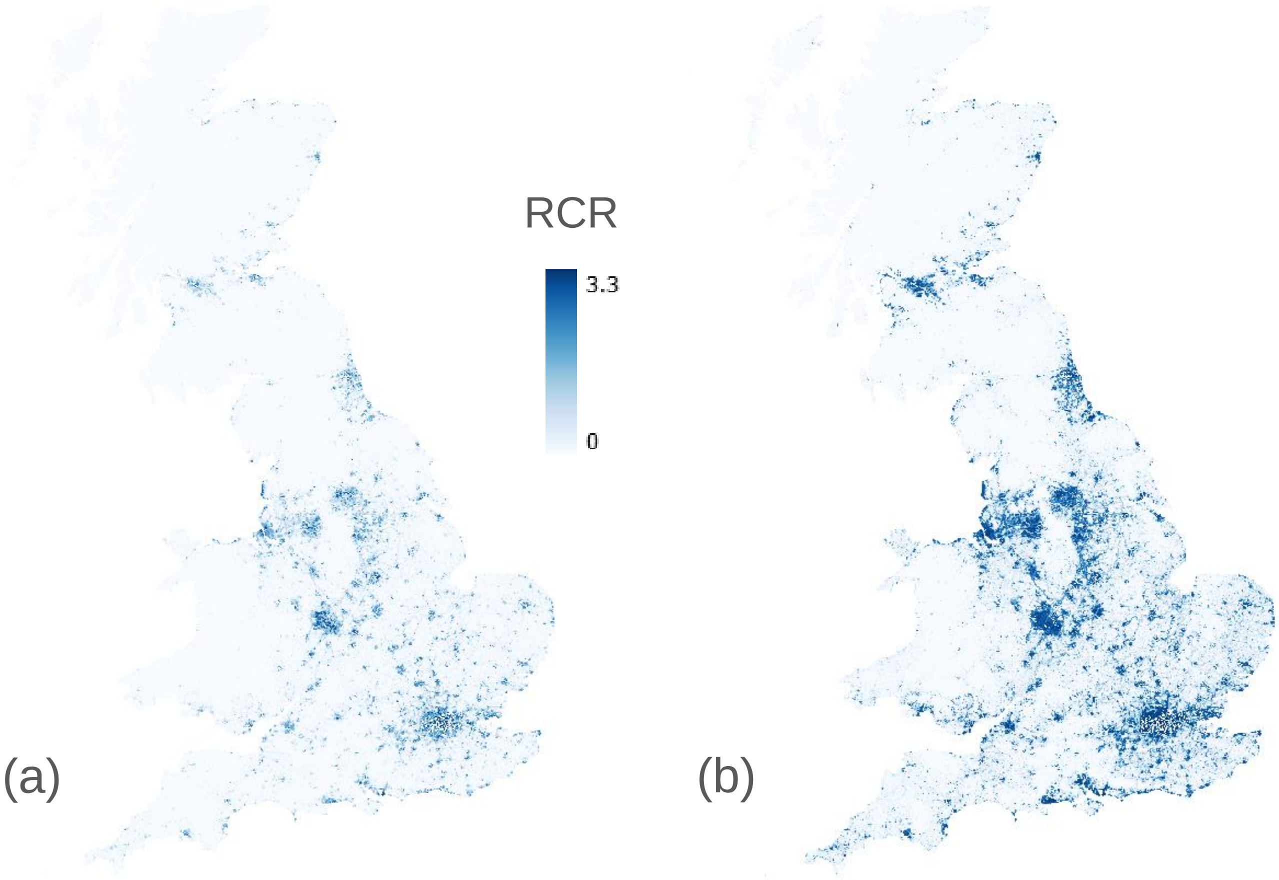


Figure 6.7 RCR_T derived from predicted concentrations of tetrachloroethylene assuming an infant exposure and conventional water treatment, for all cells shown in Figure 6.6.

Values of RCR_T for tetrachloroethylene extracted from cells containing surface water abstraction points for drinking water supply are displayed as cumulative probability distributions in Figure 6.8 for conventional water treatment trains at mean flow and Q_{95}. The percentage of abstraction points predicted to have RCR_T values greater than one for all three chemicals considered in tier 4 are shown in Table 6.8.

For conventional treatment, 15 (5.07%) and 54 (18.24%) treatment works (out of 296) were predicted to have RCR_T greater than one for tetrachloroethylene under mean flow and Q_{95} conditions, respectively.

Model predictions for the other two chemicals with top three RCR values are shown in the Appendix. In summary, for 1,4-dioxane 2.03% and 12.5% of treatment works were predicted to have RCR_T greater than one under mean flow and Q_{95} conditions, respectively. For 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride (also known as chlorendic anhydride) 0% and 4.39% of treatment works were predicted to have RCR_T greater than one under mean flow and Q_{95} conditions, respectively.

Note that predicted RCR values (exposure via drinking water only) were less than one for all abstraction points in both flow conditions for conventional treatment and RCR_T values (i.e., with an additional hypothetical five-fold exposure to these compounds from other sources) were less than one for all abstraction points in both flow conditions when advanced treatment was assumed. It is likely, therefore, that human health risks for all PMT substances associated with drinking water are currently acceptable, even if conventional treatment only is in place. If advanced treatment is in place, high margins of safety are likely be achieved for total exposure.

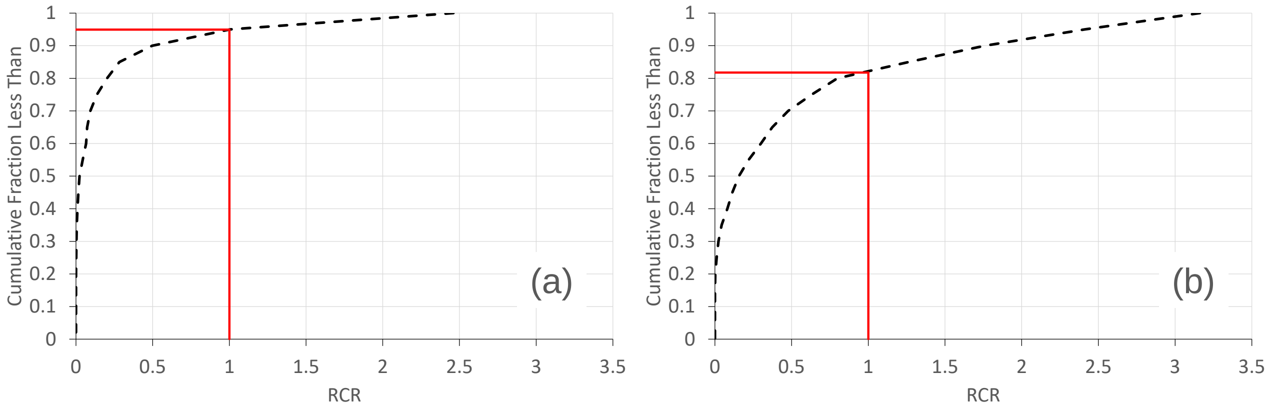


Figure 6.8 Cumulative distributions of predicted RCR_T values for tetrachloroethylene in drinking water in cells containing drinking water abstraction points assuming conventional treatment (dashed lines) under (a) mean flow and (b) Q_{95} flow. The red lines show the cumulative fraction less than $RCR_T = 1$.

Table 6.8 Predicted percentage of abstraction points with $RCR_T > 1$ for mean flow and Q95 conditions under the assumption of conventional treatment.

Chemical	Q_{mean} conditions	Q_{95} conditions
1,4-dioxane	2.03	12.50
Tetrachloroethylene	5.07	18.24
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	0	4.39

6.6 DISCUSSION OF RISK ASSESSMENT OUTPUTS

A tiered assessment of risk to human health through exposure via drinking water from surface water sources was performed for the 22 PMT/vPvM substances of interest to this project. The predominant environmental exposure pathway scenario was assumed to be wastewater emission to rivers followed by abstraction and supply. The lower tier screening assessment suggested that most of these substances pose very little risk to humans via drinking water consumption. Risk characterisation ratios (RCRs) for most substances were less than one even with highly conservative assumptions regarding use and release estimates and assuming no dilution in receiving waters and no advanced drinking water treatment.

When drinking water is assumed to be the only exposure route, *RCR* values were less than one if conventional treatment is in place, even without riverine dilution. However, RCR_T values from lower tier assessments for three substances; 1,4-dioxane, tetrachloroethylene and 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride, were high enough to indicate a potential risk. This was explored further through a spatially based higher tier assessment using a gridded model of exposure for the whole of Great Britain. The model generated estimates of surface water concentrations based on emissions which were assumed to be proportional to population density and routed through the landscape via a 1km resolution digital elevation model, under two flow scenarios: mean flow and low flow (Q_{95}).

In the higher tier assessment, all three substances; had RCRs greater than one at some abstraction sites when negligible degradation in the stream network and only conventional drinking water treatment was assumed. For tetrachloroethylene, predicted river concentrations in cells containing surface water abstraction points generated RCR_T values greater than one for approximately 5% and 18% of sites for mean flow and Q_{95} scenarios, respectively, under conventional drinking water treatment. For 1,4-dioxane the RCR_T values were greater than one for approximately 2% of surface water abstraction points at mean flow and 12.5% of points under Q_{95} conditions. For 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride, $\mathrm{RCR_T}$ values were less than one for all surface water abstraction points at mean flow and for 4.4% of points under Q_{95} conditions. However, all RCR_T values were less than one if advanced treatment was assumed. 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride hydrolyses rapidly to chlorendic acid. The hydrolysis product 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic acid (chlorendic acid). The most critical endpoint (IARC, 1990) is the same effect that can be seen with the parent compound, and for which the HBGV is based on for this substance.

If drinking water is assumed to represent the only exposure route, *RCR* values are less than one for all substances at all abstraction points under both conventional and advanced treatment. Overall, the results suggest that the consumption of these compounds via drinking water is unlikely to pose a health risk. However, drinking water may contribute to wider health risks for a small number of substances if substantial additional exposure routes exist. A more detailed assessment of the likelihood of this occurring is beyond the scope of this report.

It should be noted that the gridded exposure assessments described in this report are still very crude. Water and chemicals are routed at a 1 km resolution which is too coarse to allow detailed representation of channel networks and to describe the reality of abstraction point location with respect to rivers receiving wastewater. In any 1 km cell, there will be several rivers and streams, some of which may receive wastewater and others may not. In addition, the model assumes that chemicals are emitted in every cell in proportion to the population density. Sewage is collected in sewer networks with “sewersheds” extending over several km^2 which are emitted via WWTPs. This will result in some discrepancies between predicted and actual surface water exposure, although downstream loads should eventually be consistent for persistent chemicals.

There is a high degree of uncertainty associated with the estimates of release for all the substances assessed. For some substances, specific manufacturing site locations have been identified. However, environmental releases from these sites are uncertain and they all appear to be downstream of known surface water abstractions and thus unlikely to impact sources. Environment Agency monitoring data suggest that the top-ranked substance (by RCR) tetrachloroethylene is commonly detected in surface water in England. This suggests that the exposure assessment is conservative but that predicted concentrations are approximately of the right order of magnitude.

The HBGV for tetrachloroethene (non-cancer) is conservative, as it is based on a TDI set for inhalation exposure which was converted an oral exposure value via the addition of uncertainty factors. An alternative TDI, based on an oral study, is also available which has a higher HBGV of 14 µg/kg bw/day, versus the selected value of 4.7 µg/kg bw/day. However, this is based on a different adverse health effect and it was considered appropriate to take the more conservative approach to be fully protective of human health for all documented effects. Tetrachloroethene also has a cancer HBGV which is higher than the non-cancer HBGV; the non-cancer HBGV is therefore protective of the cancer effect.

The HBGV for 1,4-dioxane (non-cancer) is a robust TDI set by EFSA and the WHO, based on well documented studies. They are therefore considered to be the most appropriate HBGVs for these substances and the TDI used in the risk assessment for these substances is considered to be protective of human health for all individuals. As with tetrachloroethene, 1,4-dioxane has a cancer HBGV which is higher than the non-cancer HBGV with the non-cancer HBGV being protective of the cancer effect.

7. CONCLUSIONS

This project has explored the potential risk to drinking water from PMT/vPvM substances. This is needed to better understand the implications for human health and potential risk to drinking water sources from PMT substances. In turn, this will support the development of guidance for water companies on risk assessment and targeted monitoring of PMT substances to ensure drinking water supply is safe. It will also be of wider value to inform development of future UK policy on PMT substances as part of the developing Chemicals Strategy.

Substances with properties that meet the proposed EU PMT/vPvM criteria have been studied. Evidence on environmental occurrence in both raw and treated drinking waters has been collated, together with intelligence and data on the nature of use. Peer-reviewed toxicological information on each substance has been used to determine a health based guidance value (HBGV). Removal rates for each substance in both conventional drinking water treatment and advanced treatment processes have been determined. Finally, a tiered risk assessment has been performed to characterise risk to drinking water supply from surface water sources. For those substances identified as a potential risk a spatially based risk assessment was performed for England and Wales.

The substances studied in this project represent a subset of all substances that are likely to meet the proposed criteria for identification as PMT/vPvM. Substances were selected for study based on their relevance to England and Wales and a high priority for further study based on their properties, tonnage, and potential environmental emissions. We recommend that the list of PMT substances of concern for drinking water supply is regularly reviewed and updated. Many poly- and perfluoroalkylated substances (PFAS) also meet the PMT/vPvM criteria and PFAS are receiving considerable scrutiny in the scientific community, amongst regulators and in the media because of their extreme persistence, high environmental mobility, and the evidence harmful effects on health of some PFAS. We have explicitly excluded PFAS from this study because they are the subject of separate DWI funded research.

Environmental monitoring data for England and Wales show frequent detections in surface water and groundwaters for some PMT substances; these include saccharin, amantadine, 2,4,7,9-tetramethyl-5-decy-ne, melamine, 1,4-dioxane, triclosan and are most frequently detected in English surface waters. A similar pattern is observed in groundwater with 2,4,7,9-tetramethyl-5-decy-ne, trichloroethylene, saccharin and melamine most frequently detected. There are no monitoring data available for many others.

No monitoring data for any of the substances in treated drinking water in England and Wales were found. This is an evidence gap.

A wide variety of information sources have been searched to try and obtain data with which to estimate per capita release for each substance. However very little information is publicly available on amounts of each substances supplied and used in the UK.

Toxicological data for all substances covering both cancer and non-cancer endpoints have been collated and reviewed to derive HBGVs. A screening risk assessment using conservative assumptions suggest that most of the substances studied pose little risk to drinking water supply.

Whilst conventional drinking water treatment processes are moderately effective at removing most of the substances, advanced DWTPs are predicted to have a high removal efficiency.

Spatially based risk assessment were performed for three of the 22 substances studied in this project. These substances (1,4-dioxane, tetrachloroethylene and 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride) were identified as having a potential risk to drinking water in a screening level assessment.

In the higher tier assessment, all three substances; had RCRs greater than one at some surface water abstraction sites when negligible degradation in the stream network and only conventional drinking water treatment was assumed.

When advanced treatment processes are considered, none of the 22 substances had a risk characterisation greater than one and are considered to pose little risk to human health.

Most monitoring data available for England and Wales are not accurately measured and there are uncertainties associated with concentrations reported. For this reason, we have not used the data to perform any validation of model outputs. Further work to validate the model outputs using fully quantitative monitoring data for substances of interest at drinking water abstraction points would be very a useful next step.

Quantitative monitoring data for those substances with the highest potential risk in both surface water and groundwaters would be a useful additional line of evidence. None of the substances studied have been identified as a very high risk.

1,4-dioxane, tetrachloroethylene and 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride should be considered for including in targeted risk based monitoring. It would be more appropriate to monitor in water for the hydrolysis product of 1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride (chlorendic acid), than the substance itself.

Taking a precautionary approach, those substances identified as having a potential risk in the tier 2 assessment with conventional treatment (scenario 2B) could also be considered for monitoring to obtain quantitative data and better characterise typical environmental levels in English and Welsh water. This includes 2,4,7,9-tetramethyldec-5-yne-4,7-diol, trichloroethylene, melamine, dinoseb, dapsone, amantadine, tricarbonyl(methylcyclopentadienyl) manganese, 2-morpholinoethanol and 2,2'-dimethyl-2,2'-azodipropiononitrile.

Widespread environmental occurrence of melamine is reported. Potential indirect sources of melamine, such as such as the biocidal uses of cyromazine for animal health and slurry management described here should be explored further to better understand their potential for release to the environment.

The project has studied 22 substances that meet proposed criteria for identification as PMT/vPvM. However, there are likely to be other substances that meet PMT/vPvM criteria and are relevant to surface water drinking water sources in England and Wales. The list of relevant PMT substances should be reviewed and updated periodically.

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APPENDICES

APPENDIX 1 REVIEW OF PHASE 1 SUBSTANCE LIST

Supplied as separate file (ED15803_Appendix one.xls)

APPENDIX 2 INFORMATION SOURCES ON CHEMICAL USE

UK REACH

Registration of substances under UK REACH has also been considered. Currently no UK specific tonnage information is available and is unlikely to be for several years. Nordic SPIN

Since 2000, the Nordic Council have required members, (Sweden, Denmark, Finland, Norway), to declare the chemical products in use in the region. This requires importers or manufactures to annually declare the chemical products handled, the composition breakdown and the tonnage processed. Each nation, then determines the total tonnage of each substance and declares this to the SPIN system for publication. The full database from 2000 – 2019 was used in this project.

The lowest declared threshold is 0.1 tonnes. There are also rules on confidentiality, which limit the usefulness of some data. For example, if only one organisation uses a substance, the data are publicly withheld because they are commercially sensitive. Articles are not in scope along with non-chemical non-hazardous products such as cosmetics, where it is voluntary rather than mandatory to declare. Consequently, use may be under reported.

US EPA CompTox Chemical Dashboard

The US EPA have created the CompTox Chemical Dashboard – a single point of access for all the EPA's databases holding information on chemical substances.

Although there is the facility through this dashboard to obtain annual data on annual manufacture, import, usage and export of substances, extrapolated on a population basis. In general this seemed to provide an underestimate compared to other sources.

