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Environmental risk evaluation report:
Trixylenyl phosphate
(CAS no. 25155-23-1)

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This report is the result of research commissioned and funded by the Environment Agency's Science Programme.

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Steve Killeen

Head of Science

Executive summary

An environmental risk assessment has been carried out for trixylenyl phosphate (CAS no. 25155-23-1) on the basis of available information and using the methods of a European Technical Guidance Document. This substance is mainly used as a power generation fluid in Europe.

Potential risks are identified for production and from the blending of power generation fluids for some or all of the surface water (fresh and marine), sediment (fresh and marine) and soil compartments.

Emission estimates are based on information from a number of generic sources, including emission scenario documents and other risk assessments, so they could be refined with more specific information for the substance itself.

The assessment could also be refined by performing toxicity tests on sediment and terrestrial organisms. In each case, it is likely that three long-term studies would be required. The actual need for testing is closely linked with that for the other triaryl and alkyl/aryl phosphates considered as part of this project. A suggested testing strategy for the group as a whole is outlined in a separate overview document.

The risks to waste water treatment plant and air from all uses of trixylenyl phosphate are low. In addition, no risks are identified from the use of power generation fluids with trixylenyl phosphate as the base fluid.

No risk characterisation could be carried out for secondary poisoning in the absence of an adequate mammalian toxicity data set. As the substance has a relatively high bioconcentration factor (BCF) in fish (around 1,900 l/kg) and is predicted to be taken up from soil by worms, this endpoint may be important for this substance.

Trixylenyl phosphate meets the criteria for a persistent, bioaccumulative and toxic (PBT) substance on the basis of the available *screening* data only. Testing on persistence to determine a relevant environmental half-life should be considered as a priority.

Introduction

This report is one of a series of evaluations covering a group of related substances that represent the major aryl phosphate ester products used in Europe:

Triphenyl phosphate
Trixylenyl phosphate
Tricresyl phosphate
Cresyl diphenyl phosphate
Tris(isopropylphenyl) phosphate
Isopropylphenyl diphenyl phosphate
Tertbutylphenyl diphenyl phosphate
2-Ethylhexyl diphenyl phosphate
Isodecyl diphenyl phosphate
Tetraphenyl resorcinol diphosphate

A further substance is known to be commercially available, but it has already been assessed under the Notification of New Substances (NONS) Regulations. Information is also available on some (possibly obsolete) triaryl phosphates that are not thought to be supplied in the EU. This information is summarised in Annex A, but the risks from these products have not been assessed. Information for the group as a whole has also been used in this assessment, where appropriate, to fill any gaps in the database for this particular substance. Annex B discusses the read-across of data between the various phosphate esters considered.

This group was highlighted for assessment during preliminary work for a review of flame retardants (eventually published as Environment Agency 2003), particularly because they are potential replacements for other flame retardants that have already been identified as a risk to health or the environment. Regulators need to understand the potential consequences of such market switches before substantial replacement takes place. These assessments are not intended to provide a basis for comparison between the different aryl phosphates themselves; such a comparison would require consideration of a wider range of factors than are included here (such as human health risks, efficacy, recycling potential and costs). The assessments have been produced as part of the UK Coordinated Chemical Risk Management Programme (UKCCRMP) (http://www.defra.gov.uk/environment/chemicals/ukrisk.htm).

The methodology used in the report follows that given in an EU Technical Guidance Document (TGD)[1] for risk assessment of existing substances. The scientific work was mainly carried out by the Building Research Establishment Ltd (BRE), under contract to the Environment Agency. The review of mammalian toxicity data for the assessment of non-compartment specific effects was carried out by the Institute of Environment and Health, under contract to the Department for Environment, Food and Rural Affairs (Defra).

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[1] This document has recently been replaced by similar guidance for the REACH Regulation.

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1 General substance information

1.1 Identification of the substance

This assessment considers the following commercial substance.

CAS No:	25155-23-1
EINECS No:	246-677-8
EINECS Name:	Trixylenyl phosphate
Molecular formula:	$C_{24}H_{27}O_4P$
Molecular weight:	410.45 g/mol
Structural formula:	
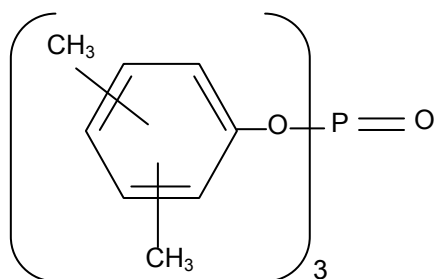
Other names, abbreviations, tradenames and registered trademarks for this substance include the following.

> Antiblaze TXP®
>
> Fyrquel 220® (historic only; the modern product is no longer based on trixylenyl phosphate)
>
> Fyrquel EHC®
>
> Kronitex TXP®
>
> Phosflex 179A®
>
> Phosphoric acid, trixylyl ester
>
> Pliabrac TXP®
>
> Reolube TXP®
>
> Tris(dimethylphenyl) phosphate
>
> Trixylyl phosphate
>
> Xylenol, phosphate ester

Some of the tradenames and trademarks may refer to older products no longer supplied to the EU, or products produced outside the EU, but these are included in the report as they are sometimes referred to in the open literature.

The name trixylenyl phosphate is used in this assessment.

1.2   Purity/impurity, additives

1.2.1   Purity/impurities

The commercial product is an isomeric mixture of phosphate esters. Hence, the actual composition will vary between different manufacturers and possibly batches.

Nobile *et al.* (1980) investigated the composition of two commercial trixylenyl phosphate products. The products investigated were a flame-retardant plasticizer and a fire-resistant hydraulic fluid. In the study, the products were quantitatively hydrolysed and the resulting phenolic products were identified. Both products yielded similar mixtures of xylenols, ethylphenols and phenol, with xylenols accounting for the majority of the products found. The xylenol isomers present were (in decreasing order of abundance) the 2,5-, 2,3-, 3,5-, 2,4- and 3,4- isomers. The 2,6-isomer was not present. The other components identified included 4-ethylphenol, p-cresol, phenol and trimethyl phenol. The commercial products were also analysed by a gas chromatographic method and tris(2,5-xylenyl) phosphate and one or both of tris-(3,5-xylenyl) or tris-(2,4-xylenyl) phosphate was found to be present in both products. The other components present could not be identified due to the complexity of the chromatograms obtained.

From the above description, the products in use (and used in tests as appropriate) consist of a mixture of components. These are rarely if ever identified in the test reports. This has implications for the interpretation of the results, and comments have been included to indicate where this has been taken into account.

1.2.2   Additives

Additives are not thought to be present in commercially supplied flame-retardant products, although some aryl phosphate ester products are sometimes supplied as blends with other (halogenated) flame retardants. Trixylenyl phosphate-based hydraulic fluids generally contain small (under 0.5 per cent) amounts of additives (Great Lakes Chemical Corporation 2003).

1.3   Physico-chemical properties

Detailed test reports were not available for review, and so the validity of many of the reported values for physico-chemical properties is not always clear.

1.3.1   Physical state (at normal temperature and pressure)

Commercial trixylenyl phosphate is a clear liquid at room temperature (Great Lakes Chemical Corporation 2002).

1.3.2   Melting point

Wightman and Malalyandi (1983) determined melting points for two pure isomers of trixylenyl phosphate. The values reported were 61°C for tris(2,3-dimethylphenyl) phosphate and 33°C or 46°C for tris(3,5-dimethylphenyl) phosphate. Muir (1984) gives a melting point of 136-138°C for the tris(2,6-dimethylphenyl) phosphate isomer, and indicates that commercial products have melting points (pour points) of around -20°C.

Wightman and Malalyandi (1983) give further values for boiling points/melting points for isomers of trixylenyl phosphate of 80-82°C at atmospheric pressure for tris(2,5-dimethylphenyl) phosphate (a literature value of 79-81°C was also quoted in the paper for this substance), 65-67°C at atmospheric pressure for tris(3,4-dimethylphenyl) phosphate (a literature value of 72°C was also quoted in the paper) and 137-139°C at atmospheric pressure for tris(2,6-dimethylphenyl) phosphate. It is not altogether clear from the paper whether these are melting points or boiling points but, by comparison with other melting point, boiling point and vapour pressure data, these values are most likely to be melting points (indeed, a literature value of 136-138°C was also quoted in the paper for tris(2,6-dimethylphenyl) phosphate and this is given as the melting point for this substance by Muir (1984)).

A melting point of -20°C is assumed for the commercial product. Pure isomers are likely to form crystals more easily, and so would be expected to have a higher melting point. However, this does not influence the outcome of this assessment.

1.3.3   Boiling point

Wightman and Malalyandi (1983) determined the boiling points of pure isomers of trixylenyl phosphate. The boiling points reported were 200-205°C at 0.2 mmHg (27 Pa) for tris(2,3-dimethylphenyl) phosphate and 195-200°C at 0.2 mmHg (27 Pa) for tris(3,5-dimethylphenyl) phosphate (a literature value of 236°C at 2 mmHg (267 Pa) was also quoted in the paper for this substance) The boiling point for tris(2,6-dimethylphenyl) phosphate given by Muir (1984) is 262-264°C at 6 mmHg (800 Pa).

IUCLID (2001) gives a boiling point for commercial trixylenyl phosphate of 243-265°C at 13.332 hPa (1,333 Pa). Further boiling points for commercial trixylenyl phosphate are reported in Boethling and Cooper (1985) as 225-295°C at 10 mmHg (1,333 Pa), 248-265°C at 4 mmHg (533 Pa) and 270°C at 3 mmHg (400 Pa).

The decomposition temperature of a commercial trixylenyl phosphate is above 300°C (Great Lakes Chemical Corporation 2002).

A boiling point of above 300°C at atmospheric pressure is assumed in the assessment.

1.3.4   Density

Shankwalkar and Cruz (1994) reported a relative density of 1.14 at 20°C for a commercial trixylenyl phosphate. A similar value of 1.13 at 20°C and 1.14 at 25°C is quoted for a commercial trixylenyl phosphate (Great Lakes Chemical Corporation 2002).

A relative density of 1.13-1.14 at 20°C is assumed in the assessment.

1.3.5   Vapour pressure

The vapour pressure at ambient temperature is an important physico-chemical property for environmental risk assessment, because it is used to estimate both the distribution of a substance in the environment and the volatile releases from products.

No reliable data appear to be available for trixylenyl phosphate at temperatures around 20-25°C. However, information on both boiling points at reduced pressure (see Section 1.3.3) and vapour pressures at elevated temperature are available for the commercial substance, with some data also available for individual pure isomers.

IUCLID (2001) gives a vapour pressure of 0.1333 hPa (13.3 Pa) at 38°C for commercial trixylenyl phosphate. Boethling and Cooper (1985) report a much lower vapour pressure of 5.2×10^{-8} mmHg (6.93×10^{-6} Pa) at 30°C for commercial trixylenyl phosphate. Muir (1984) gives vapour pressures of under 0.02 mmHg (2.7 Pa) at 150°C and 0.33 mmHg (44 Pa) at 200°C for commercial trixylenyl phosphate. Great Lakes Chemical Corporation (2003) indicates a vapour pressure of 7.05×10^{-6} mmHg (9.4×10^{-4} Pa) at 70°C for trixylenyl phosphate.

The vapour pressure or reduced pressure boiling point of a pure substance is related to the temperature within a limited temperature range according to the simplified Clapeyron-Clausius equation:

$$\log \text{ (vapour pressure)} = [\Delta H_v / 2.3RT] + \text{constant}$$

where   vapour pressure is in Pa
                 ΔH_v = heat of vapourisation in J/mol
                 R = the universal gas constant 8.314 J/mol K
                 T = temperature in K

Figure 1.1 shows a plot of log (vapour pressure or reduced pressure (Pa)) against 1/(temperature or boiling point (K)) for the data available for commercial trixylenyl phosphate. The following regression equation is derived from the plot:

$$\log \text{ (vapour pressure (Pa))} = [-4041.9 \times 1/(\text{temperature (K)})] + 10.464]$$

The value of ΔH_v for the commercial product is estimated to be -77,290 J/mol.

