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Environmental risk evaluation report: Isopropylated triphenyl phosphate (CAS nos. 28108-99-8, 26967-76-0 & 68937-41-7)

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Steve Killeen

Head of Science

Executive summary

An environmental risk assessment has been carried out for isopropylated triphenyl phosphate on the basis of available information and using the methods of a European Technical Guidance Document. The substance is a mixture of components, and the assessment considers both the low alkylated products (termed isopropylphenyl diphenyl phosphate) and the high alkylated products (termed tris(isopropylphenyl) phosphate) that are commercially available. These are used for a wide variety of applications, especially as a flame retardant plasticiser in a range of PVC products, and also polyurethanes, textile coatings, adhesives, paints and pigment dispersions. Lower alkylated products are used in thermoplastics. The lower alkylated products are used in lubricants as additives; the higher alkylated products function as both lubricant additives and base fluids.

The risks to waste water treatment plant and air from production and all uses are thought to be low. However, potential risks are identified for most or all areas of use for surface water (fresh and marine), sediment (fresh and marine) and soil compartments for both substance types, and for some uses for secondary poisoning in the freshwater and terrestrial food chains (and for the marine food chain for one use) for isopropylphenyl diphenyl phosphate (no assessment for secondary poisoning endpoints is possible for tris(isopropylphenyl) phosphate, since a suitable predicted no effect concentration (PNEC) cannot be derived).

Emission estimates are based on information from a number of generic sources, including emission scenario documents and other risk assessments, which could be refined with more specific information for the substance itself. However, some of the risk characterisation ratios are high and it is unlikely that such information by itself will be sufficient to remove all of the identified risks. Many of the predicted local concentrations (particularly for isopropylphenyl diphenyl phosphate) are dominated by the contribution of the regional water concentration. The regional emissions arise mainly from in-service losses and/or waste remaining in the environment from some PVC applications, paints, printed circuit boards, textiles and lubricant applications.

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.

No assessment of risks for humans exposed via the environment is possible for either substance type because the mammalian effects database has too much uncertainty. A more in-depth review of the available mammalian and avian toxicity data could be undertaken to better define a no observed adverse effect level (NOAEL) for both the secondary poisoning and human health assessments.

Isopropylphenyl diphenyl phosphate does not meet the criteria for a persistent, bioaccumulative and toxic (PBT) or very persistent and very bioaccumulative (vPvB) substance. However, tris(isopropylphenyl) phosphate does meet the screening PBT criteria on the basis of the available data. Testing on persistence to determine an environmental half-life should be considered.

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).

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

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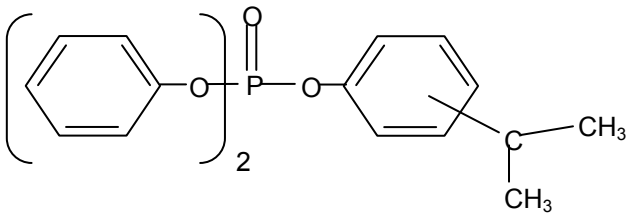
1 General substance information

1.1 Identification of the substance

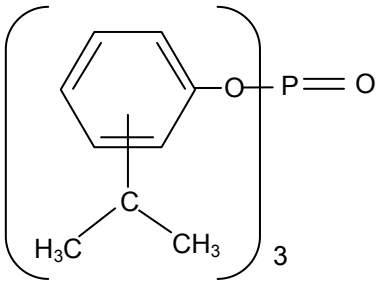
This assessment considers the following commercial substances:

CAS No: 28108-99-8
EINECS No: 248-848-2
EINECS Name: Isopropylphenyl diphenyl phosphate
Molecular formula: $C_{21}H_{21}O_4P$
Molecular weight: 368.37 g/mol
Structural formula:



CAS No: 26967-76-0
EINECS No: 248-147-1
EINECS Name: Tris(isopropylphenyl) phosphate

CAS No: 68937-41-7
EINECS No: 273-066-3
EINECS Name: Phenol, isopropylated, phosphate (3:1)
Molecular formula: $C_{27}H_{33}O_4P$
Molecular weight: 452.54 g/mol
Structural formula:



The CAS Number 68782-95-6 (EINECS Number: 272-171-1, EINECS Name: Phosphoric acid, (1-methylethyl)phenyl phenyl ester) also appears to be used.

Other names, abbreviations, trade names and registered trademarks for these substances include the following:

Durad 300®
DURAD 310M®
Isopropylated triphenyl phosphate
Kronitex 50® [2]
Kronitex 100®
Kronitex 200®
Phosflex 31 P®
Reofos 35®
Reofos 50®
Reofos 65®
Reofos 95®
Reofos 120®
Reolube HYD 46®
Triaryl phosphates isopropylated

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

Commercially supplied isopropylated triphenyl phosphates cover a range of products with differing degrees of alkylation (see Section 1.2). However, the test substance composition is not always clearly described in the available literature. In this assessment, the terms “isopropylphenyl diphenyl phosphate” and “tris(isopropylphenyl) phosphate” will be used for the lower and higher alkylated products respectively when it is clear that products of these types have been tested. The term “isopropylated triphenyl phosphate” will be used when the identity of the product is less clear, or is intermediate between the two extremes (and also to refer to the range of products in general terms). In this respect the trade name or trademark, where available, for the particular product tested is also given to provide additional clarity (even though some of these products may no longer be supplied, and the actual composition of the products may have altered over the years).

1.2 Purity/impurity, additives

1.2.1 Purity/impurities

The commercial products are complex isomeric mixtures of phosphate esters derived from phenol and isopropyl phenol. The composition of several commercial isopropylated triphenyl phosphate products is summarised in Table 1.1.The actual composition of a given product may vary slightly around these values.

[2] The Kronitex products were manufactured in the United States and were not generally available in Europe. Production of these products has now ceased.

Table 1.1 Example compositions of commercial products

Component	Commercial product										
	Kronitex 50	**Kronitex 100**	**Kronitex 200[b]**	**Phosflex 31P**	**Reofos 35[d]**	**Reofos 50[c]**	**Reofos 65[d]**	**Reofos 95[d]**	**Reofos 120[d, e]**	**Durad 300[d]**	**Durad 310M[c]**
Triphenyl phosphate	33%	18%	4-6%	28-30%	35%	28-32%	20%	9%	7.5%	5%	4%
2-Isopropylphenyl diphenyl phosphate	21%	27%	7-10%	Present	-	-	-	-	-	-	-
4-Isopropylphenyl diphenyl phosphate	12%	11%	20-25%	Present	-	-	-	-	-	-	-
Di-(2-ispropylphenyl) phenyl phosphate	6%	7%	Present	-	-	-	-	-	-	-	-
Di-(4-isopropylphenyl) phenyl phosphate	2%	5%	-	-	-	-	-	-	-	-	-
Tris(isopropylphenyl) phosphate	8%	11%	-	-	-	-	-	-	-	-	-
Isopropylated triphenyl phosphate	-	-	-	-	65%	70%	80%	91%	92.5%	95%	91%
Others	18%	21%	Minor components: di, tri- and tetra-isopropyl-substituted triphenyl phosphates.	Other components: 3-isopropylphenyl diphenyl phosphate, diisopropylphenyl diphenyl phosphate isomers (2,6-, 2,4-, 2,5- 3,5-) and trisubstituted phenol isomers.	-	-	-	-	-	-	5%

References: a) Nobile *et al.* 1980; b) Cleveland *et al.* 1986; c) Great Lakes Chemical Corporation 2002; d) IUCLID 2000.

The various products are manufactured from feedstocks containing different ratios of isopropylated phenols to phenol. The same isomers are contained in all members of the range but at different ratios, reflecting the different degrees of isopropylation. On average, the lower end of the range is approximately equivalent to an overall substitution level corresponding to mono-isopropylphenyl diphenyl phosphate, whereas the higher end of the range is equivalent to a substitution level corresponding to di-isopropylphenyl monophenyl phosphate (Great Lakes Chemical Corporation 2003).

1.2.2 Additives

Additives are not present in the flame retardant, plasticizer, fluid basestock or lubricant additive grades; however, additives may be present in the formulated fluids. The phosphate esters may also be supplied as blends with other products.

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)

Great Lakes Chemical Corporation (2002) indicate that a commercial isopropylphenyl diphenyl phosphate product (Reofos 50) is a clear liquid at room temperature and a tris(isopropylphenyl) phosphate product (Durad 310M) is a clear to amber liquid at room temperature.

1.3.2 Melting point

The melting point (pour point) of isopropylated triphenyl phosphates is reported to be in the range -26°C to -12°C (IUCLID 2000). Muir (1984) gives a pour point of -26°C for isopropylphenyl diphenyl phosphate.

A melting/pour point of -26°C will be assumed in the assessment.

1.3.3 Boiling point

Wightman and Malalyandi (1983) determined the boiling points at reduced pressure of pure isomers of isopropylphenyl diphenyl phosphate. The boiling points reported were 175°C at 0.05 mmHg (6.7 Pa) for *ortho*-isopropylphenyl diphenyl phosphate, 180°C at 0.2 mmHg (27 Pa) for *meta*-isopropylphenyl diphenyl phosphate and 185°C at 0.05 mmHg (6.7 Pa) for *para*-isopropylphenyl diphenyl phosphate.

Great Lakes Chemical Corporation report the boiling point of a commercial isopropylphenyl diphenyl phosphate product (Reofos 50) as above 300°C at 101,325 Pa, and a decomposition temperature also above 300°C.

Boethling and Cooper (1985) and Muir (1984) give a boiling point of 220-230°C at 1 mmHg (133 Pa) for commercial isopropylphenyl diphenyl phosphate.

The boiling point of a commercial tris(isopropylphenyl) phosphate product (Durad 310M) is above 300°C at 101,325 Pa (Great Lakes Chemical Corporation 2002). The decomposition temperature of the same product is given as above 300°C.

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

1.3.4 Density

Shankwalkar and Cruz (1994) reported specific gravities of 1.18, 1.165 and 1.125 at 20°C for three commercial isopropylphenyl diphenyl phosphate products. The three products had phosphorus contents of 8.3 per cent, 7.9 per cent and 7.4 per cent respectively. A specific gravity of 1.17-1.18 at 20°C has been reported for a commercial isopropylphenyl diphenyl phosphate product (Reofos 50) with a phosphorus content of 8.3 per cent (Great Lakes Chemical Corporation 2002).

IUCLID (2000) reports a density of 1.1-1.2 g/cm^3 at 25°C for commercial isopropylphenyl diphenyl phosphate products.

The specific gravity of a commercial tris(isopropylphenyl) phosphate product (Durad 310M) has been determined as 1.1 at 20°C by the ISO 3675 method (Great Lakes Chemical Corporation 2002).

A density of 1.1-1.2 g/cm^3 at 25°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 isopropylated triphenyl phosphates at temperatures around 20-25°C. However, information on boiling points at reduced pressure (see Section 0) and vapour pressure at elevated temperature are available.

A vapour pressure of 2.8×10^{-7} mmHg (3.7×10^{-5} Pa) at 30°C has been determined for commercial isopropylphenyl diphenyl phosphate (Boethling and Cooper 1985). Great Lakes Chemical Corporation (2003) indicate that the vapour pressure of isopropylated triphenyl phosphates is around 3.05×10^{-3} Pa at 70°C for a product with a relatively low degree of alkylation (such as isopropylphenyl diphenyl phosphate) and around 7.77×10^{-4} Pa at 70°C for a product with a relatively high degree of alkylation (such as tris(isopropylphenyl) 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:

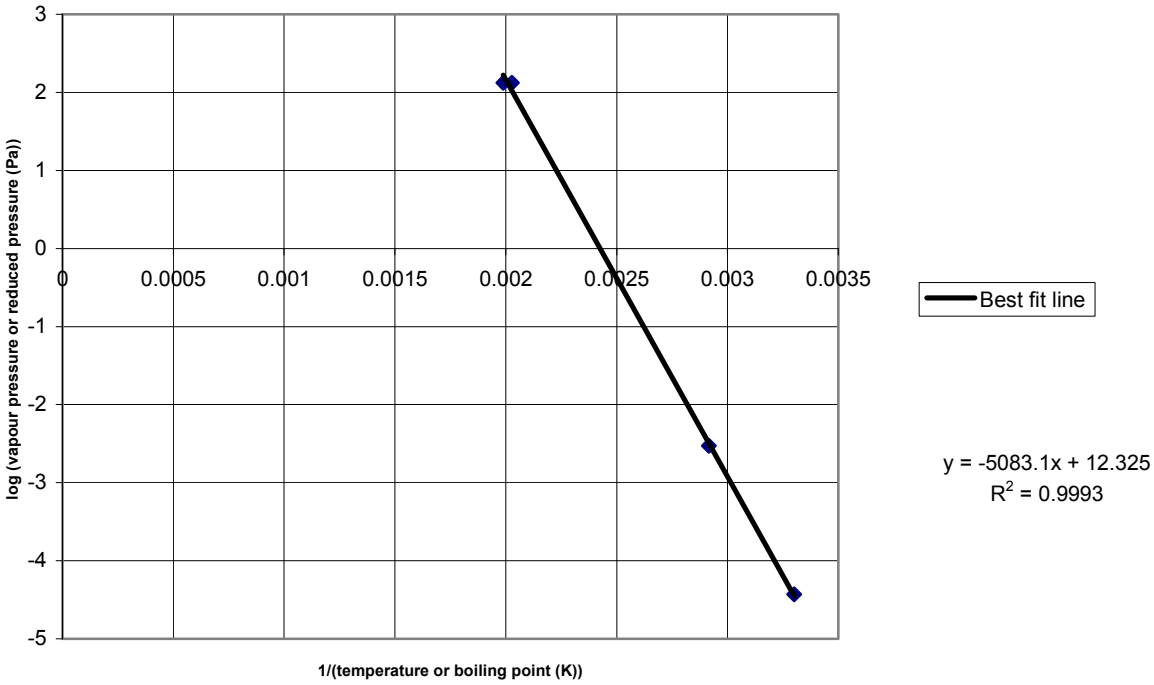
$$\log(\text{vapour pressure}) = [\underline{\Delta}H_v/2.3RT] + \text{constant}$$

where vapour pressure is in Pa
ΔH_v = heat of vapourization 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 (Pa)) against 1/(temperature or boiling point (K)) for the data available for commercial isopropylphenyl diphenyl phosphate products. The plot corresponds to the following regression equation:

log (vapour pressure (Pa)) = [-5083.1 × 1/(temperature (K))] + 12.325

Figure 1.1 Plot of log (vapour pressure or reduced pressure (Pa)) against 1/(temperature or boiling point (K)) for commercial isopropylphenyl diphenyl phosphate



From the slope of the plot, the value of ΔH_v for commercial isopropylphenyl diphenyl phosphate is estimated to be -97,200 J/mol.

Using this equation, the vapour pressure for isopropylphenyl diphenyl phosphate is estimated as 9.5×10^{-6} Pa at 20°C, 1.9×10^{-5} Pa at 25°C, 2.0 Pa at 150°C and 38 Pa at 200°C. These estimates are based on few data and so have considerable uncertainty. Te value for 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 value for ΔH_v for the pure isopropylphenyl diphenyl phosphate isomers is also around -97,200 J/mol, the following vapour pressures at 20°C can be estimated for the pure isopropylphenyl diphenyl phosphate isomers from their boiling points at reduced pressure using the simplified Clapeyron-Clausius equation:

ortho-isopropylphenyl diphenyl phosphate	6.7×10^{-6} Pa at 20°C
meta-isopropylphenyl diphenyl phosphate	2.0×10^{-5} Pa at 20°C
para-isopropylphenyl diphenyl phosphate	3.8×10^{-6} Pa at 20°C

The vapour pressure for a tris(isopropylphenyl) phosphate product is given above as 7.77×10^{-4} Pa at 70°C. Again assuming that the value for ΔH_v for this product is also around -97,200 J/mol the vapour pressure at 20°C can be estimated as 2.3×10^{-6} Pa.

A vapour pressure (at 25°C) of 4.0×10^{-8} mmHg (5.3×10^{-6} Pa) and 2.06×10^{-8} mmHg (2.7×10^{-6} Pa) can be estimated for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate from their structures 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 1.1×10^{-6} mmHg (1.5×10^{-4}) Pa from the reduced pressure boiling point of isopropylphenyl diphenyl phosphate (Grain method).

As discussed above, there are some large uncertainties in estimates of the vapour pressures of isopropylated triphenyl phosphates at room temperature. For the risk assessment the vapour pressure at 20°C is taken to be 9.5×10^{-6} Pa for isopropylphenyl diphenyl phosphate and 2.3×10^{-6} Pa for tris(isopropylphenyl) phosphate based on the estimates obtained using the Clapeyron-Clausius equation. These values are reasonably consistent with estimates provided by Great Lakes Chemical Corporation (2003) at a lower temperature of 10°C (the estimated values were 1.6×10^{-6} Pa for a lower alkylated product and 2.6×10^{-7} Pa for a higher alkylated product).

1.3.6 Water solubility

Saeger *et al.* (1979) determined the solubility of an isopropylphenyl diphenyl phosphate (Kronitex 1000) using a shake flask method. The substance used was a commercial product consisting of isopropylphenyl diphenyl phosphate along with triphenyl phosphate and bis(isopropylphenyl) phenyl 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 2.2 mg/l at room temperature. The composition of the saturated solution was found to be different to that of the commercial product, with the proportion of triphenyl phosphate elevated in solution compared with that in the commercial product. This indicates a preferential dissolution of the triphenyl phosphate component (water solubility of triphenyl phosphate itself was determined as 1.9 mg/l). As the solubility determined of 2.2 mg/l was based on the total concentration of all components of the commercial product, the actual solubility of the isopropyphenyl diphenyl phosphate may be lower than indicated by this figure.

A water solubility of around 0.026 mg/l can be estimated for isopropylphenyl diphenyl phosphate and around 2.6×10^{-5} mg/l for tris(isopropylphenyl) phosphate using the Syracuse Research Corporation WSKOW version 1.30 software (the estimate is based on an estimated log K_{ow} of 6.16 for isopropylphenyl diphenyl phosphate and 9.07 for tris(isopropylphenyl) phosphate).

A water solubility of 2.2 mg/l at room temperature (~20°C) is assumed for isopropylphenyl diphenyl phosphate in this assessment.

No measured data are available for tris(isopropylphenyl) phosphate. Annex B considers the available data for all aryl phosphates and estimates that the water solubility of tris(isopropylphenyl) phosphate would be around 0.12 mg/l. This value is used in the risk assessment, although this estimate is somewhat uncertain.

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

The octanol-water partition coefficient of an isopropylphenyl diphenyl phosphate (Kronitex 1000) was determined using a shake flask method (Saeger *et al.* 1979). The substance used was a commercial product consisting of isopropylphenyl diphenyl phosphate along with triphenyl phosphate and bis(isopropylphenyl) phenyl 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 202,000 (log K_{ow} = 5.30).

Renberg *et al.* (1980) determined the octanol-water partition coefficient for an isopropylphenyl diphenyl phosphate (the same substance as used by Saeger *et al.* 1979 above) using a high performance thin layer chromatography (HPTLC) method. Four main components of the commercial product were evident using the method and the partition coefficients determined (log values) for these components were 3.23, 4.30, 5.40 and 6.57. The mean value obtained for all components was 5.99. The component giving rise to the log K_{ow} value of 3.23 was tentatively identified as triphenyl phosphate (the log K_{ow} value for triphenyl phosphate itself was determined as 3.15 using the HPTLC method). These measured values are in reasonable agreement with the values estimated above.

A log K_{ow} of 6.16 can be estimated for isopropyl diphenyl phosphate and a log K_{ow} value of 9.07 for tris(isopropylphenyl) phosphate from their chemical structure using the Syracuse Research Corporation Log K_{ow} (version 1.60) software.

A log K_{ow} value of 5.30 is used in the assessment as representative of isopropylphenyl diphenyl phosphate.

No measured data are available for tris(isopropylphenyl) phosphate. Annex B considers the available data for all aryl phosphates and estimates that the log K_{ow} will be around 6.1 for tris(isopropylphenyl) phosphate. This value is used in this risk assessment, although there is some uncertainty in this estimate.

1.3.8 Hazardous physico-chemical properties

Flash points of above 220°C and 200°C have been reported for a commercial isopropylphenyl diphenyl phosphate product (Reofos 50) and a commercial tris(isopropylphenyl) phosphate product (Durad 310M) respectively (Great Lakes Chemical Corporation 2002). A flash point of 199°C has been reported for isopropylated triphenyl phosphates (IUCLID 2000).

The autoignition temperature of a commercial isopropylphenyl diphenyl phosphate product (Reofos 50) has been determined to be 585°C (Great Lakes Chemical Corporation 2002). The autoignition temperature of a commercial tris(isopropylphenyl) phosphate product (Durad 310M) is given as 565°C. An autoignition temperature of 551°C at 101.3 Pa is reported in IUCLID (2000) for isopropylated triphenyl phosphates.

No data could be located on explosivity or the oxidising properties.