Toxics Release Inventory

In the US, there is a requirement for annual reporting to the Toxic Release Inventory (TRI) of emissions of the 490 substances classed as toxic to humans and the environment. Reporting requirements stipulate the size and nature of industrial facilities that must meet this obligation, covering the amount of waste created and disposal methods. This provides an indication of the amount of waste emitted to the environment but also provides an indication of the likely fraction released to water. Data from 2019 and 2020 was used for this project, accessed via the TRI factsheet provided on CompTox Chemical Dashboard. For substances relevant to this project that are listed in the TRI data was extrapolated to the UK on the basis of population.

UK Trade Info

The UK Trade information database is published by HMRC. This includes a breakdown by unique commodity code of the total mass of a substance imported and exported per annum. For chemicals there is inconsistency over time in the level of detail the commodity codes provide for a chemical. However, some substances have unique commodity codes and using these, it is possible to determine the net UK border-crossings of the substance The 2018 trade data was used as the basis for estimates for this project to avoid any anomalies in data associated with disruptions to trade because of COVID from 2020.

If only a few organisations involved in trading a given commodity, the data is withheld from public declaration to protect commercial confidentiality. Similarly, the requirements for declaration were reduced prior to the UK's exit from the EU when importing goods through the EU single market system.

EuroStat Database

The EuroStat Database covers a series of Europe-wide databases including one imports, exports and production of products as defined by NACE trade codes. Some chemical substances have a unique NACE code. Codes which indicate a substance 'and it's salts' were also used, and this was treated as the substance.

In the Eurostat database, data are withheld if the production tonnage would reveal commercially sensitive information. At the time of the UK's exit from the EU, data for both the EU27 and EU28 was reported. Consequently, it is possible to estimate a value for the UK by determining the difference between these totals. The 2018 trade data was used to avoid any anomalies in data associated with disruptions to trade from COVID, although in some cases other years were selected if 2018 appeared presented obvious anomalies compared with other years. This is not a unique data source since it uses the same data as the UK TradeInfo database.

Since the total net EU position was available, this dataset also allowed for comparison with use data from phase one.

Pharmaceuticals

The Electronic Medical Communication database was searched to identify the indication of use and recommended treatment course. This was combined with information on the occurrence rate to build a scenario for use, assuming was all cases complete a full treatment course. There was no single source of occurrence rates, various journal articles were used unique to each disease / illness.

Table A2. 1 REACH Environmental Release categories (taken from ECHA guidance R16-7)

Note	No	ERC	Default worst-case release factors resulting from the conditions of use described in the ERCs		
			To air (%)	To water (before STP) (%)	To soil (%)
1,7	1	Manufacture of the substance	5	6	0.01
2,7	2	Formulation into a mixture	2.5	2	0.01
2,7	3	Formulation into a solid matrix	30	0.2	0.1
3,7	4	Use of non-reactive processing aid at industrial site (no inclusion into or onto article)	100	100	5
4,7	5	Use at industrial site leading to inclusion into/onto article	50	50	1
5,7	6A	Use of intermediate	5	2	0.1
5,7	6B	Use of reactive processing aid at industrial site (no inclusion into or onto article)	0.1	5	0.025
5,7	6C	Use of monomer in polymerisation processes at industrial site (inclusion or not into/onto article)	5	5	0
5,7	6D	Use of reactive process regulators in polymerisation processes at industrial site; (inclusion or not into/onto article)	35	0.005	0.025
6,7	7	Use of functional fluid at industrial site	5	5	5
3,7	8A	Widespread use of non-reactive processing aid (no inclusion into or onto article, indoor)	100	100	n.a.
5,7	8B	Widespread use of reactive processing aid (no inclusion into or onto article indoor)	0.1	2	n.a.
4,7	8C	Widespread use leading to inclusion into/onto article (indoor)	15	30[14]	n.a.
3,7,8	8D	Widespread use of non-reactive processing aid (no inclusion into or onto article, outdoor)	100	100	20
4,7	8E	Widespread use of reactive processing aid (no inclusion into or onto article outdoor)	0.1	2	1
4,7	8F	Widespread use leading to inclusion into/onto article (outdoor)	15	5	0.5
6,7	9A	A Widespread use of functional fluid (indoor)	5	5	n.a.

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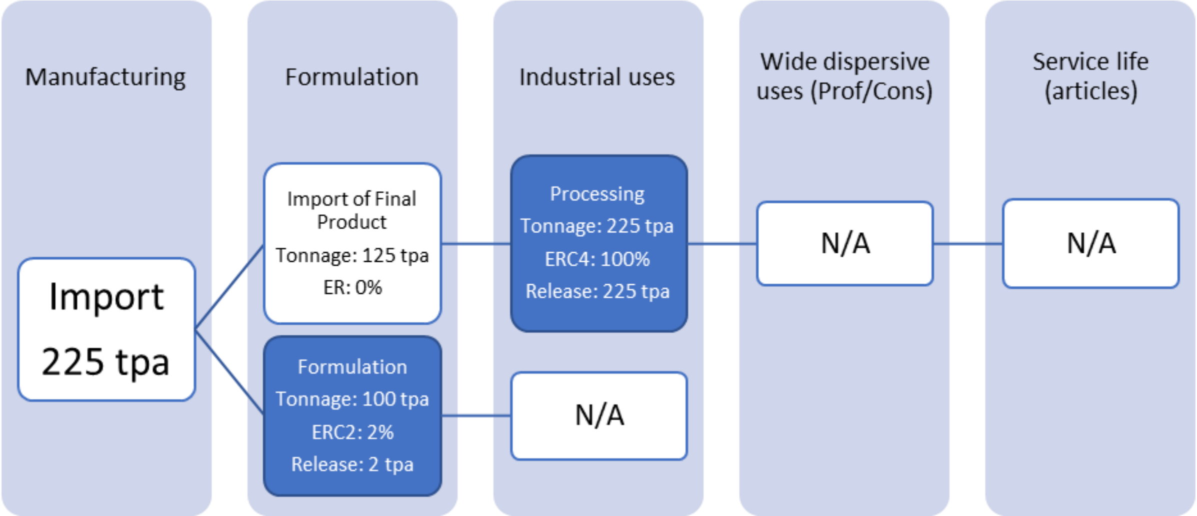
[14] The default release factor of 30% applies to activities/processes where the substance is dissolved/dispersed in a surplus of water and applied to an article via dipping/immersion or spreading (e.g. textile dyeing/finishing or application of polishes with floor cleaning water). For other widespread uses (e.g. use of paints and adhesives, including water based products) the release factor of 5% is applicable.

Note	No	ERC	Default worst-case release factors resulting from the conditions of use described in the ERCs		
			To air (%)	To water (before STP) (%)	To soil (%)
6,7	9B	Widespread use of functional fluid (outdoor)	5	5	5
8	10A	Widespread use of articles with low release (outdoor)	0.05	3.2	3.2
9,10	10B	Widespread use of articles with high or intended release (outdoor)	100	100	100
8	11A	Widespread use of articles with low release (indoor)	0.05	0.05	n.a.
9,10	11B	Widespread use of articles with high or intended release (indoor)	100	100	n.a.
10	12A	Processing of articles at industrial with low release	2.5	2.5	2.5
10	12B	Processing of articles at industrial processing with high release	20	20	20
8	12C	Use of articles at industrial sites with low release	0.05	0.05	n.a.

SUBSTANCE PROFILES

Use profiles for each substance together with details of the derivation of tier three estimates of total UK tonnage and fraction released at each life cycle stage are presented below.

1,4 - Dioxane (123-91-1)



1,4-dioxane (123-91-1) is used in a wide range of solvents to reduce irritation from other chemicals (Health Canada, 2021) but also occurs as a contaminant in alcohol ethoxylates used in cosmetics, cleaning (mostly degreasing), and personal care products. Consequently, it is a by-product present in many goods, including paint strippers, dyes, greases, antifreeze and aircraft deicing fluids, and in some consumer products (deodorants, shampoos and cosmetics) (ATSDR 2012; Mohr 2001). It is also used as processing aid.

In phase one (DWI, 2020) the upper bound of the REACH registration was identified as 1,000+tpa but assumed 1,000 tonnes exactly. EU production occurs at a single site in Germany with a capacity for manufacture of up to 2,500tpa. In the absence of additional information, we have applied the approach used in phase one estimated the UK tonnage as 9% of total EU tonnage (225tpa).

There is a single grandfathered application under UK REACH for 10-100tpa (HSE, 2021). We have assumed 1,4dioxane is not manufactured in the UK and that the UK REACH registration relates to 100tpa formulated

(ERC2) in the UK. We have assumed that an additional 125tpa are imported to the UK in finished products; the difference between total estimated UK tonnage and amount formulated in the UK.

In the absence of data to apportion the total tonnage between use as a solvent, processing aid , we have conservatively assumed the total tonnage is used in the application with greatest environmental release - use of non-reactive processing aid at industrial sites, with 100% release to the environment To account for the presence of 1,4-dioxane as a contaminant in alcohol ethoxylates we have estimated that an additional 3 tpa enter the UK environment via this route (see appendix 2 for full details), resulting in an estimated 228 tpa released to water.

It has been reported that 22% of the 25,000 cosmetic products in Skin Deep Database of cosmetics contain 1,4-dioxane. It is generally found in suds producing products, however not every product uses ethoxylation production processes most notably organic products as ethoxylation does not meet organic certifications requirements. (Campaign for Safe Cosmetics, n.d.).

The Scientific Committee on Consumer Safety conducted a study of products on sale (Scientific Committee on Consumer Safety , 2015) which provided information on the concentration, distribution and typical consumer consumption rate of 1,4-dioxane in finished products. They collated results from several small-scale sampling studies. 1,4-dioxane concentrations were measured in 170-products. 65% contained up to 1ppm, 92% contained up to 10ppm, 99% contained up to 25ppm and the maximum was 35ppm (Scientific Committee on Consumer Safety , 2015).

$$Av.ppm = [0.65 * 1] + [(0.92 - 0.65) * 10] + [(0.99 - 0.92) * 25] + [(1 - 0.99) * 35] = 5.4ppm$$

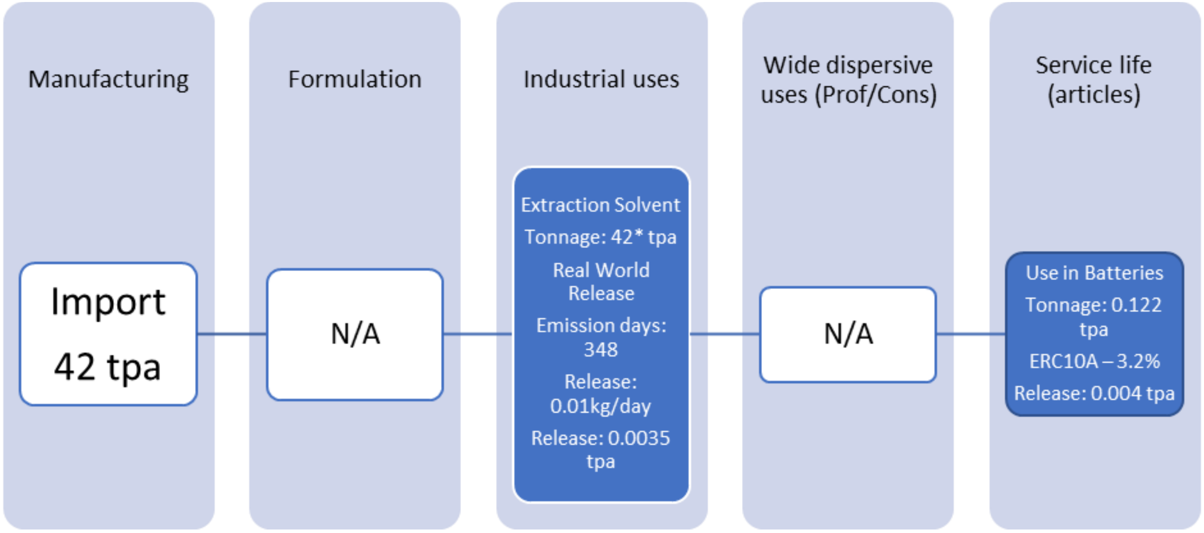
$$UK\ Useage = \left[\frac{\left(17.4g/d\ capita * \frac{5.4ppm}{1,000,000g}\right)}{1,000,000ppm/t}\right] * 365.25d/annum * 68,081,234\ capita = 2.34\ tpa$$

Using this information an average concentration in cosmetics can be derived as 5.4ppm. The Scientific Committee on Consumer Safety also determined the average cosmetic consumption is 17.4 g/day per capita. Extrapolating the per capita use to the UK population, and assuming 100% release to water through use in ‘down the drain’ personal care products, 2.34tpa of 1,4-dioxane from the cosmetics sector is assumed to be released to the water environment.

1,4-Dioxane is also a reported contaminant in ethoxylated alcohol. Using data from (HERA, 2009), and extrapolation to the UK, we estimate an additional 0.5tpa entering the UK environment via contaminated ethoxylated alcohol. This is also assumed to be 100% release to the environment.

A total release to water of 228 tpa has been derived by totalling the individual release estimates above.

Trichloroethylene (79-01-6)

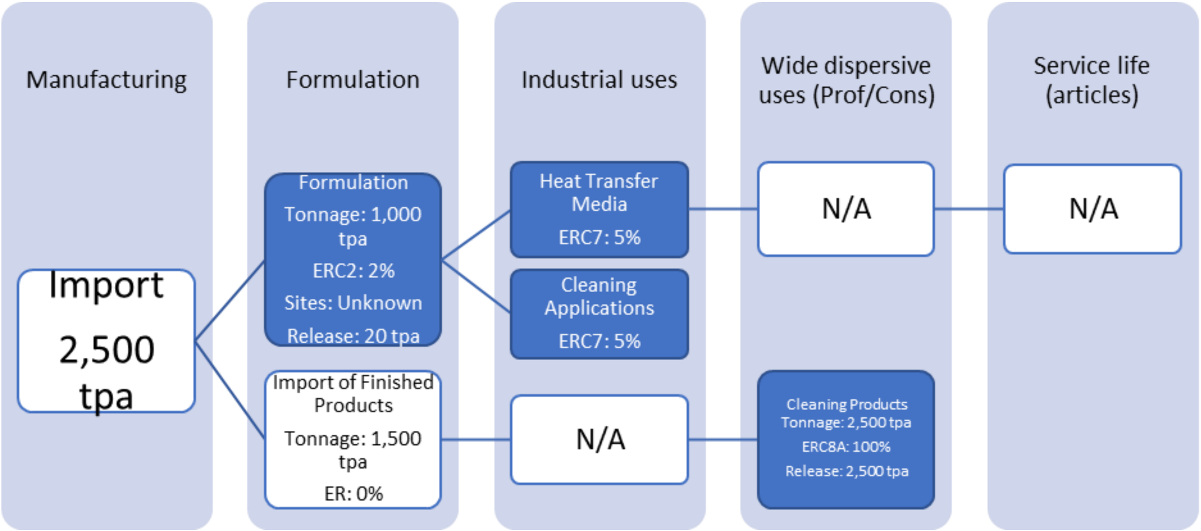


Trichloroethylene is a volatile organic solvent. It has been used in the vapour degreasing of metal parts and in consumer applications such as typewriter correction fluids, paints removers and strippers, adhesives, and spot removers (PubChem, 2022).

Trichloroethylene is a substance of very high concern (SVHC) under REACH. It is on the authorisation list with a sunset date in 2016. This means that non-exempted and non-authorised uses of the substance are now banned in the UK. A single UK application for authorisation is currently under review. Based on the regulatory status of the substance and available information, we have assumed that this is the only current UK based entity using trichloroethylene. Trichloroethylene is used at this site '*as an extraction solvent for removal of process oil and formation of the porous structure in polyethylene based separators used in lead-acid batteries*' (ECHA, 2014).

The chemical safety report (CSR) has been used for estimating amounts used and emissions, taken from the public application for authorisation documentation. The authorisation application did not cover the anticipated 0.122 tonne remaining in the final product (batteries), as this is outside of the scope of the CSR. Emissions from these articles are estimated using release factors ERC10A.

Tetrachloroethylene (127-18-4)



Tetrachloroethylene has had a wide range of uses. It is used in heat transfer media, surface cleaning, dry cleaning, and film cleaning. Use to formulate adhesives, sealants and coatings are also cited (PubChem, 2022). The major use, as listed in the Hazardous Substances Data Bank (HSDB) has been as a chemical intermediate for fluorocarbons and as a solvent for dry-cleaning. The apportionment of the total tonnage between different uses is unknown.

The UK trades tetrachloroethylene with approximately 55 countries and the net UK consumption, as reported to UK Trade Info, is approximately 1,000 tonnes annum (imports-exports). In 2018, the UK declared no production of tetrachloroethylene.

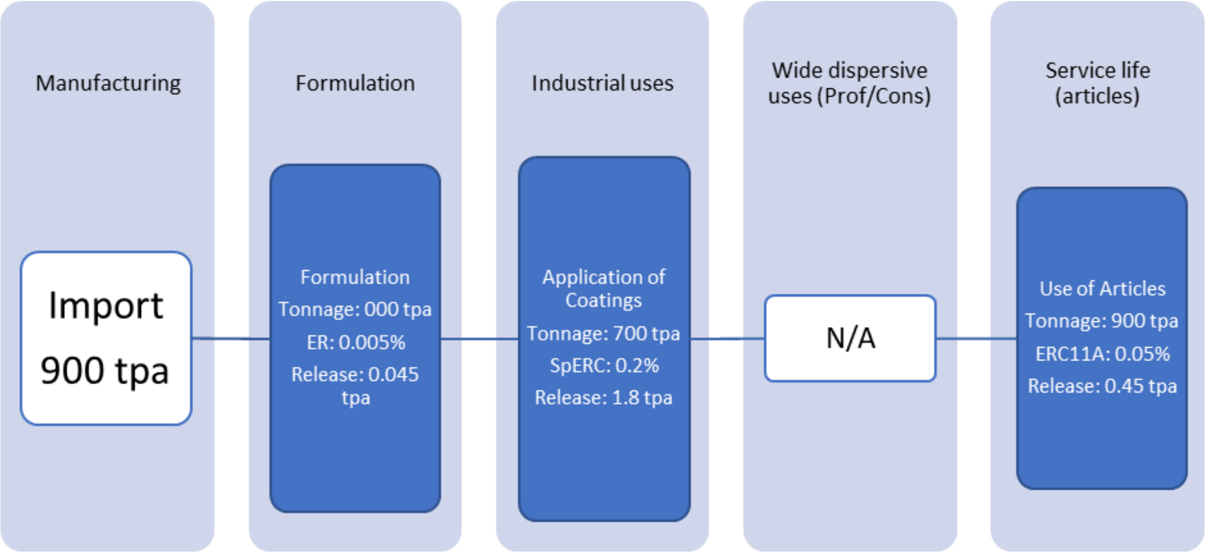
Evidence collected from REACH registration data in the phase one report suggested that the EU tonnage was between 100,000 and 1,000,000tpa. EU28 customs data (2018) has been used to estimate EU tonnage. This data reports 135,289 tonnes of tetrachloroethylene was produced, mostly for export. An overall EU net figure (production + import – export) of 27,148 tonnes remaining in the EU has been estimated. Assuming a 9% UK market share results in a UK tonnage estimate of approximately 2,500 tpa, .