Figure 1.1 Plot of log (vapour pressure or reduced pressure (Pa)) against 1/(temperature or boiling point (K)) for commercial trixylenyl phosphate.
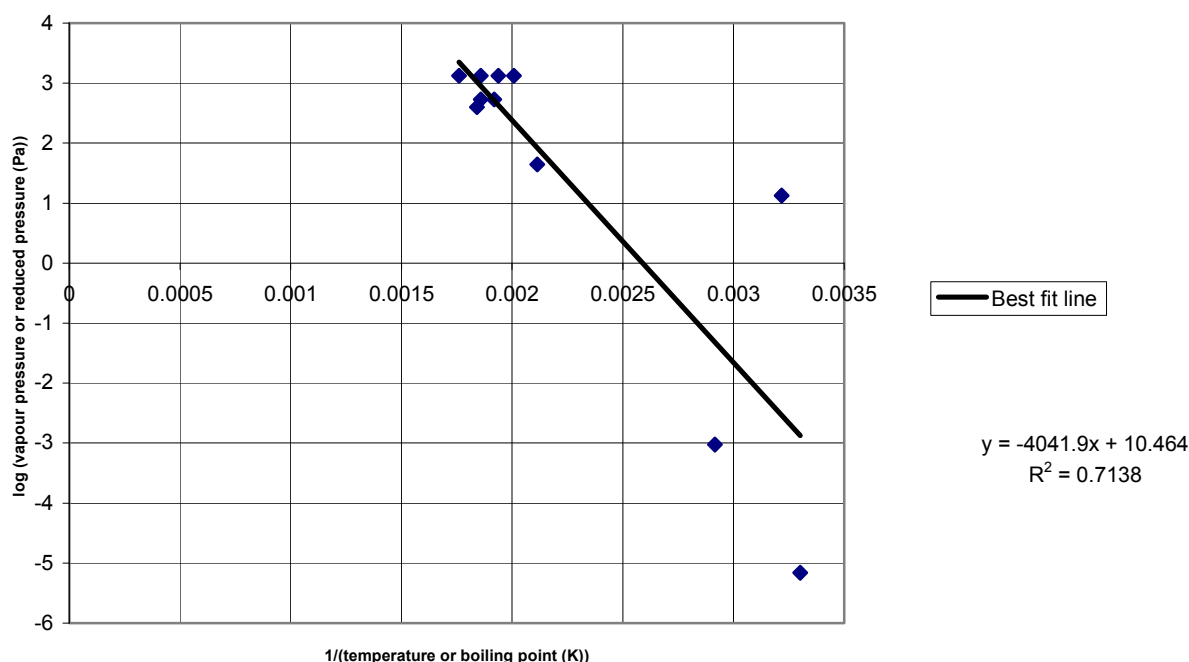
Using this equation the vapour pressure of commercial trixylenyl phosphate is estimated to be 4.7×10^{-4} Pa at 20°C, 8.0×10^{-4} Pa at 25°C, 8.1 Pa at 150°C and 83 Pa at 200°C. The correlation on the plot is, however, poor and this introduces some uncertainties in values estimated from it. The value of ΔH_v may vary with temperature

and so could introduce further errors in extrapolating the data obtained at elevated temperatures to ambient temperatures.

Assuming that the individual tris(dimethylphenyl) phosphate isomers have a similar value for ΔH_v as that estimated for the commercial trixylenyl phosphate, the following vapour pressures at 20°C can be estimated using the simplified Clapeyron-Clausius equation and their respective boiling points at reduced pressure:

tris(2,3-dimethylphenyl) phosphate	$1.2 \times 10^{-4} - 1.5 \times 10^{-4}$ Pa at 20°C
tris(2,6-dimethylphenyl) phosphate	$4.3 \times 10^{-4} - 4.6 \times 10^{-4}$ Pa at 20°C
tris(3,5-dimethylphenyl) phosphate	$1.5 \times 10^{-4} - 1.9 \times 10^{-4}$ Pa at 20°C

These values for the pure isomers are consistent with the vapour pressure estimated above for the commercial product. The pure isomers are solids at 20°C and the estimated vapour pressure is for the sub-cooled liquid.

A vapour pressure (at 25°C) of 2.06×10^{-8} mmHg (2.7×10^{-6} Pa) can be estimated for trixylenyl phosphate from its structure using the Syracuse Research Corporation MPBPWIN (version 1.28) software (modified Grain method). Boethling and Cooper (1985) estimated a vapour pressure at 25°C of 2.3×10^{-7}-5.4×10^{-6} mmHg (3.0×10^{-5}-7.2×10^{-4}) Pa from the boiling point of trixylenyl phosphate (Grain method).

The vapour pressures at 20°C estimated above for trixylenyl phosphate using the Clapeyron-Clausius equation are much higher than those estimated for other triaryl phosphates. The estimated heat of vapourisation obtained by this method for trixylenyl phosphate is much lower than that estimated for similar compounds and this may reflect the fact that relatively few data points were used in the extrapolation method for trixylenyl phosphate. Correlation on the vapour pressure plot is poor and the slope and intercept could be overly influenced by any outliers obtained at the lower temperatures.

Great Lakes Chemical Corporation (2003) quotes a vapour pressure of 2.4×10^{-9} mmHg (3.2×10^{-7} Pa) at 10°C for trixylenyl phosphate based on estimates using the Clapeyron-Clausius method.

Available vapour pressure estimates for all triaryl and alkyl/aryl phosphates are considered in Annex B and from this data a vapour pressure of around 8.7×10^{-6} Pa at 20°C appears to be more reasonable for the commercial trixylenyl phosphate. This value is used in this risk assessment for the commercial product.

1.3.6   Water solubility

Saeger *et al.* (1979) determined the solubility of a trixylenyl phosphate using a shake flask method. The substance used was a commercial product consisting mainly of a mixture of isomers of trixylenyl phosphate. In the experiment, 25 ml of the phosphate ester was added to 500 ml of purified water and shaken for 48 hours. The solution was then allowed to stand for one week in the dark before the aqueous phase was centrifuged at 20,000 g for one hour to remove droplets of undissolved substance. The aqueous phase was then extracted twice with methylene dichloride and the extracts were analysed for the commercial product by a gas chromatography method (the centrifugation/extraction/analysis steps were carried out in duplicate and gave a mean relative average deviation of 13 per cent). The solubility of the substance tested (as the commercial product) was determined to be 0.89 mg/l at room temperature.

Ofstad and Sletten (1985) determined the water solubility of a commercial tricresyl phosphate (Pliabrac 521) product using the OECD 105 column elution method using two different flow rates at 25°C. The product tested contained around 20 per cent triphenyl phosphate along with several other triaryl phosphates. The analytical method

was able to distinguish between the main components of the product and the water solubility was determined to be 3.1 mg/l (sum of all components), 0.34 mg/l for the tricresyl phosphate component (all isomers), 2.1 mg/l for the triphenyl phosphate component and 0.11 mg/l for the trixylenyl phosphate component (all isomers). The value obtained in this study for trixylenyl phosphate is slightly lower than, but in reasonable agreement with, that determined above by Saeger *et al.* (1979).

Akzo Nobel (2003) report a water solubility of 0.72 mg/l for trixylenyl phosphate obtained using the OECD 105 methodology. This value is in good agreement with the value reported by Saeger *et al.* (1979) above. Great Lakes Chemical Corporation (2003) quotes a slightly lower water solubility for trixylenyl phosphate of 0.11 mg/l (this may be the same value as determined above by Ofstad and Sledden (1985)).

A water solubility of around 4×10^{-4} mg/l can be estimated for trixylenyl phosphate using the Syracuse Research Corporation WSKOW version 1.30 software (based on an estimated log K_{ow} of 7.98).

A water solubility of 0.89 mg/l at room temperature is used in this assessment for trixylenyl phosphate[2].

1.3.7   Octanol-water partition coefficient (log K_{ow})

The octanol-water partition coefficient of a trixylenyl phosphate was determined using a shake flask method (Saeger *et al.* 1979). The test substance was a commercial product consisting mainly of a mixture of isomers of trixylenyl phosphate. In the study, the substance was dissolved in n-octanol (at least two concentrations were tested between 100 mg/kg and 10,000 mg/kg) and 100 ml of this solution was shaken with 500 ml of purified water for 48 hours in the dark. The mixture was then allowed to stand for seven days in the dark before the concentration in the water phase (based on the sum of the major components of the product found in the gas chromatography trace) was determined (as only small amounts of the test substance were found to partition into the water phase, the concentration of the substance in the n-octanol phase was taken to be the starting concentration). The K_{ow} obtained was 427,000 (log K_{ow} = 5.63).

Renberg *et al.* (1980) determined the octanol-water partition coefficient for a trixylenyl phosphate (the same substance as used by Saeger *et al.* 1979 above) using a high performance thin layer chromatography (HPTLC) method. The partition coefficient determined (log value) was 5.26, which is in good agreement with the value obtained above.

A log K_{ow} of 6.4 to 6.6 has been reported for trixylenyl phosphate (Bengtsson *et al.* 1986). The value was from an unpublished source.

Akzo Nobel (2003) determined the log K_{ow} of a commercial trixylenyl phosphate using the flask method of the OECD 117 test guideline. The log K_{ow} range determined for the various components of the product was 3.0 to 6.5.

A log K_{ow} of 7.98 can be estimated for trixylenyl phosphate from its structure using the Syracuse Research Corporation Log K_{ow} (version 1.60) software.

A log K_{ow} of 5.63 as determined by Saeger *et al.* (1979) is used in the assessment.

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[2] Further water solubility data are being generated under the US High Production Volume programme. Preliminary results indicate that the water solubility found using the generator column method was 0.0186 mg/l at 25°C which is lower than currently used in the assessment.

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1.3.8   Hazardous physico-chemical properties

The flash point for a commercial trixylenyl phosphate is given as above 220°C (Great Lakes Chemical Corporation 2002). IUCLID (2001) gives a flash point (open cup) of 246°C for another commercial product.

Great Lakes Chemical Corporation (2002) gives an autoignition temperature of 575°C for the commercial trixylenyl phosphate Kronitex TXP. A similar autoignition temperature of 566°C is given in IUCLID (2001).

Trixylenyl phosphate is not explosive (IUCLID 2001).

No data could be located on the oxidising properties of this substance.

1.3.9   Henry's law constant

A Henry's law constant of 7.19×10^{-8} atm m^3/mol (0.0073 Pa m^3/mol) at 25°C can be estimated for trixylenyl phosphate from the chemical structure of the main components (bond contribution method) using the Syracuse Research Corporation HENRYWIN (version 3.00) software. The software also gives an experimentally determined value of 3.1×10^{-8} atm m^3/mol (0.003 Pa m^3/mol) at 25°C for the same substance, but this reference has not been reviewed.

A further Henry's law constant for trixylenyl phosphate can be estimated from the vapour pressure (8.7×10^{-6} Pa) and water solubility (0.89 mg/l) at 20°C. Using these data, the Henry's law constant is estimated to be 0.004 Pa m^3/mol. This value is used in the assessment as it is consistent with the water solubility and vapour pressure data used here and is similar to the estimated and experimental values reported above.

1.3.10   Summary of physico-chemical properties

The physico-chemical properties of trixylenyl phosphate are summarised in Table 1.1. Most of the data have been obtained with commercial products and so some of the properties may vary depending on the actual composition of the product.

Table 1.1   Summary of environmentally relevant physico-chemical properties for trixylenyl phosphate

Property	Value
Melting point	-20°C
Boiling point (at atmospheric pressure)	>300°C
Relative density	1.13-1.14 at 20°C
Vapour pressure	8.7×10^{-6} Pa at 20°C
Water solubility	0.89 mg/l at room temperature
Octanol-water partition coefficient (log value)	5.63
Henry's law constant	0.004 Pa m^3/mol at 20°C

For the purposes of this assessment, the commercial substance is considered to behave as a single substance in the environment, even though it is a complex mixture.

2 General information on exposure

2.1 Production

Trixylenyl phosphate is produced through the reaction of xylenols with phosphorus oxychloride. There is only one known European production site (Chemtura (formerly Great Lakes), UK) and one additional European supplier. Information on production volume and market size is therefore confidential. It is possible that other companies may supply this substance, but no further information is available for this report.

2.2 Use

2.2.1 General introduction

Aryl phosphate flame retardants were first commercialised in the early twentieth century for use in flammable plastics such as cellulose nitrate and later for cellulose acetate (Weil 1993). Use in cellulose products is still significant, but the largest area of application is now in plasticized vinyl polymers. The main applications of these products are in wire and cable insulation, connectors, automotive interiors, vinyl moisture barriers, furniture upholstery, conveyor belts (for mining) and vinyl foams.

In addition to their use as flame retardants in polymer systems, triaryl phosphates are also used as fire-resistant hydraulic fluids, lubricants and lubricant additives (Weil 1993). Small amounts are also reported to be used as non-flammable dispersing media for peroxide catalysts.

2.2.2 Uses of trixylenyl phosphate

Information on the sales of trixylenyl phosphate into the EU has been provided by the relevant supplier companies for 2005. The specific figures are confidential; however, the major current area of use of the substance in the EU is as a power generation fluid.

This application is the only one considered in this risk assessment. Weil (1993) also reported that the lower volatility and lower extractability of this substance compared to tricresyl phosphate is advantageous for use in wire and cable insulation.

3 Environmental exposure

This assessment has been prepared in accordance with the principles of Council Regulation (EEC) 793/93 (the Existing Substances Regulation or ESR)[3] and the methods laid down in Commission Regulation (EC) 1488/94[4] , which is supported by a technical guidance document or 'TGD' (EC 2003). The European Union System for the Evaluation of Substances (EUSES) computer program[5] (v2.0.3) implements the TGD models. The EUSES output file for this assessment is confidential because of the information it contains on tonnage and use pattern.

The assessment is generic, representing a *realistic worst case approach* for a hypothetical environment that broadly reflects average European conditions. It uses a number of assumptions (such as a fixed river dilution level), and further details can be found in the TGD. The assessment is based on estimated sales figures for Europe and some site-specific information. Since these are confidential, the calculations are presented in the Confidential Annex, but they are discussed qualitatively in the report as appropriate.

3.1 Environmental fate and distribution

3.1.1 Degradation

Abiotic degradation

Atmospheric photooxidation
A rate constant for reaction of trixylenyl phosphate with atmospheric hydroxyl radicals of 4.7×10^{-11} cm^3/molecule s can be estimated from its structure using the Syracuse Research Corporation AOP (version 1.86) software. This program implements the method recommended in the TGD for estimating the rate constant.