1.3.9 Henry's law constant

A Henry's law constant of 7.74×10^{-8} atm m^3/mol (0.0078 Pa m^3/mol) at 25°C can be estimated for isopropylphenyl diphenyl phosphate from chemical structure (bond contribution method) using the Syracuse Research Corporation HENRYWIN (version 3.00) software. Using the same software a Henry's law constant of 2.93×10^{-7} atm m^3/mol (0.030 Pa m^3/mol) at 25°C can be estimated for tris(isopropylphenyl) phosphate.

A further value of Henry's law constant of 0.0016 Pa m^3/mol at 20°C can be estimated for isopropylphenyl diphenyl phosphate from a water solubility of 2.2 mg/l and vapour

pressure of 9.5×10^{-6} Pa. Similarly, a Henry's law constant of 0.0087 Pa m^3/mol at 20°C can be estimated for tris(isopropylphenyl) phosphate from its water solubility (0.12 mg/l) and vapour pressure (2.3×10^{-6} Pa). These values are in reasonable agreement with the estimates obtained above from structure alone and are used in this assessment as they are consistent with water solubility and vapour pressure data used.

1.3.10 Summary of physico-chemical properties

The physico-chemical properties of isopropylated triphenyl phosphates are summarised in Table 1.2. Most data have been obtained with commercial products and so some properties may vary depending on the actual composition of the product.

Table 1.2 Summary of environmentally relevant physico-chemical properties of isopropylated triphenyl phosphate used in the risk assessment

Property	Value	
	Isopropylphenyl diphenyl phosphate	**Tris(isopropylphenyl) phosphate**
Melting point	-26	-26
Boiling point (at atmospheric pressure)	>300	>300
Relative density	1.1-1.2	1.1-1.2
Vapour pressure	9.5×10^{-6}	2.3×10^{-6}
Water solubility	2.2	0.12
Octanol-water partition coefficient (log value)	5.3	6.1
Henry's law constant	0.0016	0.0087

For the purposes of this assessment, each of these substance types is considered to behave as a single substance in the environment, even though they are both complex mixtures.

2 General information on exposure

2.1 Production

Isopropylphenol is made by reaction of phenol with propylene. The resulting product is a mixture of mainly *ortho*- and *para*-isomers with varying degrees of alkylation (Weil 1993). The product of this reaction is then mixed with phenol and reacted with phosphorus oxychloride to produce the phosphate ester. The relative amounts of phenol and isopropylated phenol can be varied to give a range of products with a corresponding range of properties. In order to produce the higher alkylated products, less or no extra phenol would be used.

There is 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

Triaryl 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. These substances have a plasticizing effect as well as providing flame retardancy. 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 Use of isopropylated triphenyl phosphates

The substance is reported to have a similar plasticizing performance to that of tricresyl phosphate (Weil 1993). Phosphate esters containing isopropylated triphenyl groups have the widest spectrum of use among the aryl phosphates. The main area of use for all types of isopropylated triphenyl phosphates is in a range of PVC products. Both high and low alkylated products are also used in polyurethanes, textile coatings, adhesives, paints and pigment dispersions. Lower alkylated products are used in thermoplastics. Both types are used in lubricants, the lower alkylated products as additives, the higher alkylated products as both additives and base fluids.

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 photooxiation

A rate constant for reaction of isopropylphenyl diphenyl phosphate with atmospheric hydroxyl radicals of 1.8×10^{-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. Similarly, a rate constant for reaction of tris(isopropylphenyl) phosphate with atmospheric hydroxyl radicals of 3.3×10^{-11} cm^3/molecule s can be estimated using the same software.

Using an atmospheric hydroxyl radical concentration of 5×10^5 molecules/cm^3, a half-life for the reaction in air can be estimated as 21 hours for isopropylphenyl diphenyl phosphate and 12 hours for tris(isopropylphenyl) phosphate.

Hydrolysis

Wolfe (1980) developed linear free energy relationships to estimate the rate constants for neutral and alkaline hydrolysis of triaryl phosphates using the available published information on hydrolyis. 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 substitutents and the following equation was derived:

[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.ec.europa.eu/.

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

where k = second-order rate constant for hydrolysis at 30°C (l/mol s)
σ = sum of Hammet substituent constants

For the phenyl group, σ = 0 and so the second-order hydrolysis rate constant is 0.33 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 phenyl groups at this pH is around 3.3×10^{-7} s^{-1}. This is equivalent to a hydrolysis half-life of around 24 days. The value of σ for isopropylphenyl is -0.151 (for the *para*-isomer). Based on this value, the hydrolysis rate constant for the isopropylphenyl group would be 0.21 l/mol s, giving a hydrolysis half-life of around 39 days for this group at pH 8.

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 triphenyl phosphate the pKa of the leaving phenol group is around 10, and a similar value would be expected for the isopropylphenyl leaving group. 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. The alkaline hydrolysis reaction at pH 7 would have a half life of 380 days.

Great Lakes Chemical Corporation (2003) indicate that hydrolysis of aryl phosphates 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 product would be diaryl phosphates (diesters of phosphoric acid), which are acidic). The rate of hydrolysis in such a test generally increases as the acidity increases during the test. 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

There is no information on the direct photolysis reactions of isopropylated triphenyl phosphates.

Biodegradation

IUCLID (2000) summarises the results of several unpublished industry standard biodegradation tests using various commercial products. The commercial product Reolube HYD 46 was found to be readily biodegradable in an OECD 301A DOC Die-Away test. In this test, 86 per cent degradation was seen after 31 days using an activated sludge inoculum and a test concentration of 32.6 mg/l. Based on the results of this test, the substance can be considered readily biodegradable. However, the DOC Die-Away test is not currently recommended for substances of low water solubility (below 100 mg/l) and so the results of this test should be treated with caution. When the same substance was tested in an OECD 301B Modified Sturm Test at 10 mg/l and 20 mg/l, the extent of degradation was 29 per cent and 40 per cent respectively based

on CO_2 evolution. Thus, the substance was not readily biodegradable in this test system.

A further ready biodegradation test was carried out with the commercial product Reolube HYD 46 (Battersby and Bumpus 2001). This test was carried out in triplicate using the OECD 301F Manometric Respirometry test method. Biodegradation was found to occur after a lag period of 7 to 9 days and had reached 43-52 per cent degradation (mean 46 per cent; based on theoretical oxygen demand) by day 28. Again, the substance was not readily biodegradable in this test system.

Another OECD 301B test was carried out with a different commercial substance (Reofos 50) using an activated sludge inoculum (IUCLID 2000). The substance was tested at a concentration of 10 and 20 mg/l and the extent of degradation (determined as CO_2 evolution) seen after 28 days was 74 per cent at 10 mg/l and 80 per cent at 20 mg/l. Based on the results of this test, the substance can be considered readily biodegradable.

The same commercial substance (Reofos 50) was apparently shown to be readily biodegradable in another OECD 301A test, showing 94 per cent degradation after 26 days (IUCLID 2000). In this test, the concentration of test substance was 41.67 mg/l but the summary indicates that due to insolubility, a stock solution (5 g/l) of the test substance was prepared in dichloromethane and this stock solution was added directly to the aeration vessel. The summary also indicates that the test solution was fed into the aeration vessel at a rate of 8.3 ml/hour and the nutrient solution was added at a rate of 1 litre per hour. Thus, from this summary, it appears that the test protocol used was different than that currently recommended for an OECD 301A test and may actually have been an OECD 303A Coupled Units Test.

IUCLID (2000) reports the results of an unpublished biodegradation study using a commercial higher alkylated isopropylated triphenyl phosphate product (Reofos 120). The test was an OECD 301B Modified Sturm ready biodegradation test using activated sludge from a sewage treatment plant. The biodegradation seen after 28 days (determined as CO_2 evolution) was 21 per cent at a concentration of 10.6 mg/l and 13 per cent at 21.5 mg/l. Based on the results of this test, the substance is not considered readily biodegradable.

A further ready biodegradation test was carried out with the same commercial isopropylated triphenyl phosphate (Reofos 120) (Sherren 2003). The method used in this case was the OECD 301F Manommeric Respirometry method. The degradation seen (determined as percentage ThOD) was 47 per cent after 28 days. The test was extended up to 68 days and the substance was shown to be more than 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 an isopropylphenyl diphenyl phosphate (Kronitex 1000) using various test systems. The substance used was a commercial product consisting of isopropylphenyl diphenyl phosphate along with triphenyl phosphate and bis(isopropylphenyl) phenyl phosphate. The first test investigated the primary degradation of the test substance using a river die-away method. The water used in the test was settled Mississippi River water. The test substance (at a concentration of 1 mg/l) was added to the water and the test vessels (bottles) were sealed with a foil-lined cap and stored in the dark at room temperature. Sterile control solutions (containing the same concentration of test substance) and positive control solutions (containing linear alkyl benzene sulphonate) were also run. At various times during the study, a bottle was removed and the amount of the phosphate ester present was determined (a gas chromatographic method was used that analysed

the sum of the major components present in the test substance). The results showed that the test substance underwent primary degradation in the test system with around 80 per cent degradation after 28 days. No significant degradation was seen in the sterile controls.

The second 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 in the test had an operating volume of 1.5 litres. The test substance was added to the unit at a rate of either 3 mg/l or 13 mg/l per 24-hour cycle. The units were operated for a period of 15-24 weeks and samples of the mixed liquor were removed at weekly intervals and the concentration of the phosphate ester present was determined. The results indicated an equilibrium removal rate of 49 ± 8 per cent at 3 mg/l and 35 ± 11 per cent at 13 mg/l in the test system. The higher concentration was found to cause a significant decrease in the biomass present in the test system. To investigate the loss by volatilisation, the off-gases were passed through a series of scrubbers. No significant loss by volatilisation (below 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 21.5 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 9 per cent after seven days, 49 per cent after 28 days and 62 per cent after 48 days. Therefore, the substance can be considered as inherently biodegradable based on the results of this test.

The biodegradation of ^{14}C-labelled isopropylphenyl diphenyl phosphate (both di[^{14}C] phenyl- and isopropyl[^{14}C]phenyl labelled substances were used (purity of each above 99 per cent)) was studied under both aerobic and anaerobic conditions using a freshwater sediment system (Heitkamp *et al.* 1984). The test system consisted of 250 ml flasks containing 10 g (wet weight) of sediment and 90 ml of water taken from the littoral zone of a slightly eutrophic reservoir. The pH of the water was 7.1 to 7.7 and the hardness was 58-70 mg/l as $CaCO_3$. The system was allowed to stand at 22°C under aerobic conditions in the dark for several days prior to the addition of the test substance. The test substance was added as a solution in acetone. A low-exposure dose (1.56 μg/microcosm equivalent to around 15.6 μg/l) and high-exposure dose (58.5 μg/microcosm equivalent to around 585 μg/l) were used. Each experiment was replicated five times and sterile microcosms were used as controls. The aerobic or anaerobic conditions in the microcosms were maintained by continually purging the vessels with air or nitrogen. The $^{14}CO_2$ evolved from the system was determined at weekly intervals. The results are summarised in Table 3.1. These showed that the rate of mineralisation was relatively low, with only around 7 to 8 per cent mineralisation in four weeks with the isopropylphenyl diphenyl phosphate with the ^{14}C-label on the two phenyl rings, and 1 to 2 per cent mineralisation in four weeks with the isopropylphenyl

diphenyl phosphate with the ^{14}C-ring-labelled isopropylphenyl group. Similar results were found under both aerobic and anaerobic conditions. The data indicated that the phenyl and isopropylphenyl groups were mineralised at different rates. The ^{14}C-residues that could be extracted from the sediment and water (using methylene chloride with a further extraction of the sediment with methanol) were found to be mainly undegraded isopropylphenyl diphenyl phosphate along with small amounts of relatively non-polar metabolites. A more detailed analysis of the degradation products formed was carried out during the high dose experiment. This found that polar metabolites accounted for around 2.4 to 3.9 per cent of the total radioactivity added to the system. The actual identities of many of the polar metabolites were not determined due to the low concentrations present, but diphenyl phosphate was thought to be one of these products, along with methyl-substituted derivatives of diphenyl phosphate and isopropylphenyl phenyl phosphate. The main non-polar metabolite found was triphenyl phosphate, which accounted for 3.4 to 13 per cent of the total radioactivity added to the system.

Table 3.1 Biodegradation of ^{14}C-labelled isopropylphenyl diphenyl phosphate

Test system	Location of ^{14}C-ring-label	Mineralisation (as $^{14}CO_2$)				Extractable[a] ^{14}C residues from sediment/ water	Non-extractable residues from sediment/ water	Total re-covery of ^{14}C
		7 days	14 days	21 days	28 days			
Aerobic, low dose	Diphenyl groups	0.8%	2.2%	5.0%	7.1%	82.2%	5.8%	95.1%
	Isopropyl-phenyl group	0.0%	0.0%	0.5%	2.0%	86.6%	3.9%	92.5%
Anaerobic low dose	Diphenyl groups	1.4%	3.1%	5.1%	7.3%	79.7%	2.8%	90.9%
	Isopropyl-phenyl group	0.0%	0.0%	0.6%	1.1%	80.8%	Not determined	>81.9%
Aerobic high dose	Diphenyl group	0.7%	3.3%	6.0%	8.4%	76.1%	2.7%	87.2%
Aerobic sterile control	Diphenyl group				0.0%	86.7%	9.2%	95.9%

Notes: a) Extractable residues were determined by extraction of methylene chloride and further extraction of the sediment with methanol. These were found to be mainly unchanged isopropylphenyl diphenyl phosphate.

Boethling and Cooper (1985) report the results of an unpublished study using a commercial isopropylated triphenyl phosphate (main components triphenyl phosphate, 2-isopropylphenyl diphenyl phosphate and 4-isopropylphenyl diphenyl phosphate). In this study, activated sludge mixed liquor was acclimated to progressively higher concentrations of the test substance. At the start of the test, the acclimated liquor was diluted 1:10 with a mineral salts medium and the test substance was added as sole source of carbon. All three main components were found to be more than 98 per cent degraded within seven days. All components of the same substance were found to be extensively degraded in a river die-away test over seven days (the half-life for the two isopropylphenyl diphenyl phosphates was around 3 to 4 days).

Boethling and Cooper (1985) estimated that the removal of 2-isopropylphenyl diphenyl phosphate during biological waste water treatment at a production plant in the United States was 99 per cent based on the average concentration in waste water (0.63 mg/l)

and the average concentration in effluent from the treatment plant (0.009 mg/l). Similarly the removal of di-(isopropylphenyl) phenyl phosphate was estimated to be 94 per cent (concentration in waste water 0.90 mg/l and concentration in effluent 0.053 mg/l). The removal was believed 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, it was also indicated that 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 (and hence the removal lower) than indicated. The results of these studies only indicate that primary degradation may occur.

Summary of degradation

Abiotic degradation

The available information indicates that both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate will undergo hydrolysis, particularly at high and low pHs. By comparison with the data available for other triaryl phosphates (see the risk evaluation report for triphenyl phosphate in this series, for example), the products of this hydrolysis are likely to be isopropylphenol or phenol and the corresponding diaryl phosphate, which is likely to be more stable to further hydrolysis than the parent compound. The data for triphenyl phosphate are particularly relevant to this assessment, since some of the commercial forms of isopropylated triphenyl phosphates have isopropylated triphenyl phosphate present at only 65-70 per cent and contain around 30-35 per cent triphenyl phosphate (Reofos 35 and Reofos 50). Example compositions of commercial products are presented in Table 1.1 (see Section 1.2.1). The available information indicates that the rate of this hydrolysis is only likely to be significant at high pH (pH 8-9 and above) and low pH. Since the pHs found in the environment are generally outside these levels, the rate of hydrolysis of both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) 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 predicted concentrations is considered in Annex C.

There are no data on the direct photolysis reactions of isopropylated triphenyl phosphates under environmentally relevant conditions. The rate of direct photolysis is assumed to be zero in the assessment for both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate.

Atmospheric photooxidation of both isopropylated triphenyl phosphates is predicted to occur with a half-life of around 21 hours for isopropylphenyl diphenyl phosphate and 12 hours for tris(isopropylphenyl) phosphate. This reaction is taken into account in the risk assessment.

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

Isopropylphenyl diphenyl phosphate

Hydrolysis	$khydr_{water}$ = 0 d^{-1}	half-life = infinite
Photolysis	$kphoto_{water}$ = 0 d^{-1}	half-life = infinite
Atmospheric photooxidation	k_{OH} = 1.8×10^{-11} cm^3/molecule s	half-life = 21.4 h

Tris(isopropylphenyl) phosphate		
Hydrolysis	$khydr_{water}$ = 0 d^{-1}	half-life = infinite
Photolysis	$kphoto_{water}$ = 0 d^{-1}	half-life = infinite
Atmospheric photooxidation	k_{OH} = 3.3×10^{-11} cm^3/molecule s	half-life = 11.7 h

Biodegradation

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

The available standard biodegradation tests show that commercial products with lower degrees of alkylation representative of the isopropylphenyl diphenyl phosphate products that have been tested (such as Reofos 50, 70 per cent isopropylated triphenyl phosphate, 28-32 per cent triphenyl phosphate) can be considered readily biodegradable (with no information on whether the 10-day window is met). Products with higher degrees of alkylation representative of the tris(isopropylphenyl) phosphate products (such as Reofos 120, 92.5 per cent isopropylated triphenyl phosphate, 7.5 per cent triphenyl phosphate) appear to be inherently biodegradable. Given the likely degradation pathway outlined above, and the fact that isopropylphenol is likely to undergo biodegradation, tris(isopropylphenyl) phosphate is assumed to be inherently biodegradable (meeting specific criteria, as inherent biodegradability does need testing). Default degradation (mineralisation) rates estimated for isopropylphenyl diphenyl phosphate (Kp_{soil} = 117 l/kg, see Section 3.1.2) and tris(isopropylphenyl) phosphate (Kp_{soil} = 288 l/kg: see Section 3.1.2), assuming they are readily biodegradable (not meeting 10-day window) and inherently biodegradable respectively, are shown below.

Isopropylphenyl diphenyl phosphate		
Sewage treatment plant	k = 0.3 h^{-1}	half-life = 2.3 hours
Surface water	k = 1.4×10^{-2} d^{-1}	half-life = 50 days
Soil	k = 7.7×10^{-4} d^{-1}	half-life = 900 days
Sediment	k = 7.7×10^{-4} d^{-1}	half-life = 900 days

Tris(isopropylphenyl) phosphate		
Sewage treatment plant	k = 0.1 h^{-1}	half-life = 6.9 hours
Surface water	k = 4.7×10^{-3} d^{-1}	half-life = 150 days
Soil	k = 2.3×10^{-4} d^{-1}	half-life = 3,000 days
Sediment	k = 2.3×10^{-4} d^{-1}	half-life = 3,000 days

A number of screening studies are available, particularly for isopropylphenyl diphenyl phosphate, which can be considered in relation to the biodegradation rate. For surface water, around 80 per cent primary degradation of isopropylphenyl diphenyl phosphate was seen in a river die-away test at room temperature. Given that this test was carried out at room temperature, and measured only primary degradation, the results from this test are consistent with the default half-lives for surface water of 50-150 days estimated above. Similarly for sediment, up to 8 per cent mineralisation of isopropylphenyl diphenyl phosphate was seen in 28 days, which is again reasonably consistent with the default mineralisation half-lives of 300 to 3,000 days estimated above. Therefore, the default degradation half-lives estimated for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate are used in this assessment.

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 (see the risk evaluation report for triphenyl phosphate in this series, for example) suggests that

these substances may also be degraded under anaerobic conditions at a similar rate to aerobic conditions. Therefore, for this assessment, it has been assumed that the degradation rate constant (and hence half-life) in sediment will be 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

A K_{oc} value of 2.59×10^4 l/kg can be estimated for isopropylphenyl diphenyl phosphate from its structure using the Syracuse Research Corporation PCKOC version 1.63 software which employs a molecular connectivity index method. Similarly, a K_{oc} value of 6.31×10^5 l/kg can be estimated for tris(isopropylphenyl) phosphate from its structure using the software.

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

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

The log K_{ow} values for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate are 5.3 and 6.1 respectively. The resulting estimated K_{oc} values using the above equation are 5,848 l/kg for isopropylphenyl diphenyl phosphate and 14,421 l/kg for tris(isopropylphenyl) phosphate. As these values are estimated using a method recommended in the TGD, they will be used in the risk assessment. The resulting partition coefficients for soils and sediments calculated from these K_{oc} values are summarised below.

	Isopropylphenyl diphenyl phosphate	Tris(isopropylphenyl) phosphate
K_{oc}	5,848 l/kg	4,421 l/kg
Kp_{susp}	585 l/kg	1,442 l/kg
Kp_{sed}	292 l/kg	721 l/kg
Kp_{soil}	117 l/kg	288 l/kg
$K_{susp\text{-}water}$	147 m^3/m^3	361 m^3/m^3
$K_{sed\text{-}water}$	147 m^3/m^3	361 m^3/m^3
$K_{soil\text{-}water}$	176 m^3/m^3	433 m^3/m^3

These values are used in this risk assessment.