Our estimate has assumed:

- No manufacturing in the UK, based upon data reported to EuroStat
- Formulation – assumed use of the net 1,000 tonnes remaining in the UK from HMRC customs data
- Usage – importation of 1,500 tonnes in finished products, bringing the UK usage in final products to the estimated UK tonnage total of 2,500 tpa

The apportionment of the total tonnage between different uses is unknown. For the purposes of generating an estimate of use and release for this project we have assumed that all UK usage is in cleaning products (ERC8A; 100% release) as a conservative assumption.

2,4,7,9-tetramethyldec-5-yne-4,7-diol (tetramethyl decynediol) (126-86-3)



2,4,7,9-tetramethyldec-5-yne-4,7-diol has been has used in printing inks, polymerization processes and as a wetting agent and defoamer in cleaning products. Information in the REACH registration dossier and the SPIN database indicate that use in cleaning products is minor (<1%). Use in inks, coatings and formulations has been considered in the use estimates below.

An estimate of 900 tonnes per annum (tpa) was determined in phase one (DWI 2020; 9% of the upper bound of the REACH tonnage band). Prior to the UKs exit from the EU there was a single UK based REACH registrant. Comparable data under UK REACH are not yet publicly available, consequently is not included in this analysis.

HMRC customs clearance data shows that in 2018 a UK net import of 664 tonnes was reported, with 99.7% of imports coming from the USA. As this was sourced from outside the EU it should have been declared to EU REACH, it is therefore likely that the UK based registrant was responsible for this import. For estimation if has therefore been assumed 700 tonnes per annum are used in the UK. The HMRC data supports the estimated value of 900 tpa from phase one and has been used in this work, providing a degree of conservatism by allowing for sources not reflected in the HMRC data.

The estimated amount released to water was further refined by assuming all tonnage was used in printing inks and applying specific release factors specific (SpERCs), published by the European Council of the Paint, Printing, Ink and Artists' Colours Industry (ECHA 2020a,b).

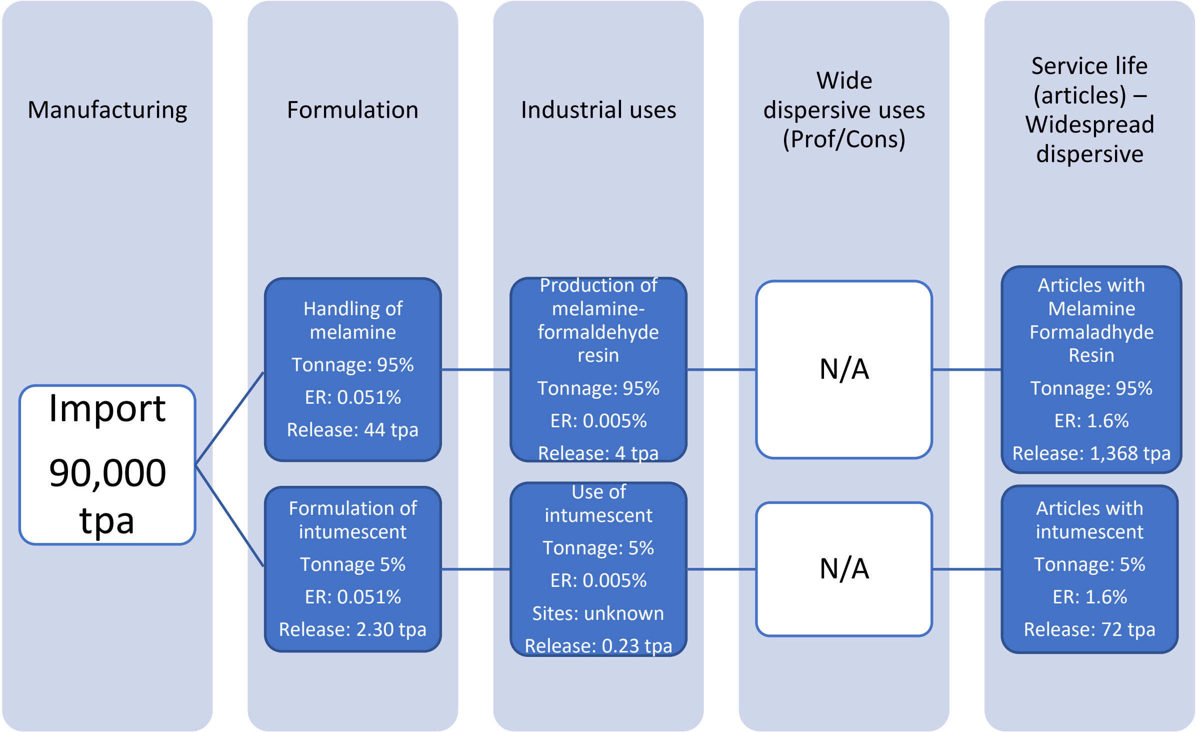
CEPE SPERC 2.4c.v2 Formulation of organic solvent and water borne coatings and inks (where specific formulation not known) – non-volatiles Water Release = 0.005% (ECHA, 2020)

CEPE SPERC 5.3.v2 Application - industrial - non-spray - indoor use – non-volatiles Water Release = 0.2% (ECHA, 2020)

Once these coatings are applied to articles the generic "Use of Articles" (ERC11A) has been assumed.

Amounts released at each life cycle stage been summed resulting in a tier 3 release of 2.3 tpa

Melamine (108-78-1)



Melamine is primarily used for melamine-formaldehyde resins, in which the melamine will be chemically bound within a polymer and generally considered unlikely to be released. There is some evidence of the release of residual melamine monomer from such articles, and it is unclear whether degradation of these polymers can lead to the release of melamine. Based on available information, 95% of melamine is used for melamine-formaldehyde resin, with release assumed to be negligible after production. The remaining five% is assumed to be used in intumescent coatings, in industrial and consumer uses.

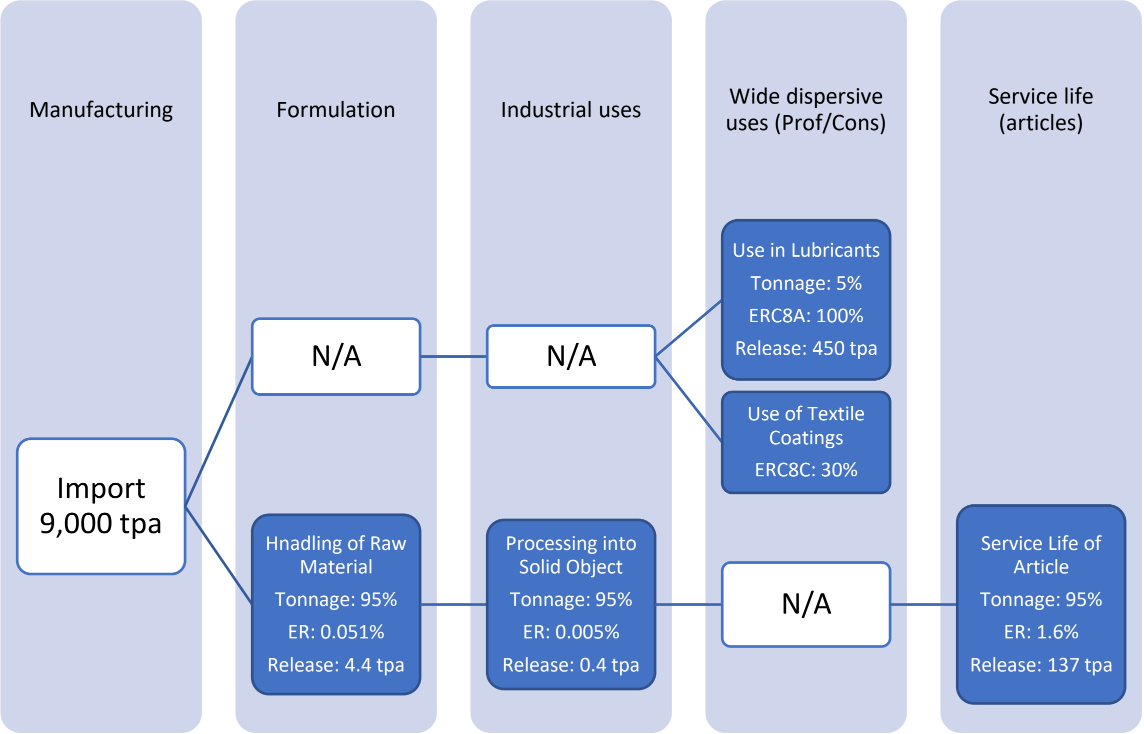
Estimates of amount released to water were determined in tier three by applying release factors reported in the OECD Emission Scenario document (OECD, 2009) (OECD 2009 using the scenario for flame retardants in plastic. The OECD have a specific scenario for use of flame retardants in polymers (OECD, 2009). For this project, release estimates have been derived by using the default low volatility at <40um particle size, scenario which assumes the following release factors.

- Handling of Raw Material, loss to water = 0.051%
- Processing, open process into solid articles = 0.005%
- Outdoor Service Life, leaching to environment = 0.16%*10 = 1.6%
    - *Expected service life ~10 years*

This results in an estimate of 1,490tpa released to the water environment.

Melamine is also identified as a major degradation product (70% of parent) of cyromazine, an insect growth regulator used as a biocide (product type 18) for the control of fly larvae in animal husbandry, outdoor manure heaps, slurry reservoirs and landfill sites and other breeding sites in animal housing. Cyromazine has also previously been used as a plant protection product (insecticide), primarily for tomato crops. As of 1st June 2022, no GB or NI Authorised Biocidal Products containing cyromazine as the active ingredient are listed. The EU Pesticides database lists cyromazine as “Not Approved” but it was previously approved for use on tomato crops from 2010 to 2019. Based on the information available no current approved use of cyromazine in the UK has been found. We have therefore been unable to consider this indirect source of melamine to the environment further. The fate of melamine resulting from the degradation of cyromazine from historical use may represent a legacy source. Further research is recommended to understand the historical use of cyromazine in the UK and its contribution to the observed levels of melamine detected in UK waters.

1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1) (melamine cyanurate) (37640-57-6)



The substance 1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1), also known as melamine cyanurate is used as a flame retardant in plastics and coatings primarily in the building industry along with use in greases and lubricants. The compound is also used in the textile industry. The substance is a high molecular weight complex, comprising one to one ratio of molecules of melamine and cyanuric acid, strongly bound in the crystal lattice (REACH registered substances fact sheet; ECHA,2022). In water, the substance is present as the two separate molecules melamine and cyanuric acid. Estimates of release have been derived for each component. As the compound is known to exist as a 1:1 molar ratio, the estimated tonnage has been split on a molar weights basis for estimating release to surface water. The melamine tonnage has been added to the melamine tonnage determined in section 2.3.5.

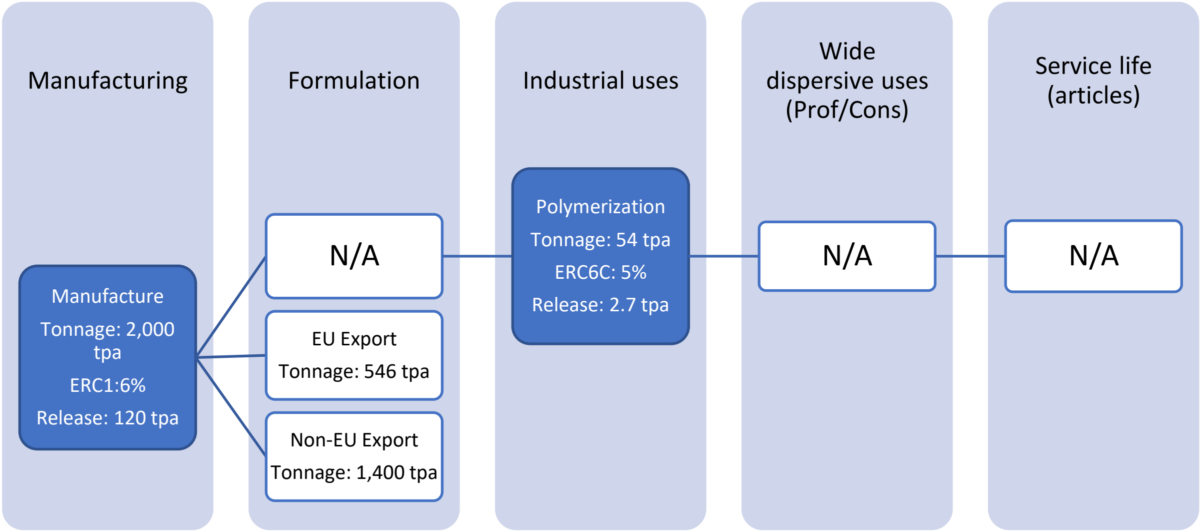
No UK based notifier was present on the REACH dossier prior to the UKs exit from the EU and no request for grandfathering under UK REACH has been submitted. This suggests that manufacture of the substance in the UK is unlikely. Consequently, only potential for release from finished products has been considered.

Data from Nordic SPIN suggest the use of melamine cyanurate as a lubricant is relatively low. A conservative estimate with an arbitrary split of use as 5% in lubricant and 95% as flame retardant was used for estimates.

As for melamine , values for fraction released from the OECD emission scenario document for flame retardants in polymers have been used to estimate quantities released (OECD, 2009).

The tonnage estimate for melamine estimated for this substances has been combined with the tonnage of melamine to provide an overall tonnage for melamine for use in exposure modelling.

Dinoseb (88-85-7)



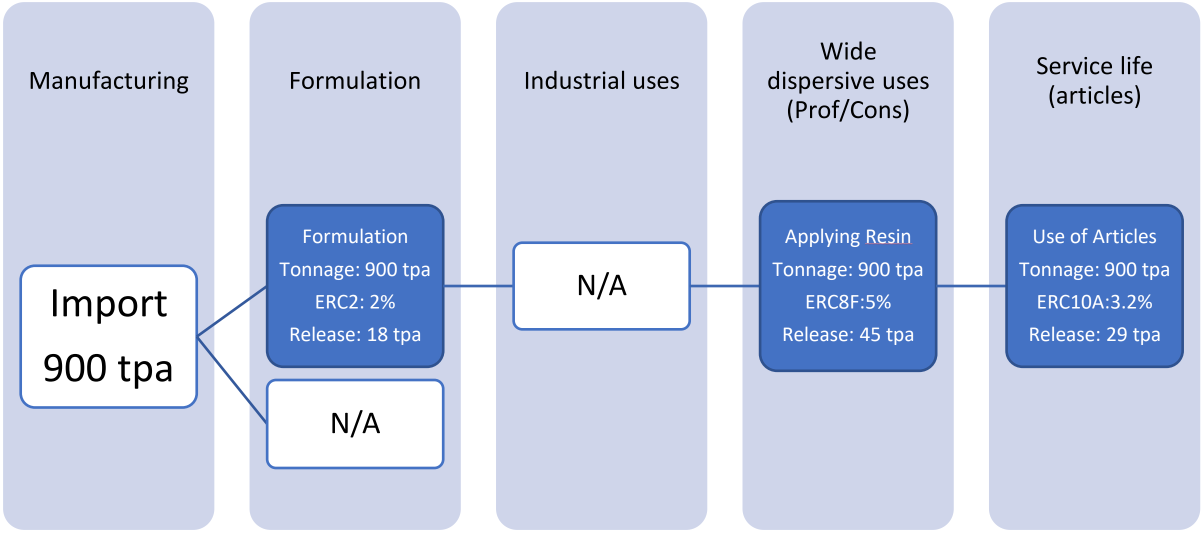
Dinoseb, also known as DNBP, is used as a polymerisation control agent (styrene retarder). REACH data and information from the manufacturer indicate that all dinoseb registered under REACH is manufactured at a single UK site. Historically dinoseb has been used as a pesticide but is not currently approved for use as a pesticide in either the UK or EU. For risk assessment and modelling we have considered releases during manufacture and industrial use.

In October 2012, Dinoseb was reviewed for potential classification as an SVHC, the manufacturer submitted a comment (ECHA, 2018) to the proposal which gave more details on their site. They stated that they were the only UK manufacturer, with a production of around 2,000tpa of which 600 tonnes was supplied to the EU, the assumption is the remaining, 1,400tpa, would be exported outside the EU region. This is supported by the UK Trade Info showing that for the 2011 calendar year, a net 602 tonnes exported from the UK to the EU with 1,714 tonnes total UK exported globally

For estimates of amounts used and released, we have based our calculations on the publicly available data shared by the manufacturer to (ECHA, 2018). We have assumed manufacture of 2,000tpa. Release to water has been calculated using the default release for manufacture (ERC1) of 6%, which results in an estimate of 120tpa release to water from the UK site during manufacture and expected to enter the water system at the local wastewater treatment works.

Assuming 600tpa in styrene production in the EU/UK, and assuming a 9% UK market share as per phase one, results in an estimate UK of 54tpa dinoseb used in styrene production. Applying the default environmental release assumptions for formulation (ERC6C (5%) – use of monomer in polymerisation processes, at an industrial site (inclusion or not onto/into article) results 2.7tpa released to water.