Using an atmospheric hydroxyl radical concentration of 5×10^5 molecules/cm^3, a half-life for the reaction in air is estimated to be eight hours.

Hydrolysis
Wolfe (1980) developed linear free energy relationships to estimate the rate constants for neutral and alkaline hydrolysis of triaryl phosphates using published information on hydrolysis. Under alkaline conditions, the second-order reaction rate constant for hydrolysis was found to correlate with the sum of the Hammett (σ) substituent constants for the aryl substituents and the following equation was derived:

$$\log k = 1.40 \times \sigma - 0.47$$

where   k = second-order rate constant for hydrolysis at 30°C (l/mol s)

         σ = sum of Hammet substituent constants

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[3] O.J. No L 084, 05/04/1993 p. 0001–0075.
[4] O.J. No L 161, 29/06/1994 p. 0003–0011.
[5] Available from the European Chemicals Bureau, http://ecb.jrc.it/.

For trixylenyl phosphate, σ = -0.069 (*meta*-) or -0.170 (*para*-) and so the second-order hydrolysis rate constant is 0.20-0.27 l/mol s. Using this value the hydrolysis half-life at any alkaline pH can be estimated. For example, at pH 8 the concentration of hydroxyl anions present is 10^{-6} mol/l and so the pseudo first-order hydrolysis reaction rate constant for trixylenyl phosphate at this pH is around 2.0×10^{-7} to 2.7×10^{-7} s^{-1}. This is equivalent to a hydrolysis half-life of around 30 to 40 days.

For hydrolysis under neutral conditions, the following equation was derived:

$$\log k = -0.95 \times pKa - 1.20$$

where k = first-order rate constant for neutral hydrolysis at 25°C (s^{-1})

pKa = $-\log_{10}$ {acid dissociation constant for the phenolic leaving group}

For trixylenyl phosphate, the pKa of the xylenol leaving group is unknown but is likely to be around 10 (the pKa of phenol is 10 and the pKa of cresols are in the range 10.01 to 10.2). This leads to an estimated value for the rate constant for the neutral hydrolysis of 2×10^{-11} s^{-1} and an estimated half-life for neutral hydrolysis of 1,100 years[6]. The half-life of the alkaline reaction at pH 7 would be 300 to 400 days.

Great Lakes Chemical Corporation (2003) indicate that hydrolysis of aryl phosphates in general can also occur under acidic conditions and packages are usually added to hydraulic fluids to delay the onset of hydrolysis during the service life of the products. The standard test for such fluids is the 'coke bottle' test. In this test, the fluid is placed in a coke bottle with distilled water (sometimes with catalytic metals such as copper) and the degradation is followed by an increase in acidity (the initial hydrolysis products would be diaryl phosphates (diesters of phosphoric acid), which are acidic). The rate of hydrolysis in such tests generally increases as the acidity increases during the test. However, although this indicates that hydrolysis of aryl phosphates can occur at acidic pHs, the autocatalysis seen in the test as a result of the formation of acidic products (resulting in an increase in acidity) is unlikely to occur in the environment owing to its natural buffering capacity.

Photolysis

No information is available on the direct photolysis reactions of trixylenyl phosphate in the environment[7].

Biodegradation

The Japanese Chemicals Evaluation and Research Institute database on degradation data (CERI 2003) reports the result of a MITI I ready biodegradation test (equivalent to OECD 301C) with trixylenyl phosphate. The test was carried out at 25°C using an activated sludge concentration of 30 mg/l and a trixylenyl phosphate concentration of 100 mg/l. The biodegradation was monitored by two methods, biochemical oxygen demand (BOD) and parent compound analysis by high performance liquid chromatography (HPLC). The degradation seen after 28 days was zero to one per cent

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[6] Further data on hydrolysis of this substance is being generated under the US HPV programme. Preliminary results indicate that hydrolysis at pH 4 was slow, the half-life at pH 7 was over one year at 25°C and the half-life at pH 9 was 219 days at 25°C.

[7] A study to determine the absorption coefficients under acidic, neutral and basic pH using ultraviolet-visible light (OECD 101 method) is being carried out under the US HPV programme. Full results from the study are not yet available.

based on BOD in three replicates and zero per cent based on HPLC analysis in three replicates. Thus, the substance is not readily biodegradable based on these results[8].

A further ready biodegradation test was carried out with a commercial trixylenyl phosphate (Sherren 2003). The method used in this case was the OECD 301F Manometric Respirometry method. The degradation seen (determined as percentage ThOD) was 29 per cent after 28 days. The test was extended up to 68 days and the substance was shown to be over 60 per cent degraded by day 68. Thus, on the basis of this test the substance is not considered to be readily biodegradable, but the fact that substantial degradation was seen over the extended time period indicates that the substance can be considered to be inherently biodegradable.

Saeger *et al.* (1979) determined the biodegradation of a trixylenyl phosphate using various test systems. The substance used was a commercial product consisting mainly of a mixture of isomers of trixylenyl phosphate.

The first part of the study investigated the primary degradation of the test substance using a semi-continuous activated sludge (SCAS) unit. The method used was based on the Soap and Detergent Association procedure (Soap and Detergent Association 1965 and 1969). The activated sludge used in the test was of domestic origin and the vessels used had an operating volume of 1.5 litres. The test substance was added to the unit at a rate of 3 or 13 mg/l per 24-hour cycle. The units were operated for a period of 14 to 25 weeks and samples of the mixed liquor were removed at weekly intervals and the concentration of the phosphate ester determined. The results indicated an equilibrium removal rate of 65 ± 18 per cent at 3 mg/l and 13 ± 9 per cent at 13 mg/l in the test system. To investigate loss by volatilisation, the off-gases were passed through a series of scrubbers. No significant loss by volatilisation (under 0.5 per cent per cycle) of the phosphate ester was seen in the experiment.

The final part of the study investigated the ultimate mineralisation of the test substance using a degradation method based on the modified Sturm method. An acclimated bacterial seed was prepared by incubation of 100 ml of settled supernatant from a SCAS unit with 20 mg of one of eleven phosphate esters (including the test substance), 50 mg of yeast extract and 900 ml of standard biological oxygen demand (BOD) water for 14 days in the dark at room temperature. At the end of the incubation period, a combined acclimated seed was prepared by mixing samples from each acclimation bottle and this was used as seed for the inherent biodegradation test. In the test, 500 ml of the composite seed was added to 5,500 ml of BOD water and the substance was then added to the bottle (initial concentration 20.2 mg/l). During the test, CO_2-free air was continually bubbled through each bottle and the CO_2 evolved from the system was determined. Control bottles (receiving no test substance) were also run. The amount of CO_2 evolved from the control bottles was around 10-15 per cent of that of the bottles containing the test substance and the results were corrected for this background CO_2 level. The CO_2 evolved from the test substance (expressed as a percentage of the maximum theoretical amount) was five per cent after seven days, 43 per cent after 28 days and 65 per cent after 48 days. Therefore, the substance can be considered as inherently biodegradable based on the results of this test.

Pickard *et al.* (1975) studied the biodegradation of a commercial triaryl phosphate (Fyrquel 220), along with triphenyl phosphate, trixylenyl phosphate and tri-ortho-cresyl phosphate, by mixed bacterial populations. The actual composition of the commercial product was not given, but it was reported that the following mixture of phenolic compounds was used to manufacture the product: 2.6 per cent phenol, 0.5 per cent ortho-cresol, 13.6 per cent meta- and para-cresol, 0.6 per cent 2-ethylphenol, 22.3 per

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[8] Further ready biodegradation testing is underway as part of the US HPV programme. Preliminary results indicate that the substance was not readily biodegradable in an OECD 301D closed bottle test. This result agrees with the other data available on ready biodegradability.

cent 2,4- and 2,5-xylenol, 49.2 per cent mixed xylenols, 8.6 per cent 3,4-xylenol, 1.3 per cent C_6-C_9 phenolics and 1.4 per cent trimethyl phenol. Based on this starting mixture, the commercial product would be a mixture of trixylenyl phosphate and tricresyl phosphates, along with other aryl phosphates. The purity of the triphenyl phosphate, trixylenyl phosphate and tri-ortho-cresyl phosphate used was not reported.

The microbial cultures used in the study were obtained by enrichment (using 0.1 per cent solutions of Fyrquel 220) of a mud sample from a lake that had been used as a seaplane base and that was rich in oil-utilizing microorganisms. The enriched mixed microbial cultures were capable of growing on Fyrquel 220, tri-ortho-cresyl phosphate and trixylenyl phosphate as sole source of carbon, but grew only poorly when triphenyl phosphate was used as the sole carbon source.

Boethling and Cooper (1985) estimated the removal of trixylenyl phosphate during biological waste water treatment at a production plant in the United States to be 89 per cent based on the average concentration in waste water (7.19 mg/l) and the average concentration in effluent from the treatment plant (0.81 mg/l). The removal was thought to be due to biodegradation since air stripping was not thought to be an important removal mechanism, and sludge wastage was not practiced at the facility. However, the results of this study should be treated with caution as the recoveries found for the effluent samples were generally much lower than found for the waste water samples (27 per cent overall versus 89 per cent overall). Thus, the concentrations in the effluent may have been higher than indicated (and hence the removal lower than indicated).

Summary of degradation

Abiotic degradation

Although no experimental studies are available on the hydrolysis of trixylenyl phosphate, the available information for triaryl phosphates as a whole indicate that they undergo hydrolysis to form diaryl phosphates which are more stable to hydrolysis than the parent compound. The rate of hydrolysis is expected to increase with increasing pH above neutral; a half-life of 30 to 40 days at pH 8 and 25°C has been estimated, and is expected to be more rapid at higher pH. The reaction is expected to be slow at neutral pH but the rate may again increase with decreasing pH. Since extremely high or low pHs are generally not found in the environment, and since biotic degradation reactions may become more important than hydrolysis at lower pHs, the rate of hydrolysis of trixylenyl phosphate is assumed to be zero in this assessment. However, in some acidic or alkaline environments, hydrolysis could become significant and so the effect of inclusion of a hydrolysis rate on the risk assessment is considered in Annex C.

No information is available on the rate of photolysis of trixylenyl phosphate in the environment, and so for the purposes of this report the rate is assumed to be zero.

Atmospheric photooxidation of trixylenyl phosphate is predicted to occur with a half-life of around eight hours. This reaction will be taken into account in the risk assessment.

In summary, the abiotic rate constants and half-lives assumed in the assessment are as follows, and the importance of hydrolysis to the overall conclusions of the risk assessment is considered further in Annex C.

Hydrolysis	$khydr_{water}$ = 0 d^{-1}	half-life = infinite
Photolysis	$kphoto_{water}$ = 0 d^{-1}	half-life = infinite
Atmospheric photooxidation	k_{OH} = 4.7×10^{-11} cm^3/molecule s	half-life = 8.2 h

Biodegradation

The most likely pathway for biodegradation of aryl phosphates is initial hydrolysis of the phosphate ester to form orthophosphate and corresponding phenolic compounds or alcohols, which then themselves undergo further biodegradation (Saeger *et al.* 1979).

Biodegradation data on trixylenyl phosphate are consistent with it being inherently biodegradable. The recommended biodegradation half-lives for surface water, soil and sediment from the TGD are summarised below (inherently biodegradable (not clear if the specific criteria are fulfilled[9]), Kp_{soil} = 170 l/kg).

Sewage treatment plant	$k = 0$ h^{-1}	half-life = infinite
Surface water	$k = 0$ h^{-1}	half-life = infinite
Sediment	$k = 2.3 \times 10^{-4}$ d^{-1}	half-life = 3,000 days
Soil	$k = 2.3 \times 10^{-4}$ d^{-1}	half-life = 3,000 days

For sediment, the TGD recommends that the default rate constant should be ten times lower than that for soil to reflect the fact that the deeper sediment layers are anaerobic (this calculation assumes that degradation under anaerobic conditions does not occur). However, the available information for some other triaryl phosphates (for example, see the risk evaluation report for triphenyl phosphate in this series) suggests that these substances may also be degraded under anaerobic conditions at a similar rate to aerobic conditions. Therefore, for this assessment, it is assumed that the degradation rate constant (and hence half-life) in sediment is the same as in soil.

Although the phenolic part of the triaryl phosphate will undergo mineralisation, orthophosphate/phosphoric acid will also be produced as a result of the degradation. The fate, behaviour and effects of this substance are beyond the scope of this assessment.

3.1.2   Environmental partitioning

Adsorption

No measured K_{oc} values are available for trixylenyl phosphate.

A K_{oc} value of 1.0×10^5 l/kg can be estimated for trixylenyl phosphate from its structure using the Syracuse Research Corporation PCKOC version 1.63 software, which employs a molecular connectivity index method.

Chapter 4 of the TGD recommends the following equation for estimating K_{oc} from log K_{ow} for phosphates:

$$\log K_{oc} = 0.49 \log K_{ow} + 1.17$$

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[9]Criteria given in the TGD are: a) elimination can be ascribed to biodegradation; b) no recalcitrant metabolites are formed; c) adaptation time is limited. These criteria relate to the interpretation of standard inherent biodegradation tests. For trixylenyl phosphate, there are no such tests and so it is difficult to relate these criteria directly to the test results. However, the following points should be considered. From OECD 301F and the test based on the modified Sturm method, it is clear that over 60% degradation was reached only after extended periods (up to 68 days) and so it is difficult to argue that the limit adaptation criterion is met. In addition, there is some uncertainty in the extent of removal in the Boethling and Cooper (1985) study using an industrial treatment plant and actual removal could be lower than the 89% quoted. Removal in the SCAS test (65% at a concentration of 3 mg/l and 13% at 13 mg/l) was relatively low, particularly at the higher concentration. Therefore, the rate constants chosen here assume that the substance is inherently biodegradable but that the criteria are not met.