It is possible to use some of the measured levels data in Section 3.3.1 (from Boethling and Cooper 1985) for water and sediment to estimate the sediment-water sorption coefficient. This estimate is somewhat higher than the value estimated above, at 1,670 l/kg. This is limited to one pair of values giving one coefficient value; other limit values in sediment would lead to lower values and the relationship between the water data and sediment data is not specific. As a result, this is not used in this assessment. However, higher sorption coefficients than predicted have been indicated for triphenyl phosphate, and this will be considered in general terms in the overview to this series.

Volatilisation

No studies are available on the volatilisation of isopropylated triphenyl phosphates from water or soil. The Henry's law constant (at 20°C) is estimated as 0.0016 Pa m^3/mol for isopropylphenyl diphenyl phosphate and 0.0087 Pa m^3/mol for tris(isopropylphenyl) phosphate. These values indicate that volatilisation from water is likely to be limited.

Fugacity modelling

The potential environmental distribution of both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) 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 3.2.

The results of the model show that the distribution behaviour of both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate in the environment will be broadly similar. Only a small amount of the substances released to the environment will be in the air compartment at steady state. When the substances are released to air they distribute mainly to the soil compartment, presumably by atmospheric deposition. When they are released to soil, the substances generally remain in the soil, with only a small fraction distributing to the water and sediment compartment. When released to water, the substances are likely to distribute to the sediment and to a lesser extent the water phase at steady state.

The behaviour of both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate during waste water treatment was estimated using the EUSES 2.0 model. The results are summarised below.

	Isopropylphenyl diphenyl phosphate	Tris(isopropylphenyl) phosphate
Degraded	43.7%	16.3%
Adsorbed to sludge	33.8%	56.1%
Volatilised to air	1.58×10^{-3}%	4.31×10^{-3}%
To effluent	22.5%	27.5%

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

Table 3.2 Results of generic level III fugacity model for isopropylated triphenyl phosphates

Input data	Value	
	Isopropylphenyl diphenyl phosphate	Tris(isopropylphenyl) phosphate
Vapour pressure	9.5×10^{-6} Pa at 20°C	2.3×10^{-6} Pa at 20°C
Water solubility	2.2 mg/l	0.12 mg/l
Henry's law constant	0.0016 Pa m^3/mol at 20°C	0.0087 Pa m^3/mol at 20°C
Log K_{ow}	5.3	6.1
Atmospheric half-life	21.4 hours	11.7 hours
Half-life in water	50 days	150 days
Half-life in soil and sediment	900 days	3,000 days

Emission rate	Model results at steady state									
	Isopropylphenyl diphenyl phosphate					Tris(isopropylphenyl) phosphate				
	Amount in air	Amount in soil	Amount in water	Amount in sediment	Overall residence time/ persistence	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	0.025%	90.7%	1.10%	8.19%	680 days	6.8×10^{-3}%	87.6%	0.29%	12.1%	2,070 days
1,000 kg/hour to air 0 kg/hour to soil 0 kg/hour to water	0.089%	98.3%	0.19%	1.43%	570 days	0.035%	97.9%	0.048%	2.04%	1,189 days
0 kg/hour to air 1,000 kg/hour to soil 0 kg/hour to water	7.6×10^{-6}%	99.9%	0.012%	0.086%	1,291 days	2.6×10^{-6}%	99.8%	4.9×10^{-3}%	0.21%	4,284 days
0 kg/hour to air 0 kg/hour to soil 1,000 kg/hour to water	2.1×10^{-5}%	0.023%	11.8%	88.1%	179 days	1.1×10^{-5}%	0.031%	2.31%	97.7%	738 days

3.1.3 Bioaccumulation and metabolism

Measured data

The uptake and accumulation of two commercial isopropylphenyl diphenyl phosphate products (Kronitex 200 and Phosflex 31P) by fathead minnows (*Pimephales promelas*) was studied as part of a 90-day partial life-cycle toxicity study (Cleveland *et al.* 1986; details of the toxicity study are reported in Section 4.1.1). The composition of Kronitex 200 was given as four to six per cent triphenyl phosphate, seven to 10 per cent 2-isopropylphenyl diphenyl phosphate, 20-25 per cent 4-isopropylphenyl diphenyl phosphate, along with bis-(2-isopropylphenyl) phenyl phosphate and minor amounts of di-, tri- and tetra-isopropyl-substituted triphenyl phosphates. The composition of Phosflex 31P was given as 28-30 per cent triphenyl phosphate, along with isomers of isopropylphenyl diphenyl phosphate, isomers of diisopropylphenyl diphenyl phosphate and tri-substituted phenol phosphates. Fish were exposed to five concentrations of the test substance for up to 90 days in a flow-through system. At 30, 60 and 90 days of exposure, a composite sample of ten fish was removed from each treatment group and analysed for the concentration of both isopropylphenyl diphenyl phosphates and triphenyl phosphate. The concentrations of these two components in the water were also determined at fortnightly intervals. The results are summarised in Table 3.3.

Table 3.3 Bioconcentration of a commercial isodecyl diphenyl phosphate in fathead minnow

Product	Mean measured concentration in water (mg/l)		Mean measured concentration in fish (mg/kg wet weight)						BCF at 90 days (l/kg)	
			30 days		60 days		90 days			
	TPP	IPDP	TPP	IPDP	TPP	IPDP	TPP	IPDP	TPP	IPDP
Kronitex 200	0.002	0.003	1	33	2	67	3	23	1,500	7,667
	0.003	0.004	2	29	2	42	3	37	1,000	9,250
	0.005	0.008	3	34	4	141	5	57	1,000	7,125
	0.009	0.015	5	61	14	264	15	92	1,667	6,133
	0.036	0.052	15	285	16	470	31	320	861	6,154
	Control		<1	16	<1	9	<1	3		
Phosflex 31P	0.005	0.003	2	8	3	17	4	23	800	7,667
	0.008	0.006	4	17	5	22	8	37	1,000	6,167
	0.013	0.008	6	25	20	50	16	66	1,231	8,250
	0.014	0.015	12	65	28	122	56	100	4,000	6,667
	Control		<0.8	<2	<0.2	<2	<0.2	<2		

Source: Cleveland *et al.* (1986).
Notes: TPP = Triphenyl phosphate.
IPDP = Isopropylphenyl diphenyl phosphate.

The paper reported that the mean BCF determined at 90 days in this study was 7,266 ± 1,288 l/kg for isopropylphenyl diphenyl phosphate and 1,206 ± 355 l/kg for triphenyl phosphate for experiments using the Kronitex 200 product, and 7,188±1,506 l/kg for isopropylphenyl diphenyl phosphate and 1,758±1,506 l/kg for triphenyl phosphate for the experiments using the Phosflex 31P product. When placed in clean water, depuration of both components from the fish was found to be rapid, with half-lives of less than seven days. The control survival was relatively poor in the series of experiments with Kronitex 200, and treatment-related toxic effects, including effects on

growth, were seen in some of the studies, particularly at the higher concentrations tested. This adds some uncertainty to the BCFs determined in this study.

Muir (1984) and Boethling and Cooper (1985) report the results of unpublished work by Huckins and Petty (1982) that showed that the major route of metabolism of isopropylphenyl diphenyl phosphate in rainbow trout (*Oncorhynchus mykiss*) was O-dearylation to yield diphenyl phosphate. The diphenyl phosphate is then eliminated either as the compound itself or as a conjugate. The same authors determined a bioconcentration factor of 495 l/kg for ^{14}C-labelled isopropylphenyl diphenyl phosphate in fathead minnow (*Pimephales promelas*). The fish were exposed to a concentration of 2.5 μg/l for 28 days using a flow-through system.

No data appear to be available on the uptake of tris(isopropylphenyl) phosphate from water, or the uptake of isopropylated triphenyl phosphates from food.

Calculated data

In addition to a BCF, the TGD also requires a biomagnification factor (BMF) to be taken into account. For both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate, the default BMF would be one based on the BCF values determined above.

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 value 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} value of 5.3 (isopropylphenyl diphenyl phosphate) or 6.1 (tris(isopropylphenyl) phosphate), the $BCF_{earthworm}$ is estimated to be 2,395 (isopropylphenyl diphenyl phosphate) or 15,108. These values are used in this assessment, although their reliability is unknown.

Summary of accumulation

Two studies have investigated the bioconcentration of isopropylphenyl diphenyl phosphate in fish. One series of experiments using commercial products found the BCF to be around 7,188 to 7,266 l/kg, whereas the second series found the BCF to be around 495 l/kg using ^{14}C-labelled isopropylphenyl diphenyl phosphate. There is no obvious explanation for the large difference between the values obtained in the two series of experiments, although the higher values were determined in a toxicity study and so the results may have been affected by the toxicity of the substance to the fish, particularly at the higher concentrations.

No bioconcentration data appear to be available for tris(isopropylphenyl) phosphate.

The log K_{ow} values of isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate are 5.3 and 6.1 respectively. Using the methods recommended in the TGD, a fish BCF value of 6,383 l/kg for isopropylphenyl diphenyl phosphate and 30,549 l/kg for tris(isopropylphenyl) phosphate can be estimated. However, this approach has been shown to overestimate the actual BCF for some triaryl phosphates (for example, see the risk evaluation report for triphenyl phosphate in this series); probably because it assumes that little or no metabolism is occurring.

Annex B considers the available bioconcentration data for triaryl and trialkyl/aryl phosphates as a whole. Based on this information, a BCF of around 564 l/kg for isopropylphenyl phosphate and 1,986 l/kg for tris(isopropylphenyl) phosphate appear to

be appropriate. These values will be used in the risk assessment as they are consistent with the other data available for triaryl and alkyl/aryl phosphates.

However, these values are much lower than have been determined in some studies with isopropylphenyl diphenyl phosphate, and although the results from these studies are considered to be uncertain due to treatment-related toxicity seen at the higher concentrations, the effect of this toxicity on the determined BCF remains unclear.

In addition to a BCF, the TGD also requires a biomagnification factor (BMF) to be taken into account. For both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate, the default BMF would be one based on the BCF values determined above.

Using the methods outlined in the TGD and a log K_{ow} value of 5.3 (isopropylphenyl diphenyl phosphate) or 6.1 (tris(isopropylphenyl) phosphate), the $BCF_{earthworm}$ is estimated as 2,395 (isopropylphenyl diphenyl phosphate) or 15,108. The reliability of these estimates is unknown.

3.2 Environmental releases

3.2.1 General discussion

Releases from the production and use of isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate were estimated using a number of sources such as the default methods from the TGD, the Emission Scenario Document (ESD) on plastics additives (OECD 2004a), the Emission Scenario Document on lubricants (OECD 2004b) and scenarios developed under the Existing Substances Regulation for other substances with similar uses. In the absence of specific information on the substance, the ESDs and the scenarios for other substances are 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 isopropylated triphenyl 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 3.5 and Table 3.6.

3.2.3 Releases from use (processing)

This section contains information on the methods and factors used to estimate emissions from the processing (use) of the substance. This also includes formulation steps where appropriate.

PVC

Emissions from the use in PVC were estimated using the methods outlined in the ESD on plastics additives (OECD 2004a). The ESD provides methods for estimating the releases from three stages:

- handling of raw materials;
- compounding – the blending into the polymer of additives;
- conversion – the forming of the polymer into finished articles.

The first two stages are assumed to always take place together. There are companies which compound the plastics and then sell them on to converters, so separate calculations are carried out for the two as well as for the case where compounding and conversion take place together. The emission factors in the ESD are derived from information on a model substance, di(2-ethylhexyl)phthalate (DEHP), and are modified according to the relative properties of this substance and the substance of interest. The main property affecting the emissions is the vapour pressure of the substance. Both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate have a lower vapour pressure than DEHP at the processing temperatures, and are classed as of low volatility according to the criteria in the ESD[6]. The ESD also uses the particle size or form of the substance in estimating the possible releases from raw materials handling. Both substances are liquids (Section 1.3.1).

The emission factors derived using the ESD methods are (depending on the type of PVC product):

Isopropylphenyl diphenyl phosphate:

- Compounding (including raw materials handling): 0-0.001 per cent to air, 0.01-0.011 per cent to waste water.
- Conversion: 0.001-0.005 per cent to air, 0.001-0.005 per cent to waste water.

Tris(isopropylphenyl) phosphate:

- Compounding (including raw materials handling): 0.001 per cent to air, 0.011 per cent to waste water.
- Conversion: 0.001-0.005 per cent to air, 0.001-0.005 per cent to waste water.

Thermoplastics and polyurethane

Methods from the ESD are also used for these polymeric materials. For these, the emission factors are as follows (the same factors for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate apply where both are used in the type of polymer):

- Compounding (including raw materials handling): 0.001 per cent to air, 0.011 per cent to waste water.
- Conversion: 0.001 per cent to air, 0.001 per cent to waste water.

Textile coating

This use produces PVC coatings on fabrics, and as such can be considered a plastics process. The ESD on plastics additives (OECD 2004a) provides information on release factors for this use and these are used here. The emission factors used are:

[6] 'Low volatility' is used in comparison to DEHP which is of 'medium volatility'. All phosphates assessed in this series have vapour pressures considered low in terms of organic substances.l.

- Compounding (including raw materials handling): 0.01 per cent to water.
- Conversion: 0.005 per cent to air, 0.005 per cent to water

Lubricants

Emissions from the use of the substance in lubricants (from the blending step) were estimated using the methods outlined in the ESD on lubricants (OECD 2004b). Estimates were made for use as an additive in lubricants for both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate. The estimated emissions to air from lubricant blending are very low. The emission factors for releases to water from blending are 1.4×10^{-5} kg/tonne lubricant for isopropylphenyl diphenyl phosphate and 8.6×10^{-6} kg/tonne lubricant for tris(isopropylphenyl) phosphate.

Tris(isopropylphenyl) phosphate is also used as a base fluid for hydraulic fluids. The emission factor to air for this use is estimated using the ESD methods to be 3×10^{-3} kg/tonne lubricant, and the emission factor to water is 5.1×10^{-4} kg/tonne lubricant. These factors are not in fact used, as the emissions are included with those for a production site.

Pigment dispersions

Emissions from this use were estimated using the plastics additives ESD (OECD 2004a), considering a compounding step only. The emission factors are the same as those for thermoplastics and polyurethanes above.

Paints

Emissions from the blending (formulation) of paints and their application were estimated using the TGD default values, which are 0.1 per cent to air and 0.3 per cent to water for formulation, and 0.1 per cent to water for application. This assumes that paints containing the substance are used in industry rather than by the general public.

Adhesives

Information from risk assessments on other substances were used to estimate emissions from formulation into adhesives. These are considered to be negligible.

3.2.4 Releases over lifetime of products

Isopropylated triphenyl phosphates are used in products which are expected to have extended service lives (more than one year). These are therefore potentially important sources of emission. Possible losses from PVC and other polymeric materials through leaching and volatilisation are considered in this section. A limited amount of information on the release of isopropylated triphenyl phosphates is available, and has been included here, but the estimates are based on the methods outlined in the Emission Scenario Document (OECD 2004a) and also take into account the approaches used in the risk assessment of other substances (for example, the risk assessment on medium-chain chlorinated paraffins carried out under the Existing Substances Regulation (ECB 2005)). The approach taken also considers the release of polymer particulates (waste remaining in the environment) over the lifetime of products and at disposal as appropriate; this is based on the treatment of this area in other risk assessments, such as that on medium-chain chlorinated paraffins.

Releases from the service life of lubricants are estimated using the methods in the ESD (OECD 2004b). Where the substance is used as an additive, the emission estimates are those for hydraulic fluids of types HM and HV, leading to releases of eight per cent

to soil and two per cent to water. Where the use is as a base fluid in hydraulic fluids, type HFD fluids have been assumed and the factors are 0.6 per cent to water and 1.4 per cent to soil. For use as a base fluid in power generation fluids, information from the industry indicates that the losses from the use of these fluids are negligible.

Isopropylphenyl diphenyl phosphate is used as a process solvent in the manufacture of adhesives, and none remains in the adhesive at the point of sale. Therefore, there are no emissions from the use of the adhesives.

In the absence of information on the types of polymeric materials in which the pigment dispersions are used, a release of five per cent to cover the service life and losses on disposal (see below) is assumed.

Leaching loss

No information appears to be available on the leaching of isopropylated triphenyl phosphate from products.

Factors from the ESD on plastics additives are used in the assessment for emissions from PVC products and adhesives. Compared to the model substance DEHP in the ESD, isopropylphenyl diphenyl phosphate is classed as a high solubility substance and tris(isopropylphenyl) phosphate is classed as a medium solubility substance, and the factors are increased accordingly from those for DEHP (which is considered to be of low solubility). The factors also depend on the nature of the products and how they are used. A factor of 0.5 per cent over the lifetime of the product is the most widely used value, but higher factors of up to 30 per cent are used for some external uses.

Polyurethane and thermoplastic articles (and some PVC articles) are considered not to come into contact with water on a regular basis in their lifetime and so emissions to water from these uses are considered to be negligible.

Emission factors for paints are also based on the ESD, with leaching of 0.75 per cent per year for tris(isopropylphenyl) phosphate and 1.5 per cent per year for isopropylphenyl diphenyl phosphate (these are based on external use of the paints).

For textiles, the emission estimates are based on the method used in the medium-chain chlorinated paraffins assessment (ECB 2005). This is based on data for the model substance DEHP; hence, the factors are adjusted for solubility as noted above. The factors are 0.25 per cent for tris(isopropylphenyl) phosphate and 0.5 per cent for isopropylphenyl diphenyl phosphate, both over the lifetime of the product and assuming internal use.

Volatile loss

The stability of, and volatile loss from, several commercial aryl and alkyl/aryl phosphate products has been studied using a combination of differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) under both a nitrogen atmosphere (Shankwalkar and Cruz 1994) and an oxygen atmosphere (Shankwalkar and Placek 1992). The results of the studies are summarised in

Table 3.4.

The results under a nitrogen atmosphere show that the triaryl phosphates start to decompose at temperatures of around 310-350°C, whereas the alkyl diphenyl phosphates tested start to decompose at a temperature of around 260°C. The decomposition temperatures under an oxygen atmosphere are significantly lower. For

all the substances tested, significant weight loss occurred at temperatures below that at which decomposition starts indicating a loss of the substance by volatilisation at elevated temperatures.

Table 3.4 Thermal degradation temperature and weight loss of aryl and alkyl/aryl phosphates

Phosphate ester	Experiments under an oxygen atmosphere				Experiments under a nitrogen atmosphere		
	Start of thermal degradation	1% weight loss	5% weight loss	10% weight loss	Start of thermal degradation	5% weight loss	10% weight loss
Triphenyl phosphate	>400°C	188°C	236°C	252°C			
Tricresyl phosphate	215°C	184°C	255°C	252°C	333°C	272°C	306°C
Trixylenyl phosphate	210°C	224°C	268 °C	286°C	311°C	276°C	302°C
Isopropylphenyl diphenyl phosphate[a]	210-215°C	200-218°C	239-265 °C	263-288°C	311-314°C	264-282°C	293-307°C
Tertbutylphenyl diphenyl phosphate[a]	295-305°C	213-234°C	262-277°C	280-295°C	338-347°C	274-278°C	305-306°C
2-Ethylhexyl diphenyl phosphate	200°C	90°C	220°C	229°C	257°C	226°C	231°C
Isodecyl diphenyl phosphate	165°C	93°C	213°C	235°C	264°C	233°C	246°C

Notes: a) Data for three (nitrogen atmosphere) or four (oxygen atmosphere) different grades.

Although isopropylated triphenyl phosphates themselves were not studied in this test, it can be inferred that the weight loss likely from this substance at elevated temperature would be similar to that seen from other triaryl phosphates with similar properties.

The weight loss on heating a 10 mg sample of a commercial isopropylphenyl diphenyl phosphate (Reofos 50) at a rate of 10°C per minute under nitrogen atmosphere has been determined as five per cent at 216°C, ten per cent at 235°C and 50 per cent at 284°C by thermogravimetric analysis (Great Lakes Chemical Corporation 2002).

These data do not allow emission factors for the service life to be estimated. Factors from the ESD on plastics additives are used, as applied in the risk assessment of medium-chain chlorinated paraffins as appropriate. These are applied to articles from PVC, thermoplastics, polyurethane, adhesives and textiles. Volatile losses from products occur at ambient temperatures, and at these temperatures isopropylated triphenyl phosphates are considered to have a low vapour pressure in relation to DEHP, the reference compound. The appropriate factor from the ESD is therefore that for low volatility substances or 0.01 per cent over the lifetime of the product. An exception to this is where the use is in thin films, where a higher value of 0.55 per cent (for isopropylphenyl diphenyl phosphate) or 0.15 per cent (for tris(isopropylphenyl) phosphate) over the lifetime was used. These factors were also used for volatile losses from paints in service.