Dapsone (80-08-0)



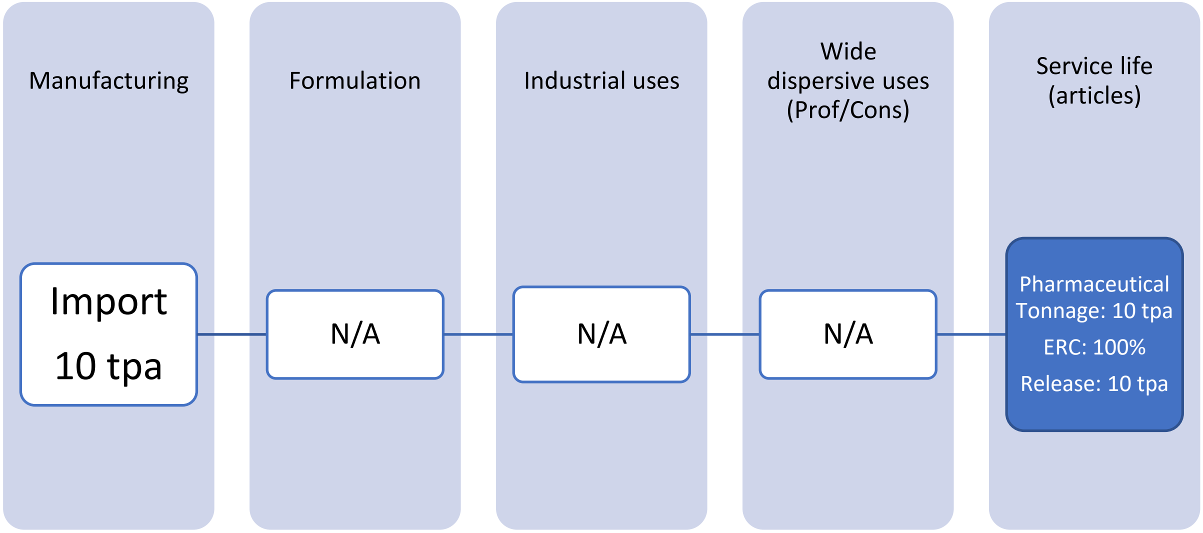
Dapsone has a wide variety of uses; as a resin in articles, as an intermediate in the manufacture of polymers, and as a pharmaceutical indicated for use as an anti-infective for treatment of leprosy, dermatitis herpetiformis and prevention of pneumonia.

For industrial uses, it was not possible to refine tonnage estimates further than previous phase one estimates (DWI 2020) and this value was carried forward to the current project. As a conservative assumption the total REACH tonnage has been applied to the use of dapsone the use as a resin in articles as this has greater potential for environmental release than its use as a chemical intermediate.

Pharmaceutical use in the UK is not reflected in the REACH tonnage data. Use as a pharmaceutical has been estimated by combining the average UK case rate and recommended treatment plan, resulting in an estimated. Additional 2tpa. This is maybe an underestimate as dapsone could be prescribed for other conditions. As a conservative assumption we have assumed no metabolism of dapsone following administration and excretion.

The estimated pharmaceutical use has been added to the estimate for industrial uses to give a tier 3 estimate of 94tpa

Amantadine (768-94-5)

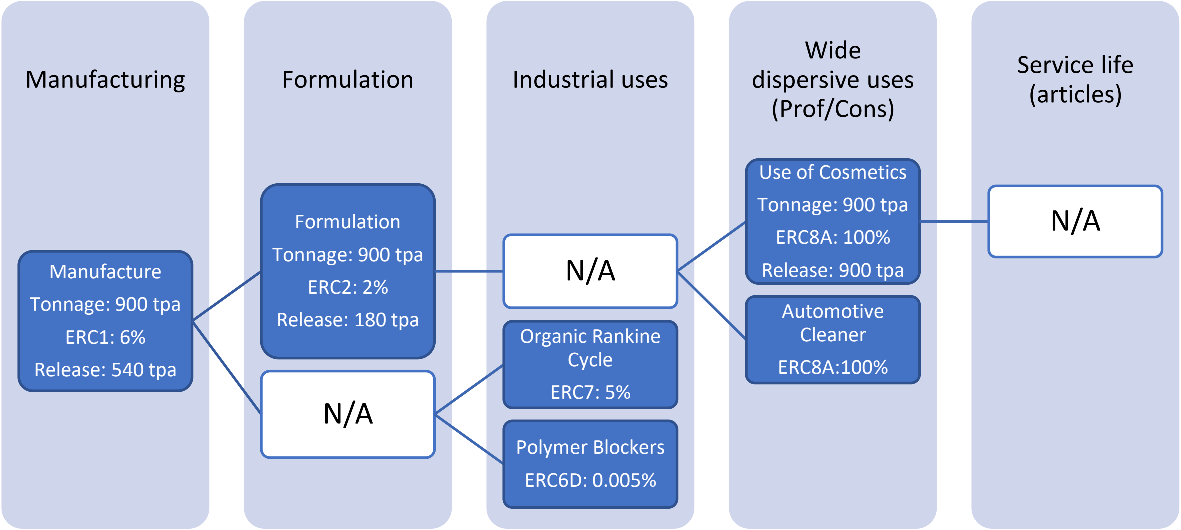


Amantadine is primarily used as an active pharmaceutical ingredient (API). Tonnage information reported under REACH does not cover its use as a pharmaceutical. Amantadine, as amantadine hydrochloride is used for treatments of Influenza A, Parkinson's disease, and Herpes zoster.

Consequently, estimates based on REACH tonnage could reflect an underestimate of the total tonnage. The only REACH dossier in the public ECHA database reports intermediate usage by BASF in Germany. During phase one (DWI, 2020), the intermediate use reported under REACH was assumed to reflect use in a closed system with no environmental release. Expanding our review to consider other databases, we found no other reported uses of amantadine in Nordic SPIN or documented in the US EPA CompTox Dashboard.

UK case rates for Parkinson's disease have been used to conservatively estimate usage in the UK and we have assumed the primary form of treatment is amantadine. Amantadine is also used for treatment of influenza and Herpes zoster, but the contribution is negligible in comparison, mostly due to the treatment cycles on the order of days, as opposed to years in the case of Parkinson's disease. As a conservative assumption we have assumed no metabolism once administered. The off-licence use of amantadine in veterinary medicine is anecdotally reported as a treatment for pain management in cats and dogs. There are no data publicly available to indicate the scale of use in this manner and we have been unable to include this in our estimate. The anticipated use of amantadine in veterinary medicine is a knowledge gap that should be explored further an any subsequent studies.

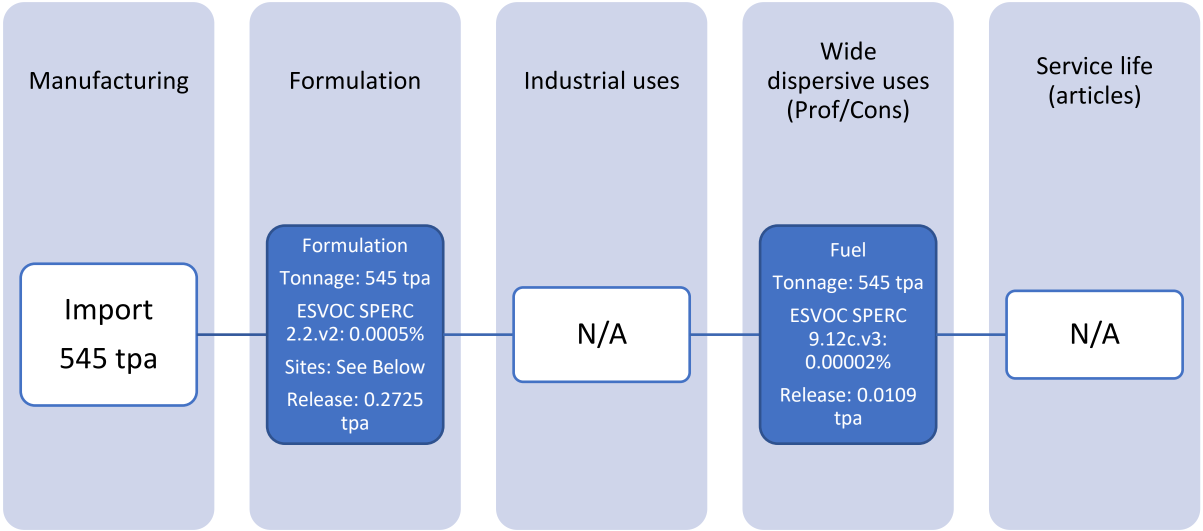
Hexamethyldisiloxane (107-46-0)



Hexamethyldisiloxane has a variety of uses, mostly in personal care products, automotive cleaning products, pharmaceuticals and cosmetics but also in industrial applications with reported uses as an intermediate and within polymers. We have been unable to refine the tonnage further from the estimate in phase 1 project (900tpa). Tonnage reported under REACH will not account for pharmaceutical use, for which no data has been found.

The substance has been grandfathered under UK REACH, suggesting that manufacture and/or import from outside EU/EEA may be occurring in the UK. We have not found any data that could be used to attribute the distribution of tonnage across different use scenarios so as a conservative estimate we have assumed that all hexamethyldisiloxane is used in down the drain personal care products.

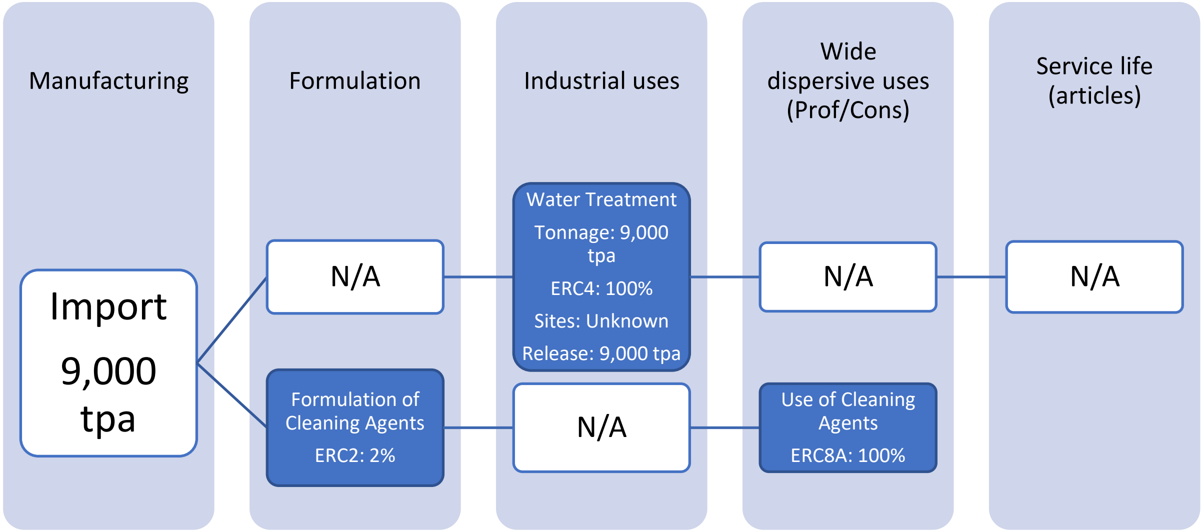
Tricarbonyl(methylcyclopentadienyl) manganese (12108-13-3)



Tricarbonyl(methylcyclopentadienyl) manganese is used as a fuel additive to improve the octane number in unleaded petrol. The substance has been grandfathered under UK REACH. No evidence of UK manufacture has been identified. We have assumed that formulation into fuels and use of fuels are the main emission pathways.

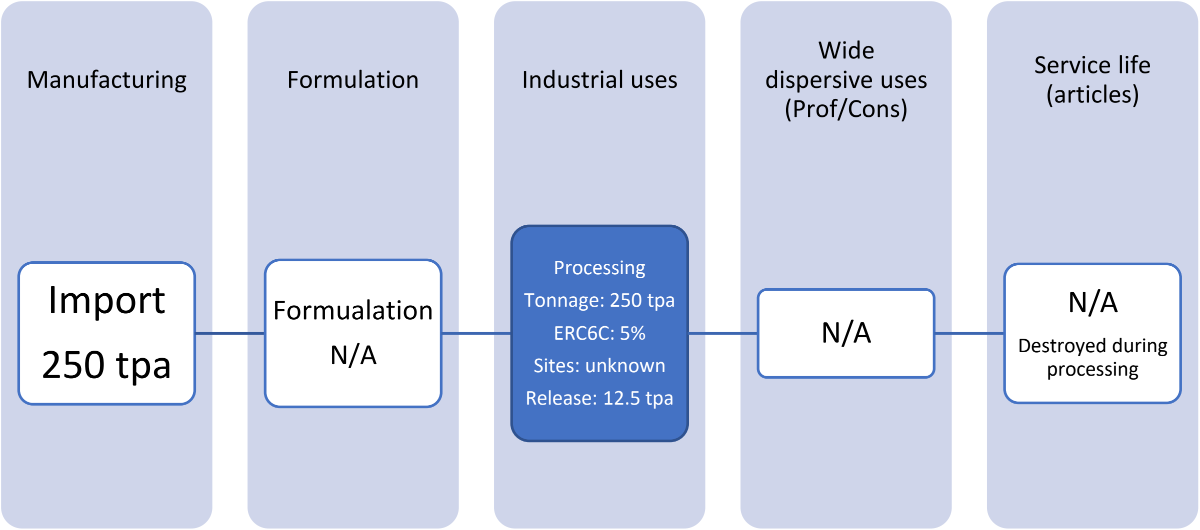
Tonnage has been estimated using known values of consumption of unleaded petrol in the UK (17 billion litres per year) and permitted concentration of manganese in fuel (8mg/L), which results in an estimate of 545 tpa. Specific environmental release categories are available for this sector and have been applied to the tonnage estimate to provide the estimated fraction released during formulation and use (ESIG, 2019).

2-phosphonobutane-1,2,4-tricarboxylic acid (37971-36-1)



2-Phosphonobutane-1,2,4-tricarboxylic acid is used in water treatment for its anti-scale properties in industrial uses of reverse osmosis water in industrial cooling or circulatory systems. It is also reported with widespread use in cleaning agents & drinking water treatment processes. We have been unable to obtain data to apportion total tonnage between different uses. Consequently, we have assumed the total estimated tonnage from phase one (DWI, 2020), is used in the ERC with greatest release (100% release).

1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride (chlorendric anhydride; 115-27-5)

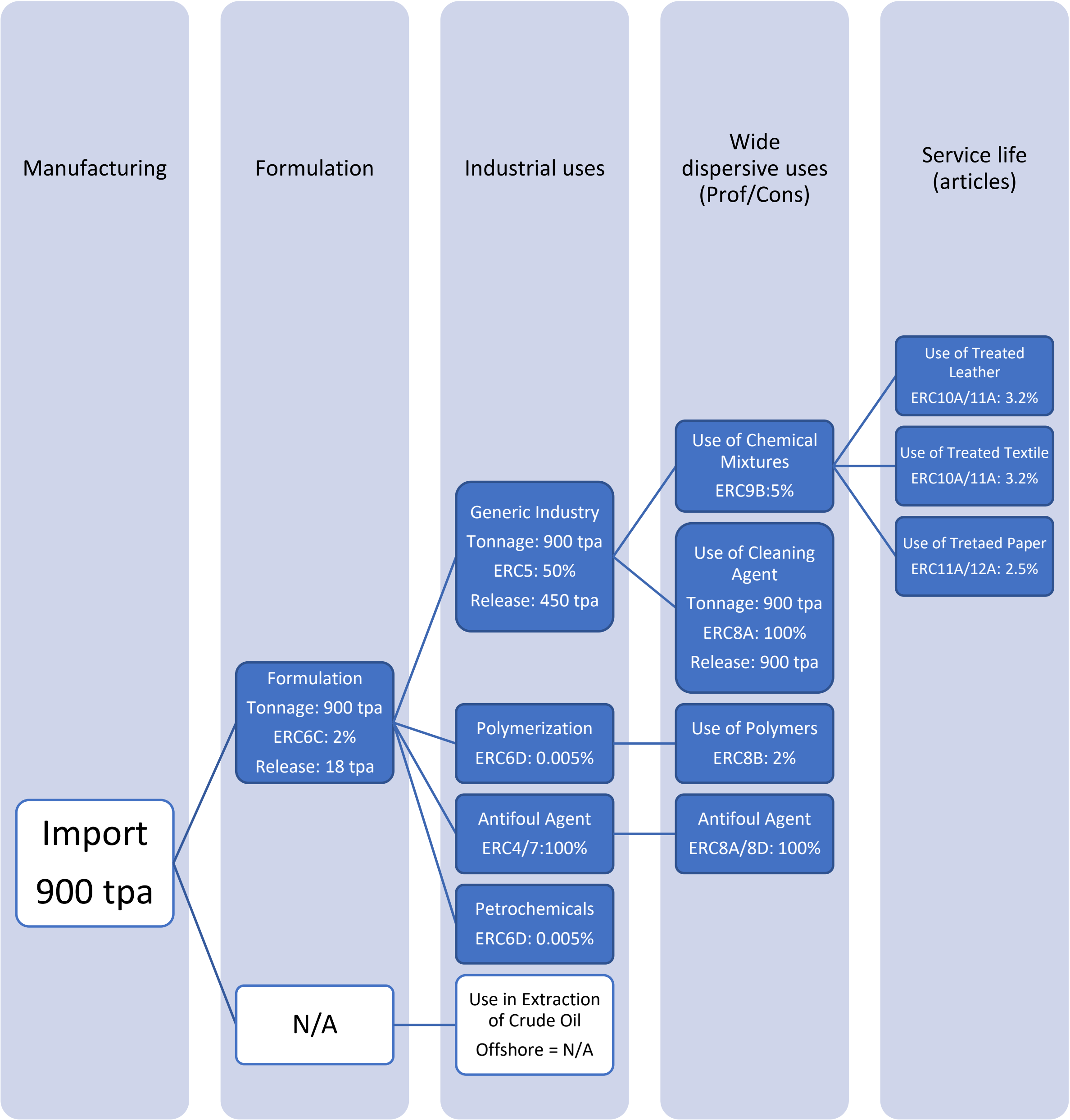


The substance is used in resin formation in polymer and plastic products manufacture. Release to the environment is anticipated to occur from industrial use in the production of articles and from thermoplastic manufacture. The substance has been grandfathered under UK REACH.