Using this equation for trixylenyl phosphate (log K_{ow} of 5.63) results in an estimated K_{oc} of 8,486 l/kg. Since this value is obtained using the method recommended in the TGD, it is used in the risk assessment. The resulting partition coefficients for soils and sediments calculated using the methods given in the TGD are shown below.

K_{oc}	8,486 l/kg		
Kp_{susp}	849 l/kg	$K_{susp\text{-}water}$	213 m^3/m^3
Kp_{sed}	424 l/kg	$K_{sed\text{-}water}$	213 m^3/m^3
Kp_{soil}	170 l/kg	$K_{soil\text{-}water}$	255 m^3/m^3

These values are used in the risk assessment.

Volatilisation

No studies are available on the volatilisation of trixylenyl phosphate from water. The Henry's law constant estimated for trixylenyl phosphate is 0.004 Pa m^3/mol at 20°C. This indicates that volatilisation from water is likely to be limited.

Fugacity modelling

The potential environmental distribution of trixylenyl phosphate has been studied using a generic level III fugacity model. The model used was a four-compartment model (EQC version 1.01, May 1997) that has been circulated for use within the Organisation for Economic Cooperation and Development (OECD) High Production Volume (HPV) programme. The model was run four times with a nominal release rate of 1,000 kg/hour initially entering the air, soil or water compartments in different proportions. The physico-chemical properties used and the results of the modelling exercise are shown in Table 3.1.

The results of the model show that only a small amount of trixylenyl phosphate released to the environment will be in the air compartment at steady state. When the substance is released to air it distributes mainly to the soil compartment, presumably by atmospheric deposition. When it is released to soil, the substance generally remains in soil, with only a small fraction distributing to the water and sediment compartment. When released to water, the substance is likely to distribute mainly to the sediment phase at steady state, but a small fraction is also predicted to remain in water.

Table 3.1   Results of generic level III fugacity model for trixylenyl phosphate

Input data	Value
Vapour pressure	8.7×10^{-6} Pa at 20°C
Water solubility	0.89 mg/l
Henry's law constant	0.004 at 20°C
Log Kow	5.63
Atmospheric half-life	8.2 hours
Half-life in water	infinite
Half-life in soil and sediment	3,000 days

Emission rate	Model results at steady state				
	Amount in air	Amount in soil	Amount in water	Amount in sediment	Overall residence time/ persistence
1,000 kg/hour to air 1,000 kg/hour to soil 1,000 kg/hour to water	5.7×10^{-3}%	90.0%	0.47%	9.5%	1,938 days
1,000 kg/hour to air 0 kg/hour to soil 0 kg/hour to water	0.033%	98.3%	0.077%	1.57%	993 days
0 kg/hour to air 1,000 kg/hour to soil 0 kg/hour to water	4.2×10^{-6}%	99.8%	9.9×10^{-3}%	0.20%	4,266 days
0 kg/hour to air 0 kg/hour to soil 1,000 kg/hour to water	1.2×10^{-5}%	0.034%	4.67%	95.3%	556 days

The behaviour of trixylenyl phosphate during waste water treatment was estimated using the EUSES model. Using a degradation rate constant of 0.3 h^{-1} (see Section 3.1.1), a K$_{oc}$ of 8,486 l/kg (see above) and a vapour pressure of 8.7×10^{-6} Pa at 20°C (see Section 1.3.5), the following behaviour is predicted.

Degraded	0%
Adsorbed to sludge	49.4%
Volatilised to air	3.7×10^{-3}%
To effluent	50.6%

These values are used in predicted environmental concentration (PEC) calculations.

3.1.3   Bioaccumulation and metabolism

Measured data

Uptake from water

The bioconcentration of a commercial triaryl phosphate product in bleak (*Alburnus alburnus*) was investigated (Bengtsson *et al.* 1986). The product tested contained triphenyl phosphate, cresyl diphenyl phosphate (two main components), tricresyl phosphate (three main components) and trixylenyl phosphate (three main components). The tests were carried out using a flow-though system with natural brackish water (7‰ salinity) at 10°C. The fish used in the test had an average weight of five grams (53 fish were used in 60 litres of water) and were fed twice daily (once daily

at weekends) with a 0.25 g portion of commercial food. The pH of the water was 7.6 to 7.9 and the dissolved oxygen concentration remained above 90 per cent of saturation throughout the study. The experiment consisted of a 14-day uptake period where the fish were exposed to a nominal concentration of 50 μg/l of the triaryl phosphate product, followed by a 14-day depuration period in clean flowing water. Samples of both fish (three fish per sample time except at day 14 and 28 where five groups of three fish were sampled) and water were analysed for the concentrations of the main components (as determined by gas chromatographic analysis) of the triaryl phosphate product on days zero, one, two, four, seven, 14, 17, 18, 21 and 28 of the experiment. No mortality or evidence for abnormal behaviour was seen in the fish during the experiment. Steady state was reached within the 14-day exposure period (steady state was actually attained within two days) for triphenyl phosphate, the cresyl diphenyl phosphate components and two of the tricresyl phosphate components of the mixture. Steady-state bioconcentration factors (BCFs) were determined as 400 l/kg, 100-220 l/kg and 800 l/kg for these components respectively. For the other components, steady state was approached, but had not been reached by the end of the 14-day uptake period and the non-steady state BCFs estimated at 14 days were 400 l/kg for the remaining tricresyl phosphate component and 1,300-1,900 l/kg for the three trixylenyl phosphate components. All components were found to be rapidly eliminated from the fish, with a depuration half-life of four days or less. Triphenyl phosphate, cresyl diphenyl phosphate and tricresyl phosphate components were almost completely eliminated from the fish within 14 days but the trixylenyl phosphate components were still evident in the fish after 14 days.

Uptake from food

A long-term dietary accumulation study with a commercial triaryl phosphate product was carried out with minnows (*Phoxinus phoxinus*) (Bengtsson *et al.* 1986). The substance tested contained triphenyl phosphate, cresyl diphenyl phosphate (two main components), tricresyl phosphate (three main components) and trixylenyl phosphate (three main components). The test was carried out using a flow-through system with six groups of 30 fish (average body weight 1.9 g), each in 50 litres of natural brackish water (7‰ salinity). The test was started in January and was carried out for 163 days (although the resulting concentrations in fish were determined after four months only) and the water temperature followed the natural seasonal fluctuations (3.6-4.5°C from January to April, 7°C by the end of April, 13°C by the end of May and 12.to 15°C from June until the end of the experiment). The dissolved oxygen concentration in the test was always above 90 per cent of saturation and the pH of the water was 7.7 to 8.0. Five concentrations of the test substance were used (100, 300, 1,000, 3,000 and 10,000 mg/kg food) and a control using uncontaminated food was run. The test used a commercial fish food which was spiked by adding the triaryl phosphate as a solution in acetone and evaporating off the solvent. The fish were given two 0.25 g portions of food per day. The total amount of food given to the fish by four months of the experiment was two grams per fish. No mortalities or abnormal behaviour were seen in any of the fish, and all food given to the fish was eaten. The concentrations of the various components in the fish after four months exposure are shown in Table 3.2.

Overall, only around 0.017-0.14 per cent of the total amount of test substance fed to fish was found to be present in the fish at the end of the study. The bioaccumulation factors, based on the estimated concentration in fish and concentration in food, are all very much less than one.

Table 3.2   Concentrations in minnows after four months exposure to contaminated food

Food concentration	Total concentration in fish (mg/kg fresh weight)			
	Cresyl diphenyl phosphate (sum of two components)	Tricresyl phosphate (sum of three components)	Trixylenyl phosphate (sum of three components)	Triphenyl phosphate
Control	0.005	Not detected	0.005	Not detected
100 mg/kg	0.030	0.023	0.053	0.094
300 mg/kg	0.020	0.016	0.085	0.47
1,000 mg/kg	0.225	0.019	0.225	0.896
3,000 mg/kg	0.12	0.016	0.88	2.01
10,000 mg/kg	0.73	0.043	1.39	2.05

Calculated data

For the terrestrial food chain, the TGD requires a BCF for earthworms. No experimental data are available for this endpoint and so an earthworm BCF is estimated using the following equation given in the TGD:

$$BCF_{earthworm} = 0.84 + 0.012 \, K_{ow}/RHO_{earthworm}$$

where $RHO_{earthworm}$ = density of the earthworm = 1 kg/l
              K_{ow} = octanol-water partition coefficient

Using a log K_{ow} of 5.63 and the methods given in the TGD, the $BCF_{earthworm}$ is estimated to be 5,120 l/kg. This value is used in the assessment, though its reliability is unknown.

Summary of accumulation

One study looked at the bioconcentration of trixylenyl phosphate from a commercial product in a brackish water fish. The BCF in this study was of the order of 1,300-1,900 l/kg; steady state was approached, but had not been reached by the end of the study.

The log K_{ow} for trixylenyl phosphate is 5.63. Using the methods recommended in the TGD, a BCF for fish of 12,176 can be estimated. This method clearly overestimates the actual BCF for this substance.

Annex B considers the available data for all triaryl phosphate esters and, based on a read-across of these data, the BCF for trixylenyl phosphate would be expected to be around 1,240 l/kg. This is consistent with the data available for triaryl phosphates as a whole and also the measured data obtained for trixylenyl phosphate.

A BCF of around 1,900 l/kg is used in the assessment for trixylenyl phosphate. This value represents the upper limit of the available experimental data and is used here as a "reasonable worst case" approach.

In addition to a BCF, the revised TGD also requires a biomagnification factor (BMF) to be taken into account. For trixylenyl phosphate, the default BMF would be one (BCF around 1,900 l/kg). This is consistent with the available feeding study data that showed bioaccumulation from food was low.

Using a log K_{ow} value of 5.63, the $BCF_{earthworm}$ is estimated to be 5,120 l/kg.

3.2   Environmental releases

3.2.1   General discussion

Releases from the production and use of trixylenyl phosphate were estimated using a number of sources such as the default methods from the TGD and the Emission Scenario Document (ESD) on lubricants (OECD 2004). In the absence of specific information on the substance, the ESD is considered to be a reasonable basis for emission estimation; the TGD default values are intended for use as realistic worst case values in the absence of other data. Hence the estimates from these sources will have some degree of uncertainty. The actual calculations are considered confidential as they are based on confidential production and use figures.

The producers of trixylenyl phosphate provided information on the amounts used by representative large customers, and this was used in the local estimates of emissions from use.

3.2.2   Releases from production

Releases from production sites were estimated from specific information provided by the producing companies. The results are included in Table 3.3.

3.2.3   Releases from use (processing)

Emissions from the use of the substance in power generation fluids (from the blending step) were estimated using the methods outlined in the ESD on lubricants (OECD 2004). Estimated emissions to air from lubricant blending are low. Emission factors for releases to water from blending are 5.9×10^{-4} kg/tonne lubricant for use as a base fluid.

3.2.4   Releases over lifetime of products

Trixylenyl phosphate is used in products that are expected to have extended service lives (more than one year), and so these might be a source of emission to the environment. However, information from the industry relating to the use of power generation fluids indicates that losses from the use of these fluids are negligible.

3.2.5   Summary of environmental releases

Estimated environmental releases of trixylenyl phosphate are summarised in Table 3.3.

Table 3.3   Summary of estimated environmental release of trixylenyl phosphate

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	Water	Soil	Air	Water[a]	Soil	Air	Water[a]	Soil
Production			3.5			1,040 to surface water[b]				
Power generation fluids	Blending	0.018	2.78×10^{-3}		0.47	0.07		3.24	0.5	
	Use	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible
Total					0.47	1,040		3.24	0.5	

Notes: a) Regional and continental emissions to water are split 80:20 between waste water treatment and direct discharge to surface water, except where noted.

b) Emissions calculated from site-specific data, after waste water treatment (sludges from production sites are incinerated, calculating the values after treatment allows this to be reflected in the emission estimates).

3.3 Environmental concentrations

3.3.1 Aquatic environment (surface water, sediment and wastewater treatment plant)

Calculation of PECs

PECs for surface water and sediment were estimated with the EUSES 2.0.3 program using the data summarised in the previous sections as input. The concentrations predicted for surface water and sediment are shown in Table 3.4.

Table 3.4 Summary of predicted local concentrations for the aquatic compartment

Scenario		PEC$_{local}$			
		Microorganisms in sewage treatment plant (mg/l)	Surface water - emission episode (μg/l)	Surface water - annual average (μg/l)	Sediment (mg/kg wet wt.)
Production of trixylenyl phosphate		0.04	1.06	0.88	0.2
Power generation fluid	Lubricant blending	0.70	0.09	0.08	0.02
	Use of fluid	negligible	negligible	negligible	negligible

The predicted regional concentrations are 0.02 μg/l for surface water and 6.88×10^{-3} mg/kg wet weight for sediment.