Waste in the environment

This considers the loss of substance in particles of plastic material from articles in use. The approach is the same as that used in the risk assessment for medium-chain chlorinated paraffins. For use in PVC a loss of zero to five per cent is assumed, depending on the use of the products. For textiles and adhesives, a loss of two per cent of the material over the lifetime of the products or articles is assumed and for paints, a loss of five per cent. For other use areas (thermoplastics and polyurethane), no waste generation during the lifetime is assumed. Losses may also occur on disposal at the end of the service life. A figure of two per cent loss on disposal is assumed for all plastic materials (including textiles) and adhesives. For paints, a loss of five per cent on disposal is assumed. As noted above, losses of pigment dispersions are taken as five per cent across the whole of service life and disposal. In the calculations, the substance in these particles is assumed to be available in the environment; this is likely to be an overestimate, but there are no data to indicate how much may be available.

Other sources of release

A small quantity of isopropylated triphenyl phosphates is not allocated to one of the use areas. It has been assumed that this amount is in fact used in these areas, but passes through a longer supply chain and hence its use is not known to the major producers and suppliers who provided the information. To deal with this, an overall emission factor has been derived from the estimated releases from the quantity allocated to specific uses. This factor has been applied to the unallocated tonnage, and the release divided between the different compartments in the same ratio as for the allocated tonnage. These releases appear in the summary tables (Table 3.5 and Table 3.6) under miscellaneous uses.

3.2.5 Summary of environmental releases

The estimated environmental releases are summarised in Table 3.5 (isopropylphenyl diphenyl phosphate) and Table 3.6 (tris(isopropylphenyl) phosphate).

Table 3.5 Summary of estimated environmental release of isopropylphenyl diphenyl 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			23			1,811 to surface water[c]				
Paints and coatings	Formulation	0.58	1.74							
	Processing		0.018							
	Losses during service life[d]				190	1,710 to surface water		3,717	33,453 to surface water	
	Waste remaining in the environment[d]				3.4	857 to surface water	2,582	31	7,715 to surface water	23,238
Lubricant additive	Blending	1.05×10^{-9}	7.93×10^{-4}		2.7×10^{-7}	0.21		4.77×10^{-7}	0.36	
	Losses in use[d]					476 to surface water	1,904		4,284 to surface water	17,136
Hydraulic fluid	Blending	5.18×10^{-10}	4.37×10^{-4}		3.37×10^{-8}	0.03		3.37×10^{-8}	0.03	
	Losses in use[d]					48 to surface water	192		432 to surface water	1,728
Pigment dispersions	Raw materials handling and compounding	0.002	0.022		e	e				
	In service losses/waste in environment[d]				0.04	8.7 to surface water	26.25	0.32	78.4 to surface water	236
Adhesives		negligible	negligible	neg.	negligible	negligible	negligible	negligible	negligible	negligible

Table 3.5 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	**Water**	**Soil**	**Air**	**Water[a]**	**Soil**	**Air**	**Water[a]**	**Soil**
Textiles/ fabric coating	Raw materials handling and compounding		0.06							
	Conversion	0.03	0.03							
	Raw materials handling, compounding and application	0.03	0.09		e	e		e	e	
	In service losses				4.66	233		41.9	2,097	
	Waste remaining in the environment[d]				1.8	458 to surface water	1,380	16.6	4,124 to surface water	12,423
Thermo-plastics and styrenics	Raw materials handling and compounding	0.001	0.011							
	Conversion	0.001	0.001							
	Raw materials handling, compounding and conversion	0.002	0.012		e	e		e	e	
	In service losses				4.8×10^{-4}			4.3×10^{-3}		
	Waste in the environment[d]				2.0×10^{-3}	0.5 to surface water	1.5	0.02	4.48 to surface water	13.5
Miscellaneous	Unallocated tonnage				15	1,206 + 296 to surface water	927	139	10,858 + 2,665 to surface water	8,346

Table 3.5 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	**Water**	**Soil**	**Air**	**Water[a]**	**Soil**	**Air**	**Water[a]**	**Soil**
PVC – 1[b]	Raw materials handling and compounding		0.032							
	Conversion	0.016	0.016							
	Raw materials handling, compounding and conversion	0.016	0.048		e	e		e	e	
	In service losses				0.96	48		8.64	432	
	Waste in the environment[d]				0.48	121 to surface water	364	4.36	1,087 to surface water	3,274
PVC – 2[b]	Raw materials handling and compounding	0.0025	0.0275							
	Conversion	0.0125	0.0125							
	Raw materials handling, compounding and conversion	0.015	0.040		e	e		e	e	
	In service losses				1.43	71.5		12.87	643.5	
	Waste in the environment[d]				0.28	70.8 to surface water	213	2.56	638 to surface water	1,920

Table 3.5 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	**Water**	**Soil**	**Air**	**Water[a]**	**Soil**	**Air**	**Water[a]**	**Soil**
PVC – 3[b]	Raw materials handling and compounding	0.0031	0.034							
	Conversion	0.0157	0.0157							
	Raw materials handling, compounding and conversion	0.0188	0.050		e	e		e	e	
	In service losses				130	118		1,168	1,062	
	Waste in the environment[d]				0.47	116 to surface water	350	4.2	1046 to surface water	3,152
PVC – 4[b]	Raw materials handling and compounding	0.0025	0.0275							
	Conversion	0.0025	0.0025							
	Raw materials handling, compounding and conversion	0.005	0.030		e	e		e	e	
	In service losses				0.42			3.78		
	Waste in the environment[d]				0.02	4.18 to surface water	12.6	0.15	37.6 to surface water	113

Table 3.5 continued

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	**Water**	**Soil**	**Air**	**Water[a]**	**Soil**	**Air**	**Water[a]**	**Soil**
PVC – 5[b]	Raw materials handling and compounding	0.0025	0.0275							
	Conversion	0.0025	0.0025							
	Raw materials handling, compounding and conversion	0.005	0.03		e	e		e	e	
	In service losses[d]				112	1,568		10.1	14,112	
	Waste in the environment[d]				0.41	103 to surface water	309	3.71	924 to surface water	2,782
PVC – 6[b]	Raw materials handling and compounding	0.0018	0.02							
	Conversion	0.0092	0.0092							
	Raw materials handling, compounding and conversion	0.011	0.029		e	e		e	e	
	In service losses[d]				2.4	6,240 to surface water		21.6	56,160 to surface water	
	Waste in the environment[d]				1.53	381 to surface water	1,148	13.8	3,431 to surface water	10,335

Table 3.5 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	Water	Soil	Air	Water[a]	Soil	Air	Water[a]	Soil
PVC – 7[b]	Raw materials handling and compounding	0.013	0.14							
	Conversion	0.065	0.065							
	Raw materials handling, compounding and conversion	0.08	0.21		e	e		e	e	
	In service losses[d]				6.28	8,792		56.5	79,128	
	Waste in the environment[d]				4.16	1,035 to surface water	3,118	37.4	9,316 to surface water	28,060
Polyurethane	Raw materials handling and compounding	0.015	0.16							
	Conversion	0.015	0.015							
	Raw materials handling, compounding and conversion	0.03	0.178		e	e		e	e	
	In service losses				11.1			99.9		
	Waste in the environment[d]				2.2	552 to surface water	1,662	19.9	4,965 to surface water	14,954
Total					613	27,083	14,199	5,658	239,805	127,750

Notes: a) Regional and continental emissions to water are split 80:20 between waste water treatment and direct discharge to surface water, unless noted.
b) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to that used for tris(isopropylphenyl) phosphate.
c) 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).
d) Releases from the service life for these uses and as waste in the environment are assumed to go directly to surface water.
e) Values for individual steps are confidential, but are included in the total figure.

Table 3.6 Summary of estimated environmental release of tris(isopropylphenyl) 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			7.9			760 to surface water[c]				
Lubricant additive	Blending	2.38×10^{-10}	3.84×10^{-4}		5.38×10^{-8}	0.09		8.07×10^{-8}	0.13	
	Losses in use[d]					304 to surface water	1,216		2,736 to surface water	10,944
Hydraulic fluid	Blending	0.018	2.32×10^{-3}		0.46	0.06		0.7	0.09	
	Losses in use[d]					70 to surface water	162		626 to surface water	1,462
Power generation fluid	Blending	0.018	4.08×10^{-4}		0.45	0.01				
	Losses in use				negligible	negligible	negligible	negligible	negligible	negligible
Paints and coatings	Formulation	0.013	0.04		e	e		e	e	
	Processing		0.015			4				
	Losses during service life[d]				0.58	21 to surface water		5.2	189 to surface water	
	Waste remaining in the environment[d]				0.04	9.69 to surface water	29.2	0.35	87.2 to surface water	263
Pigment dispersions	Raw materials handling and compounding	0.005	0.055							
	In service losses/waste in environment[d]				0.46	115 to surface water	345	4.14	1,031 to surface water	3,105

Table 3.6 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	**Water**	**Soil**	**Air**	**Water[a]**	**Soil**	**Air**	**Water[a]**	**Soil**
Textile/fabric coating	Raw materials handling and compounding		0.05							
	Application of coating	0.025	0.025							
	Raw materials handling, compounding and application	0.025	0.075		e	e				
	In service losses				1.37	34.25		12.3	308	
	Waste remaining in the environment[d]				0.54	135 to surface water	406	4.88	1,214 to surface water	3,657
PVC – 1[b]	Raw materials handling and compounding	0.001	0.011							
	Conversion	0.005	0.005							
	Raw materials handling, compounding and conversion	0.006	0.016		e	e		e	e	
	In service losses				0.15	0.25		1.35	2.25	
	Waste in the environment[d]				1.99×10^{-8}	0.5 to surface water	1.49	0.02	4.5 to surface water	13.4

Table 3.6 continued

Life cycle stage		Local (kg/day)			Regional (kg/year			Continental (kg/year)		
		Air	Water	Soil	Air	Water[a]	Soil	Air	Water[a]	Soil
PVC – 2[b]	Raw materials handling and compounding	0.0073	0.0793							
	Conversion	0.0073	0.0073							
	Raw materials handling, compounding and conversion	0.014	0.085		e	e		e	e	
	In service losses				5.8			52.2		
	Waste in the environment[d]				0.23	57.8 to surface water	174	2.1	520 to surface water	1,566
PVC – 3[b]	Raw materials handling and compounding	0.0025	0.0275							
	Conversion	0.0025	0.0025							
	Raw materials handling, compounding and conversion	0.005	0.03		e	e		e	e	
	In service losses[d]				0.72	522		6.48	4,698	
	Waste in the environment[d]				0.27	68.4 to surface water	206	2.47	616 to surface water	1,854

Table 3.6 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	Water	Soil	Air	Water[a]	Soil	Air	Water[a]	Soil
Polyurethane	Raw materials handling and compounding	0.005	0.055							
	Conversion	0.005	0.005							
	Raw materials handling, compounding and conversion	0.01	0.06		e	e		e	e	
	In service losses				0.31			2.79		
	Waste in the environment[d]				0.06	15.4 to surface water	46.5	0.56	139 to surface water	418
Adhesives	In service losses				0.18	364 to surface water		1.62	3,276 to surface water	
	Waste in the environment[d]				0.06	15.9 to surface water	48	0.58	143 to surface water	432
Miscellaneous	Unallocated tonnage				1.3	43.5 + 89.9 to surface water	201	9.28	392 + 809 to surface water	1,812
Total					26	2,686	2,836	119	16,863	25,514

Notes: a) Regional and continental emissions to water are split 80:20 between waste water treatment and direct discharge to surface water, unless noted.
b) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to that used for tris(isopropylphenyl) phosphate.
c) 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).
d) Releases from the service life for these uses and as waste in the environment are assumed to go directly to surface water.
e) Values for individual steps are confidential, but are included in the total figure.

3.3 Environmental concentrations

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

Calculation of PECs

The PECs for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate in 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 water and sediment are shown in Table 3.7.

The predicted regional concentrations for isopropylphenyl diphenyl phosphate are 0.337 μg/l for surface water and 0.062mg/kg wet weight for sediment. The predicted regional concentrations for tris(isopropylphenyl) phosphate are 0.066 µg/l for surface water and 0.037 mg/kg wet weight for sediment.

Predicted concentrations were also calculated for the marine environment using the EUSES program. These are included in Table 3.8. Note that production is not included in the table as the production sites do not discharge into the marine environment.

Measured levels in water and sediment

Water

Muir (1984) reported that isopropylphenyl diphenyl phosphate was found in surface water near a triaryl phosphate manufacturing plant in the United States at a concentration of below 0.1 μg/l.

Boethling and Cooper (1985) reported that isopropylphenyl diphenyl phosphate was not detected (detection limit 10 μg/l) in water samples collected near an aryl phosphate production site and a large user of hydraulic fluids in the United States in the late 1970s.

Boethling and Cooper (1985) reported the results of a later (early 1980s) survey of the levels of isopropylphenyl diphenyl phosphate in surface water in the United States. The substance was found at 0.4-0.45 μg/l in all four samples from Saginaw River (industrialised area), at 0.25 μg/l in one out seven samples from Kanawha River (industrialised area near to aryl phosphate manufacturer) and at 0.45-0.65 μg/l in three out of four samples from Eastern Lake Superior (remote area) but was not detected (detection limit 0.1-0.5 μg/l) in four samples from Baltimore Harbour (industrialised area), three samples from Detroit River (industrialised area), and four samples from Delaware River (industrialised area near to aryl phosphate manufacturer).

A survey of the levels of tris(isopropylphenyl) phosphate in surface waters from all over Japan has been carried out by Environment Agency Japan (1996). The substance was not detected in 24 samples analysed in 1978 (detection limit in the range 0.05-2 µg/l).

Table 3.7 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 weight)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
Production of isopropylated diphenyl phosphate		0.12	0.05	3.39	1.33	3.27	1.28	0.43	0.42
Lubricant additive	Blending of lubricant	8.93×10^{-5}	5.29×10^{-5}	0.35	0.07	0.34	0.07	0.04	0.02
Hydraulic fluid	Blending of fluid	4.92×10^{-5}	3.19×10^{-4}	0.34	0.10	0.34	0.07	0.04	0.03
Power generation fluid	Blending of fluid Use at power station		5.62×10^{-5} negligible		0.07 negligible		0.07 negligible		0.02 negligible
Adhesives		negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible
Paints	Formulation Application	0.20 1.99×10^{-3}	5.51×10^{-3} 2.07×10^{-3}	19.8 0.53	0.61 0.27	16.3 0.50	0.51 0.10	2.53 0.07	0.19 0.08
Textile/ fabric coating	Compounding Application of coating Combined compounding and application of coating	6.76×10^{-3} 3.38×10^{-3} 0.01	6.89×10^{-3} 3.44×10^{-3} 0.01	1.01 0.67 1.34	0.74 0.40 1.08	0.89 0.61 1.16	0.16 0.11 0.21	0.13 0.09 0.17	0.23 0.13 0.34
Thermo-plastics and styrenics	Compounding Conversion Combined compounding and conversion	1.24×10^{-3} 1.13×10^{-4} 1.35×10^{-3}		0.46 0.35 0.47		0.34 0.35 0.45		0.06 0.04 0.06	

Table 3.7 continued.

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 weight)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
PVC – 1[a]	Compounding	3.6×10^{-3}	1.51×10^{-3}	0.69	0.21	0.63	0.12	0.09	0.07
	Conversion	1.8×10^{-3}	6.89×10^{-4}	0.52	0.13	0.48	0.09	0.07	0.04
	Combined compounding and conversion	5.41×10^{-3}	2.2×10^{-3}	0.87	0.28	0.78	0.15	0.11	0.09
PVC – 2[a]	Compounding	3.1×10^{-3}	0.01	0.64	1.14	0.36	0.95	0.08	0.36
	Conversion	1.41×10^{-3}	1.01×10^{-3}	0.48	0.17	0.35	0.15	0.06	0.05
	Combined compounding and conversion	4.51×10^{-3}	0.01	0.78	1.21	0.38	1.01	0.10	0.38
PVC – 3[a]	Compounding	3.83×10^{-3}	3.79×10^{-3}	0.72	0.44	0.65	0.37	0.09	0.14
	Conversion	1.77×10^{-3}	3.44×10^{-4}	0.51	0.1	0.48	0.09	0.07	0.03
	Combined compounding and conversion	5.63×10^{-3}	4.13×10^{-3}	0.90	0.47	0.80	0.40	0.11	0.15
PVC – 4[a]	Compounding	3.1×10^{-3}		0.64		0.59		0.08	
	Conversion	2.82×10^{-4}		0.37		0.36		0.05	
	Combined compounding and conversion	3.38×10^{-3}		0.67		0.61		0.09	
PVC – 5[a]	Compounding	3.1×10^{-3}		0.64		0.59		0.08	
	Conversion	2.82×10^{-4}		0.37		0.36		0.05	
	Combined compounding and conversion	3.38×10^{-3}		0.67		0.61		0.09	

Table 3.7 continued.

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 weight)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
PVC – 6[a]	Compounding	2.25×10^{-3}		0.56		0.52		0.07	
	Conversion	1.04×10^{-3}		0.44		0.42		0.06	
	Combined compounding and conversion	3.27×10^{-3}		0.66		0.60		0.08	
PVC – 7[a]	Compounding	0.02		1.9		1.62		0.24	
	Conversion	7.32×10^{-3}		1.06		0.93		0.14	
	Combined compounding and conversion	0.02		2.68		2.26		0.34	
Poly-urethane	Compounding	0.02	7.57×10^{-3}	2.12	0.81	1.8	0.20	0.27	0.25
	Conversion	1.69×10^{-3}	6.89×10^{-4}	0.50	0.13	0.47	0.08	0.06	0.04
	Combined compounding and conversion	0.02	8.26×10^{-3}	2.32	0.88	1.97	0.22	0.30	0.28
Pigment dispersions	Production of dispersions	2.48×10^{-3}	7.57×10^{-3}	0.58	0.81	0.37	0.68	0.07	0.25

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

Table 3.8 Summary of predicted local concentrations for the marine compartment

Scenario		PEC_{local}					
		Marine water - emission episode (μg/l)		Marine water - annual average (μg/l)		Marine sediment (mg/kg wet weight)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
Lubricant additive	Blending of lubricant	0.04	8.27×10^{-3}	0.03	7.51×10^{-3}	4.47×10^{-3}	2.6×10^{-3}
Hydraulic fluid	Blending of fluid	0.03	0.02	0.03	7.2×10^{-3}	4.24×10^{-3}	5.58×10^{-3}
Power generation fluid	Blending of fluid		8.39×10^{-3}		8.04×10^{-3}		2.64×10^{-3}
	Use at power station		negligible		negligible		negligible
Adhesives		negligible	negligible	negligible	negligible	negligible	negligible
Paints	Formulation	8.66	0.20	7.12	0.17	1.11	0.06
	Application	0.12	0.08	0.10	0.02	0.02	0.03
Textile/fabric coating	Compounding	0.33	0.25	0.28	0.04	0.04	0.08
	Application of coating	0.18	0.13	0.15	0.02	0.02	0.04
	Combined compounding and application of coating	0.48	0.37	0.40	0.06	0.06	0.12
Thermoplastics and styrenics	Compounding	0.09		0.03		0.01	
	Conversion	0.04		0.04		4.6×10^{-3}	
	Combined compounding and conversion	0.09		0.08		0.01	

Table 3.8 continued.

Scenario		PEC_{local}					
		Marine water - emission episode (μg/l)		Marine water - annual average (μg/l)		Marine sediment (mg/kg wet weight)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
PVC – 1	Compounding	0.19	0.06	0.16	0.03	0.02	0.02
	Conversion	0.11	0.03	0.10	0.02	0.01	9.7×10^{-3}
	Combined compounding and conversion	0.27	0.08	0.23	0.04	0.03	0.03
PVC – 2	Compounding	0.17	0.39	0.04	0.33	0.02	0.12
	Conversion	0.09	0.04	0.04	0.04	0.01	0.01
	Combined compounding and conversion	0.23	0.42	0.05	0.35	0.03	0.13
PVC – 3	Compounding	0.20	0.14	0.17	0.12	0.03	0.04
	Conversion	0.11	0.02	0.10	0.02	0.01	5.85×10^{-3}
	Combined compounding and conversion	0.28	0.15	0.24	0.13	0.04	0.05
PVC – 4	Compounding	0.17		0.14		0.02	
	Conversion	0.04		0.04		5.55×10^{-3}	
	Combined compounding and conversion	0.18		0.15		0.02	
PVC – 5	Compounding	0.17		0.14		0.02	
	Conversion	0.04		0.04		5.55×10^{-3}	
	Combined compounding and conversion	0.18		0.15		0.02	

Table 3.8 continued.