Extrapolation of datasets gathered through REACH, SPIN & the US EPA CompTox Dashboard suggest 72-121 tpa chlorendric anhydride are used in the UK.

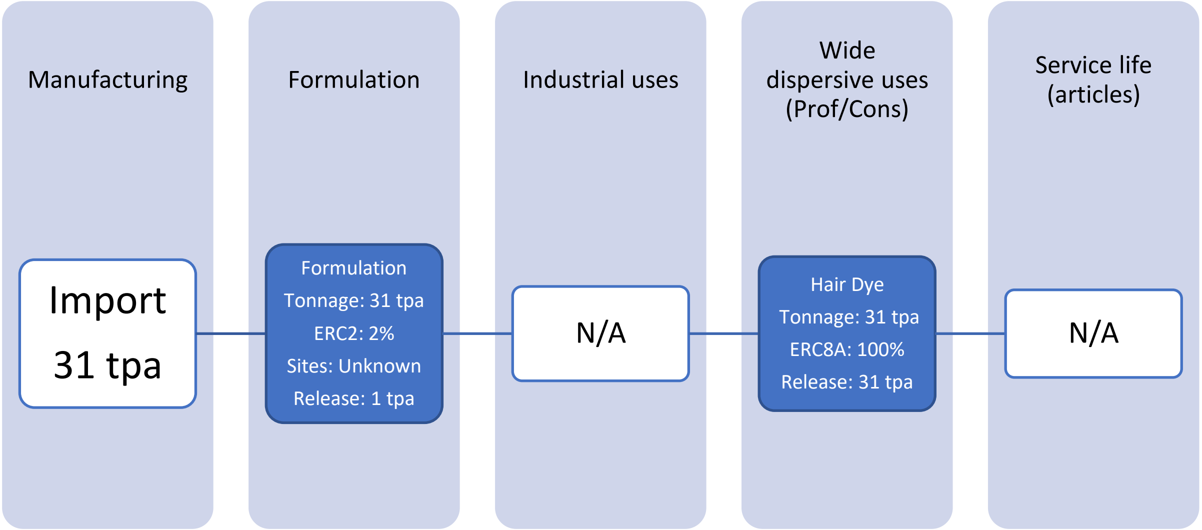
An e-SDS produced by a REACH notifier describes an exposure scenario for a generic 250 tpa downstream user processing, ERC 6D - Use of reactive process regulators in polymerisation processes at industrial site (inclusion or not into/onto article). The operations handling chlorendic anhydride in the UK are unknown, however for estimation we have assumed one of these downstream users is based in the UK. For estimates of release during manufacture, we have used ERC6C (5%). It has been assumed that as the substance is a reactive component, destruction of material would occur during the production.

4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl (2226-96-2)



4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl was identified in a wide range of products in phase one. Information from the REACH registration (ECHA, 2022) reports that it is used by downstream consumers, professional workers (widespread uses), in formulation or repacking, at industrial sites and in manufacturing. Data reported to the Nordic SPIN database suggests that extraction of crude petroleum and natural gas and manufacture of chemicals and chemical products are the main uses. It has not been possible to refine the previous phase one tonnage estimate (900tpa). In the absence of additional data, a conservative estimate of release assuming the total tonnage is used as a cleaning agent (environmental release category ERC 8A;100%) has been used.

4-aminophenol (123-30-8)



4-aminophenol is primarily used in hair dye. No UK manufactures of 4-aminophenol have been identified during our research. For predicting environmental emissions we have assumed only formulation and use occur in the UK. To refine the phase one tonnage estimate we have estimated a per capita per day release using information on the proportion of hair dye products containing 4-aminophenol and weight fraction inclusion levels. The frequency of hair dye use in the UK and the proportion of the population using hair dye have also been considered. Using this approach described in detail below, we have estimated an annual release of 31 tpa.

4-Aminophenol is primarily used in permanent hair dyes, where it is a primary intermediate, with functional groups added to provide the colour (Compound Intrest, 2015) (Goebel, 2017).

The release has been calculated as follows

UK population over 15 (Aged over 15/16)	= 59,597,300 * (100% - 17.4%) = 49,227,000 People
Number of Female Users (popn x % females x % using hair dye)	= 49,227,000 * 50.8% * 59% = 14,754,000 People
Female Population using Hair Dye containing 4-aminophenol	= 14,754,000 * 37.6% = 5,549,000 People
Number of Male Users (popn x % males x % using hair dye)	= 49,227,000 * 49.2% * 21% = 5,086,000 People
Male Population using hair dye containing 4-aminophenol	= 5,086,000 * 51.7% = 2,629,000 People
Total Number of Users of 4-Aminophenol Hair Dye	= 5,549,000 + 2,629,000 = 8,178,000 People
Total Usage of 4-Aminophenol containing Hair Dye	= 8,178,000 * 100g/app * 7.99 app/annum = 6,534,000,000 g/annum = 6,534 tpa
Average Concentration 4-Aminophenol	= 53%*0.9% + 47%*0.1% = 0.47%
Predicted Usage of 4-Aminophenol	= 6,534* 0.47% = **31 tpa**

Using the following assumptions

It has been assumed all products on the UK market comply with the regulations. It has been assumed hair dye containing 4-Aminophenol uses up-to the maximum permittable concentration of 0.9% 4-Aminophenol.

4-Aminophenol is featured in EC 1197/2013, Table III, *List of Substances Which Cosmetic Products Must Not Contain Except Subject to The Restrictions Laid Down* and states use as a colourant in Hair Dye & Eyelash colourant. Other cosmetic uses such as nail polish & body lotion, are therefore not assumed. Use of eyelash colourant dye has been assumed negligible compared to hair dye.

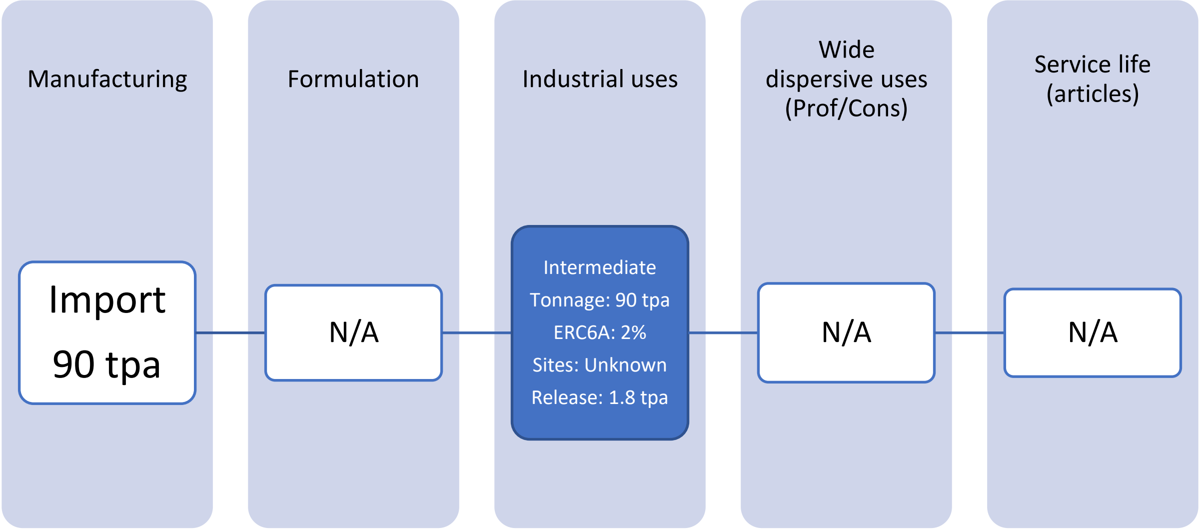
A 1981 study found that 396 of 811 of hair dyes sampled (49%) contained p-Aminophenol. Of these 184 (46%) contained 0.1-1% and 212 (53%) contained <0.1% p-Aminophenol (Anon., 1988). We have used the assumption 46% of hair dyes contain 0.9% 4-aminophenol the legal limit, and 53% of hair dyes contain 0.1% of 4-aminophenol.

A French-based database (INCI Beauty, n.d.) providing analysis of cosmetic products indicates there are around 4,000 hair colouring products, 80 Men's hair colouring products and 400 vegetable hair dying products (INCI Beauty, n.d.) that 4-aminophenol is present in 51.69% of Men's hair colouring products and 37.61% of Hair colouring products. For the estimate it assumed all products have an equal market share, i.e. 51.69% of male users will use a hair dye containing 4-aminophenol.

Based on published market research surveys assumed hair dye use is: 59% female, 21% male

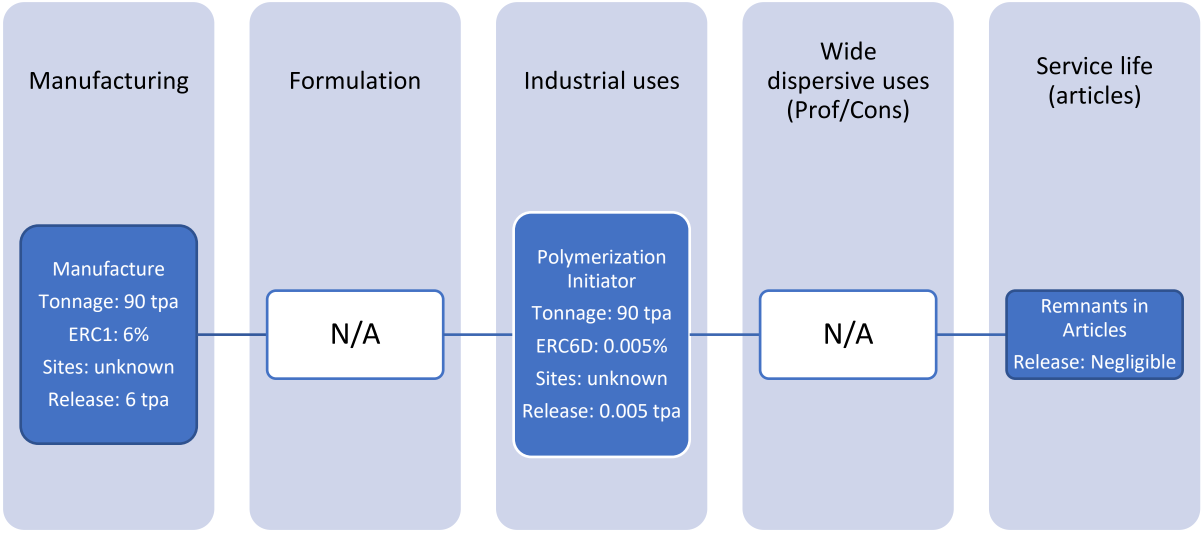
The 2021 England & Wales Census showed that the population was 59,597,300, of which 17.4% were under 15, with a 50.8% Female to 49.2 Male Population (Office for National Statistics, 2022). For our estimate we have assumed people under 15 will not use hair dye.

2-morpholinoethanol (622-40-2)



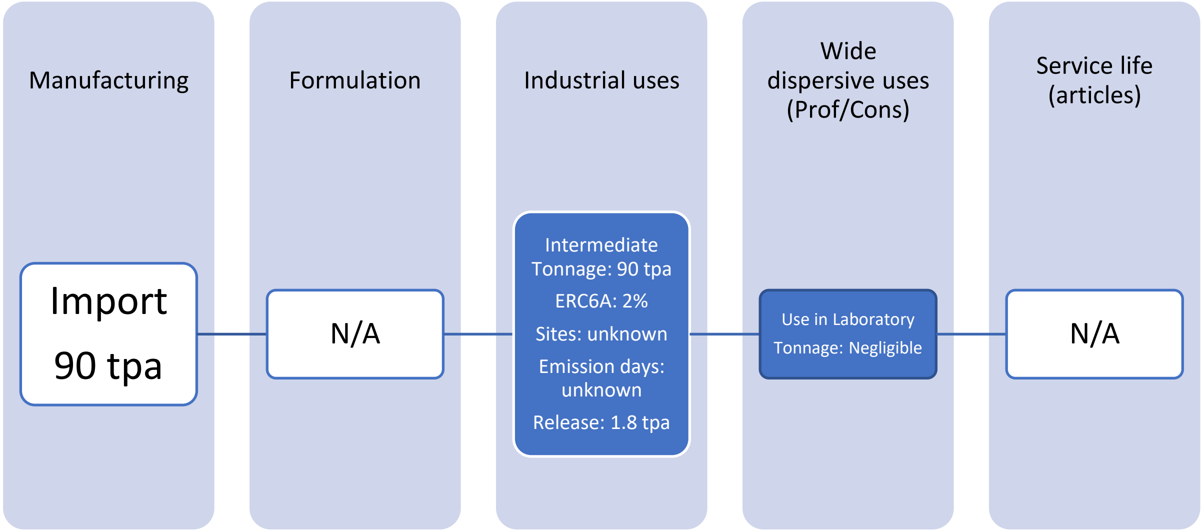
2-morpholinoethanol is used as an intermediate in the manufacture of fine chemicals (small scale production, high purity, high value chemicals) and as an intermediate in pharmaceuticals, where it is used as a base from which to make more complex substances. It has not been grandfathered under UK REACH. We have therefore assumed it is not manufactured in the UK, however it is possible that it could be used in the UK under a downstream user import notification, details of which are not publicly available. No additional data on amounts used with which to refine the phase one tonnage estimate have been found.
The tier two estimate (9% of upper bound of REACH tonnage band) has been carried forward to this project, and ERC6A (Industrial use resulting in manufacture of another substance; 2% release to wastewater during formulation) applied to estimate release of 1.8tpa.

2,2'-azobis[2-methylbutyronitrile] (13472-08-7)



Information obtained from the REACH registration indicates that 2,2'-azobis[2-methylbutyronitrile] is used as a polymerization initiator. The substance has been grandfathered into UK REACH. As an initiator, complete destruction is expected so although remnants in articles are expected, for estimation purposes negligible release has been assumed during this life cycle stage.

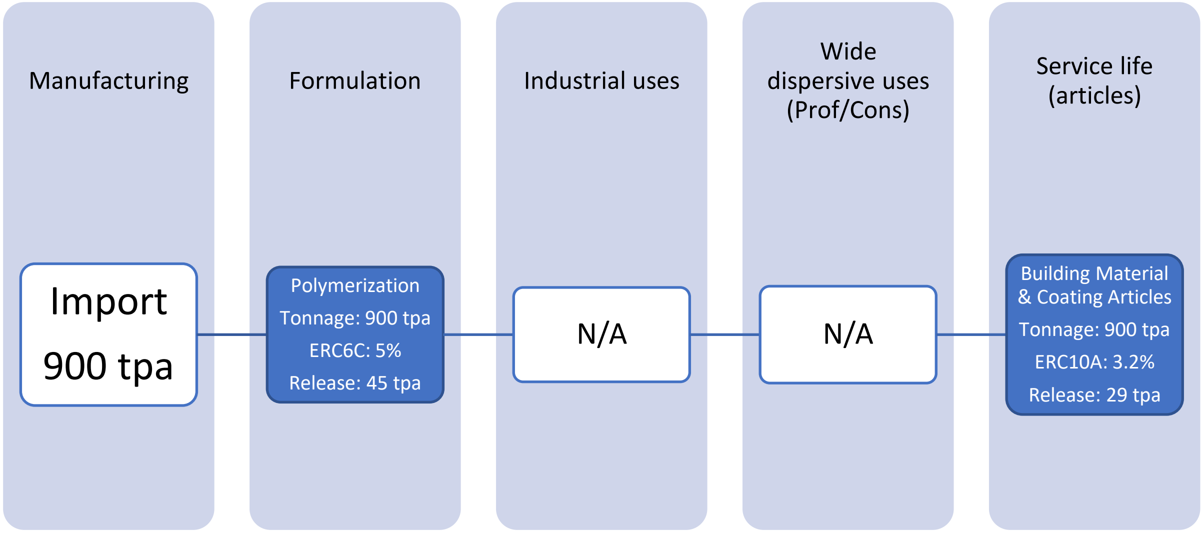
1,3-dichlorobenzene (541-73-1)



1,3-dichlorobenzene is used as a chemical intermediate with REACH registrants identified in Germany and Italy. It has not been grandfathered under UK REACH. No further insights on nature of use or amounts used were available from the Nordic SPIN database or US EPA CompTox. The estimates for this project only consider known usage of the isomer 1,3-dichlorobenzene. Several products only specify the use of 'dichlorobenzene', but we have been unable to use this data in this project because it is unclear if it is referring to 1,3-dichlorobenzene. Our estimate may therefore underestimate the proportion of 1,3-dichlorobenzene released.

The estimate of release for this project considers reported use of the isomer 1,3-dichlorobenzene. Several products only specify 'dichlorobenzene'. We have been unable to use this data here project because it is unclear if it is referring to 1,3-dichlorobenzene. Our tier three estimate may therefore underestimate the amount of 1,3-dichlorobenzene released.