Predicted concentrations were also calculated for the marine environment using the EUSES program. These are included in Table 3.5. Note that production is not included in the table as the production sites do not discharge into the marine environment.

Table 3.5 Summary of predicted concentrations for the marine environment

Scenario		PEC$_{local}$		
		Marine water - emission episode (μg/l)	Marine water - annual average (μg/l)	Marine sediment (mg/kg wet wt.)
Power generation fluid	Lubricant blending	0.02	0.01	2.9×10^{-3}
	Use of fluid	negligible	negligible	negligible

Measured levels in water and sediment

Water

Trixylenyl phosphate was monitored in England and Wales over the period November 2007 to April 2008 as part of the Environment Agency's Targeted Risk Based Monitoring (TRBM) initiative. Six samples were collected at approximately weekly intervals from 15 paired WWTP effluent/receiving water sites across all eight Environment Agency Regions. The site selection criteria are not specified – it is likely that most were reasonably large WWTP with mixed industrial/household influent. One WWTP (Davyhulme) collects wastewater from an industrial complex that is known to include a production site.

The limit of detection was 0.062 µg/l. The substance was detected on a few occasions, as indicated in Table 3.6.

Table 3.6   Positive detections of trixylenyl phosphate associated with WWTP in England and Wales during 2007/8

Sampling location	EA Region	Date of sampling	Measured concentration, µg/l
Non-tidal River Trent at Gunthorpe	Midlands	19/1/08	0.107
Huddersfield WWTP	North east	22/1/08	0.141
River Calder at Mirfield	North east	22/1/08	0.0871
		14/2/08	0.125
Davyhulme WWTP	North west	27/11/07	0.331
		6/12/07	4.31
		11/12/07	1.05
		18/12/07	0.975
		22/1/08	0.626
		1/2/08	1.21
Manchester Ship Canal	North west	27/11/07	0.198
		6/12/07	0.26
		12/12/07	0.375
		7/1/08	2.26
		21/1/08	2.82
		5/2/08	0.671
Great Stour	Southern	22/11/07	1.48

Data from other countries

A survey of the levels of trixylenyl phosphate in surface waters from all over Japan was carried out by Environment Agency Japan (1996). The substance was not detected in 63 samples analysed in 1981 (detection limit was 0.2 µg/l).

Boethling and Cooper (1985) reported the results of an early 1980s survey of the levels of trixylenyl phosphate in surface water in the United States. The substance was not found (detection limit of the method was 0.5 µg/l) in four samples from Saginaw River (industrialised area), four samples from Baltimore Harbour (industrialised area), three samples from Detroit River (industrialised area), four samples from Delaware River (industrialised area near to aryl phosphate manufacturer), seven samples from

Kanawha River (industrialised area near to aryl phosphate manufacturer) and four samples from Eastern Lake Superior (remote area).

Sediment

No European monitoring data have been located.

Boethling and Cooper (1985) report the results of monitoring studies carried out in the late 1970s near to an aryl phosphate production site in the United States. The substances included in the studies were triphenyl phosphate, tricresyl phosphate, isopropylphenyl diphenyl phosphate and aryl phosphates with molecular weights above 410 (which included trixylenyl phosphate and di-(isopropylphenyl) phenyl phosphate). The concentration of total aryl phosphates found in the sediment was 229 mg/kg at the outfall and 4.4 mg/kg at a location eight miles downstream from the outfall. A further twelve sediment samples were also analysed and were found to contain total aryl phosphate concentrations of 0.07 to 1,032 mg/kg. As a result of these findings, a more comprehensive survey was undertaken. This found total aryl phosphate concentrations of seven to 6,320 mg/kg at locations less than 100 yards downstream of the plant. Levels further downstream were much lower than these, but concentrations above 1 mg/kg were found in some samples ten miles downstream. The report states that the actual concentration in sediments could have been much higher than indicated by these data, as the analytical recovery from spiked sediment was around six per cent. The mixed aryl phosphates with molecular weights above 452 were thought to be present at the highest concentrations and triphenyl phosphate was thought to be present at the lowest concentrations in these samples.

Boethling and Cooper (1985) reported the results of a later (early 1980s) survey of the levels of trixylenyl phosphate in sediments from the United States. Trixylenyl phosphate was found at 0.38-0.4 mg/kg in three out of four samples from Saginaw River (industrialised area), at 0.18-0.9 mg/kg in three samples from Baltimore Harbour (industrialised area), at below 0.24 mg/kg in two samples from Detroit River (industrialised area), at 0.16 mg/kg in one of two samples from Delaware River (industrialised area near to aryl phosphate manufacturer), at under 0.9 mg/kg in one out of six samples from Kanawha River (industrialised area near to aryl phosphate manufacturer) and at 0.15 in one of two samples from Eastern Lake Superior (remote area). The detection limit of the method was in the range 0.03-0.2 mg/kg but some interferences occurred in some samples, making determination of the precise concentration of trixylenyl phosphate difficult.

Hoke *et al.* (1993) determined the levels of trixylenyl phosphate in sediment from the Grand Calumet River, Indiana (industrialised area). In all, ten composite sediment samples were collected during 1988-1990 and trixylenyl phosphate was not detected (detection limit 0.01 mg/kg dry weight) in any of the samples.

A survey of the levels of trixylenyl phosphate in sediments from all over Japan was carried out by Environment Agency Japan (1996). The substance was detected in 13 out of 63 samples analysed in 1981 at a concentration of 0.07 to 3.7 mg/kg dry weight (the detection limit was 0.050 mg/kg dry weight).

Comparison of measured levels with predicted levels

There are insufficient monitoring data to compare with predicted concentrations in surface water. Trixylenyl phosphate was detected on all six sampling occasions in the Manchester Ship Canal (in the range 0.198 to 2.82 µg/l). These could be linked to the

production site, but there might be other local sources too. The monitoring data are of a similar order of magnitude to the local freshwater PEC for production (1.06 µg/l).

Trixylenyl phosphate has also been detected in rivers in three other English regions (once or twice out of six samples, between 0.087 and 1.48 µg/l). This is presumably linked to local industrial activity, although no further investigations have taken place to identify the source(s). In two cases there were no positive detections in the associated WWTP effluent, which suggests that the emissions occurred upstream. The reasonable worst case PEC for the blending of power generation fluid is 0.09 µg/l, whilst regional background concentrations are expected to be around 0.02 µg/l. The monitoring data suggest that these PECs may not be unrealistic.

For sediment, concentrations of trixylenyl phosphate up to 3.7 mg/kg dry weight were determined in a Japanese sample collected in 1981. This concentration is higher than predicted concentrations but the actual source of trixylenyl phosphate related to this sample is unknown and could relate to historic emissions or uses not considered in this assessment. The other monitoring data generally show levels of trixylenyl phosphate lower than this value and more in line with the concentrations predicted in this assessment.

The predicted concentrations are used in the risk characterisation.

3.3.2   Terrestrial compartment

Calculation of PECs

PECs for the soil compartment were estimated using EUSES 2.0.3 and are summarised in Table 3.7.

Table 3.7   Summary of predicted local concentrations for the terrestrial compartment

Scenario		PEC_{local}			
		Annual average conc. in air (mg/m^3)	Agricultural soil – 30 day average (mg/kg wet wt.)	Agricultural soil – 180 day average (mg/kg wet wt.)	Groundwater under agricultural soil (µg/l)
Production of trixylenyl phosphate		2.96×10^{-8}	8.99×10^{-6a}	9.07×10^{-6a}	6.05×10^{-5a}
Power generation fluid	Lubricant blending	4.14×10^{-6}	0.02	0.02	0.12
	Use of fluid	negligible	negligible	negligible	negligible

Notes: a) Sewage sludge from the production site is not applied to land.

The estimated regional concentrations for the soil compartment are summarised below.

$PEC_{regional}$ = 5.48×10^{-4} mg/kg wet weight. for agricultural soil

= 3.65×10^{-3} µg/l for pore water of agricultural soil

= 2.19×10^{-6} mg/kg wet weight for natural soil

= 2.19×10^{-6} mg/kg wet weight for industrial soil

Measured levels

Boethling and Cooper (1985) report the results of monitoring studies carried out in the late 1970s near to an aryl phosphate production site in the United States. The substances included in the studies were triphenyl phosphate, tricresyl phosphate, isopropylphenyl diphenyl phosphate and aryl phosphates with molecular weights above 410 (which included trixylenyl phosphate and di-(isopropylphenyl) phenyl phosphate. The concentration of total aryl phosphates found in a soil sample collected from the plant yard was 26,550 mg/kg. This sample was collected in an area subject to frequent spills. The total aryl phosphate concentration found in river bank soil (collected from an area known to have received discarded soil from the plant yard) was 37 mg/kg.

Comparison of measured levels with predicted levels

There are insufficient data to compare with predicted concentrations. The available monitoring data refer to spillage whereas the main route to soil assumed in predicted levels is from spreading of sewage sludge. The predicted concentrations are used in the risk characterisation.

3.3.3 Air compartment

Calculation of PECs

Concentrations of trixylenyl phosphate in air were estimated using EUSES 2.0.3. The PECs calculated are summarised in Table 3.7.

The predicted regional concentration in air is 1.11×10^{-10} mg/m^3.

As no measured data are available on the actual levels of trixylenyl phospahte in air, the predicted concentrations are used in the risk characterisation.

3.3.4 Non-compartment specific exposure relevant for the food chain

Predicted concentrations in biota and food

Predicted concentrations of trixylenyl phosphate in fish and earthworms are shown in Table 3.8 and predicted concentrations in food for human consumption are shown in Table 3.9. The concentrations were calculated using EUSES 2.0.3.

Table 3.8   Summary of predicted local concentrations for secondary poisoning

Scenario		Predicted concentration			
		Fish (mg/kg)	Earthworms (mg/kg)	Marine fish[b] (mg/kg)	Marine top[b] predators (mg/kg)
Production of trixylenyl phosphate		0.85	8.57×10^{-3a}	n/a	n/a
Power generation fluid	Lubricant blending	0.09	0.29	0.01	5.85×10^{-3}
	Use of fluid	negligible	negligible	negligible	negligible

Notes: a) Sewage sludge from the production site is not applied to land.
b) No production emissions to marine waters.

Measured levels in biota and food

Lombardo and Egry (1979) found trixylenyl phosphate at a concentration of 80 µg/kg in sturgeon from the Columbia River, USA, from an area downstream of several metal processing plants.

Gilbert *et al.* (1986) carried out a survey of the levels of total trialkyl and triaryl phosphates, including trixylenyl phosphate, in composite total diet samples (covering 15 commodity food types) representing an average adult diet for eight regions of the United Kingdom. The mean total dietary intake of total organic phosphates was estimated to be 0.072-0.105 mg/day. In general, the highest concentrations of total phosphate esters (total triaryl and trialkyl) were in offal and nuts (these food groups have only a low relative importance in the diet). Trixylenyl phosphate was found to occur in only minor amounts in isolated samples.

Comparison of measured levels with predicted levels

The available monitoring data for trixylenyl phosphate are limited in their coverage. The substance has been found in fish near sources of release and in small amounts in some food samples.

The predicted concentrations are used in the risk characterisation.

Table 3.9   Summary of predicted local concentrations in food for human consumption

Scenario		Concentration							
		Fish (mg/kg)	Root crops (mg/kg)	Leaf crops (mg/kg)	Drinking water (mg/l)	Meat (mg/kg)	Milk (mg/kg)	Air (mg/m^3)	Total daily human intake (mg/kg bw/day)
Production of trixylenyl phosphate		1.66	1.93×10^{-4}	2.84×10^{-5}	2.19×10^{-4}	1.5×10^{-4}	4.74×10^{-5}	2.9×10^{-8}	2.74×10^{-3}
Power generation fluid	Lubricant blending	0.15	0.39	4.1×10^{-3}	1.2×10^{-4}	3.0×10^{-3}	9.6×10^{-4}	4.1×10^{-6}	2.48×10^{-3}
	Use of fluid	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible
Regional sources		0.04	0.01	2.9×10^{-6}	5.0×10^{-6}	7.8×10^{-6}	2.5×10^{-6}	1.1×10^{-10}	1.26×10^{-4}

4 Effects assessment: Hazard identification and dose (concentration) – response (effect) assessment

4.1 Aquatic compartment

The following sections review the available toxicity data for trixylenyl phosphate with aquatic organisms. Where possible, a validity marking is given for each study (this appears in the summary tables within each section). The following validity markings have been used:

1. **Valid without restriction.** The test is carried out to internationally recognised protocols (or equivalent protocols) and all or most of the important experimental details are available.

2. **Use with care.** The test is carried out to internationally recognised protocols (or equivalent protocols) but some important experimental details are missing, or the method used, or endpoint studied, in the test means that interpretation of the results is not straightforward.

3. **Not valid.** There is a clear deficiency in the test that means the results cannot be considered valid.

4. **Not assignable.** Insufficient detail is available on the method used to allow a decision to be made on the validity of the study.

In terms of the risk assessment, toxicity data assigned a validity marking of one or two are considered of acceptable quality when deriving the predicted no effect concentration (PNEC).

One important property when considering the aquatic toxicity data is water solubility. The water solubility of trixylenyl phosphate is 0.89 mg/l. Some studies have been carried out at concentrations greater than this water solubility and, although this in itself does not necessarily invalidate the test (for example, co-solvents or solubility aids could have been used in the test to aid dispersion of the substance in the test media), this does introduce some uncertainty over the concentration to which the organisms were actually exposed in the test.