Scenario		PEC_{local}					
		Marine water - emission episode (μg/l)		Marine water - annual average (μg/l)		Marine sediment (mg/kg wet weight)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
PVC – 6	Compounding	0.13		0.11		0.02	
	Conversion	0.08		0.07		9.8×10^{-3}	
	Combined compounding and conversion	0.18		0.15		0.02	
PVC – 7	Compounding	0.73		0.6		0.09	
	Conversion	0.35		0.3		0.05	
	Combined compounding and conversion	1.07		0.89		0.14	
Polyurethane	Compounding	0.82	0.28	0.68	0.06	0.11	0.09
	Conversion	0.11	0.03	0.09	0.01	0.01	9.7×10^{-3}
	Combined compounding and conversion	0.91	0.3	0.76	0.06	0.12	0.09
Pigment dispersions	Production of dispersions	0.14	0.28	0.04	0.23	0.02	0.09

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

Sediment

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. 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 survey 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 one mg/kg were found in some samples ten miles downstream. The report indicates that the actual concentration present in the 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 also indicate that isopropylphenyl diphenyl phosphate itself was found to be present at 8 mg/kg in a single sediment sample collected earlier from the same area.

Boethling and Cooper (1985) reported the results of a later (early 1980s) survey of the levels of isopropylphenyl diphenyl phosphate in sediments from the United States. The substance was found at 0.6-0.75 mg/kg in three out of four samples from Saginaw River (industrialised area), at 0.13-0.98 mg/kg in three out of three samples from Baltimore Harbour (industrialised area), below 1.3 mg/kg in two samples from Detroit River (industrialised area) and below 0.4 mg/kg in one out of six samples from Kanawha River (industrialised area near to aryl phosphate manufacturer), but was not found (detection limit 0.03-0.2 mg/kg) in two samples from Delaware River (industrialised area near to aryl phosphate manufacturer) and four samples from Eastern Lake Superior (remote area).

A survey of the levels of tris(isopropylphenyl) phosphate in sediments from all over Japan was carried out by Environment Agency Japan (1996). The substance was detected in three out of 24 samples analysed in 1978 at a concentration of 100 μg/kg dry weight (the detection limit was in the range 10 to 100 μg/kg dry weight).

Comparison of measured levels with predicted levels

The available monitoring data is limited in its scope. Much of the data is from the 1970s and early 1980s in North America and it is not known if the levels found are representative of the current situation in Europe. Nevertheless, concentrations in the range up to one mg/kg have been found in sediments in industrial areas in the United States, and a concentration of 8 mg/kg was reported in a sediment sample close to a production site in the United States. These values are reasonably consistent with the predicted levels. Predicted levels 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 3.9.

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

Isopropylphenyl diphenyl phosphate	$PEC_{regional}$	= 2.21×10^{-3} mg/kg wet weight for agricultural soil
		= 0.02 μg/l for pore water of agricultural soil
		= 1.62×10^{-4} mg/kg wet weight for natural soil
		= 0.13 mg/kg wet weight for industrial soil
Tris(isopropylphenyl) phosphate	$PEC_{regional}$	= 4.26×10^{-4} mg/kg wet weight for agricultural soil
		= 1.67×10^{-3} μg/l for pore water agricultural soil
		= 6.30×10^{-5} mg/kg wet weight for natural soil
		= 0.08 mg/kg wet weight for industrial soil

Measured levels

Boethling and Cooper (1985) reported that isopropylphenyl diphenyl phosphate was not detected (detection limit 0.1 mg/kg) in soil samples collected near to an aryl phosphate production site and a large user of hydraulic fluids in the United States.

In a further study reported in Boethling and Cooper (1985), isopropylphenyl diphenyl phosphate was present at a concentration of up to 4,000 μg/kg in soil samples collected near a production plant in the United States in 1979. The area sampled was reported to be subject to spills. Isopropylphenyl diphenyl phosphate was also found at 0.1 mg/kg in soil from another production plant, at up to 0.5 mg/kg in soil near a steel works and at up to one mg/kg in soil from near a PVC processor.

Boethling and Cooper (1985) report the results of monitoring studies carried out in the late 1970s near 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

The measured data appear to refer mainly to spillages. The predicted levels are calculated based on aerial deposition and application of sewage sludge as the main routes to soil and so are not directly comparable to the measured levels. Predicted levels are therefore used in the risk characterisation.

Table 3.9 Summary of predicted local concentrations for the terrestrial compartment

Scenario		PEC_{local}					
		Agricultural soil – 30 day average (mg/kg wet wt.)		Agricultural soil – 180 day average (mg/kg wet wt.)		Ground water under agricultural soil (μg/l)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
Production of isopropylated diphenyl phosphate		1.73×10^{-4}[b]	8.56×10^{-5}[b]	1.73×10^{-4}[b]	8.59×10^{-5}[b]	1.67×10^{-3}[b]	3.38×10^{-4}
Lubricant additive	Blending of lubricant	2.03×10^{-3}	2.85×10^{-3}	1.92×10^{-3}	2.81×10^{-3}	0.02	0.01
Hydraulic fluid	Blending of fluid	1.19×10^{-3}	0.02	1.13×10^{-3}	0.02	0.01	0.07
Power generation fluid	Blending of fluid		4.06×10^{-3}		4.02×10^{-3}		0.02
	Use at power station		negligible		negligible		negligible
Adhesives		negligible	negligible	negligible	negligible	negligible	negligible
Paints	Formulation	4.11	0.29	3.88	0.29	37.5	1.13
	Application	0.04	0.11	0.04	0.11	0.38	0.42
Textile/fabric coating	Compounding	0.14	0.36	0.13	0.36	1.29	1.4
	Application of coating	0.07	0.18	0.07	0.18	0.65	0.70
	Combined compounding and application of coating	0.21	0.55	0.20	0.54	1.94	2.11
Thermo-plastics and styrenics	Compounding	0.03		0.02		0.24	
	Conversion	2.55×10^{-3}		2.41×10^{-3}		0.02	
	Combined compounding and conversion	0.03		0.03		0.26	

Table 3.9 continued.

Scenario		PEC_{local}					
		Agricultural soil – 30 day average (mg/kg wet wt.)		Agricultural soil – 180 day average (mg/kg wet wt.)		Ground water under agricultural soil (μg/l)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
PVC – 1[a]	Compounding	0.08	0.08	0.07	0.08	0.69	0.31
	Conversion	0.04	0.04	0.04	0.04	0.35	0.14
	Combined compounding and conversion	0.11	0.12	0.11	0.11	1.04	0.45
PVC – 2[a]	Compounding	0.07	0.58	0.06	0.57	0.59	2.23
	Conversion	0.03	0.05	0.03	0.05	0.27	0.21
	Combined compounding and conversion	0.09	0.62	0.09	0.61	0.86	2.39
PVC – 3[a]	Compounding	0.08	0.20	0.08	0.20	0.73	0.77
	Conversion	0.04	0.02	0.04	0.02	0.34	0.07
	Combined compounding and conversion	0.12	0.22	0.11	0.22	1.08	0.84
PVC – 4[a]	Compounding	0.07		0.06		0.59	
	Conversion	6.11×10^{-3}		5.78×10^{-3}		0.06	
	Combined compounding and conversion	0.07		0.07		0.65	

Table 3.9 continued.

Scenario		PEC_{local}					
		Agricultural soil – 30 day average (mg/kg wet wt.)		Agricultural soil – 180 day average (mg/kg wet wt.)		Ground water under agricultural soil (μg/l)	
		Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)	Isopropyl phenyl diphenyl	Tris(iso-propyl phenyl)
PVC – 5[a]	Compounding	0.06		0.06		0.59	
	Conversion	6.11×10^{-3}		5.78×10^{-3}		0.06	
	Combined compounding and conversion	0.07		0.07		0.65	
PVC – 6[a]	Compounding	0.05		0.04		0.43	
	Conversion	0.02		0.02		0.20	
	Combined compounding and conversion	0.07		0.06		0.63	
PVC – 7[a]	Compounding	0.33		0.31		3.01	
	Conversion	0.16		0.15		1.41	
	Combined compounding and conversion	0.50		0.47		4.54	
Polyurethane	Compounding	0.38	0.40	0.36	0.39	3.44	1.54
	Conversion	0.04	0.04	0.03	0.04	0.33	0.14
	Combined compounding and conversion	0.42	0.44	0.40	0.43	3.84	1.68
Pigment dispersions	Production of dispersions	0.05	0.40	0.05	0.39	0.48	1.54

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used from tris(isopropylphenyl) phosphate.
b) Sludge from the production sites is not applied to agricultural land.

3.3.3 Air compartment

Calculation of PECs

The concentrations in air were estimated using EUSES 2.0.3. The PECs calculated are summarised in Table 3.10.

The predicted regional concentration is 1.88×10^{-8} mg/m^3 for isopropylphenyl diphenyl phosphate and 3.24×10^{-9} mg/m^3 for tris(isopropylphenyl) phosphate.

Table 3.10 Summary of predicted local concentrations for the air compartment

Scenario		Local concentrations	
		Annual average concentration in air (mg/m^3)	
		Isopropylphenyl diphenyl	Tris(isopropyl phenyl)
Production of isopropylated diphenyl phosphate		1.15×10^{-7}	9.35×10^{-8}
Lubricant additive	Blending of lubricant	1.88×10^{-8}	3.25×10^{-9}
Hydraulic fluid	Blending of fluid	1.88×10^{-8}	3.6×10^{-7}
Power generation fluid	Blending of fluid Use at power station		4.12×10^{-6} negligible
Adhesives		negligible	negligible
Paints	Formulation Application	1.33×10^{-4} 1.88×10^{-8}	2.97×10^{-6} 3.27×10^{-9}
Textile/fabric coating	Compounding Application of coating Combined compounding and application of coating	1.9×10^{-8} 6.87×10^{-6} 6.87×10^{-6}	3.33×10^{-9} 9.93×10^{-7} 9.93×10^{-7}
Thermo-plastics and styrenics	Compounding Conversion Combined compounding and conversion	1.95×10^{-8} 2.97×10^{-7} 4.76×10^{-7}	
PVC – 1[a]	Compounding Conversion Combined compounding and conversion	1.89×10^{-8} 3.67×10^{-6} 3.67×10^{-6}	1.07×10^{-7} 5.21×10^{-7} 6.25×10^{-7}
PVC – 2[a]	Compounding Conversion Combined compounding and conversion	7.97×10^{-8} 3.23×10^{-7} 3.84×10^{-7}	1.67×10^{-6} 1.67×10^{-6} 3.2×10^{-6}
PVC – 3[a]	Compounding Conversion Combined compounding and conversion	7.27×10^{-7} 3.61×10^{-6} 4.31×10^{-6}	5.74×10^{-7} 5.74×10^{-7} 1.15×10^{-6}

Table 3.10 continued.

Scenario		Local concentrations	
		Annual average concentration in air (mg/m^3)	
		Isopropyl phenyl diphenyl	Tris(isopropyl phenyl)
PVC – 4[a]	Compounding	5.9×10^{-7}	
	Conversion	5.9×10^{-7}	
	Combined compounding and conversion	1.16×10^{-6}	
PVC – 5[a]	Compounding	5.9×10^{-7}	
	Conversion	5.9×10^{-7}	
	Combined compounding and conversion	1.16×10^{-6}	
PVC – 6[a]	Compounding	4.3×10^{-7}	
	Conversion	2.12×10^{-6}	
	Combined compounding and conversion	2.53×10^{-6}	
PVC – 7[a]	Compounding	2.99×10^{-6}	
	Conversion	1.49×10^{-5}	
	Combined compounding and conversion	1.83×10^{-5}	
Polyurethane	Compounding	3.45×10^{-6}	2.62×10^{-7}
	Conversion	3.45×10^{-6}	2.62×10^{-7}
	Combined compounding and conversion	6.87×10^{-6}	5.21×10^{-7}
Pigment dispersions	Production of dispersions	8.58×10^{-8}	1.15×10^{-6}

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

Measured levels

Boethling and Cooper (1985) reported that isopropylphenyl diphenyl phosphate was not detected (detection limit 2 μg/m^3) in air samples collected near an aryl phosphate production site and a large user of hydraulic fluids in the United States.

Boethling and Cooper also report the results of a more extensive investigation of the levels of isopropylphenyl diphenyl phosphate in air close to two aryl phosphate producer sites, an aryl phosphate formulation site, and three user sites (two steel works and a PVC processor). Isopropylphenyl diphenyl phosphate was found in air from one of the production sites at a concentration up to 0.05 ng/m^3, in air from the formulation site at up to 0.0001 ng/m^3 and at air from one steel works at 0.005-0.040 ng/m^3.

Sjödin *et al.* (2001) investigated the levels of isopropylphenyl phosphate in indoor and outdoor air at various locations in Sweden. Indoor air samples were taken from an electronics equipment recycling plant (samples taken on two working days at three locations in the dismantling hall and one close to the shredder), a printed circuit board manufacturing plant (samples taken on one working day at three locations within the plant), a computer repair facility (samples taken on one day at one location), from a computer teaching hall with 20 computers (samples taken on one day at one location) and two offices equipped with two or three computers (samples taken on one day in two different offices). The outdoor air sample was taken from a suburban area close to Stockholm. Samples were collected using personal sampling equipment and were

collected over a 500-minute period at a flow rate of 3.0 l/minute (corresponding to a total air sample of 1.5 m^3) or a 400-minute period at a flow rate of 9.0 l/minute (corresponding to a total air sample of 3.6 m^3). Two duplicate samplers were used at each location investigated. Isopropylphenyl phosphate was found in air samples from the electronics equipment recycling facility at 3.4 to 15 ng/m^3 (mean 7.7 ng/m^3) in the dismantling hall and 54 to 100 ng/m^3 in the shredder room. The isopropyldiphenyl phenyl phosphate was found to be associated mainly with the particulate phase. In addition to isopropylphenyl diphenyl phosphate, the study also found two isomers of propylphenyl diphenyl phosphate to be present in the samples (1.3-5.1 ng/m^3 (mean 3.1 ng/m^3) and 0.7-3.1 ng/m^3 (mean 1.9 ng/m^3) for the two isomers respectively in the dismantling hall and 20-39 ng/m^3 and 16-26 ng/m^3 respectively in the shredder room). No data were reported for the levels of isopropylphenyl diphenyl phosphate or propylphenyl diphenyl phosphate in air from the other locations sampled.

IUCLID (2000) reports that isopropylated triphenyl phosphates were found at two out of 24 sites in the United States at a concentration of 0.4-0.5 μg/l. No further details of this study are available.

Comparison of measured levels with predicted levels

The measured levels in air are all very low. Isopropylphenyl diphenyl phosphate has been detected in air near to production sites, and in air at an electronics equipment recycling facility. However, the coverage of the available measured data is limited in relation to the scenarios considered in this assessment and so the predicted concentrations will be used in the risk characterisation.

3.3.4 Non-compartment specific exposure relevant for the food chain

Predicted concentrations in biota and food

The predicted concentrations of both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate in fish and earthworms are shown in Table 3.11 and predicted concentrations in marine fish for marine predators and marine top predators are shown in Table 3.12. Predicted concentrations in food for human consumption are shown in Table 3.13 for isopropylphenyl diphenyl phosphate and Table 3.14 for tris(isopropylphenyl) phosphate. Concentrations were calculated using EUSES 2.0.

Measured levels in biota and food

Muir (1984) found isopropylphenyl diphenyl phosphate in fish near a triaryl phosphate manufacturing plant in the United States at a concentration of 0.1 to 8 μg/kg.

Boethling and Cooper report that components of a commercial triaryl phosphate functional fluid product (Houghto-Safe 1120) that contained mixed isopropylated triphenyl phosphates were found in bottom-feeding fish collected downstream (100 feet to 1.5 miles downstream) of a steel mill discharge. The total triaryl phosphate concentrations found were in the range 0.1 to 0.3 mg/kg muscle.

Total diet studies carried out in the United States between April 1982 and April 1984 indicated that the mean total daily intake of isopropylated triphenyl phosphate was

0.1 ng/kg body weight in infants, 0.7 ng/kg body weight for toddlers, 0.2-0.4 ng/kg body weight for 14-16 year olds and 0.4-0.8 ng/kg body weight for adults (Gunderson 1988).

Gilbert *et al.* (1986) carried out a survey of the levels of total trialkyl and triaryl phosphates, including isopropylphenyl diphenyl 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 diet). Isopropylphenyl diphenyl phosphate, bis(2-isopropylphenyl) phenyl phosphate and bis(4-isopropylphenyl) phenyl phosphate were all included in the survey but were not found to be present in any of the samples analysed.

Boethling and Cooper (1985) reported that isopropylphenyl diphenyl phosphate was present at a concentration of 1,000-5,000 μg/kg in four vegetation samples collected near to three users of triaryl phosphates (two steel works and a PVC processor) in the United States in 1979.

Comparison of measured levels with predicted levels

The available measured data indicate that isopropylphenyl diphenyl phosphate has been found in fish and plants near to sources of release. A survey of the levels in food for human consumption in the United Kingdom found that the substance was generally not present in the food sampled, whereas the substance was found in samples from the United States. As the available monitoring data are limited in their coverage of the scenarios considered in this assessment, predicted levels are used in the assessment.

Table 3.11 Summary of predicted local concentrations for secondary poisoning

Scenario		Predicted concentration			
		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		Fish (mg/kg)	Earthworms (mg/kg)	Fish (mg/kg)	Earthworms (mg/kg)
Production of isopropylated diphenyl phosphate		1.02	0.03	1.34	0.01[a]
Lubricant additive	Blending of lubricant	0.19	0.04	0.14	0.09
Hydraulic fluid	Blending of fluid	0.19	0.03	0.13	0.46
Power generation fluid	Blending of fluid Use at power station			0.14 negligible	0.12 negligible
Adhesives		negligible	negligible	negligible	negligible
Paints	Formulation Application	4.69 0.24	40.6 0.44	0.57 0.16	7.66 2.87
Textile/fabric coating	Compounding Application of coating Combined compounding and application of coating	0.35 0.27 0.42	1.42 0.73 2.12	0.23 0.18 0.27	9.55 4.79 14.3
Thermoplastics and styrenics	Compounding Conversion Combined compounding and conversion	0.19 0.19 0.22	0.28 0.05 0.30		
PVC – 1[a]	Compounding Conversion Combined compounding and conversion	0.27 0.23 0.31	0.77 0.40 1.14	0.19 0.16 0.21	2.11 0.97 3.07
PVC – 2[a]	Compounding Conversion Combined compounding and conversion	0.20 0.19 0.20	0.66 0.32 0.96	1.0 0.21 1.07	15.1 1.42 16.2

Table 3.11 continued.

Scenario		Predicted concentration			
		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		Fish (mg/kg)	Earthworms (mg/kg)	Fish (mg/kg)	Earthworms (mg/kg)
PVC – 3[a]	Compounding	0.28	0.82	0.43	5.26
	Conversion	0.23	0.39	0.16	0.49
	Combined compounding and conversion	0.32	1.19	0.46	5.74
PVC – 4[a]	Compounding	0.26	0.66		
	Conversion	0.20	0.08		
	Combined compounding and conversion	0.27	0.72		
PVC – 5[a]	Compounding	0.26	0.66		
	Conversion	0.20	0.08		
	Combined compounding and conversion	0.27	0.72		
PVC – 6[a]	Compounding	0.24	0.49		
	Conversion	0.21	0.24		
	Combined compounding and conversion	0.27	0.70		
PVC – 7[a]	Compounding	0.55	3.28		
	Conversion	0.36	1.55		
	Combined compounding and conversion	0.73	4.93		
Polyurethane	Compounding	0.60	3.75	0.27	10.5
	Conversion	0.23	0.38	0.14	1.0
	Combined compounding and conversion	0.65	4.17	0.28	11.5
Pigment disp.	Production of dispersions	0.20	0.54	0.74	10.5

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.
b) Sludge from the production site is not spread onto land.

Table 3.12 Summary of predicted concentrations for secondary poisoning (marine compartment)

Scenario		Predicted concentration			
		Isopropyl phenyl diphenyl		Tris(isopropyl phenyl)	
		Marine fish (mg/kg)	Marine top predators (mg/kg)	Marine fish (mg/kg)	Marine top predators (mg/kg)
Lubricant additive	Blending of lubricant	0.02	0.02	0.01	0.01
Hydraulic fluid	Blending of fluid	0.02	0.02	0.01	0.01
Power generation fluid	Blending of fluid			0.01	0.01
	Use at power station			negligible	negligible
Adhesives		negligible	negligible	negligible	negligible
Paints	Formulation	2.02	0.42	0.17	0.04
	Application	0.04	0.02	0.02	0.01
Textile/fabric coating	Compounding	0.09	0.03	0.05	0.02
	Application of coating	0.05	0.02	0.03	0.02
	Combined compounding and application of coating	0.12	0.04	0.06	0.02
Thermoplastics and styrenics	Compounding	0.02	0.02		
	Conversion	0.02	0.02		
	Combined compounding and conversion	0.03	0.02		
PVC – 1[a]	Compounding	0.05	0.02	0.03	0.02
	Conversion	0.04	0.02	0.02	0.01
	Combined compounding and conversion	0.07	0.03	0.04	0.02
PVC – 2[a]	Compounding	0.02	0.02	0.33	0.08
	Conversion	0.02	0.02	0.04	0.02
	Combined compounding and conversion	0.02	0.02	0.35	0.08

Table 3.12 continued.