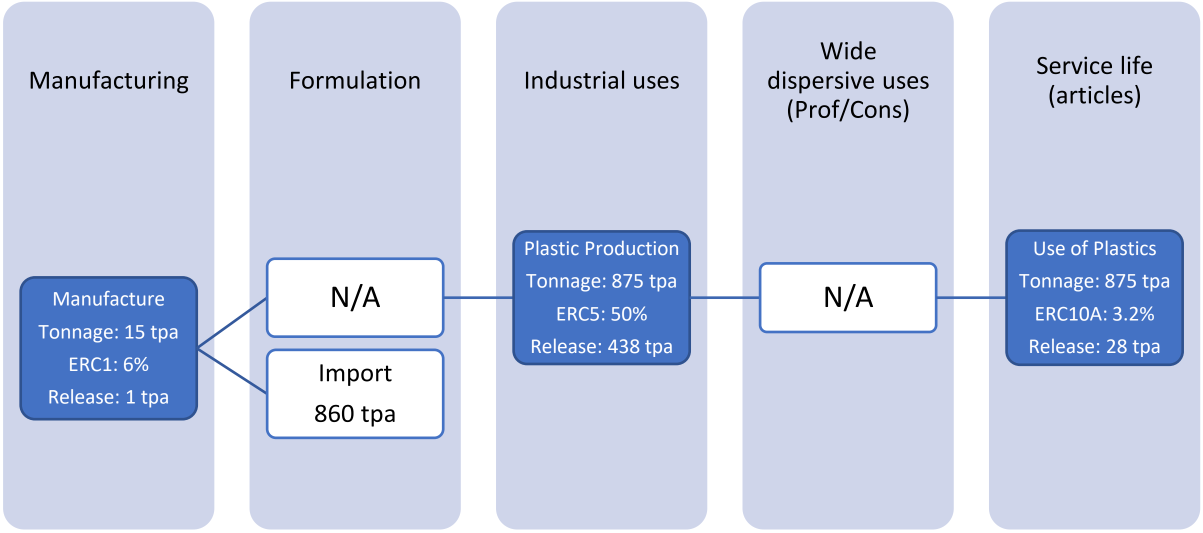
2,2'-dimethyl-2,2'-azodipropiononitrile (APN) (78-67-1)



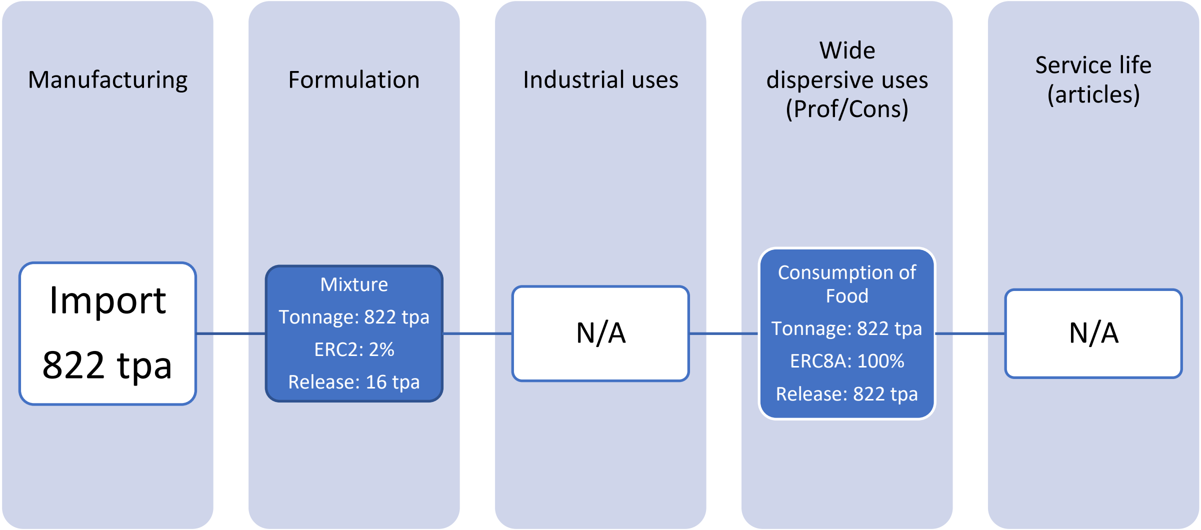
2,2'-dimethyl-2,2'-azodipropiononitrile (APN) is used in polymerization processes. There are no data to indicate it is manufactured in the UK. Information from the Nordic SPIN database suggests use in coating and building materials. With limited data available regarding use and presence in finished articles, the phase one estimate of 900 tpa has been used for tier 3. Environmental release categories applicable for formulation as a monomer for polymerization (ERC6C) and widespread use of articles outdoors with low intended release (ERC10A) have been applied to estimate environmental release.

N-butylbenzenesulphonamide (3622-84-2)

N-butylbenzenesulphonamide (BBSA) is used in the production of plastics for the automotive sector. EU REACH has a registered tonnage of 10,000 tonnes, and sulphonamides have a EuroStat declared production of 6,000 – 7,000 tonnes in the EU. In 2018, approximately 1,300 tonnes were imported into the UK, 440 tonnes were exported, and 15 tonnes were produced. Data from Eurostat indicates that in 2018, approximately 1,300 tonnes of sulphonamides were imported, 440 tonnes were exported resulting in a net import of 860 tonnes and 15 tonnes were manufactured in the UK. We have conservatively assumed that the total tonnage of sulphonamides reported in Eurostat is all BBSA.



1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin) (81-07-2)



1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin) is used in pharmaceuticals, polymer modifiers, adhesives, cosmetics, and food sweeteners. Pharmaceutical use appears to be as part of the formulation, possibly for flavouring oral medicines, as no active ingredient declaration has been obtained. No UK organisations are named in REACH dossiers and there has been no UK REACH grandfathering. Saccharin and its salts are recognised as a unique commodity through customs. Eurostat indicates no production in the UK, but UK Trade Info reports a net 822 tonnes was imported into the UK in 2018, with 33 traders identified. This value is higher than the tier estimate derived in (DWI, 2020). Consequently, this higher estimate, based on customs data has been used as the tier 3 estimate in this project. It is possible that is still an underestimate, since saccharin may be present in imported food items but not declared as a chemical.

APPENDIX 3 SAMPLE CODES & WIMS PURPOSE CODES USED FOR ANALYSIS OF MONITORING DATA

1. Environment Agency LC-MS/GC-MS targeted scan data.

‘Useable data’, included in the analysis below has been defined as:

- Purpose code is Monitoring (defined as a code starting M)
- Sampling point descriptor is relevant (defined as starting freshwater or groundwater respectively)

2. Environment Agency Water Quality data archive [Open WIMS data](#) (accessed December 2022)

Useable data Defined as:

- Purpose is Monitoring, defined as one of
    - ENVIRONMENTAL MONITORING STATUTORY (EU DIRECTIVES)
    - WATER QUALITY OPERATOR SELF MONITORING COMPLIANCE DATA
    - MONITORING (UK GOVT POLICY - NOT GQA OR RE)
    - WATER QUALITY UWWTD MONITORING DATA
    - COMPLIANCE AUDIT (PERMIT)
    - MONITORING (NATIONAL AGENCY POLICY)
    - COMPLIANCE FORMAL (PERMIT)
    - PLANNED FORMAL NON-STATUTORY (PERMIT/ENV MON)
    - OTA COMPLIANCE CATCHMENT PERMITTING (OPERATOR DATA)
    - IPPC/IPC MONITORING (AGENCY AUDIT - PERMIT)
    - IPPC/IPC MONITORING (FORMAL SAMPLE)
    - STATUTORY AUDIT (OPERATOR DATA)
    - ENVIRONMENTAL MONITORING (GQA & RE ONLY)
    - WASTE MONITORING (OPERATOR SELF-MONITORING DATA)
    - IPPC/IPC MONITORING (OPERATOR SELF MONITORING DATA)
- Sampling point descriptor is relevant
    - Groundwater
    - Freshwater incorporates: RIVER / RUNNING SURFACE WATER/ POND / LAKE / RESERVOIR WATER / CANAL WATER

- Unit is or convertible to µg/L of sample (for mass basis 1L of sample = 1kg)

APPENDIX 4 QSR SEARCH PROTOCOL AND OUTCOME

Table A4. 1 Search terms, scope and criteria for inclusion/exclusion

	Description	Inclusion criteria	Exclusion criteria
Population	Persistent, mobile, toxic substances/chemicals PMT PM [substances– see list include CAS,EC number synonyms]		
Outcome	Reported occurrence in environmental waters (surface water, ground water) and treated drinking water in England and Wales. England/ English Wales UK water water quality drinking water tap water surface water river groundwater aquifer environment	Substance (confirmed identity) on agreed list detected in ground or surface waters in England or Wales Drinking water (tap water) Detection – yes/no Reported concentration Include all UK waters & Eire (highest priority given to E & W) Published in English	PMT substances not on agreed list Other environmental media (air, soil, sediment, biota, WWTW sludge, WWTW effluent) Marine, estuarine, and coastal waters Detections in human biological samples Studies before 2000 unless no other data available[15]. Analytical method development Not published in English

Data sources

PubMed, PubChem, Full text Science Direct, Google Scholar,

(the USEPAs PubMed Abstract sifter will be used for search and retrieval of information available here)

Screening criteria Search results will be screened, first, using the title and applying criteria summarised in the table above. Details of accepted papers will be recorded in a spreadsheet and then screened again by reading the abstract or first paragraph. Papers will then be placed into two categories: included and excluded.

Data capture. We will record the date, search engine used, the search string (combinations of key words) and the number of records returned, the results of each search will be saved as a list of references. If an unmanageable number of papers are identified, the exclusion criteria and the focus of research and search terms will be reviewed.

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[15] Recent number of literature searches and synthesis reviews have been conducted and reporting concentrations of PMT substances in raw and treated waters (e.g. Arp & Hale, 2019; Schulz et al., 2019; Initial focus will be on most recent publications initially.

A spreadsheet will be used to record this information trail. The column headings will include information about the publication (authors, year, title, source).

Occurrence data will be captured in Excel spreadsheet summarising substance, reference, sample type, sampling month & year, number of samples, minimum, maximum and mean concentrations, analytical limits of detection (if reported). For many substances, any data reported may simply be as presence/absence with no associated concentration.

Validity/QA

A second person will independently screen a sample of documents to check that there is no bias. If necessary, remedial actions will be taken to ensure the criteria are applied appropriately.

A proportion of all data entries will be reviewed by Emma Pemberton to confirm the information extracted by the data analysis team. The proportion of data to be reviewed will be confirmed once the search has been undertaken but is anticipated to be range of 10% of all data entries.

Members of the review team

Simon Cook, Megan Griffiths, Eleonore Delouvrier, Chesney Swansborough

Table A4. 2 Table of outcomes for literature search carried out

Substance	Search engine	Date of search	Search string used	Total number of papers found	Total number of relevant papers
2,4,7,9-tetramethyldec-5-yne-4,7-diol	PubMed (Abstract Sifter)	20/01/2022	(2,4,7,9-tetramethyldec-5-yne-4,7-diol OR 204-809-1 OR 126-86-3 or 2,4,7,9-tetramethyl-5-decyne-4,7-diol) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	11	1
	Science Direct	14/02/2022	(2,4,7,9-tetramethyldec-5-yne-4,7-diol OR 2,4,7,9-Tetramethyl-5-decyne-4,7-diol OR 204-809-1 OR 126-86-3) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*)	9,560	2
1,4-dioxane	PubMed (Abstract Sifter)	21/01/2022	(1,4-dioxane OR 204-661-8 OR 123-91-1 or dioxane or dioxan or p-dioxane or diethylene dioxide or diethylene oxide or diethylene ether or glycol ethylene ether) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	717	0
	Science Direct	14/02/2022	(1,4-dioxane OR 204-661-8 OR 123-91-1) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*)	10,174	11
Trichloroethylene	PubMed (Abstract Sifter)	21/01/2022	(trichloroethylene OR 201-167-4 OR 79-01-6 or TCE or acetylene trichloride) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	811	5
	Science Direct	14/02/2022	(trichloroethylene OR 201-167-4 OR 79-01-6 or TCE or acetylene trichloride) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*)	16,278	6
Tetrachloroethylene	PubMed (Abstract Sifter)	26/01/2022	(Tetrachloroethylene OR 204-825-9 OR 127-18-4 OR Perchloroethylene OR PCE OR perc OR tetrachloroethene OR perclene OR perchlor) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	530	5
	Science Direct	14/02/2022	(Tetrachloroethylene OR 204-825-9 OR 127-18-4 OR Perchloroethylene OR PCE OR tetrachloroethene) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*)	46,794	3
Melamine	PubMed (Abstract Sifter)	21/01/2022	(melamine OR 203-615-4 OR 108-78-1 or cyanuramide or traminotriazine) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	182	1
	Science Direct	14/02/2022	(melamine OR 203-615-4 OR 108-78-1 or cyanuramide or traminotriazine) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	2,220	2

Substance	Search engine	Date of search	Search string used	Total number of papers found	Total number of relevant papers
Dinoseb	PubMed (Abstract Sifter)	21/01/2022	(Dinoseb OR 201-861-7 OR 88-85-7 or 6-sec-butyl-2,4-dinitrophenol) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	15	0
	Science Direct	14/02/2022	(Dinoseb OR 201-861-7 OR 88-85-7 or 6-sec-butyl-2,4-dinitrophenol) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	773	0
Ametryn	PubMed (Abstract Sifter)	26/01/2022	(Ametryn OR 212-634-7 OR 834-12-8 OR Ametrex OR Ametryne) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	84	4
	Science Direct	16/02/2022	(Ametryn OR 212-634-7 OR 834-12-8 OR Ametrex) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	2,080	1
Dapsone	PubMed (Abstract Sifter)	26/01/2022	(Dapsone OR 201-248-4 OR 80-08-0 OR Avlosulfon OR Diaminodiphenylsulfone OR DDS OR 4-[(4-aminobenzene)sulfonyl]aniline) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) (Dapsone OR 201-248-4 OR 80-08-0 OR Avlosulfon OR Diaminodiphenylsulfone OR DDS OR 4-[(4-aminobenzene)sulfonyl]aniline) AND (water OR groundwater OR drinking water OR river OR surface water)	0	0
	Science Direct	16/02/2022	(Dapsone OR DDS OR 80-08-0 OR diaminodiphenyl sulfone) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	5,207	0
Amantadine	PubMed (Abstract Sifter)	26/01/2022	(Amantadine OR 212-201-2 OR 768-94-5 OR Gocovri OR Symadine OR Symmetrel OR 1-adamantylamine OR 1-aminoadamantane) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	54	2
	Science Direct	16/02/2022	(Amantadine OR 768-94-5 OR Gocovri) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	1,294	4
Hexamethyldisiloxane	PubMed (Abstract Sifter)	26/01/2022	(Hexamethyldisiloxane OR 203-492-7 OR 107-46-0 OR HMDSO) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	21	0
	Science Direct	16/02/2022	(Hexamethyldisiloxane OR 203-492-7 OR 107-46-0 OR HMDSO) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	9,777	0
Tricarbonyl(methylcyclopentadienyl) manganese	PubMed (Abstract Sifter)	26/01/2022	(Tricarbonyl(methylcyclopentadienyl) manganese OR 235-166-5 OR 12108-13-3 OR Ethyl MMT OR MCMT OR MMT) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	123	0

Substance	Search engine	Date of search	Search string used	Total number of papers found	Total number of relevant papers
	Science Direct	16/02/2022	(Tricarbonyl(methylcyclopentadienyl) manganese OR 235-166-5 OR 12108-13-3 OR MMT) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	50	0
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1)	PubMed (Abstract Sifter)	26/01/2022	(1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1) OR 253-575-7 OR 37640-57-6 OR Melamine cyanurate) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) (1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1) OR 253-575-7 OR 37640-57-6 OR Melamine cyanurate) AND (water OR groundwater OR drinking water OR river OR surface water)	2 5	0
	Science Direct	16/02/2022	(1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6- triamine (1:1) OR 253-575-7 OR 37640-57-6 OR Melamine cyanurate) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	2	0
2-phosphonobutane-1,2,4-tricarboxylic acid	PubMed (Abstract Sifter)	26/01/2022	(2-phosphonobutane-1,2,4-tricarboxylic acid OR 253-733-5 OR 37971-36-1 OR PBTC) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	12	1
	Science Direct	16/02/2022	(2-phosphonobutane-1,2,4-tricarboxylic acid OR 253-733-5 OR 37971-36-1 OR PBTC) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	793	0
4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	PubMed (Abstract Sifter)	26/01/2022	(4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl OR 218-760-9 OR 2226-96-2) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	37	0
	Science Direct	16/02/2022	(4-hydroxy-2,2,6,6- tetramethylpiperidinoxyl OR 218-760-9 OR 2226-96-2 OR TEMPOL) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	1,176	0
4-aminophenol	PubMed (Abstract Sifter)	21/01/2022	(4-aminophenol or 123-30-8 or 204-616-2) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	69	4
	Science Direct	04/02/2022	(4-aminophenol or 123-30-8 or 204-616-2) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental)	35	0
2-morpholinoethanol	PubMed (Abstract Sifter)	21/01/2022	(2-morpholinoethanol OR 4-morpholineethanol OR 210-734-5 OR 622-40-2) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) (2-morpholinoethanol OR 4-morpholineethanol OR 210-734-5 OR 622-40-2) AND (water OR groundwater OR drinking water OR river OR surface water)	0	0

Substance	Search engine	Date of search	Search string used	Total number of papers found	Total number of relevant papers
	Science Direct	04/02/2022	(2-morpholinoethanol OR 4-morpholineethanol OR 210-734-5 OR 622-40-2) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility)	1,582	1
Sulisobenzone	PubMed (Abstract Sifter)	21/01/2022	(Sulisobenzone OR 223-772-2 OR 4065-45-6) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	16	1
	Science Direct	04/02/2022	(Sulisobenzone OR 223-772-2 OR 4065-45-6) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility)	487	11
2,2'-azobis[2-methylbutyronitrile]	PubMed (Abstract Sifter)	25/01/2022	(2,2'-azobis[2-methylbutyronitrile] OR 236-740-8 OR 13472-08-7) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	107	0
	Science Direct	04/02/2022	(2,2'-azobis[2-methylbutyronitrile] OR 236-740-8 OR 13472-08-7) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility)	557	0
1,3-dichlorobenzene	PubMed (Abstract Sifter)	25/01/2022	(1,3-dichlorobenzene OR 208-792-1 OR 541-73-1) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	14	0
	Science Direct	04/02/2022	(1,3-dichlorobenzene OR 208-792-1 OR 541-73-1) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility)	1,494	6
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	PubMed (Abstract Sifter)	25/01/2022	(2,2'-dimethyl-2,2'-azodipropiononitrile OR APN OR 201-132-3 OR 78-67-1) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	22	0
	Science Direct	04/02/2022	(2,2'-dimethyl-2,2'-azodipropiononitrile OR APN OR 201-132-3 OR 78-67-1) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility)	13,032	0
N-butylbenzenesulphonamide	PubMed (Abstract Sifter)	25/01/2022	(N-butylbenzenesulphonamide OR 222-823-6 OR 3622-84-2) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	6	0
	Science Direct	04/02/2022	(N-butylbenzenesulphonamide OR 222-823-6 OR 3622-84-2) AND (detected OR concentration OR occurrence) AND (freshwater OR groundwater OR "drinking water" OR river OR "surface water") AND (environment OR environmental) AND (PMT OR mobile OR mobility)	459	3
4-nitrotoluene	PubMed (Abstract Sifter)	18/02/2022	(4-nitrotoluene OR 202-808-0 OR 99-99-0) AND ((detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	17	0