A further consideration in interpreting the results for trixylenyl phosphate is that the commercial product is an isomeric mixture of phosphate esters, where the composition of the product may vary between manufacturers. Small amounts of triphenyl phosphate and other aryl phosphates may also be present in (older) commercial products tested.

4.1.1 Toxicity to fish

Short-term studies

The results of short-term toxicity tests with freshwater fish are given in Table 4.1[10].

A flow-through acute toxicity study with rainbow trout (*Oncorhynchus mykiss*) was carried out with a commercial trixylenyl phosphate (Union Carbide 1979). In the study, groups of ten rainbow trout were exposed to a range of five trixylenyl phosphate concentrations for 96 hours. The tank volume and flow-rate used in the test was 180 litres and 24 litres per hour respectively. No fish died during the study and the 96-hour LC_{50} was determined to be above 100 mg/l based on nominal concentrations. Concentrations in this study (6.3 to 100 mg/l) were well above the water solubility of the substance tested, and the test report indicates that oily droplets were formed on the water surface at all concentrations tested. In addition, the biological loading in this study was 8.3 g/l, which is higher than recommended in the current OECD test guidelines (this higher loading will, however, have been partly offset by the use of a flow-through system, and the dissolved oxygen concentration was maintained throughout the test by gentle aeration). The results of this test are best interpreted as the substance showing no toxic effects at its limit of solubility in the test media.

A fish 96-hour LC_{50} and a 14-day LC_{50} of 0.71 and 0.38 mg/l respectively can be estimated for trixylenyl phosphate using the US EPA ECOSAR (version 0.99h) software (the program used the selected log K_{ow} of 5.63 in the calculations).

Using the methods given in the TGD, a 96-hour LC_{50} of 0.22 mg/l can be estimated using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.63.

No data are available on the short-term toxicity of trixylenyl phosphate to marine fish.

Long-term studies

No data are available on the long-term toxicity of trixylenyl phosphate to freshwater or marine fish. The USEPA ECOSAR program estimates a long-term no effect concentration of 0.024 mg/l for fish.

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[10] Further acute toxicity testing with fish for this substance is being carried out under the US HPV programme. Preliminary results indicate that the 96-hour LC_{50} for fathead minnows (*Pimephales promelas*) is above 1.12 mg/l based on measured concentrations using a flow-through system. The results from this test also appear to show no effects at solubility.

Table 4.1   Short-term toxicity of trixylenyl phosphate to freshwater fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Oncorhynchus mykiss	USEPA 1975	One replicate of 10 fish in 180 l, the loading was 8.3 g/l	149 g	Acetone	6.3, 12.5, 25, 50 and 100 plus control (no solvent control was run)	N	Well water	10°C	222	7.5	Flow	8.3-10	Mortality	0% Mortality	96h-LC$_{50}$ >100 mg/l	IUCLID 2001	2

Notes: N = Nominal concentration.
M = Measured concentration.
Temp. = Temperature.
Hard. = Water hardness as mg CaCO$_3$/l.
D.O. = Dissolved oxygen (given as mg O$_2$/l or per cent saturation).
Val. = Validity rating (see Section 4.1): 1) Valid without restriction; 2) Use with care; 3) Not valid; 4) Not assignable.

4.1.2 Toxicity to aquatic invertebrates

Short-term studies

No data are available on the short-term toxicity of trixylenyl phosphate to freshwater invertebrates[11].

Using the methods given in the TGD, a 48-hour EC_{50} of 0.47 mg/l can be estimated for *Daphnia magna* using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.63. The USEPA ECOSAR program (v0.99h) estimates a value of 0.16 mg/l for the same endpoint.

The acute toxicity of trixylenyl phosphate (no information on purity) to the brackish water harpacticoid copepod *Nitocra spinipes* was determined by Bengtsson and Tarkpea (1983) (results are summarised in Table 4.2). The 96-hour LC_{50} was reported to be 1.9 mg/l. The method used was reported to be the same as that used by Lindén *et al.* (1979). Few other details of the specific test for trixylenyl phosphate were reported. This value is close to, but above, the water solubility of trixylenyl phosphate assumed for this assessment.

Long-term studies

No long-term toxicity data for trixylenyl phosphate are available for freshwater or marine invertebrates.

4.1.3 Toxicity to algae

The results of toxicity tests with freshwater algae are summarised in Table 4.3[12].

Wong and Chau (1984) investigated the toxicity of trixylenyl phosphate (no information on purity) to algae. The experiments investigated the effects on the primary production (as measured by ^{14}C-uptake from ^{14}C-carbonate) in cultures of *Ankistrodesmus falcatus* over a four-hour period. The tests were carried out by inoculating 13.9 ml of growth medium with one ml of algal cell culture (7×10^5 cells per ml giving an initial inoculum concentration of 4.7×10^4 cells per ml in the test solution; algal cells were in the logarithmic growth phase) and incubating for 24 hours with the test substance. The substance was added as a solution in acetone (final acetone concentration in the test solution was under 0.05 per cent and an acetone control was also run at this concentration).

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[11] Further acute toxicity testing with *Daphnia magna* is being carried out under the US HPV programme. Preliminary results indicate that the 48-hour EC_{50} is 0.06 mg/l based on measured concentrations using a semi-static method. This value is lower than the predicted value.

[12] Further toxicity testing with freshwater algae is being carried out under the US HPV programme. Preliminary results indicate that the 96-hour EC_{50} for *Selenastrum capricornutum* (now *Pseudokirchneriella subcapitata*) is above 1.01 mg/l based on biomass. The 96-hour NOEC is 0.112 mg/l for biomass. The results are based on initial measured concentrations (at 82-101% of the nominal); by the end, concentrations had fallen to 51-62% of the nominal.

Table 4.2   Short-term toxicity of trixylenyl phosphate to marine invertebrates

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. tested	N or M	Media	Temp.	Sal.	pH	Static/ flow	D.O.	Endpoint	Control resp.	Effect conc.	Ref.	Val.
Nitocra spinipes	Lindén *et al.* 1979	Two replicates of 10 per treatment, in 10 ml solution	3-6 week old	Acetone may have been used at 500 μl/l.	Six concs. plus control.	N	Natural brackish seawater	20-22°C	7‰	7.8	Static		Mortality		96h-LC_{50} = 1.9 mg/l	Bengt-sson and Tarkpea 1983	2

Notes:
N = Nominal concentration.
M = Measured concentration.
Temp. = Temperature.
Sal. = Water salinity (given as parts per thousand (‰)).
D.O. = Dissolved oxygen (given as mg O_2/l or per cent saturation).
Val. = Validity rating (see Section 4.1): 1) Valid without restriction; 2) Use with care; 3) Not valid; 4) Not assignable.

Table 4.3   Toxicity of trixylenyl phosphate to freshwater algae

Species	Test guide-line	Initial inoculum conc.	Co-solvent	Concs. tested	N or M	Test conditions				Endpoint	Control response	Effect concentration	Reference	Val.
						Media	Temp.	Hard.	pH					
Ankistrodesmus falcatus		4.7×10^4 cells/ml	Acetone at $\leq0.05\%$.	Solvent control and dark control run.	N	CHU-10 medium	20°C			Primary production (uptake of ^{14}C)	Uptake in dark control was <5% of total seen in solvent control.	4h-$IC_{50} \geq 5$ mg/l	Wong and Chau 1984	2

Notes:
N = Nominal concentration.
M = Measured concentration.
Temp. = Temperature.
Hard. = Water hardness (given as mg $CaCO_3$/l).
D.O. = Dissolved oxygen (given as mg O_2/l or per cent saturation).
Val. = Validity rating (see Section 4.1): 1) Valid without restriction; 2) Use with care; 3) Not valid; 4) Not assignable.

After the initial 24-hour incubation, 0.1 ml of a sodium ^{14}C-carbonate solution was added and the solution was incubated for a further four hours. At the end of four hours, the amount of radioactivity taken up by the cells (corrected for uptake in dark controls) was determined and the concentration causing a 50 per cent reduction in primary production (IC_{50}) was found to be above 5.0 mg/l for *A. falcatus*. These results are best interpreted as the substance showing little or no effect at its limit of solubility in the test media.

The USEPA ECOSAR program (v0.99.h) estimates a 96-hour EC_{50} of 0.065 mg/l. and a no effect concentration of 0.054 mg/l.

There are no toxicity data for trixylenyl phosphate with marine algae.

4.1.4   Toxicity to microorganisms

Yoshioka *et al.* (1985) determined the toxicity of trixylenyl phosphate (no information on purity) to the protozoan *Tetrahymena pyriformis*. Dimethyl sulphoxide was used as a co-solvent at a concentration below 5,000 mg/l (this solvent did not affect the growth of *T. pyriformis* at a concentration of 10,000 mg/l). The tests were carried out at 30°C in sterile growth medium containing two per cent protease, and a series of concentrations were tested (a factor of 1.8 between each concentration was used). The growth of the organisms over 24 hours was determined (the number of cells present was determined by microscope or Coulter counter). The 24-hour EC_{50} for trixylenyl phosphate was over 160 mg/l based on the growth rate of the organisms. The actual toxicity for trixylenyl phosphate could not be determined due to its low solubility in the test medium (the test appears to have been carried out using a fine dispersion of the test substance rather than a true solution), and so the actual EC_{50} reported in the paper is uncertain. However, the substance probably did not cause effects at its solubility limit in this test.

4.1.5   Toxicity to sediment organisms

No toxicity data are available for trixylenyl phosphate with sediment-dwelling organisms.

4.1.6   Predicted no effect concentration (PNEC) for the aquatic compartment

Surface water

A limited amount of acute toxicity data is available for trixylenyl phosphate. The fish and (non-standard) algal tests show no effects at concentrations up to the water solubility of the substance, whereas a 96-hour EC_{50} of 1.9 mg/l was determined for a marine invertebrate (this concentration is slightly higher than the assumed water solubility of the substance of 0.89 mg/l). Ongoing work indicates that the 48-hour EC_{50} for *Daphnia magna* may be around 0.06 mg/l. No long-term toxicity data are available for trixylenyl phosphate.

The acute toxicity of trixylenyl phosphate is predicted to be in the range 0.22-0.71 mg/l and, by comparison with other triaryl phosphates, effects at concentrations below the water solubility of the substance cannot be ruled out over long-term exposure.

Annex B considers the available toxicity data for all triaryl phosphates and based on a read-across of these data, the expected long-term toxicity of trixylenyl phosphate is outlined below:

- Long-term no observed effect concentration (NOEC) for fish of 0.017 mg/l.
- Long-term NOEC for invertebrates of around 0.007 mg/l.
- Long-term NOEC for algae is likely to be greater than those for fish and invertebrates

The long-term no effect concentrations predicted using ECOSAR are 0.024 mg/l and 0.054 mg/l for fish and algae respectively. No prediction for a long-term no effect concentration for invertebrates is available from this program.

An assessment factor of 1,000 could be applied to the marine invertebrate result, giving a PNEC of 1.9 µg/l. Alternatively, a PNEC of 0.7 µg/l could be derived from the predicted long-term no effect concentration for invertebrates using a factor of 10. Both of these values are considered to be provisional given the lack of reliable data. The lower value is used in the risk characterisation; the effect of using the value derived from the measured result is also considered.

Limited data are available on marine species. All of the available data is used for the freshwater PNEC, and the same approach is used for the marine PNEC. This gives a PNEC of 0.07 µg/l using an assessment factor of 100.

Microorganisms

There is one toxicity result for trixylenyl phosphate for microorganisms. This is a 24-hour EC_{50} of above 160 mg/l for the protozoan *Tetrahymena pyriformis*. The solubility of the test substance was exceeded in this test and so the results are best interpreted in terms of no effects at solubility. According to the TGD, the NOEC from a study with *Tetrahymena pyriformis* can be used directly as the $PNEC_{microorganisms}$, and so the $PNEC_{microorganisms}$ could be taken as 0.89 mg/l (the water solubility of the substance). This approach may overestimate the actual toxicity of the substance to sewage treatment processes since the actual solubility in pure water may not be relevant to the exposure of microorganisms during waste water treatment. In this respect, no significant effects would be seen at 160 mg/l and so this is used as the $PNEC_{microorganisms}$ in the assessment.

Sediment

No sediment toxicity data are available for trixylenyl phosphate. In the absence of data, the equilibrium partitioning method can be used to estimate the PNEC.

$$PNEC_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \times PNEC_{water} \times 1000$$

where $K_{susp-water}$ = suspended sediment-water partition coefficient = 213 m^3/m^3 (see Section 3.1.2).
RHO_{susp} = bulk density of suspended sediment = 1,150 kg/m^3.

Using the indicative concentration of 0.7 µg/l for surface water, the $PNEC_{sed}$ can tentatively be estimated as 0.130 mg/kg wet weight. This value is used in the provisional risk characterisation.

As the log K_{ow} of this substance is above five, the resulting PEC/PNEC ratios should be increased by a factor of 10 according to the TGD, to take into account the possibility of direct ingestion of sediment-bound substance.

The same approach is applied for the marine sediment PNEC, using the marine PNEC to give a value of 0.013 mg/kg wet weight for sediment. As for freshwater, the risk ratios are increased by a factor of ten.