Scenario		Predicted concentration			
		Isopropyl phenyl diphenyl		Tris(isopropyl phenyl)	
		Marine fish (mg/kg)	Marine top predators (mg/kg)	Marine fish (mg/kg)	Marine top predators (mg/kg)
PVC – 3 [a]	Compounding	0.06	0.03	0.12	0.03
	Conversion	0.04	0.02	0.02	0.01
	Combined compounding and conversion	0.07	0.03	0.13	0.04
PVC – 4 [a]	Compounding	0.05	0.02		
	Conversion	0.02	0.02		
	Combined compounding and conversion	0.05	0.02		
PVC – 5 [a]	Compounding	0.05	0.02		
	Conversion	0.02	0.02		
	Combined compounding and conversion	0.05	0.02		
PVC – 6 [a]	Compounding	0.04	0.02		
	Conversion	0.03	0.02		
	Combined compounding and conversion	0.05	0.02		
PVC – 7 [a]	Compounding	0.18	0.05		
	Conversion	0.09	0.03		
	Combined compounding and conversion	0.26	0.07		
Polyurethane	Compounding	0.20	0.05	0.06	0.02
	Conversion	0.03	0.02	0.02	0.01
	Combined compounding and conversion	0.22	0.06	0.07	0.02
Pigment disp.	Production of dispersions	0.02	0.02	0.23	0.06

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

Table 3.13 Summary of predicted local concentrations in food for human consumption for isopropylphenyl diphenyl phosphate

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 isopropylated diphenyl phosphate		1.84	2.59×10^{-3}	1.62×10^{-4}	8.17×10^{-4}	2.81×10^{-4}	8.87×10^{-5}	9.6×10^{-8}	3.07×10^{-3}
Lubricant additive	Blending of lubricant	0.19	0.03	4.05×10^{-5}	8.58×10^{-5}	3.67×10^{-5}	1.16×10^{-5}	2.52×10^{-12}	4.8×10^{-4}
Hydraulic fluid	Blending of fluid	0.19	0.02	3.46×10^{-5}	8.44×10^{-5}	3.48×10^{-5}	1.1×10^{-5}	3.31×10^{-13}	4.09×10^{-4}
Adhesives		negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible
Paints	Formulation	9.2	58.2	0.21	0.04	0.08	0.03	1.33×10^{-4}	0.34
	Application	0.28	0.59	3.19×10^{-4}	3.82×10^{-4}	1.9×10^{-4}	6.01×10^{-5}	6.37×10^{-11}	3.73×10^{-3}
Textile/ fabric coating	Compounding	0.5	2.0	1.02×10^{-3}	1.29×10^{-3}	6.2×10^{-4}	1.96×10^{-4}	2.16×10^{-10}	0.01
	Application of coating	0.35	1.01	0.01	6.54×10^{-4}	3.57×10^{-3}	1.13×10^{-3}	6.85×10^{-6}	6.34×10^{-3}
	Combined compounding and application of coating	0.66	3.01	0.01	1.94×10^{-3}	4.18×10^{-3}	1.32×10^{-3}	6.85×10^{-6}	0.02
Thermo-plastics and styrenics	Compounding	0.19	0.37	2.1×10^{-4}	2.38×10^{-4}	1.22×10^{-4}	3.87×10^{-5}	7.62×10^{-10}	2.35×10^{-3}
	Conversion	0.20	0.04	4.32×10^{-4}	8.7×10^{-5}	1.7×10^{-4}	5.37×10^{-5}	2.78×10^{-7}	5.32×10^{-4}
	Combined compounding and conversion	0.25	0.40	8.64×10^{-4}	2.6×10^{-4}	3.49×10^{-4}	1.1×10^{-4}	4.57×10^{-7}	2.65×10^{-3}

Table 3.13 continued.

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)
PVC – 1[a]	Compounding	0.36	1.07	5.54×10^{-4}	6.89×10^{-4}	3.35×10^{-4}	1.06×10^{-4}	1.15×10^{-10}	6.48×10^{-3}
	Conversion	0.27	0.54	5.4×10^{-3}	3.49×10^{-4}	$1.91x10^{-3}$	6.04×10^{-4}	3.66×10^{-6}	3.53×10^{-3}
	Combined compounding and conversion	0.44	1.61	5.93×10^{-3}	1.04×10^{-3}	2.24×10^{-3}	7.07×10^{-4}	3.66×10^{-6}	9.68×10^{-3}
PVC – 2[a]	Compounding	0.21	0.92	5.65×10^{-4}	5.93×10^{-4}	3.19×10^{-4}	1.01×10^{-4}	6.09×10^{-8}	5.4×10^{-3}
	Conversion	0.2	0.42	6.59×10^{-4}	2.71×10^{-4}	2.82×10^{-4}	8.92×10^{-5}	3.05×10^{-7}	2.64×10^{-3}
	Combined compounding and conversion	0.21	1.34	1.2×10^{-3}	8.62×10^{-4}	5.9×10^{-4}	1.87×10^{-4}	3.66×10^{-7}	7.72×10^{-3}
PVC – 3[a]	Compounding	0.37	1.14	1.58×10^{-3}	7.33×10^{-4}	6.92×10^{-4}	2.19×10^{-4}	7.08×10^{-7}	6.89×10^{-3}
	Conversion	0.27	0.53	5.3×10^{-3}	3.43×10^{-4}	1.87×10^{-3}	5.93×10^{-4}	3.59×10^{-6}	
	Combined compounding and conversion	0.45	1.67	6.85×10^{-3}	1.08×10^{-3}	2.56×10^{-3}	8.09×10^{-4}	4.3×10^{-6}	0.01
PVC – 4[a]	Compounding	0.33	0.92	1.28×10^{-3}	5.93×10^{-4}	5.61×10^{-4}	1.77×10^{-4}	5.71×10^{-7}	5.63×10^{-3}
	Conversion	0.20	0.09	8.67×10^{-4}	8.99×10^{-5}	$3.16x10^{-4}$	1.0×10^{-4}	5.71×10^{-7}	
	Combined compounding and conversion	0.35	1.0	2.12×10^{-3}	6.48×10^{-4}	8.58×10^{-4}	2.71×10^{-4}	1.14×10^{-6}	6.13×10^{-3}

Table 3.13 continued.

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)
PVC – 5[a]	Compounding	0.33	0.92	1.28×10^{-3}	5.93×10^{-4}	5.61×10^{-4}	1.77×10^{-4}	5.71×10^{-7}	5.63×10^{-3}
	Conversion	0.20	0.09	8.67×10^{-4}	8.99×10^{-5}	3.16×10^{-4}	1.0×10^{-4}	5.71×10^{-7}	8.28×10^{-4}
	Combined compounding and conversion	0.35	1.0	2.12×10^{-3}	6.48×10^{-4}	8.58×10^{-4}	2.71×10^{-4}	1.14×10^{-6}	6.13×10^{-3}
PVC – 6[a]	Compounding	0.29	0.67	9.31×10^{-4}	4.32×10^{-4}	4.09×10^{-4}	1.29×10^{-4}	4.11×10^{-7}	4.18×10^{-3}
	Conversion	0.24	0.31	3.12×10^{-3}	2.02×10^{-4}	1.1×10^{-3}	3.49×10^{-4}	2.1×10^{-6}	2.17×10^{-3}
	Combined compounding and conversion	0.34	0.97	4.02×10^{-3}	6.28×10^{-4}	1.5×10^{-3}	4.74×10^{-4}	2.51×10^{-6}	5.99×10^{-3}
PVC – 7[a]	Compounding	0.92	4.67	6.48×10^{-3}	3.01×10^{-3}	2.84×10^{-3}	9.0×10^{-4}	2.97×10^{-6}	0.03
	Conversion	0.53	2.19	0.02	1.41×10^{-3}	7.73×10^{-3}	2.44×10^{-3}	1.49×10^{-5}	0.01
	Combined compounding and conversion	1.28	7.03	0.03	4.54×10^{-3}	0.01	3.43×10^{-3}	1.83×10^{-5}	0.04
Poly-urethane	Compounding	1.02	5.34	7.45×10^{-3}	3.44×10^{-3}	3.27×10^{-3}	1.03×10^{-4}	3.43×10^{-6}	0.03
	Conversion	0.27	0.51	5.07×10^{-3}	3.28×10^{-4}	1.79×10^{-3}	5.66×10^{-4}	3.43×10^{-6}	
	Combined compounding and conversion	1.11	5.94	0.01	3.84×10^{-3}	5.08×10^{-3}	1.61×10^{-3}	6.85×10^{-6}	0.03
Pigment dispersion	Production of dispersions	0.21	0.74	4.83×10^{-4}	4.75×10^{-4}	2.66×10^{-4}	8.4×10^{-5}	6.7×10^{-8}	4.4×10^{-3}
Regional sources		0.19	0.03	4.26×10^{-5}	8.42×10^{-5}	4.28×10^{-5}	1.35×10^{-5}	1.88×10^{-8}	4.97×10^{-4}

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

Table 3.14 Summary of predicted local concentrations in food for human consumption for tris(isopropylphenyl) phosphate

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 isopropylated diphenyl phosphate		2.55	3.01×10^{-3}	2.93×10^{-5}	3.2×10^{-4}	6.22×10^{-4}	1.97×10^{-4}	9.03×10^{-8}	4.21×10^{-3}
Lubricant additive	Blending of lubricant	0.14	0.10	9.48×10^{-6}	1.73×10^{-5}	5.66×10^{-5}	1.79×10^{-5}	2.73×10^{-12}	7.66×10^{-4}
Hydraulic fluid	Blending of fluid	0.14	0.59	1.62×10^{-4}	6.57×10^{-5}	4.99×10^{-4}	1.58×10^{-4}	3.56×10^{-7}	3.44×10^{-3}
Power generation fluid	Blending of fluid	0.14	0.14	1.29×10^{-3}	1.77×10^{-5}	2.85×10^{-3}	9.02×10^{-4}	4.11×10^{-6}	1.05×10^{-3}
	Use at power station	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible
Paints	Formulation	1.01	10	1.79×10^{-3}	1.13×10^{-3}	6.37×10^{-3}	2.02×10^{-3}	2.97×10^{-6}	0.06
	Application	0.19	3.75	3.25×10^{-4}	4.21×10^{-4}	1.63×10^{-3}	5.17×10^{-4}	2.66×10^{-11}	0.02
Textile/ fabric coating	Compounding	0.32	12.5	1.08×10^{-3}	1.4×10^{-3}	5.44×10^{-3}	1.72×10^{-3}	8.54×10^{-11}	0.07
	Application of coating	0.23	6.26	8.49×10^{-4}	7.03×10^{-4}	3.4×10^{-3}	1.07×10^{-3}	9.9×10^{-7}	0.03
	Combined compounding and application of coating	0.42	18.8	1.93×10^{-3}	2.11×10^{-3}	8.83×10^{-3}	2.79×10^{-3}	9.9×10^{-7}	0.10
PVC – 1[a]	Compounding	0.24	2.75	2.71×10^{-4}	3.09×10^{-4}	1.27×10^{-3}	4.02×10^{-3}	1.04×10^{-7}	0.02
	Conversion	0.18	1.26	2.7×10^{-4}	1.41×10^{-4}	9.0×10^{-3}	2.85×10^{-4}	5.18×10^{-7}	7.21×10^{-3}
	Combined compounding and conversion	0.29	4.01	5.4×10^{-4}	4.5×10^{-4}	2.17×10^{-3}	6.85×10^{-4}	6.22×10^{-7}	

Table 3.14 continued

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)
PVC – 2[a]	Compounding	1.88	19.8	2.23×10^{-3}	2.23×10^{-3}	9.76×10^{-3}	3.09×10^{-3}	1.67×10^{-6}	0.11
	Conversion	0.29	1.84	6.78×10^{-4}	2.07×10^{-4}	1.93×10^{-3}	6.11×10^{-4}	1.67×10^{-6}	0.01
	Combined compounding and conversion	2.0	21.3	2.83×10^{-3}	2.39×10^{-3}	0.01	3.61×10^{-3}	3.2×10^{-6}	0.12
PVC – 3[a]	Compounding	0.74	6.88	7.72×10^{-4}	7.72×10^{-4}	3.38×10^{-3}	1.07×10^{-3}	5.71×10^{-7}	0.04
	Conversion	0.19	0.63	2.33×10^{-4}	7.1×10^{-5}	6.65×10^{-4}	2.1×10^{-4}	5.71×10^{-7}	3.79×10^{-3}
	Combined compounding and conversion	0.79	7.51	1.0×10^{-3}	8.43×10^{-4}	4.04×10^{-4}	1.28×10^{-3}	1.14×10^{-6}	0.04
Poly-urethane	Compounding	0.41	13.8	1.27×10^{-3}	1.54×10^{-3}	6.16×10^{-3}	1.95×10^{-3}	2.59×10^{-7}	0.08
	Conversion	0.16	1.25	1.9×10^{-4}	1.41×10^{-4}	7.24×10^{-4}	2.29×10^{-4}	2.59×10^{-7}	7.15×10^{-3}
	Combined compounding and conversion	0.43	15	1.46×10^{-3}	1.68×10^{-3}	6.88×10^{-3}	2.18×10^{-3}	5.18×10^{-7}	0.08
Pigment dispersion	Production of dispersions	1.34	13.8	1.54×10^{-3}	1.54×10^{-3}	6.76×10^{-3}	2.14×10^{-3}	1.14×10^{-6}	0.08
Regional sources		0.13	0.02	2.3×10^{-6}	1.65×10^{-5}	4.0×10^{-5}	1.26×10^{-5}	3.24×10^{-9}	2.99×10^{-4}

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

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

4.1 Aquatic compartment

The following sections review the available toxicity data for isopropylated triphenyl 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 PNEC.

Several of the tests are unpublished studies carried out by industry. It has not been possible to validate all of these tests within the scope of this report and these are assigned a validity marking of four unless it is clear that some aspects of the test invalidate the results (for these a validity marking of three is given). The studies given a validity marking of four have been considered along with the studies assigned a validity marking of one and two when deriving the PNEC.

One important property when considering the aquatic toxicity data is water solubility. The water solubility of isopropylphenyl diphenyl phosphate is around 2.2 mg/l and that of tris(isopropylphenyl) phosphate is around 0.12 mg/l. Several studies have been carried out at concentrations greater than these values and, although this in itself does not necessarily invalidate the test (for example, cosolvents 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. In cases where it is clear that undissolved test substance was present in the test media, the tests have been marked as not valid.

A further consideration when considering the aquatic effects data is that a range of commercial isopropylated triphenyl phosphate products are produced. These products contain various isopropylated triphenyl phosphates (ranging from isopropylphenyl diphenyl phosphate to tris(isopropylphenyl) phosphate) along with triphenyl phosphate.

The amount of triphenyl phosphate present in the commercial products generally decreases as the degree of alkylation of the products increases, but is up to around 30 per cent in some of the products tested. This is particularly relevant for the assessment of aquatic effects data as triphenyl phosphate itself has been shown to be toxic to aquatic organisms (see the risk evaluation report for triphenyl phosphate in this series). The actual composition of the various isopropylated triphenyl phosphate products tested is frequently not given in the available literature, but any relevant information on the identity (such as trade name) or composition of the tested product is included in the following study descriptions. Table 1.1 in Section 1.2.1 gives further information on the composition of some of the (possibly older) commercial products.

4.1.1 Toxicity to fish

Short-term studies

The short-term toxicity of isopropylated triphenyl phosphates to freshwater fish is summarised in Table 4.1.

Cleveland *et al.* (1986) determined the acute toxicity of two commercial isopropylphenyl diphenyl phosphate products (Kronitex 200 and Phosflex 31P) to rainbow trout (*Oncorhynchus mykiss*) and bluegill sunfish (*Lepomis macrochirus*) and also fathead minnow (*Pimephales promelas*) and channel catfish (*Ictalurus punctatus*) in the case of Phosflex 31P. The composition of Kronitex 200 was given as four to six per cent triphenyl phosphate, seven to 10 per cent 2-isopropylphenyl diphenyl phosphate, 20-25 per cent 4-isopropylphenyl diphenyl phosphate, along with bis-(2-isopropylphenyl) phenyl phosphate and minor amounts of di-, tri- and tetraisopropyl-substituted triphenyl phosphates. The composition of Phosflex 31P was given as 28-30 per cent triphenyl phosphate, along with isomers of isopropylphenyl diphenyl phosphate, isomers of diisopropylphenyl diphenyl phosphate and tri-substituted phenol phosphates.

The tests were all carried out using a static test system using acetone as co-solvent. In the tests with Kronitex 200, the 96-hour LC_{50} was determined as 4.5 mg/l for *O. mykiss* and 29 mg/l for *L. macrochirus*. Phosflex 31P appeared to be more acutely toxic and the 96-hour LC_{50} for this substance was determined as 0.9 mg/l for *O. mykiss*, 2.6 mg/l for *L. macrochirus*, 1.7 mg/l for *P. promelas* and below 0.3 mg/l for *I. punctatus*. Tests were also carried out to investigate the effects of varying the water hardness (in the range 40 mg/l to 320 mg/l as $CaCO_3$), pH (in the range 6.5 to 8.5) and temperature (in the range 7°C to 17°C for *O. mykiss* and 12°C to 22°C for *L. macrochirus*) on the toxicity. None of these parameters were found to have a significant effect on the 96-hour LC_{50} determined for either species with either substance. Most of these LC_{50} values are close to or above the water solubility of the substance.

Great Lakes Chemical Corporation (2002) give an unpublished 96-hour LC_{50} of 1.6 mg/l for fish (unspecified species) for a commercial isopropylphenyl diphenyl phosphate (Reofos 50) product containing 28-32 per cent triphenyl phosphate. This may be the same study reported below in IUCLID (2000) with rainbow trout. The reported value is close to the water solubility of the test substance.

Table 4.1 Short-term toxicity of isopropylated triphenyl phosphates to freshwater fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
?													Mortality		96h-LC_{50} = 1.6 mg/l (Reofos 50)	Great Lakes Chemical Corp. 2002	4
					Water accomm. fraction	N							Mortality		96h-LC_{50} >1,000 mg/l (Durad 310M)	Great Lakes Chemical Corporation 2002	4
Brachydanio rerio	OECD 203			Lecithin used to form an emulsion	48, 80, 130, 220, 370, 620 and 1,000 mg/l	N							Mortality		96h-LC_{50} >1,000 mg/l (Reolube HYD 46)	IUCLID 2000	3
	OECD 2003					N									96h-LC_{50} =1,000 mg/l (Reofos 120)	IUCLID 2000	3
Ictalurus punctatus	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artificial water	22°C	38-46	7.2-7.6	Static		Mortality		96h-LC_{50} >0.3 mg/l (Phosflex 31P)	Cleveland *et al.* 1986	2
	USEPA 1975	10 in 15 litres		Acetone at ≤0.67 ml/l	At least 8 concs.	N	Artificial water	20°C	44	7.4	Static		Mortality		96h-LC_{50} = 43 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2
	USEPA 1975	20 in 41 litres		Acetone at ≤0.20 ml/l	At least 8 concs.	N	Well water	17°C	272	7.4	Flow		Mortality		96h-LC_{50} = >15 mg/l 30d-LC_{50} = 4.5 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2

Table 4.1 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Lepomis macro-chirus	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artifi-cial water	22°C	38-46	7.2-7.6	Static		Mortality		96h-LC_{50} = 29 mg/l (Kronitex 200)	Cleveland *et al.* 1986	2
	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artifi-cial water	22°C	38-46	7.2-7.6	Static		Mortality		96h-LC_{50} = 2.6 mg/l (Phosflex 31P)	Cleveland *et al.* 1986	2
	USEPA 1975	10 in 15 litres		Acetone at ≤0.67 ml/l.	At least 8 concs.	N	Artifi-cial water	20°C	44	7.4	Static		Mortality		96h-LC_{50} = 12 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2
	USEPA 1975	20 in 41 litres		Acetone at ≤0.20 ml/l.	At least 8 concs.	N	Well water	20°C	272	7.4	Flow		Mortality		96h-LC_{50} = 11 mg/l 17d-LC_{50} = 5.0 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2
Oncorhyn-chus mykiss	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artifi-cial water	12°C	38-47	7.2-7.6	Static		Mortality		96h-LC_{50} = 4.5 mg/l (Kronitex 200)	Cleveland *et al.* 1986	2
	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artifi-cial water	12°C	38-47	7.2-7.6	Static		Mortality		96h-LC_{50} = 0.9 mg/l (Phosflex 31P)	Cleveland *et al.* 1986	2

Table 4.1 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Oncorhyn-chus mykiss (continued)	OECD 203					Y					Semi-static		Mortality		96h-LC_{50} = 1.15 mg/l (Reofos 50)	IUCLID 2000	4
		10		Yes	1.0, 1.8, 3.2, 5.6 and 10 mg/l plus control and solvent control	N	Artifi-cial water	11.4°C	44	7.37	Static		Mortality		96h-LC_{50} = 1.6 mg/l (Reofos 50 or Kronitex 50?)	IUCLID 2000, IUCLID 2001	3
		10		Yes	1.0, 1.8, 3.2, 5.6 and 10 mg/l plus control and solvent control	N			44	7.35	Static		Mortality		96h-LC_{50} = 2.4 mg/l (Kronitex 100?)	IUCLID 2001	4
		10		Yes	0.56, 1.0, 1.9, 3.2 and 5.6 plus control and solvent control	N			42	7.44	Static		Mortality		96h-LC_{50} = 4.46 mg/l (Kronitex 200?)	IUCLID 2001	4
	USEPA 1975	10 in 15 litres		Acetone at ≤0.67 ml/l.	At least 8 concs.	N	Artifi-cial water	10°C	44	7.4	Static		Mortality		96h-LC_{50} = 1.7 mg/l (Houghto-Safe 1120	Nevins and Johnson 1978	2
	USEPA 1975	20 in 41 litres		Acetone ≤0.20 ml/l.	At least 8 concs.	N	Well water	17°C	272	7.4	Flow		Mortality		96h-LC_{50} = 0.65 mg/l 8d-LC_{50} = 0.59 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2

Table 4.1 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Pimephales promelas	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artifi-cial water	22°C	38-47	7.2-7.6	Static		Mortality		96h-LC_{50} = 1.7 mg/l	Cleveland *et al.* 1986	2
				Yes	1.8, 3.2, 5.6, 10.0 and 18 mg/l plus control and solvent control.	N			43	7.42	Static		Mortality		96h-LC_{50} = 10.8 mg/l (Reofos 50)	IUCLID 2000	3
		10		Acetone	5.6, 10, 18, 32 and 56 mg/l plus control and solvent control.	N					Static		Mortality		96h-LC_{50} = 14.9 mg/l (Reofos 65 or Kronitex 50?) 96h-LC_{50} = 50.1 mg/l (Kronitex 200?)	IUCLID 2000 IUCLID 2001	4
	USEPA 1975	10 in 15 litres		Acetone at ≤0.67 ml/l.	At least 8 concs.	N	Artifi-cial water	17°C	44	7.4	Static		Mortality		96h-LC_{50} = 35 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2
	USEPA 1975	20 in 41 litres		Acetone at ≤0.20 ml/l.	At least 8 concs.	N	Well water	17°C	272	7.4	Static		Mortality		96h-LC_{50} = 17 mg/l 20d-LC_{50} = 8.5 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	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.