Substance	Search engine	Date of search	Search string used	Total number of papers found	Total number of relevant papers
	Science Direct	18/02/2022	(4-nitrotoluene OR 201-321-0 OR 81-07-2 OR p-nitrotoluene) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	4,310	0
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	PubMed (Abstract Sifter)	18/02/2022	(1,2-benzisothiazol-3(2H)-one1,1-dioxide OR 201-321-0 OR 81-07-2 OR Sodium Saccharin) AND ((detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	282	6
	Science Direct	18/02/2022	(1,2-benzisothiazol-3(2H)-one1,1-dioxide OR 201-321-0 OR 81-07-2 OR Sodium Saccharin) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	12	0
Carbon tetrachloride (CTC)	PubMed (Abstract Sifter)	18/02/2022	(Carbon tetrachloride OR 200-262-8 OR 56-23-5 OR CTC) AND ((detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	375	0
	Science Direct	18/02/2022	(Carbon tetrachloride OR 200-262-8 OR 56-23-5 OR CTC) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	37,256	0
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride (PE1+) (chlorendric anhydride)	PubMed (Abstract Sifter)	26/01/2022	(1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride OR 204-077-3 OR 115-27-5 OR Chlorendic Anhydride) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) (1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride OR 204-077-3 OR 115-27-5 OR Chlorendic Anhydride) AND (water OR groundwater OR drinking water OR river OR surface water)	0	0
	Science Direct	16/02/2022	(1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride OR 204-077-3 OR 115-27-5 OR Chlorendic Anhydride) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	15,028	0
Chloroform	PubMed (Abstract Sifter)	18/02/2022	(Chloroform OR 200-663-8 OR 67-66-3 OR trichloromethane) AND ((detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	1,868	8
	Science Direct	18/02/2022	(Chloroform OR 200-663-8 OR 67-66-3 OR trichloromethane) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	30,653	1
Triclosan	PubMed (Abstract Sifter)	18/02/2022	(Triclosan OR 222-182-2 OR 67-66-3) AND ((detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	816	113
	Science Direct	18/02/2022	(Triclosan OR 222-182-2 OR 67-66-3) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	23,179	8

Substance	Search engine	Date of search	Search string used	Total number of papers found	Total number of relevant papers
Tris(2-chloro-1-methylethyl) phosphate (TCPP)	PubMed (Abstract Sifter)	18/02/2022	(Tris(2-chloro-1-methylethyl) phosphate OR TCPP OR 237-158-7 OR 13674-84-5) AND ((detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water)	109	14
	Science Direct	18/02/2022	(Tris(2-chloro-1-methylethyl) phosphate OR TCPP OR 237-158-7 OR 13674-84-5) AND (detected OR concentration OR occurrence) AND (water OR groundwater OR drinking water OR river OR surface water) AND (environment OR environmental) AND (PMT OR mobile OR mobility OR persisten*) AND (UK OR Engl* OR Wales)	77	2

APPENDIX 5 ENVIRONMENT AGENCY MONITORING DATA

Table A5. 1 Summary of PMT substances detected in English surface waters. Source data: Environment Agency, LCMS & GCMS water quality semi-quantitative monitoring screen. Accessed December 2021.

substance	CAS	No. of sites[16]	No. of samples[17]	Date range	Min conc. (µg/L)	Max conc. (µg/L)	Average conc. (µg/L)
2,4,7,9-tetramethyldec-5-yne-4,7-diol	126-86-3	440	5,686	2011 - 2021	0.006	48	0.6
1,4-dioxane	123-91-1	315	4,717	2007 - 2021	0.02	31[18]	0.4
trichloroethylene	79-01-6	191	1,637	2007 - 2021	0.002	53	0.4
tetrachloroethylene	127-18-4	191	871	2007 - 2021	0.015	650[19]	2.0
triclosan	3380-34-5	157	1,657	2007 -2021	0.002	20	0.2
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	81-07-2	108	1,240	2014 - 2021	0.02	0.025	0.02
1,3-dichlorobenzene	541-73-1	108	655	2007 – 2021	0.02	0.015	0.02
melamine	108-78-1	87	266	2019 – 2021	0.006	13	0.7
amantadine	768-94-5	69	360	2019 - 2021	0.0001	0.11	0.004
dinoseb	88-85-7	4	9	2008 - 2021	0.01	0.13	0.05
dapsone	80-08-0	3	9	2014 - 2020	0.0005	0.02	0.003
N-butylbenzenesulphonamide	3622-84-2	2	2	2017	0.002	0.16	
hexamethyldisiloxane	107-46-0	2	2	2017	0.015	0.025	

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[16] Number of 'useable' sites where substance was detected

[17] Number of useable samples where substance was detected

[18] Excludes results of 2.35 g/L & 2.78 g/L which were removed as outliers, suspected error in reporting units

[19] Excludes a result of 0.244 g/L which was removed as an outlier, suspected error in reporting units

The temporal and spatial sampling frequency varies significantly between substances. Consequently, summary data for each substance detected have been aggregated nationally and reported as a range (minimum to maximum) plus an average value. Values reported as less than limit of detection (LOD) have been treated as a value half LOD when calculating the average. This is a standard approach to treatment of data, but may lead to an overestimation of average concentration, and the numeric value should be treated cautiously. Samples clearly associated with waste sites, effluent or pollution incidents have been excluded from the analysis. Data reported as a total load on a passive monitoring device such as semi-permeable membrane device (SPMD) or POCIS have been excluded as we are unable to derive a concentration in water from the raw data available. Sample purpose codes and sampling point descriptors used to identify relevant data are also listed in Appendix 3.

Site details for groundwater data were unavailable in the GC-MS/LC-MS screening dataset. Consequently, it was not possible to report the number of groundwater sites at which substances were detected and so this is omitted from Table A5. 2

Table A5. 2 Summary of PMT substances detected in English groundwater. Source data: Environment Agency, LCMS & GCMS water quality semi-quantitative monitoring screen. Accessed December 2021. Number of sites unknown (information redacted from dataset)

Substance	CAS	No. of samples	Date range	Min conc. (µg/L)	Max conc. (µg/L)	Average conc. (µg/L)
2,4,7,9-tetramethyldec-5-yne-4,7-diol	126-86-3	620	2011 - 2020	0.008	4	0.09
1,4-dioxane	123-91-1	495	2009 - 2020	0.01	63[20]	1.4
trichloroethylene	79-01-6	969	2009 - 2020	0.005	184	1.4
triclosan	3380-34-5	104	2009 - 2021	0.0003	2.6	0.05
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	81-07-2	200	2017 - 2021	0.0004	0.88	0.04
tetrachloroethylene	127-18-4	580	2009 - 2020	0.02	180	4.0
1,3-dichlorobenzene	541-73-1	105	2009 – 2020	0.002	3.7	0.1
amantadine	768-94-5	8	2019 - 2020	0.0001	0.007	0.002
melamine	108-78-1	47	2019 - 2020	0.006	2.5	0.1

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[20] Excludes a result of 0.15 g/L which was removed as an outlier, suspected error in reporting units

dinoseb	88-85-7	14	2009 - 2014	0.01	0.7	0.1
dapsone	80-08-0	4	2017 - 2020	0.0002	0.0003	
hexamethyldisiloxane	107-46-0	1	2017	0.02	0.02	
N-butylbenzenesulphonamide	3622-84-2	1	2017	0.02	0.02	

Table A5. 3 Summary of other names and identifiers used in the search of the WIMS monitoring data

Substance	CAS no.	Search included
Tetrachloroethylene	127-18-4	“Tetrachloroethylene :- {Perchloroethylene}” & “Tetrachloroethylene : Dry Wt :- {Perchloroethylene}”
Trichloroethylene	79-01-6	“Trichloroethylene :- {Trichloroethene}” & “Trichloroethylene : Dry Wt :- {Trichloroethene}”
Dinoseb	88-85-7	“Dinoseb :- {2-Methyl-n-propyl-4,6-dinitrophenol} :- {DNBP}” & “Dinoseb : Dry Wt :- {2-Methyl-n-propyl-4,6-dinitrophenol} :- {DNBP}”

APPENDIX 6 PHYSICO-CHEMICAL PROPERTIES

Table A6. 1 Physico-chemical properties of the 22 identified PMTs used to estimate removal by different drinking water treatment processes (DWTP)

Compound	CAS No.	Smiles notation	No. of H bond acceptors (from ACD/Labs	No of H bond donors (from ACD/Labs)	C (from ACD/ Labs)	H (from ACD/ Labs)	C:H ratio (calculated)	Molecular weight (from ACD/Labs)	log D (pH 4/5.5) (from ACD/Labs)	Experimental logKow (from EPISUITE)	Estimated LogKow (from EPISUITE)	LogP (from ACD/ Labs)	logD (pH 7) (from ACD/ Labs)	Charge at pH 7 (from Chemicalize or via logD at different pH*)	Removal in Wastewater Treatment (%) from EPISUITE
2,4,7,9-tetramethyldec-5-yne-4,7-diol	126-86-3	CC(C)CC(C)(C#CC(C)(CC(C)C)O)O	2	2	14	16	0.9	226.355	2.94	NR	3.61	3.11	2.94	0*	15.80
1,4-dioxane	123-91-1	C1COCCO1	2	0	4	8	0.5	88.105	-0.29	-0.32	-0.27	-0.27	-0.29	0	2.12
Trichloroethylene	79-01-6	C(=C(Cl)Cl)Cl	0	0	2	1	2.0	131.388	2.57	2.47	2.42	2.26	2.57	0	79.58
Tetrachloroethylene	127-18-4	C(=C(Cl)Cl)(Cl)Cl	0	0	2	0	NA	165.833	3.30	2.97	3.4	2.95	3.30	0	87.91
Melamine	108-78-1	C1(=NC(=NC(=N1)N)N)N	6	6	3	6	0.5	126.120	-1.48	-0.38	-1.37	-1.37	-1.18	0	1.85
Dinoseb	88-85-7	CCC(C)C1=C(C(=CC(=C1)[N+](=O)[O-])[N+](=O)[O-])O	7	1	10	12	0.8	240.213	1.89	3.67	3.56	3.61	0.39	neg*	14.49
Dapsone	80-08-0	C1=CC(=CC=C1N)S(=O)(=O)C2=CC=C(C=C2)N	4	4	12	12	1.0	248.301	1.08	0.77	0.97	0.94	1.08	0*	1.88
Amantadine	768-94-5	C1C2CC3CC1CC(C2)(C3)N	1	2	10	17	0.6	151.249	-0.56	2.43	2.44	2.22	-0.31	0	3.39
Hexamethyldisiloxane	107-46-0	C[Si](C)(C)O[Si](C)(C)C	1	0	6	18	0.3	162.378	4.03	4.76	4.2	4.2	4.03	0	99.95
Tricarbonyl(methylcyclopentadienyl) manganese	12108-13-3	CC1C=C[C-]=C1.[C-]#[O+].[C-]#[O+].[C-]#[O+].[Mn]	NR	NR	9	7	1.3	218.089	NR	NR	1.75	NR	NR	NR	2.07

Compound	**CAS No.**	**Smiles notation**	**No. of H bond acceptors (from ACD/Labs**	**No of H bond donors (from ACD/Labs)**	**C (from ACD/ Labs)**	**H (from ACD/ Labs)**	**C:H ratio (calculated)**	**Molecular weight (from ACD/Labs)**	**log D (pH 4/5.5) (from ACD/Labs)**	**Experimental logKow (from EPISUITE)**	**Estimated LogKow (from EPISUITE)**	**LogP (from ACD/ Labs)**	**logD (pH 7) (from ACD/ Labs)**	**Charge at pH 7 (from Chemicalize or via logD at different pH*)**	**Removal in Wastewater Treatment (%) from EPISUITE**
1,3,5-triazine-2,4,6(1H,3H,5H)-trione, compound with 1,3,5-triazine-2,4,6-triamine (1:1)	37640-57-6	C1(=NC(=NC(=N1)N)N)N.C1(=O)NC(=O)NC(=O)N1	NR	NR	6	9	0.7	255.198	NR	NR	NR	NR	NR	NR	NR
2-phosphonobutane-1,2,4-tricarboxylic acid	37971-36-1	C(CC(CC(=O)O)(C(=O)O)P(=O)(O)O)C(=O)O	9	5	7	11	0.6	270.131	-8.10	NR	-1.36	-2.09	-9.06	0*	1.85
1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride	115-27-5	C12C(C(=O)OC1=O)C3(C(=C(C2(C3(Cl)Cl)Cl)Cl)Cl)Cl	3	0	9	2	4.5	370.828	3.66	NR	4.37	4.06	3.66	0*	49.06
4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl	2226-96-2	CC1(CC(CC(N1[O])(C)C)O)C	1	3	9	18	0.5	172.245	NR	NR	0.56	NR	NR	0	1.86
4-aminophenol	123-30-8	C1=CC(=CC=C1N)O	2	3	6	7	0.9	109.126	-0.04	0.04	0.24	-0.29	0.16	0	1.85
2-morpholinoethanol	622-40-2	C1COCCN1CCO	3	1	6	13	0.5	131.173	-1.83	NR	-1.32	-0.6	-0.71	0	1.85
2,2'-azobis[2-methylbutyronitrile]	13472-08-7	CCC(C)(C#N)N=NC(C)(CC)C#N	4	0	10	16	0.6	192.261	2.36	NR	3.86	2.32	2.36	0*	24.11
1,3-dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	0	0	6	4	1.5	147.002	3.27	3.53	3.28	3.42	3.27	0	56.05
2,2'-dimethyl-2,2'-azodipropiononitrile (APN)	78-67-1	CC(C)(C#N)N=NC(C)(C)C#N	4	0	8	12	0.7	164.208	1.74	1.1	2.87	1.26	1.74	0*	2.13

Compound	CAS No.	Smiles notation	No. of H bond acceptors (from ACD/Labs	No of H bond donors (from ACD/Labs)	C (from ACD/ Labs)	H (from ACD/ Labs)	C:H ratio (calculated)	Molecular weight (from ACD/Labs)	log D (pH 4/5.5) (from ACD/Labs)	Experimental logKow (from EPISUITE)	Estimated LogKow (from EPISUITE)	LogP (from ACD/ Labs)	logD (pH 7) (from ACD/ Labs)	Charge at pH 7 (from Chemicalize or via logD at different pH*)	Removal in Wastewater Treatment (%) from EPISUITE
N-butylbenzenesulphonamide	3622-84-2	CCCCNS(=O)(=O)C1=CC=CC=C1	3	1	10	15	0.7	213.297	1.85	NR	2.31	2.57	1.85	0*	2.78
1,2-benzisothiazol-3(2H)-one 1,1-dioxide (saccharin)	81-07-2	C1=CC=C2C(=C1)C(=O)NS2(=O)=O	4	1	7	5	1.4	182.184	-1.29	0.91	0.45	0.91	-1.29	0	1.88
Triclosan	3380-34-5	C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl	2	1	12	7	1.7	289.542	5.27	4.76	4.66	5.17	5.13	0*	68.67

APPENDIX 7 RISK ASSESSMENT OUTPUTS

Table A7. 1 Predicted drinking water concentrations (*C*) in μg L^{-1} and RCRs for chemicals with both a cancer-based (c) and a non-cancer-based (nc) HBGV, using the HBGV not used in the main risk assessment. HBGVs are expressed in μg kg^{-1} d^{-1}. The tonnage employed here was at **Tier 3**. Note RCRs are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR>1. Cells coloured green have RCR<1. RCRs calculated assuming exposure only via drinking water. Concentrations shown as 0.0 indicate values <0.01 μg L^{-1} RCR values shown as 0.00 indicate values < 0.001.

	No DW Treatment Tier 3A		Conventional Tier 3B		Advanced Tier 3C		
Compound	**C**	**RCR**	**C**	**RCR**	**C**	**RCR**	**HBGV used**
1,4-dioxane	225.0	0.10	12.1	0.08	1.3	0.01	96 (nc)
Trichloroethylene	61.5	0.00	52.1	0.00	1.6	0.00	0.5 (nc)
Tetrachloroethylene	0.0	**1.05**	0.0	0.55	0.0	0.03	5.7 (c)

Table A7. 2 Predicted drinking water concentrations (*C*) in μg L^{-1} and RCR_T values for chemicals with both a cancer-based (c) and a non-cancer-based (nc) HBGV, using the HBGV not used in the main risk assessment. HBGVs are expressed in μg kg^{-1} d^{-1}. The tonnage employed here was at **Tier 3**. Note RCRs are shown here for infants. Values for children and adults are lower. Cells coloured orange with bold text have RCR_T >1. Cells coloured green have RCR_T<1. RCR_T calculated assuming exposure via drinking water is 20% of total exposure (i.e. assumed exposure is 5 x higher than that predicted via drinking water). Concentrations shown as 0.0 indicate values <0.01 μg L^{-1}. RCR_T values shown as 0.00 indicate values < 0.001.

	No DW Treatment Tier 3A		Conventional Tier 3B		Advanced Tier 3C		
Compound	**C**	**RCR**	**C**	**RCR**	**C**	**RCR**	**HBGV used**
1,4-dioxane	225.0	0.48	12.1	0.41	1.3	0.05	96 (nc)
Trichloroethylene	61.5	0.00	52.1	0.00	1.6	0.00	0.5 (nc)
Tetrachloroethylene	0.0	**5.25**	0.0	**2.74**	0.0	0.15	5.7 (c)

The Appendix shows (a) Spatial patterns of predicted chemical concentrations in river water under Q_{mean} and Q_{95} conditions for the remaining two chemicals with RCR_T values greater than one in Tier 3B (scaled against the values shown for tetrachloroethylene in Figure 5); (b) Spatial patterns of RCR_T values for these chemicals, assuming conventional treatment for all cells, under Q_{mean} and Q_{95} conditions (scaled against the values shown for tetrachloroethylene in Figure 6) and (c) Cumulative probability distributions of RCR_T for each chemical at drinking water abstraction points, illustrating the fraction of cells containing abstractions with $RCR_T > 1$.