4.2   Terrestrial compartment

No terrestrial toxicity data are suitable for determining a PNEC for trixylenyl phosphate. In the absence of data, the equilibrium partitioning method can be used to estimate the PNEC:

$$PNEC_{soil} = \frac{K_{soil-water}}{RHO_{soil}} \times PNEC_{water} \times 1000$$

where $K_{soil-water}$ = soil-water partition coefficient = 255 m^3/m^3 (see Section 3.1.2).
RHO$_{soil}$ = bulk density of wet soil = 1,700 kg/m^3.

Using the indicative concentration of 0.7 μg/l derived for surface water, the PNEC$_{soil}$ can tentatively be estimated as 0.105 mg/kg wet weight. This value is used in the provisional risk characterisation.

As the log K_{ow} of this substance is above five, according to the TGD, the resulting PEC/PNEC ratios should be increased by a factor of 10 when using this PNEC to take into account the possibility of direct ingestion of sediment-bound substance.

4.3   Atmosphere

No information is available on the toxicity of trixylenyl phosphate to plants and other organisms exposed via air. The low vapour pressure of the substance means that volatilisation to the atmosphere is likely to be limited and the resulting concentrations are likely to be low. The possibility of trixylenyl phosphate contributing to atmospheric effects such as global warming and acid rain is thus likely to be small. In addition, as the substance does not contain halogen atoms, it will not contribute to ozone depletion.

4.4   Mammalian toxicity

4.4.1   Available data

Table 4.4 summarises the limited data included in the IUCLID from 2001 (IUCLID 2001). In a letter dated May 2002 from Akzo Nobel under the US HPV programme (Akzo Nobel 2002), there is a commitment to conduct an OECD TG 422 study to address data gaps for repeated dose, reproductive and developmental toxicity. There is also a commitment to conduct *in vitro* genotoxicity studies. However, the results of this testing have not yet been added to the HPV website. This same letter states: "*A substantial number of aromatic phosphate esters exist and they show very different toxicological properties. Certain of these aryl phosphates are neurotoxic and adversely affect reproduction. Others do not show target organ toxicity. It is thus impossible to use structure-activity relationships to accurately predict the toxicological potential of an*

aryl phosphate. The Sponsor Company believes that trixylenyl phosphate should be independently tested because it consists of a complex mixture of at least 50 isomers and its toxicological properties cannot be predicted from data on other aryl phosphates." Primary references were not consulted here.

4.4.2 NOAEL and Margins of Safety (MOS) for assessment of human exposure via the environment

There are no data for acute inhalation, sensitisation, repeated dose toxicity, *in vitro* chromosomal aberrations, *in vivo* genetic toxicity, carcinogenicity and reproductive toxicity[13]. There are currently insufficient data to derive a repeat dose/long-term no observed adverse effect level (NOAEL) for trixylenyl phosphate.

The potential for acute toxicity following oral and dermal exposure is low. A dose of 20,000 mg/kg bodyweight did not cause any deaths in a group of ten Sprague-Dawley rats (Hazleton Wisconsin 1995, cited in IUCLID 2001). However, neurotoxicity was observed in hens exposed to a single oral dose of 11,350 mg/kg bodyweight trixylenyl phosphate (Stauffer Chemical Company 1980, cited in IUCLID 2001).

It is not possible to identify a suitable NOAEL on which to base an acceptable margin of safety. The mixed component nature of the commercial products means that it may be difficult to identify results which can be considered representative.

4.4.3 PNEC for secondary poisoning

It is not possible to calculate a PNEC for secondary poisoning due to the lack of adequate toxicity data.

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[13] It is understood that an OECD 422 study (repeated dose and reproduction/developmental toxicity screening study) has been conducted but the results are not yet available.

Table 4.4   Summary of key representative toxicological data for trixylenyl phosphate

Endpoint		Study type	Species	Duration of exposure	Data quality	Result/comment	Reference
Acute toxicity	Oral	OECD TG 401	Sprague-Dawley rat	Single dose	Valid without restrictions	LD_{50}>20,000 mg/kg bw	Hazleton Wisconsin 1995 cited IUCLID 2001
	Inhalation	-	-	-	-	No data	-
	Dermal	LD_{50}	New Zealand white rabbit	Single dose	Valid without restrictions	LD_{50}>2,000 mg/kg bw	Stauffer Chemical Company 1984 cited IUCLID 2001
Irritation		Skin and eye irritation	Rabbit	As per guideline	Valid without restrictions	Skin – mildly irritating Eye – mildly irritating	IUCLID 2001
Sensitisation		-	-	-	-	Data gap	-
Repeated dose toxicity		-	-	-	-	Data gap	-
Genetic toxicity *in vitro*	Tests for gene mutations	Two Ames tests	*Salmonella typhimurium*		Not assignable	Negative	IUCLID 2001
	Tests for chromosomal aberrations	-	-	-	-	Data gap	-
Genetic toxicity *in vivo*		-	-	-	-	Data gap	-
Carcinogenicity		-	-	-	-	Data gap	-
Reproductive toxicity		-	-	-	-	Data gap	-
Neurotoxicity		Acute neurotoxicity	White leghorn hen	Single oral gavage dose	Valid without restrictions	LD_{50}>11,350 mg/kg bw neurotoxicity observed after nine days	Stauffer Chemical Company 1980 cited IUCLID 2001

4.5　Hazard classification

4.5.1　Classification for human health

Trixylenyl phosphate is not classified in Annex I of Directive 67/548/EEC. There are insufficient data to propose a classification at present.

4.5.2　Classification for the environment

Trixylenyl phosphate is currently not classified as dangerous to the environment.

The fish bioconcentration factor (BCF) is around 1,900 l/kg and the substance is not readily biodegradable.

Limited data are available on the acute toxicity of trixylenyl phosphate to aquatic organisms. A single fish study showed no effects at concentrations in excess of the substance's water solubility. Similarly, no effects were seen over four hours with algae at concentrations in excess of the water solubility (no standard 72 hour study is available). No acute toxicity data are available for freshwater invertebrates[14], but a 96-hour LC_{50} of 1.9 mg/l was determined for the brackish water copepod *Nitrocra spinipes* (this value is slightly above the water solubility of the test substance assumed for this assessment). Based on this result, the following classification could be considered:

> N:　　　　Dangerous for the environment.
> R51/53:　Toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment.

4.6　PBT assessment

The criteria for persistence (P and vP), bioaccumulation potential (B and vB) and toxicity (T) included in the TGD are shown in Table 4.5.

Table 4.5　Criteria for identification of PBT and vPvB substances

Criterion	PBT criteria	vPvB criteria
P	Half-life above 60 days in marine water or above 40 days in freshwater* or half-life above 180 days in marine sediment or above 120 days in freshwater sediment*	Half-life above 60 days in marine water or freshwater or above 180 days in marine or freshwater sediment
B	BCF above 2,000	BCF above 5,000
T	Chronic NOEC below 0.01 mg/l or classification for certain human health end points, or endocrine-disrupting effects	Not applicable

Notes:　* For the purpose of marine environment risk assessment, half-life data in freshwater and freshwater sediment can be overruled by data obtained under marine conditions.

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[14] Further acute toxicity data are being generated under the US HPV programme. Preliminary results indicated that the 48-hour EC_{50} for *Daphnia magna* is 0.06 mg/l. Based on this result, the proposed classification would be N: R50/53.

Persistence: trixylenyl phosphate is considered to be inherently biodegradable but it is not possible to determine if the specific criteria are met (Section 3.1.3). Hence the substance meets the first stage screening criteria for P and vP.

Bioconcentration: a value of 1,900 l/kg is estimated in Section 3.1.3. Hence the substance narrowly fails to meet the B criterion.

Toxicity: the lowest estimated NOEC value is 0.007 mg/l, which would meet the criterion.

The overall conclusion is that the substance meets two of the criteria on the basis of screening data, and only narrowly misses the third. It is therefore considered to be a candidate for further investigation. Persistence testing to determine a half-life under environmentally relevant conditions should be considered.

5   Risk characterisation

This section identifies the potential risks that trixylenyl phosphate might pose for the freshwater and marine aquatic compartments, terrestrial compartment, air compartment and predatory organisms through secondary poisoning. The risk characterisation is performed by comparing the PECs with the PNECs to derive a risk characterisation ratio (RCR). An RCR of less than one implies that any risk resulting from that level of exposure is acceptable. An RCR above one implies a potential risk, and all such values are highlighted in bold in the following tables. Annex C considers the effect of a faster hydrolysis rate on the overall conclusions.

As discussed in Section 3.1.2, the adsorption potential of the substance (represented by the K_{oc}) is estimated, and this has a significant influence on its predicted partitioning behaviour in the environment. There is some evidence for triphenyl phosphate (see the risk evaluation report of that substance in this series) that the prediction method might underestimate the K_{oc} for this type of substance. A sensitivity analysis has been performed in Annex D, and this shows that a higher K_{oc} value would affect the conclusions, but not necessarily in a straightforward (or especially significant) way. Further testing for sediment sorption coefficient is suggested for triphenyl phosphate, and this could indicate a need for further studies with this substance.

5.1   Freshwater compartment

5.1.1   Surface water

An indicative PNEC for surface water was estimated to be 0.7 μg/l. The resulting worst case risk characterisation ratios are summarised in Table 5.1.

Table 5.1   Summary of risk characterisation ratios for surface water

Scenario		Predicted concentration (μg/l)	Risk characterisation ratio
Production of trixylenyl phosphate		1.06	**1.52**
Power generation fluid	Lubricant blending	0.09	0.13
	Use of fluid	negligible	negligible
Regional sources		0.02	0.03

The PEC/PNEC is above one for production of trixylenyl phosphate. There are also potential risks at the Manchester Ship Canal and the Great Stour near Ashford, based on the results of an initial Environment Agency monitoring survey (see Section 3.3.1). These may require further investigation at the local level. Further monitoring for trixylenyl phosphate is taking place, at one WWTP per Environment Agency region, in both final effluent and associated receiving waters (6 samples at 4 week intervals). The sites are different from those used in the previous monitoring exercise. Sampling is expected to take place from September 2008 until March 2009.

No risk to surface water was identified from the use of trixylenyl phosphate in power generation fluids or from regional sources based on the approach taken.

The sensitivity analysis in Annex C suggests that a faster hydrolysis rate than assumed here would only have a small impact on surface water concentrations.

There is some uncertainty over the PNEC for this endpoint (being based on extrapolated data). The alternative PNEC derived from the one aquatic test result available is 1.9 µg/l. This PNEC would show no risks in any of the life cycle scenarios considered (although some concentrations measured in the Manchester Ship Canal did exceed this value). The LC_{50} from which it is derived is above the solubility selected for the substance, and so it too is subject to some uncertainty.[15]

In view of the uncertainty in the acute toxicity values, consideration could be given to carrying out long-term aquatic toxicity tests to establish a more reliable PNEC. However, only one life cycle scenario gives rise to risks and the other ratios are at least a factor of four below the lowest PNEC value used, so revision of the exposure assessment for this scenario would seem more relevant in the first instance. Further information is needed on emissions and/or the local environmental characteristics for production sites.

Data to revise the aquatic PNEC would also revise the sediment and soil PNECs, which are derived here using the equilibrium partition method. However, as the risk characterisation for these two compartments includes an additional factor of 10 due to the method used to derive the PNECs, testing on organisms for those compartments would be more valuable.

5.1.2   Waste water treatment

The PNEC for waste water treatment processes is 160 mg/l. The resulting risk characterisation ratios are summarised in Table 5.2.

Table 5.2   Summary of risk characterisation ratios for waste water treatment plants

Scenario		Predicted concentration (mg/l)	Risk characterisation ratio
Production of trixylenyl phosphate		0.04	<0.01
Power generation fluid	Lubricant blending	7.03×10^{-4}	<0.01
	Use of fluid	negligible	negligible

PEC/PNEC ratios are all less than one. On this basis, no risk to waste water treatment plants would be expected from the production and use of trixylenyl phosphate.

None of the measured WWTP effluent concentrations exceed 5 µg/l, and so these do not suggest any risks either.

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[15] Preliminary results indicate that the 48-hour EC_{50} for *Daphnia magna* is 0.06 mg/l. Applying an assessment factor of 1,000 would give a PNEC of 0.06 µg/l. On this basis, lubricant blending would also give rise to a potential risk (with an RCR of 1.5). The RCR for production would become 17. Risks would also be identified for the non-tidal River Trent at Gunthorpe and River Calder at Mirfield based on monitoring data.

5.1.3   Sediment

The PNEC for sediment was tentatively estimated as 0.13 mg/kg wet weight. The resulting PEC/PNEC ratios, increased by a factor of 10 to take into account the possibility of direct ingestion of sediment-bound substance, are given in Table 5.3.

Table 5.3   Summary of risk characterisation ratios for sediment

Scenario		Predicted concentration (mg/kg wet wt.)	Risk characterisation ratio
Production of trixylenyl phosphate		0.20	**15.2**
Power generation fluid	Lubricant blending	0.02	**1.28**
	Use of fluid	negligible	negligible
Regional sources		6.88×10^{-3}	0.53

The PEC/PNEC ratios for sediment are greater than one for production and blending of power generation fluids. The information for production noted for the water compartment would also be relevant here.

No risks to sediment are identified from use in power generation fluids and from regional sources based on the approach taken.