Several unpublished studies on the toxicity of isopropylated triphenyl phosphates to fish were reported in IUCLID (2000) and IUCLID (2001). Tests were carried out with the commercial product Reofos 50. The 96-hour LC_{50} for this substance was determined to be 1.15 mg/l and 1.6 mg/l with rainbow trout (*Oncorhynchus mykiss*) and 10.8 mg/l with fathead minnows (*Pimephales promelas*). IUCLID (2000) indicates that in the study with fathead minnow and one of the studies with rainbow trout (96-hour LC_{50} =1.6 mg/l), the test substance formed oily drops on the surface of the water at most or all concentrations tested and so the results cannot be considered valid. Few other details are available to assess the validity of the remaining rainbow trout data, although the result is reportedly based on measured concentrations. Reported LC_{50}s are generally close to the solubility of the test substance.

IUCLID (2000) gives a fathead minnow (*Pimephales promelas*) 96-hour LC_{50} of 14.9 mg/l for another commercial product (Reofos 65). The same study is reported in IUCLID (2001) but here the 96-hour LC_{50} is given as 50.1 mg/l. These values appear to be well above the water solubility of the test substance.

Two other unpublished studies using commercial isopropylated triphenyl phosphate products with rainbow trout (*Oncorhynchus mykiss*) are reported in IUCLID (2001). These studies found 96-hour LC_{50}s of 2.4 mg/l and 4.46 mg/l for two commercial products. These values are close to, but above, the water solubility of the test substance.

A final unpublished study reported in IUCLID (2000) is for the commercial product Reolube HYD 46 with zebrafish (*Brachydanio rerio*). The 96-hour LC_{50} determined was reported to be above 1,000 mg/l. However, in this test the test substance was mixed with lecithin using ultrasonication to form an emulsion and the test solutions were reported to be turbid. Therefore the results cannot be considered to be valid.

Further acute toxicity tests were carried out by Nevins and Johnson (1978). The substance tested was a commercial product (Houghto-Safe 1120) with isopropylphenyl diphenyl phosphate as the principal component. The 96-hour LC_{50}s were 1.7 mg/l with rainbow trout (*Oncorhynchus mykiss*), 12 mg/l with bluegill (*Lepomis macrochirus*), 35 mg/l with fathead minnow (*Pimephales promelas*) and 43 mg/l with channel catfish (*Ictalurus puctatus*). Temperatures used in this study (10°C for *O. mykiss*, 17°C for *P. promelas* and 20°C for *L. macrochirus* and) are slightly below those currently recommended in the OECD test guidelines (13-17°C for *O. mykiss* and generally 21-25°C for warm water species). It is not known what effect this will have had on the results. With the exception of the *O. mykiss* result, all LC_{50} values are above the water solubility of the test substance.

Nevins and Johnson (1978) also determined the 96-hour LC_{50} and asymptotic LC_{50} value for *O. mykiss, P. promelas, L. macrochirus* and *I. punctatus* using flow-through tests of between eight and thirty days duration. The 96-hour LC_{50} values in this series of tests were 0.65 mg/l for *O. mykiss*, 17 mg/l for *P. promelas,* 11 mg/l for *L. macrochirus* and above 15 mg/l for *I. punctatus.* The LC_{50} values determined at the end of the study were 8-day LC_{50} = 0.59 mg/l for *O. mykiss*, 20-day LC_{50} = 8.5 mg/l for *P. promelas*, 17-day LC_{50} = 5.0 mg/l for *L macrochirus* and 30-day LC_{50} = 4.5 mg/l for *I. punctatus*. Based on these data, the authors estimated the asymptotic LC_{50} value to be 0.54 mg/l for *O. mykiss*, 6.6 mg/l for *P. promelas* and 3.4 mg/l for *L. macrochirus* (no value could be estimated for *I. punctatus*). Again, with the exception of *O. mykiss*, the LC_{50}s reported are above the water solubility of the test substance and temperatures used in these tests (17-20°C) are generally lower than is currently recommended for warm water species by the OECD.

Sublethal effects were noted in most of the fish tests carried out by Nevins and Johnson (1978), including poorer feeding, hypersensitivity to disturbance, development

of hemorrhagic areas around the dorsal fin and development of impaired swimming ability. These effects were most pronounced in the longer flow-through tests.

Great Lakes Chemical Corporation (2002) gives a 96-hour LC_{50} for fish (species unknown) of above 1,000 mg/l (as water accommodated fraction). The result was from an unpublished study with a commercial tris(isopropylphenyl) phosphate product (Durad 310M), that consisted of five per cent dodecyl phosphate, four per cent triphenyl phosphate, with the remainder made up of isopropylated triaryl phosphates. This result appears to show no effect of the commercial product at its limit of solubility (although details of how the water accommodated fraction was prepared were not checked).

IUCLID (2000) reports the results of an unpublished OECD 203 test on zebrafish (*Brachydanio rerio*) using a commercial isopropylated triphenyl phosphate product (Reofos 120). This showed a LC_0 of 580 mg/l and an LC_{50} of 1,000 mg/l. The report indicates that the test substance was added directly to the water in the tanks and so this test cannot be considered valid, as there would be a significant amount of undissolved substance present.

A fish 96-hour LC_{50} and a 14-day LC_{50} of 0.0.17 and 52 mg/l respectively can be estimated for isopropylphenyl diphenyl phosphate from the log K_{ow} value of 5.3 using the USEPA ECOSAR (version 0.99h) software. Similarly, a fish 96-hour LC_{50} and a 14-day LC_{50} of 0.44 and 0.16 mg/l respectively can be estimated for tris(isopropylphenyl) phosphate from its log K_{ow} of 6.1 using the same software.

Using the methods given in the TGD, a 96-hour LC_{50} of 0.34 mg/l can be estimated for isopropylphenyl diphenyl phosphate using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.3. This is in reasonable agreement with the available data for the more sensitive species tested. Similarly, a 96-hour LC_{50} of 0.11 mg/l can be estimated for tris(isopropylphenyl) phosphate from a log K_{ow} of 6.1.

No data are available of the acute toxicity of isopropylated triphenyl phosphates to marine fish.

Long-term studies

The long-term toxicity of isopropylated triphenyl phosphate to freshwater fish is summarised in Table 4.2.

Two 90-day partial life-cycle toxicity studies were carried out for two commercial isopropylphenyl diphenyl phosphate products (Kronitex 200 and Phosflex 31P) using fathead minnows (*Pimephales promelas*) (Cleveland *et al.* 1986). The composition of Kronitex 200 was given as four to six per cent triphenyl phosphate, seven to 10 per cent 2-isopropylphenyl diphenyl phosphate, 20-25 per cent 4-isopropylphenyl diphenyl phosphate, along with bis-(2-isopropylphenyl) phenyl phosphate and minor amounts of di-, tri- and tetraisopropyl-substituted triphenyl phosphates. The composition of Phosflex 31P was given as 28-30 per cent triphenyl phosphate, along with isomers of isopropylphenyl diphenyl phosphate, isomers of diisopropylphenyl diphenyl phosphate and tri-substituted phenol phosphates. The study was carried out using a flow-through test system. The nominal concentrations of the test substance used were 0.06, 0.12, 0.25, 0.50 and 1.0 mg/l. Analyses of the water concentrations were carried out every two weeks and the mean measured concentrations in the various exposure groups (expressed as the sum of the isopropylphenyl diphenyl phosphate and the triphenyl phosphate components of the product) were 0.005, 0.007, 0.013, 0.024 and 0.088 mg/l respectively for the Kronitex 200 product (corresponding to around five to nine per cent of the nominal values) and 0.008, 0.014, 0.021, 0.029 and 0.205 mg/l (corresponding to around six to 21 per cent of the nominal values for Phosflex 31P. The actual

concentrations present in these tests will be higher than implied by these measured data, as not all components of the commercial substance were analysed.

For the tests with Kronitex 200, the survival of the fish was not statistically significantly different (p=0.05) in any treatment group when compared with the control group. However, survival in the control group was relatively low (around 80 per cent survival at 30 days falling to 68 per cent survival at 60 days and 65 per cent survival at 90 days). Growth of the fish was found to be statistically significantly (p=0.01) reduced when compared to the control group only at the highest concentration (nominal concentration of one mg/l) tested at 30 days. No statistically significant (p=0.05) reductions in growth were seen in any other treatment group or time period compared with the control group (a statistically significant increase in the length of fish was seen in some treatments at 90 days compared with the control group, and the mean length in the nominal one mg/l treatment group was similar to or slightly larger than the control group at both day 60 and day 90). Overall, little or no effect on survival and growth appears to have been seen in this study. The no observed effect concentration (NOEC) for survival is therefore one mg/l based on the nominal concentration or 0.088 mg/l based on the measured concentration. The 30-day NOEC for growth is 0.5 mg/l (nominal value) or 0.024 mg/l (measured value), and the 60- and 90-day NOEC for growth is one mg/l (nominal value) or 0.088 mg/l (measured value). Relatively poor survival in the control population indicates that the conditions used in this particular test may not have been optimum for survival and growth. Measured concentration data for this substance are likely to underestimate the actual exposure concentration, as not all components of the commercial substance were included in the analysis.

The Phosflex 31P product appeared to be more toxic to fathead minnows. The highest concentration tested (1 mg/l nominal or 0.21 mg/l measured) caused almost complete mortality (98 per cent) within 30 days. The mortality seen in the other treatment groups was not statistically different (p=0.05) to that seen in the control population. Growth of the fish was found to be statistically significantly (p=0.01) reduced compared with the control population at day 30 at the highest concentration tested (1 mg/l nominal or 0.21 mg/l measured). No statistically significant reductions in growth were seen in any other treatment group at any other time period, although again the mean length seen in some treatment groups was statistically significantly (p=0.01) greater than in the control group (it was not possible to determine the effects on growth at the highest concentration tested at day 60 and day 90 owing to the high mortality rate seen). Overall, the NOEC for mortality for this substance was determined as 0.5 mg/l (nominal) or 0.029 mg/l (measured) and the NOEC for growth was 0.5 mg/l (nominal) or 0.029 mg/l (measured). The measured concentration data for this substance are likely to underestimate the actual exposure concentration, as not all components of the commercial substance were included in the analysis.

In addition, Mayer *et al.* (1986) report unpublished MATCs for Phosflex 31P with fathead minnow (*Pimephales promelas*) as follows:

90-day MATC = 77 μg/l for survival
= 77 μg/l for growth
= >200 μg/l for gross pathology (cataracts)

Few other details of this study are available, but it is likely that these are the same results reported by Cleveland *et al.* (1986) above (the NOEC and LOEC from the Cleveland *et al.* (1986) study are 0.029 and 0.21 mg/l; the geometric mean (MATC) of these two values is 0.077 mg/l).

The USEPA ECOSAR program (v0.99h) predicts a long-term no effect concentration of 0.038 mg/l for isopropylphenyl diphenyl phosphate and 0.011 mg/l for tris(isopropylphenyl) phosphate.

Table 4.2 Long-term toxicity of isopropyl diphenyl phosphate to freshwater fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control response	Effect conc.	Refer ence	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Pimephales promelas		20 per replicate, four replicates per treatment. Loading was 40 fry in 60 litres, which was reduced to 20 fry in 60 litres at day 30.	Fry about one week old.	Cosolvent used at 0.05 ml/l.	Nominal concs. of 0.06, 0.12, 0.25, 0.5 and 1.0 mg/l plus solvent control. Measured concs. 0.005, 0.007, 0.013, 0.024 and 0.088 mg/l.	M	Artifi-cial water	25°C	40	7.2-7.4	Flow		Growth	Mean length at 30 days = 24.8±2.9 mm. Mean length at 60 days = 31.4±3.8 mm. Mean length at 90 days = 36.8±5.3 mm.	30d-NOEC = 0.024 mg/l (Kronitex 200) 60d-NOEC ≥0.088 mg/l (Kronitex 200) 90d-NOEC ≥0.088 mg/l (Kronitex 200)l	Cleve-land *et al*. 1986	2
													Mortality	Mortality was 20% at day 30, 32% at day 60 and 35% at day 90.	30d-NOEC ≥0.088 mg/l 60d-NOEC ≥0.088 mg/l 90d-NOEC ≥0.088 mg/l (Kronitex 200)l		

Table 4.2 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. Tested	N or M	Test conditions						End-point	Control response	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Pimephales promelas (continued)		20 per replicate, four replicates per treatment. Loading was 40 fry in 60 litres, which was reduced to 20 fry in 60 litres at day 30.	Fry about one week old.	Cosolvent used at 0.05 ml/l.	Nominal concs. of 0.06, 0.12, 0.25, 0.5 and 1.0 mg/ plus solvent control. Measured concs. 0.008, 0.014, 0.021, 0.029 and 0.205 mg/l.	M	Artifi-cial water	25°C	40	7.2-7.4	Flow		Growth	Mean length at 30 days = 27.7±2.7 mm. Mean length at 60 days = 30.3±2.6 mm. Mean length at 90 days = 38.4±2.7 mm.	30d-NOEC =0.029 mg/l (Phosflex 31P) 60d-NOEC =0.029 mg/l (Phosflex 31P) 90d-NOEC =0.029 mg/l (Phosflex 31P)	Cleve-land *et al.* 1986	2
													Mortality	Mortality was 16% at 30 days, 16% at 60 days and 18% at 90 days.	30d-NOEC = 0. 029 mg/l 60d-NOEC = 0.029 mg/l 90d-NOEC = 0.029 mg/l (Phosflex 31P)		

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.

There are no toxicity data available on the long-term toxicity of isopropylated triphenyl phosphates to marine fish.

4.1.2 Toxicity to aquatic invertebrates

Short-term studies

Freshwater

The short-term toxicity of isopropylated triphenyl phosphates to freshwater aquatic invertebrates is summarised in Table 4.3.

Ziegenfuss *et al.* (1986) determined the acute toxicity of isopropylphenyl diphenyl phosphate (purity not given) to both the daphnid *Daphnia magna* and the midge *Chironomus tentans.* The test method was based on ASTM (1980). The 48-hour LC_{50} values determined were 0.25 mg/l for *D. magna* and 0.61 mg/l for *C. tentans.*

Great Lakes Chemical Corporation (2002) give a 48-hour EC_{50} of 2.44 mg/l for *Daphnia magna* using a commercial isopropylphenyl diphenyl phosphate (Reofos 50) containing 28-32 per cent triphenyl phosphate from an unpublished study. This value is close to the solubility limit of the test substance.

IUCLID (2000) reports the results from several other unpublished studies. A 48-hour EC_{50} of 14 mg/l was determined for *Daphnia magna* using a commercial product (Reolube HYD 46). The substance appears to have been tested as an emulsion (using lecithin and ultrasonic dispersion) and a shallow dose-response appears to have been seen in this study (such as 48-hour NOEC=0.3 mg/l, 48-hour EC_{50}=14 mg/l and 96-hour EC_{50}=167 mg/l, all based on nominal concentrations). Thus, the results from this test are questionable as the test substance may not have been in true solution.

A second unpublished study with *Daphnia magna* is reported in IUCLID (2000). The 48-hour EC_{50} in this study was reported to be 31.3 mg/l for the commercial product Reofos 50. Analytical monitoring of the concentration appears to have been carried out in this study but it is not currently possible to further validate the results from this study. The value reported is well above the water solubility of the test substance.

The results of further unpublished studies with *Daphnia magna* using commercial isopropylated triphenyl phosphate products are reported in IUCLID (2001). These give 48-hour EC_{50} values of 0.83 mg/l, 1.5 mg/l and 2.44 mg/l for three different products. These values are close to the water solubility of the test substance.

Sanders *et al.* (1985) determined the acute toxicity of two commercial isopropylphenyl diphenyl phosphate products (Krontex 200 and Phosflex 31P; purities not given) to *Daphnia magna*, midge (*Chironomus plumosus*) and an amphipod (*Gammarus pseudolimnaeus*). The tests were carried out using static test systems. The toxicity values obtained for Kronitex 200 were a 48-hour EC_{50} of 3.2 mg/l with *D. magna*, a 48-hour EC_{50} of 2.4 mg/l with *C. plumosus* and a 96-hour LC_{50} of 1.1 mg/l with *G. pseudolimnaeus*. The equivalent toxicity values obtained using Phosflex 31P were a 48-hour EC_{50} of 6.8 mg/l with *D. magna*, a 48-hour EC_{50} of 1.8 mg/l with *C. plumosus* and a 96-hour LC_{50} of 2.2 mg/l with *G. pseudolimnaeus*. These values are close to the water solubility of the test substance.

Further acute toxicity tests using *Gammarus pseudolimnaeus* have been carried out by Nevins and Johnson (1978). The substance tested was a commercial product (Houghto-Safe 1120) with isopropylphenyl diphenyl phosphate as the principal component. The 96-hour LC_{50} was 0.7 mg/l.