Note that predicted *RCR* was not greater than one at any abstraction points under conventional treatment when drinking water was assumed to be the only exposure route. Furthermore, RCR_T was not greater than one for any substance at any abstraction point if advanced treatment is assumed.

1,4-dioxane

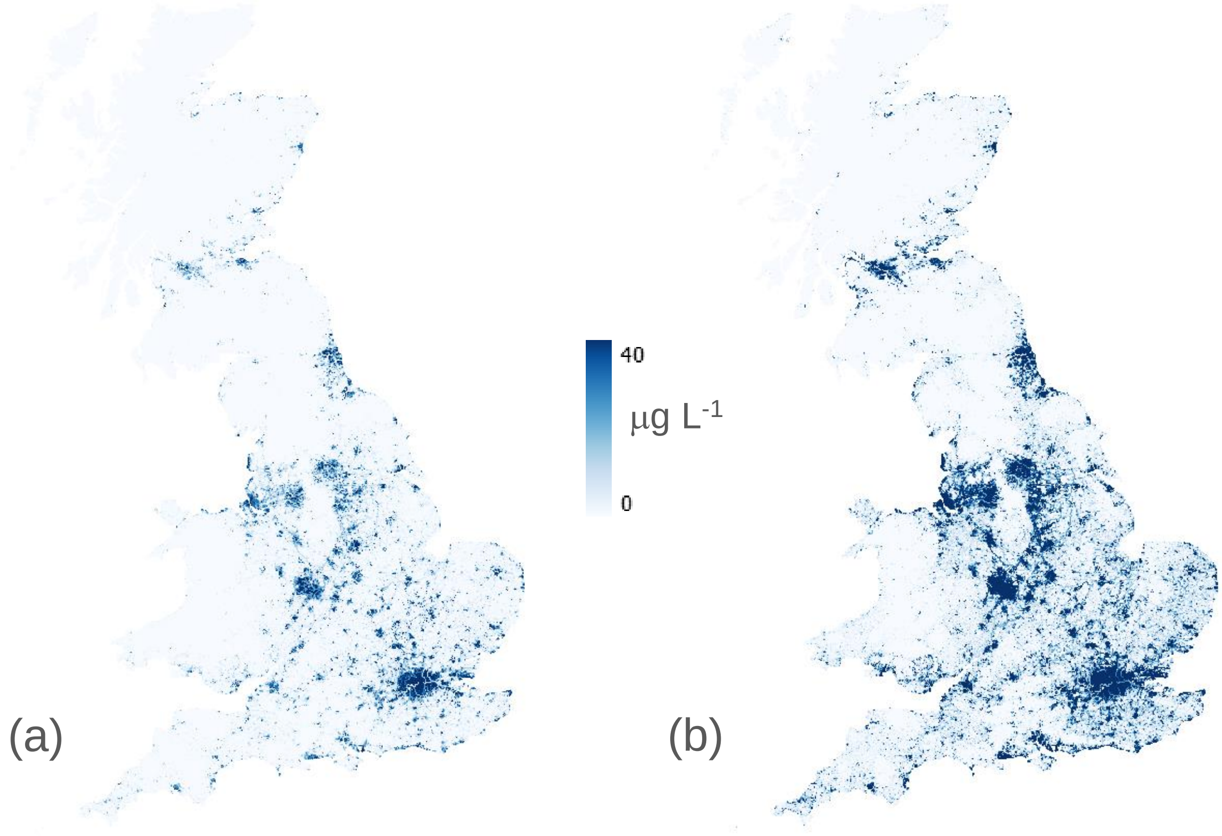

Figure A7. 1 Predicted spatial patterns of the concentrations of 1,4-dioxane in river water for Great Britain under (a) mean flow and (b) Q_{95} conditions. Note scale is the same as for tetrachloroethylene in Figure 5.

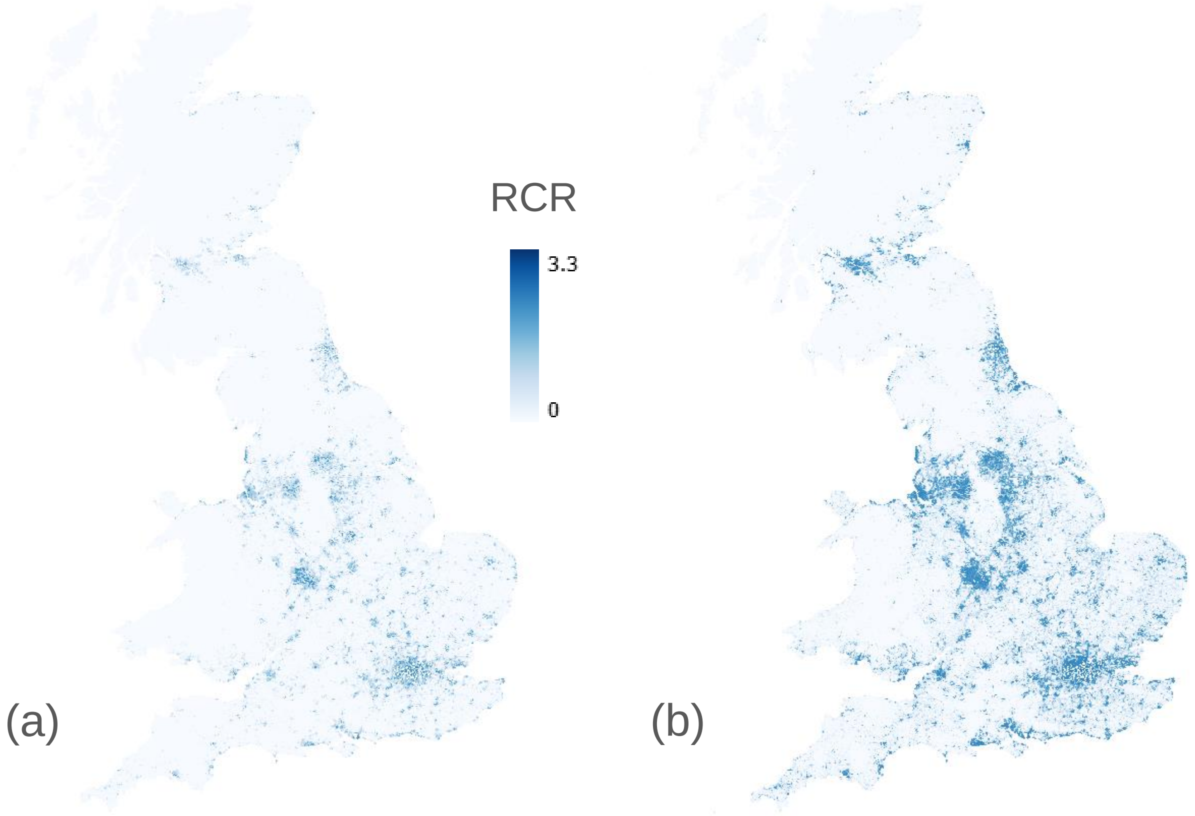

Figure A7. 2 Predicted spatial patterns of the RCR_T for 1,4-dioxane in drinking water following conventional treatment for Great Britain under (a) mean flow and (b) Q_{95} conditions. Note the scale is the same as for and (b) Q_{95} conditions. Note scale is the same as for tetrachloroethylene in Figure 6.

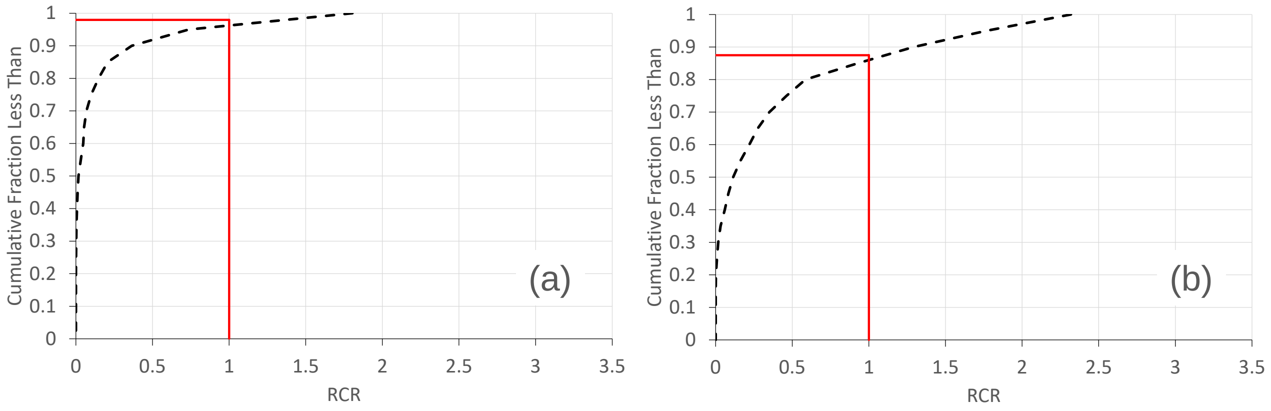

Figure A7. 3 Cumulative distributions of predicted RCR_T values for 1,4-dioxane in drinking water in cells containing drinking water abstraction points assuming conventional treatment (dashed lines) under (a) mean flow and (b) Q_{95} flow. The red lines show the cumulative fraction less than $RCR_T = 1$.

1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride

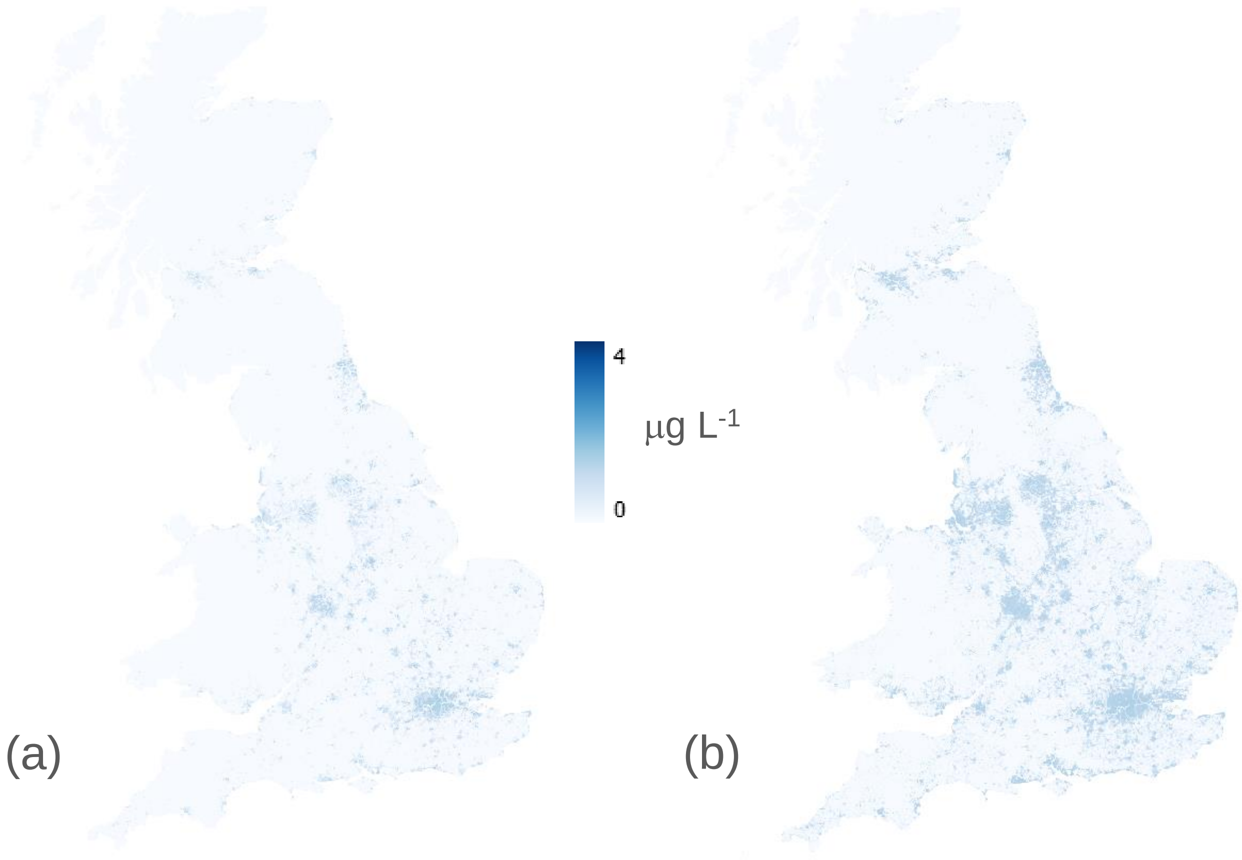

Figure A7. 4 Predicted spatial patterns of the concentrations of 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride in river water for Great Britain under (a) mean flow and (b) Q_{95} conditions. Note scale is 10 x lower than for tetrachloroethylene in Figure 5.

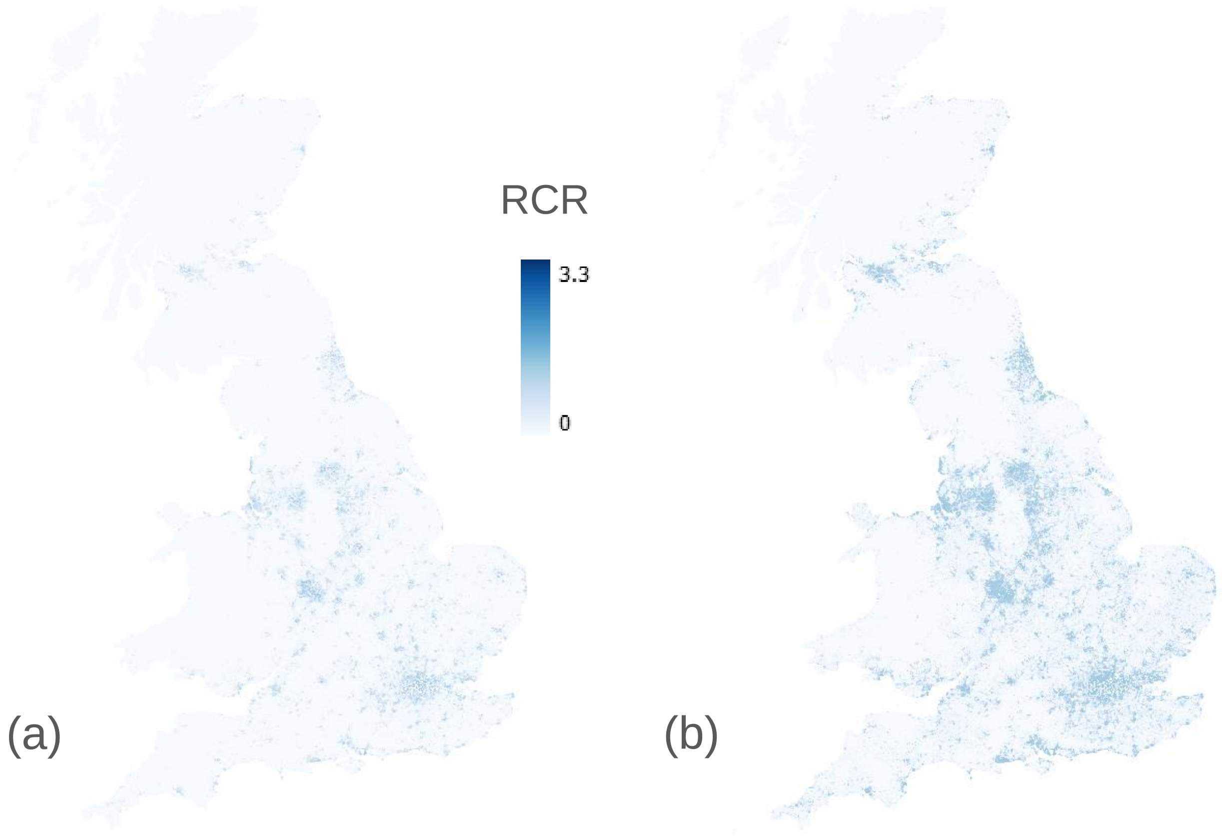

Figure A7. 5 Predicted spatial patterns of the RCR_T for 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride in drinking water following conventional treatment for Great Britain under (a) mean flow and (b) Q_{95} conditions. Note the scale is the same as for tetrachloroethylene in Figure 6.

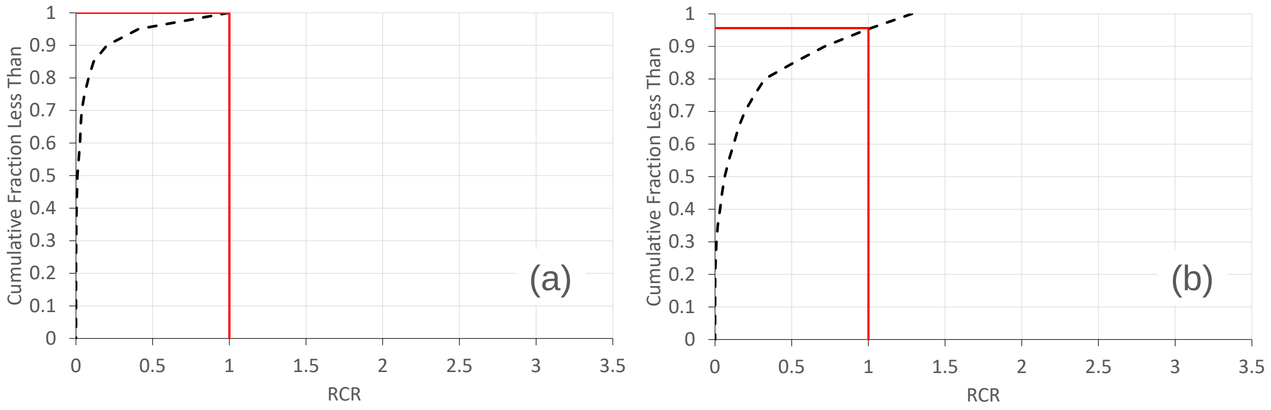

Figure A7. 6 Cumulative distributions of predicted RCR_T values for 1,4,5,6,7,7-hexachloro-8,9,10- trinorborn-5-ene-2,3-dicarboxylic anhydride in drinking water in cells containing drinking water abstraction points assuming conventional treatment (dashed lines) under (a) mean flow and (b) Q_{95} flow. The red lines show the cumulative fraction less than $RCR_T = 1$.

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