The sensitivity analysis in Annex C suggests that a faster hydrolysis rate than assumed here could have a significant effect on the local and regional sediment PECs. It may therefore be possible to refine the PECs by carrying out further testing to investigate the actual degradation (mineralization) half-life in sediment under relevant environmental conditions[16].

The PNEC for sediment is based on the equilibrium partitioning approach. Sediment toxicity tests could be carried out to refine the PNEC for this endpoint if it is not possible to revise the exposure assessment. It is likely that three long-term tests would be required.

5.2   Terrestrial compartment

The PNEC for soil is tentatively estimated to be 0.105 mg/kg wet weight. The resulting PEC/PNEC ratios, increased by a factor of 10 to take into account the possibility of direct ingestion of sediment-bound substance, are summarised in Table 5.4.

The PEC/PNEC ratio for blending of power generation fluids is greater than one. Further information is needed on process emissions to refine PECs for this scenario.

No risks to soil are identified for production or from regional sources, based on the approach taken.

Like sediment, the sensitivity analysis in Annex C suggests that a faster hydrolysis rate than assumed here could have a significant effect on the local and regional soil PECs. It may therefore be possible to refine the PECs by carrying out further testing to investigate the actual degradation (mineralization) half-life in soil under relevant environmental conditions.

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[16] The half-life determined in such a test would be the result of degradation by both biodegradation and hydrolysis to biodegradable substances.

Table 5.4   Summary of risk characterisation ratios for the terrestrial compartment

Scenario		Predicted concentration (mg/kg wet wt.)	PEC/PNEC ratio
Production of trixylenyl phosphate		8.99×10^{-6a}	<0.01
Power generation fluid	Lubricant blending	0.02	**1.78**
	Use of fluid	negligible	negligible
Regional sources	Agricultural soil	5.48×10^{-4}	0.05
	Natural soil	2.19×10^{-6}	<0.01
	Industrial soil	2.19×10^{-6}	<0.01

Notes: a) Sewage sludge from the production site is not applied to land.

The PNEC for soil is based on the equilibrium partitioning approach. Toxicity tests with soil organisms would allow the PNEC for this endpoint to be refined. As for sediment, testing on three species in long-term tests would probably be required.

5.3   Atmosphere

No information is available on the toxicity of trixylenyl phosphate to plants and other organisms exposed via air. The low vapour pressure of the substance means that volatilisation to the atmosphere is likely to be limited and the resulting concentrations are likely to be low (predicted concentrations are all below 3×10^{-7} mg/m^3). The possibility of trixylenyl phosphate contributing to atmospheric effects such as global warming and acid rain is thus likely to be small. In addition, as the substance does not contain halogen atoms, it will not contribute to ozone depletion.

5.4   Secondary poisoning

No PNEC for secondary poisoning could be derived for trixylenyl phosphate and so a risk characterisation for this endpoint cannot be performed. As the substance has a relatively high BCF in fish (around 1,900 l/kg) and is predicted to be taken up from soil by worms, this endpoint may be important for this substance. The lowest PNEC derived for secondary poisoning among the phosphates assessed in this series is 0.16 mg/kg for isodecylphenyl diphenyl phosphate. A PNEC of this order would indicate possible risks for production for the freshwater food chain, and for blending of power generation fluids for the terrestrial food chain (a low risk would be predicted for marine food chains). No conclusions can be drawn at the present time, and the situation should be reconsidered once appropriate mammalian toxicity data become available.

5.5   Risks to human health following environmental exposure

As noted in Section 4.4.2, the available data do not allow a suitable NOAEL to be identified on which to base an assessment for humans exposed through the environment, and therefore no risk characterisation has been carried out.

5.6   Marine compartment

Although a PEC/PNEC approach can be applied to the marine environment, there are additional concerns which may not be adequately addressed using the same methods as above. Chief among these concerns is the possibility that hazardous substances may accumulate in parts of the marine environment. The effects of such accumulation are unpredictable in the long term, and once such accumulation has occurred it may be practically difficult to reverse. The properties which lead to substances behaving in this way also lead to greater uncertainty in estimating exposures and/or effect concentrations, and so make a quantitative risk assessment more difficult. In order to identify substances which are likely to behave in this way, criteria have been developed relating to the persistence, accumulation and toxicity of the substance. The first part of the marine assessment is therefore a comparison of the properties of the substance with these criteria. This is presented in Section 4.5.

The PEC values for the marine assessment are presented in Sections 3.3.1 and 3.3.4. These were calculated using EUSES. PNECs for marine aquatic species are included in Section 4.1.6. The resulting PEC/PNEC ratios are presented in Table 5.5.

Table 5.5   Summary of risk characterisation ratios for the marine compartment

Scenario		Local marine compartment	Local marine sediment compartment	Fish-eating birds and mammals[a]	Top predators[a]
		PEC/PNEC ratio	PEC/PNEC ratio	PEC/PNEC ratio	PEC/PNEC ratio
Power generation fluid	Lubricant blending	**1.12**	**11.2**	-	-
	Use of fluid	negligible	negligible	-	-

Notes: No PNEC for secondary poisoning as no suitable data available.

The only risk identified is for marine water and sediment from lubricant blending. Further information on emissions from this process as indicated in the freshwater sediment assessment would also help to refine the result. More specifically for the marine assessment, information is needed on whether lubricant blending using trixylenyl phosphate takes place at any locations which discharge to the marine environment, and if so whether they only do so after effluent treatment (the calculations above assume a direct discharge to the marine environment without waste water treatment).

Testing on freshwater organisms would also affect the marine PNEC, although as noted in Section 5.1.1 such testing is not considered a priority for that part of the assessment. Testing on sediment organisms would be of more value for the sediment assessment. There is also the possibility of testing on marine species, which would allow the assessment factor to be reduced.

6   Conclusions

Trixylenyl phosphate can enter the environment from its production and use, and from the use of articles made from materials containing it. Although the commercial substance is a complex mixture, it is assumed to behave as a single substance for the purposes of this assessment.

Based on the available information, potential risks are identified for one or more of the protection goals. The overall conclusions are summarised in Table 6.1 in a simplified form. Section 5 should be consulted for the detailed results.

Table 6.1   Summarised potential environmental risks identified for cresyl diphenyl phosphate

Life cycle stage	Surface water	Sediment	WWTP	Air	Soil	Marine water	Marine sediment
Production	✳	✳	-	-	-	-	-
Power generation fluids – manufacture	-	✳	-	-	✳	✳	✳
Power generation fluids – use	-	-	-	-	-	-	-
Regional	-	-	-	-	-	-	-

No risk assessment for food chain exposure or humans exposed via the environment is currently possible in the absence of an adequate mammalian toxicity data set.

Trixylenyl phosphate meets the PBT criteria on the basis of the available *screening* data. Testing on persistence to determine an environmental half-life should be considered for this substance before any revision of other parts of the assessment is carried out.

The potential risks identified could be reassessed following further work, in particular:

- Collation of further site and industry-specific information on releases of trixylenyl phosphate from use in power generation fluids. This work could include:

  - An improved description of practices at sites blending power generation fluids using trixylenyl phosphate, to determine the realism of the emission estimates, ideally through surveys of representative sites.

  - Targeted monitoring to confirm or replace the calculated PEC values (especially in sediments and WWTP sludge). As noted in Section 5.1.1, some further monitoring is planned by the Environment Agency for this substance in 2009.

  - Information on the fate of sludges from sites using the substance.

  - Surveys to locate user sites, especially in relation to marine discharges.

- Long-term sediment and soil organism toxicity testing.

- Studies on the fate of the substance in WWTP (municipal and industrial).

- Further testing to investigate the actual degradation (mineralization) half-life in sediment and soil under relevant environmental conditions.

The possible risks identified for production sites could also be addressed by some aspects of the work above, but as there are only a small number of production sites these are considered to be better addressed by local authorities. The same may be true for power generation fluid manufacture.

There may be opportunities to read across information and test results from this substance to the other aryl phosphates assessed in this group (and vice versa). Therefore, the additional work indicated above should be considered in relation to that proposed for other members of the group. The overview document should be consulted for more information on this.

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8   Glossary of terms

Term	Description
Biochemical oxygen demand (BOD)	A measure of degradation potential
Bioconcentration factor (BCF)	A measure of chemical uptake, being the ratio between the concentration in an organism and the concentration in an environmental compartment (usually water)
CAS number (no.)	An identifying code number assigned to chemicals by the Chemical Abstract Services. The CAS number is a generally recognised identification reference for a chemical; a substance can have more than one such number
Inherently biodegradable	Some potential for environmental degradation to carbon dioxide and water, and so on, as measured by laboratory screening tests involving microorganisms
Lowest observed effect concentration (LOEC)	The lowest concentration in a toxicity test that gives rise to adverse effects (relative to a control)
Median effective concentration (EC_{50})	The concentration in a toxicity test at which a particular effect is observed in half of the organisms exposed for a specified time
Median lethal loading (LL_{50})	The loading of substance in a water-accommodated fraction that leads to death in half of the organisms exposed for a specified time
Median lethal concentration/dose (LC/D_{50})	The concentration in a toxicity test that can be expected to cause death in half of the organisms exposed for a specified time
No observed effect concentration (NOEC)	The highest concentration in a toxicity test that does not give rise to adverse effects (relative to a control)
Octanol-water partition coefficient (K_{ow})	This parameter gives an indication of the partitioning behaviour of a substance between water and lipid-containing materials such as cell membranes or organic matter in soils and sediments
Readily biodegradable	Rapid environmental degradation to carbon dioxide and water, and so on, as measured by laboratory screening tests involving microorganisms

9   Abbreviations

Acronym	Description
B	Bioaccumulative
BCF	Bioconcentration factor
BMF	Biomagnification factor
BOD	Biochemical oxygen demand
bw	Bodyweight
CAS	Chemical Abstract Services
CMR	Carcinogenic, mutagenic and toxic to reproduction
EC	European Communities
EC_{50}	Median effect concentration
EC_x	As EC_{50}, but for x% effect; x usually being 0, 10, or 100
ECB	European Chemicals Bureau
EEC	European Economic Communities
EINECS	European Inventory of Existing Commercial Chemical Substances – this lists all chemical substances that were supplied to the market prior to 18th September 1981
EPA	Environmental Protection Agency (USA)
ESD	Emission Scenario Document
ESR	The Existing Substances Regulation – Council Regulation (EEC) 793/93 on the evaluation and control of the risks of 'existing' substances.
EU	European Union
EUSES	European Union System for the Evaluation of Substances (software tool in support of the TGD on risk assessment)
HPLC	High performance liquid chromatography
HPV	High Production Volume (supply above 1,000 tonnes per year)
IUCLID	International Uniform Chemical Information Database: contains non-validated tonnage, use pattern, property and hazard information for chemicals, submitted by industry under the Existing Substances Regulation (ESR)
K_{oc}	Organic carbon normalised distribution coefficient
K_{ow}	Octanol-water partition coefficient
Kp	Solids-water partition coefficient
$L(E)C_{50}$	Median lethal (effect) concentration
LD_{50}	Median lethal dose
LL_{50}	Median lethal loading
$\log K_{ow}$	Log of the octanol-water partition coefficient (K_{ow})
NO(A)EL	No observed (adverse) effect level

Acronym	Description
NOEC	No observed effect concentration
n.t.p.	Normal temperature and pressure
OECD	Organisation for Economic Cooperation and Development
P	Persistent
PBT	Persistent, bioaccumulative and toxic
PEC	Predicted environmental concentration
pH	Logarithm (to the base 10) of the hydrogen ion concentration [H+]
pK$_a$	Logarithm (to the base 10) of the acid dissociation constant
PNEC	Predicted no effect concentration
TGD	Technical Guidance Document
TXP	Trixylenyl phosphate
USEPA	Environmental Protection Agency, USA
UV	Ultraviolet region of the electromagnetic spectrum
vB	Very bioaccumulative
vP	Very persistent
vPvB	Very persistent and very bioaccumulative
wt	Weight
wwt	Wet weight
WWTP	Wastewater treatment plant

10 Data collection and peer review process

This report has been produced using publicly available data gathered and assessed by the contractor for the Environment Agency. Additional information has been submitted voluntarily by member companies of the Phosphate Ester Flame Retardant Consortium (PEFRC, http://www.pefrcnet.org/), and the Environment Agency would like to thank them for their co-operation.

The Environment Agency has been keen to ensure that the data used in this report are as complete and accurate as possible. Original reports and literature articles for key studies were retrieved and assessed for reliability wherever possible (it is clearly indicated where this was not the case).

The main scientific literature search was performed in 2002, with some further limited searching to consider specific issues up to 2007.

Drafts of this report have been circulated to key stakeholders in UK and European Industry for comment on several occasions, as well as members of the UK and European chemical regulatory community in July 2007. The Advisory Committee on Hazardous Substances has also provided helpful comments as part of its own deliberations on this substance group (their last review was in September 2007).

In addition, certain technical aspects of the report were peer-reviewed by an independent expert group set up by the Environment Agency for this purpose in April 2007. The experts were:

- Dr Kay Fox (independent consultant);
- Dr Tamara Galloway (University of Plymouth).

Their comments have not been published but are available on request. All comments received have been addressed in the final report where appropriate.

The Institute for Environment and Health wrote the human health effects assessment, and this was peer-reviewed by colleagues at the Health and Safety Executive and Health Protection Agency.

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