Table 4.3 Short-term toxicity of isopropyl diphenyl phosphate to freshwater invertebrates

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Chironomus plumosus	USEPA 1975		4th instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	22°C	270	7.2-7.4	Static		Immobil. mortality		48h-EC_{50} = 2.4 mg/l (Kronitex 200)	Sanders *et al.* 1985	2
	USEPA 1975		4th instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	22°C	270	7.2-7.4	Static		Immobil. mortality		48h-EC_{50} = 1.8 mg/l (Phosflex 31P)	Sanders *et al.* 1985	2
Chironomus tentans	ASTM 1980		2nd instar (10-14 day)				Well water				Static		Immobil. mortality		48h-EC_{50} = 0.61 mg/l	Ziegen-fuss *et al.* 1986	2
Daphnia magna	ASTM 1980		<24 h				Well water				Static		Immobil. mortality		48h-EC_{50} = 0.25 mg/l	Ziegen-fuss *et al.* 1986	2
													Immobil. mortality		48h-EC_{50} = 2.44 mg/l	Great Lakes Chem. Corp. 2002	4
	OECD 202			Lecithin used as emulsifier along with ultrasonic dispersion	0.14, 0.26, 0.47, 0.84, 1.5, 2.7, 4.9, 8.8, 16, 29, 52, 93 and 167 mg/l	N							Immobil. mortality		48h-EC_{50} = 14 mg/l (Reolube HYD 46)	IUCLID 2000	3
	OECD 202					M							Immobil. mortality		48h-EC_{50} = 31.3 mg/l (Reofos 50)	IUCLID 2000	4

Table 4.3 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Daphnia magna (continued)	OECD 202					N							Immobil. mortality		48h-EC_{50} = 29 mg/l (Reofos 120)	IUCLID 2000	3
	OECD 202	Five per replicate, four replicates per treatment	<24 h	No	Water accomm. fraction – limit test with initial loading of 1,000 mg/l plus control	N	Synth. Elendt M7	20.3-20.8°C	196	7.38 - 8.01		≥77 % sat.	Immobil. mortality	0% immobile	48h-EC_{50} >1,000 mg/l (Durad 310M)	Knight and Allan 2002	2
						N					Static		Immobil. mortality		48h-EC_{50} = 0.83 mg/l (Kronitex 100?)	IUCLID 2001	4
		Five per replicate, four replicates per treatment		Yes	1.0, 1.8, 3.2, 5.6, 10 and 18 mg/l plus control and solvent control	N					Static		Immobil. mortality		48h-EC_{50} = 1.5 mg/l (Kronitex 200?)	IUCLID 2001	4
						N					Static		Immobil. mortality		48h-EC_{50} = 2.44 mg/l (Kronitex 50?)	IUCLID 2001	4
	USEPA 1975		<24h	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-7.4	Static		Immobil. mortality		48h-EC_{50} = 3.2 mg/l (Kronitex 200)	Sanders *et al.* 1985	2
	USEPA 1975		<24h	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-7.4	Static		Immobil. mortality		48h-EC_{50} = 6.8 mg/l (Phosflex 31P)	Sanders *et al.* 1985	2

Table 4.3 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Gammarus pseudolim-naeus	USEPA 1975		Early instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-7.4	Static		Mortality		96h-LC_{50} = 1.1 mg/l (Kronitex 200)	Sanders *et al.* 1985	2
	USEPA 1975		Early instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-7.4	Static		Mortality		96h-LC_{50} = 2.2 mg/l (Phosflex 31P)	Sanders *et al.* 1985	2
	USEPA 1975	10 in 15 litres		Acetone at up to 0.67 ml/l.	At least 8 concs.	N	Well water	20°C	272	7.4	Static		Mortality		96h-LC_{50} = 0.70 mg/l (Houghto-Safe 1120)	Nevins and Johnson 1978	2

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

Knight and Allan (2002) determined a 48-hour EC_{50} for *Daphnia magna* of above 1,000 mg/l (as water accommodated fraction, WAF). The result was from a study with a commercial tris(isopropylphenyl) phosphate product (Durad 310M) that consisted of five per cent dodecyl phosphate, four per cent triphenyl phosphate, with the remainder made up of isopropylated triaryl phosphates. The test was carried out using a semi-static method (renewal every 24 hours). The WAF was prepared from a single initial loading of 1,000 mg/l. In order to prepare the WAF, a weighed amount of the test substance was added directly to the test medium and stirred in the dark for one hour (preliminary work had shown that this method of preparation resulted in the maximum achievable concentration of the test substance and minimised degradation). Following stirring, the solution was centrifuged and the supernatant was used as the test solution (to ensure that *Daphnia* were only exposed to the water-soluble fraction). The test solution was analysed for the concentration of the test substance during the test. Both the freshly prepared solutions and the solution just prior to renewal (24-hours old) were analysed. The concentrations measured were 0.710-1.274 mg/l in the freshly prepared solutions and 0.436-0.671 mg/l in the 24-hour solutions. The arithmetic mean exposure concentration was therefore 0.77 mg/l. However, the test substance was also reported to have been detected (detection limit 0.404 mg/l) in the freshly prepared control test solutions but not the 24-hour-old control solutions (the reason for this was unknown and was attributed to an artefact of the system). It was visually noted that the exposed *Daphnia* had test material adhering to their bodies at 24 hours and that this was impeding normal movement. By 48 hours, the amount of adhering material had increased, and one *Daphnia* was found to be immobile (encased with test material) at 48 hours. Overall, although there are some uncertainties with this test (such as the possible presence of test substance in the controls and the adherence of the substance to the *Daphnia*), it can be concluded from this test that the test substance was not acutely toxic to *Daphnia* at concentrations up to the solubility limit (0.77 mg/l).

IUCLID (2000) report the results of an unpublished OECD 202 test with *Daphnia magna* using a commercial isopropylated triphenyl phosphate product (Reofos 120). This showed a 24-hour EC_{50} of 29 mg/l. The report indicates that the test substance was added as a homogeneous suspension (using sorbitan fatty acid ester polyglycolether) in water to the tanks and so this test cannot be considered valid, as there would be a significant amount of undissolved substance present.

Using the methods given in the TGD, a 48-hour EC_{50} for *Daphnia magna* of 0.64 mg/l can be estimated for isopropylphenyl diphenyl phosphate using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.3. This is in reasonable agreement with available data for the more sensitive species tested. Similarly, a 96-hour LC_{50} of 0.28 mg/l can be estimated for tris(isopropylphenyl) phosphate from a log K_{ow} of 6.1. The USEPA ECOSAR program (v0.99h) predicts values of 0.23 mg/l for isopropylphenyl diphenyl phosphate and 0.067 mg/l for tris(isopropylphenyl) phosphate for the same endpoint.

Marine

The short-term toxicity of isopropyl diphenyl phosphate to marine invertebrates is summarised in Table 4.4.

Table 4.4 Short-term toxicity of isopropyl diphenyl phosphate to marine invertebrates

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. tested	N or M	Test conditions						End-point	Control response	Effect concentration	Reference	Val.
							Media	Temp.	Sal.	pH	Static/ flow	D.O.					
Crangon crangon		20			10 and 50 mg/l	N							Mortality		96h-LC_{50} > 50 mg/l (Durad 300)	IUCLID 2000	4
		20			10 and 50 mg/l	N							Mortality		96h-LC_{50} >50 mg/l (Reofos 95)	IUCLID 2000	4
		20			10 and 50 mg/l	N							Mortality		96h-LC_{50} > 50 mg/l (12% triphenyl phosphate & 88% isopropylated triaryl phosphates)	IUCLID 2000	4
		20			10 and 50 mg/l	N							Mortality		96h-LC_{50} >50 mg/l (15% triphenyl phosphate & 85% isopropylated triaryl phosphates)	IUCLID 2000	4

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.

IUCLID (2000) reports the results of unpublished industry screening studies with brown shrimp (*Crangon crangon*). The 96-hour LC_{50} values reported were all above 50 mg/l for a number of commercial products including Durad 300 (five per cent triphenyl phosphate and 95 per cent isopropylated triaryl phosphates), Reofos 95 (7.5 per cent triphenyl phosphate and 93.5 per cent isopropylated triaryl phosphates) and two unnamed products (consisting of 12 per cent triphenyl phosphate and 88 per cent isopropylated triaryl phosphates and 15 per cent triphenyl phosphate and 85 per cent isopropylated triaryl phosphates respectively). The results are based on nominal concentrations and only two concentrations were tested (10 and 50 mg/l). The tests were apparently carried out under constant agitation, implying that the substances were present as a suspension. Since the reported LC_{50} values are well above the water solubility of the substances, the results should be treated with caution.

Long-term studies

The long-term toxicity of isopropyl diphenyl phosphate to freshwater invertebrates is summarised in Table 4.5.

Sanders *et al.* (1985) investigated the effects of two commercial isopropylphenyl diphenyl phosphate products (Kronitex 200 and Phosflex 31P, compositions not given) on the survival and reproduction of *Daphnia magna* over 21 days. The test was carried out using a flow-through system using nominal exposure concentrations. The 21-day NOEC values based on survival were 0.027 mg/l for Kronitex 200 and 0.028 mg/l for Phosflex 31P (for Phosflex 31P, survival was reported to be only 45 per cent at 0.0035 mg/l compared with the control survival of 80 per cent (the survival at 0.007, 0.014 and 0.028 mg/l was similar to the control) but the significance of this finding is not commented on in the paper). The 21-day NOEC values based on reproduction were determined to be 0.006 mg/l for Kronitex 200 and 0.028 mg/l for Phosflex 31P. The experiment with Kronitex 200 used quite widely spaced concentrations (the actual concentrations tested were 0.006, 0.027, 0.072 and 0.154 mg/l) and so it is possible that the actual NOEC could be higher than indicated by this result. However, the reduction in the mean number of offspring/adult was quite severe at 0.027 mg/l (39 compared with 915 in the controls: the mean number of offspring/adults at 0.006 mg/l was 127 but this was apparently not statistically significantly different from the control population, which suggests significant variations in the numbers in the controls). There are a number of uncertainties in this study. It is not clear whether the figures presented for numbers of offspring are per adult, as stated in the paper, or are totals for each exposure, which appears more likely from the size of the values. The number of offspring in the controls was below that indicated in the current OECD test guideline (but would have been sufficient for the guideline at the time the test was performed) and there are some variations between the controls used for these tests and ones with other substances at the same time. Overall, the study is valid with restrictions.

Sanders *et al.* (1985) also investigated the effects of the same two commercial products on the survival and growth of amphipods (*Gammarus pseudolimnaeus*) over 90 days using a flow-through system. The NOECs for survival were determined to be 0.011 μg/l for Kronitex 200 and 0.019 μg/l for Phosflex 31P (for Kronitex 200, survival was found to be statistically significantly reduced (p=0.05) at 0.031 mg/l and 0.128 mg/l but not at 0.063 mg/l, indicating a relatively poor dose-response, and the survival of the control population in this series was only 75 per cent). For growth, the mean length of the organisms at 90 days was found to be statistically significantly reduced at a concentration of 0.128 mg/l for Kronitex 200, giving a 90-day NOEC of 0.063 mg/l, but no statistically significant reductions in growth were seen at any concentration tested for Phosflex 31P (90-day NOEC above 0.088 mg/l).

A final study carried out by Sanders *et al.* (1985) investigated the effects of the same commercial products on the emergence of midges (*Chironomus plumosus*) over 30 days using a flow-through system. In this test, 100 first-instar larvae were placed in a test chamber (10 × 20 × 10 cm) containing one litre of water, and 13 g of washed sand and 0.3 g of commercial dog candy were added to provide a substrate for the larvae to build a case. The organisms were fed 0.3 g of dog candy every fifth day until they had transformed into the pupal stage. The emergence of midges was less than the control at all concentrations tested, but these differences were only statistically significant (p=0.05) at concentrations of 0.319 mg/l and above for both substances. The NOECs, based on the percentage emergence after 30 days, were therefore determined as 0.184 mg/l for both products. However, the control response in the Kronitex 200 series of experiments was low (70 per cent emergence compared with 95 per cent emergence in the control for the Phosflex 31P experiments). The significance of this for the results is not clear.

There are no long-term toxicity data for isopropylated triphenyl phosphates with marine invertebrates.

4.1.3 Toxicity to algae

The toxicity of isopropyl diphenyl phosphate to fresh water algae is summarised in Table 4.6 .

Sanders *et al.* (1985) determined the toxicity of two commercial isopropylphenyl diphenyl phosphate products (Kronitex 200 and Phosflex 31P, compositions not given) to *Selenastrum capricornutum*[7] over 14 days. The growth of the alga was determined by dry weight measurements. The concentrations tested were 0.1, 1.0, 10 and 100 mg/l and statistically significant (p=0.05) reductions in cell growth (dry weight) were seen at concentrations of 1.0 mg/l and above for Kronitex 200 and at all concentrations for Phosflex 31P. Thus, the NOEC for Kronitex 200 was 0.1 mg/l and it was not possible to determine a NOEC for Phosflex 31P. However, the length of this study (14 days rather than the normal 72 hours for an algal growth study) means that the results from this test are uncertain.

Great Lakes Chemical Corporation (2002) give a 72-hour IC_{50} for alga (species unknown) of above 1,000 mg/l (as water accommodated fraction). The result was from an unpublished study with the commercial tris(isopropylphenyl) phosphate product Durad 310M, that consisted of five per cent dodecyl phosphate, four per cent triphenyl phosphate, with the remainder made up of isopropylated triaryl phosphates.

The USEPA ECOSAR program (v0.99h) predicts a 96-hour EC_{50} of 0.17 mg/l and a long term no-effect concentration of 0.12 mg/l for isopropylphenyl diphenyl phosphate. The predicted values for tris(isopropylphenyl) phosphate are 0.041 mg/l (96-hour EC_{50}) and 0.034 mg/l (long-term no effect concentration).

No toxicity data are available for isopropylated triphenyl phosphates with marine algae.

[7] Now called *Pseudokirchneriella subcapitata*.

Table 4.5 Long-term toxicity of isopropyl diphenyl phosphate to freshwater invertebrates

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. tested	N or M	Test conditions						End-point	Control response	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Chironomus plumosus		100 per replicate, two replicates per treatment	1st instar		18, 36, 64, 184, 319, 718 and 1,500 µg/l plus control	N	Well water	22°C	270	7.2-7.4	Flow		Emerge.	70% emerged at day 30	30d-NOEC = 0.184 mg/l (Kronitex 200)	Sanders *et al.* 1985	2
		100 per replicate, two replicates per treatment	1st instar		18, 36, 64, 184, 319, 718 and 1,500 µg/l plus control	N	Well water	22°C	270	7.2-7.4	Flow		Emerge.	95% emerged at day 30	30d-NOEC = 0.184 mg/l (Phosflex 31P)	Sanders *et al.* 1985	2
Daphnia magna		10 per replicate, two replicates per treatment	<24 h		6, 27, 72 and 154 µg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	95% survival	21d-NOEC = 0.027 mg/l (Kronitex 200)	Sanders *et al.* 1985	2
													Repro.	Mean offspring/ adult = 915	21d-NOEC = 0.006 mg/l (Kronitex 200)		
		10 per replicate, two replicates per treatment	<24 h		0.85, 1.7, 3.5, 7.0, 14, 28 and 56 µg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	80% survival	21d-NOEC = 0.028 mg/l (Phosflex 31P)	Sanders *et al.* 1985	2
													Repro.	Mean offspring/ adult = 329	21d-NOEC = 0.028 mg/l (Phosflex 31P)		

Table 4.5 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. tested	N or M	Test conditions						End-point	Control response	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Gammarus pseudolim-naeus		10 per replicate, four replicates per treatment	5-10 day old		0.5, 1.0, 9.0, 11, 31, 63 and 128 μg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	75% survival	90d-NOEC = 0.011 mg/l (Kronitex 200)	Sanders *et al*. 1985	2
													Growth	Mean length 10.7 mm	90d-NOEC = 0.063 mg/l (Kronitex 200)		
		10 per replicate, four replicates per treatment	5-10 day old		5, 10, 19, 38 and 88 μg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	90% survival	90d-NOEC = 0.019 mg/l (Phosflex 31P)	Sanders *et al*. 1985	2
													Growth	Mean length 9.4 mm	90d-NOEC ≥0.088 mg/l (Phosflex 31P)		

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.

Table 4.6 Toxicity of isopropyl diphenyl 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					
?				Water accommodated fraction	N							72h-IC_{50} >1,000 mg/l (Durad 310M)	Great Lakes Chemical Corporation 2002	4
Selenastrum capricornutum			Acetone at up to 0.1 ml/l	0.1, 1.0, 10 and 100 mg/l plus control – each run in triplicate	N	Well water	24°C	270	7.2-7.4	Biomass (dry weight)		14d-NOEC = 0.1 mg/l (Kronitex 200)	Sanders *et al*. 1985	3
			Acetone at up to 0.1 ml/l	0.1, 1.0, 10 and 100 mg/l plus control – each run in triplicate	N	Well water	24°C	270	7.2-7.4	Biomass (dry weight)		14d-NOEC = <0.1 mg/l (Phosflex 31P)	Sanders *et al*. 1985	3

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.

4.1.4 Toxicity to microorganisms

IUCLID (2000) reports a three-hour EC_0 of 1,000 mg/l for a commercial isopropylphenyl diphenyl phosphate product (Reolube HYD 46) from an unpublished OECD 209 activated sludge respiration inhibition test (no significant inhibition of respiration was seen at the highest concentration tested). The substance was tested as an emulsion in this study.

IUCLID (2000) also reports the results of an unpublished OECD 209 activated sludge respiration inhibition test using a commercial isopropylated triphenyl phosphate product (Reofos 120). The three-hour IC_{20} was determined to be 44 mg/l and the three-hour IC_{50} was above 100 mg/l.

Armstrong (year unknown) gives a further a three-hour EC_{50} for inhibition of activated sludge of above 1,000 mg/l. The result was from an OECD 209 activated sludge respiration inhibition test with a commercial tris(isopropylphenyl) phosphate product (Durad 310M), that consisted of five per cent dodecyl phosphate, four per cent triphenyl phosphate, with the remainder made up of isopropylated triaryl phosphates. The report indicates that the substance was tested at concentrations of 10, 31.6, 100, 316 and 1,000 mg/l and globules of test material were seen in the vessels at concentrations of 100 mg/l and above. These globules were dispersed throughout the test medium by aeration throughout the three-hour the incubation period. No inhibitory effect was seen at any concentration tested. The three-hour EC_{50} determined for the positive control (3,5-dichlorophenol) was 7.71 mg/l, which is within the recommended range given in the test guideline.

4.1.5 Toxicity to sediment organisms

No toxicity data are available for sediment organisms.

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

Surface water

Acute toxicity data are available for fish, invertebrates and algae. The lowest results from the more reliable standard tests are a 96-hour LC_{50} of 0.65 mg/l for fish (*Oncorhynchus mykiss*), a 48-hour LC_{50} of 0.25 mg/l for invertebrates (*Daphnia magna*) but there is some uncertainty over the actual 96-hour IC_{50} for algae (one study showed no effects above 1,000 mg/l when tested as a water-accommodated fraction).

In general terms, although a range of acute toxicity values have been determined, there is no obvious pattern between the toxicity and the actual product tested. This implies that most of the isopropylated triphenyl phosphate products can be considered to have similar acute toxicities. Quantitative structure activity relationship (QSAR) estimates of the acute toxicity to fish (96-hour LC_{50} is estimated to be 0.34 mg/l for isopropylphenyl diphenyl phosphate and 0.11 mg/l for tris(isopropylphenyl) phosphate) and *Daphnia magna* (48-hour EC_{50} is estimated to be 0.64 mg/l for isopropylphenyl diphenyl phosphate and 0.28 mg/l for tris(isopropylphenyl) phosphate) also suggest that the acute toxicity of the various products should be broadly similar.

Long-term data are also available for fish and invertebrates. Again, there is no obvious pattern between the toxicity seen and the substance tested, although the database is relatively small. The lowest NOECs obtained from the more reliable studies were a 30-day NOEC of 0.024 mg/l for fish (*Pimephales promelas*) in a fry growth study and a 21-day NOEC of 0.006 mg/l in a *Daphnia magna* reproduction test. No reliable NOEC is available for algae.

Available long-term data for fish cover only growth and mortality of fry and not the embryo-larval stages. Annex B considers the available data for triaryl phosphates as a whole and this would indicate that, when all the available long-term fish toxicity data are considered (data for both mortality and growth of fry and effects on early lifestages), the NOECs would be around 0.01 mg/l for isopropylphenyl diphenyl phosphate and 0.019 mg/l for tris(isopropylphenyl) phosphate, which indicates the substance would be expected to be slightly less toxic to fish than was found for *Daphnia*. In addition, the analysis given in Annex B indicates that the long-term NOEC of alga would also be expected to be higher than found for both fish and *Daphnia*. Long-term no effect concentrations for algae predicted using the USEPA ECOSAR program are higher than the experimental result for *Daphnia*.

On this basis, a $PNEC_{water}$ of 0.6 μg/l is derived by applying an assessment factor of 10 to the lowest available long-term NOEC for *Daphnia magna.* This value is assumed to hold for both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate. For the marine environment, an assessment factor of 100 is used on the same data, giving a PNEC of 0.06 µg/l. The uncertainty in the Daphnia NOEC is recognised, but there are other experimental and predicted values which are similar.

An IC_{50} of above 100 mg/l was determined for an isopropylated triphenyl phosphate product in an activated sludge respiration inhibition test. According to the TGD, an assessment factor of 100 is appropriate for this type of test result, and so the $PNEC_{microorganisms}$ is estimated to be above one mg/l. Although the water solubility of the test substance was exceeded in this test, the actual solubility in pure water may not be relevant to the exposure of microorganism during waste water treatment.

Sediment

No sediment toxicity data are available for isopropylated triphenyl phosphate. In the absence of data, the equilibrium partitioning method is used to estimate the PNEC:

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

where $K_{susp\text{-}water}$ = suspended sediment-water partition coefficient, 147 m^3/m^3 for isopropylphenyl diphenyl phosphate or 361 m^3/m^3 for tris(isopropylphenyl) phosphate (see Section 3.1.2).

RHO_{susp} = bulk density of suspended sediment = 1,150 kg/m^3.

Using the $PNEC_{water}$ of 0.6 μg/l, the $PNEC_{sed}$ is estimated to be 0.077 mg/kg wet weight using the properties of isopropylphenyl diphenyl phosphate or 0.188 mg/kg wet weight using the properties of tris(isopropylphenyl) phosphate. These values are used in the risk characterisation.

As the log K_{ow} of these substances 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.

The PNECs for the marine sediment compartment are calculated in the same way, giving values of 7.7 µg/kg wet weight for isopropylphenyl diphenyl phosphate and 0.019 mg/kg wet weight for tris(isopropylphenyl) phosphate.

4.2 Terrestrial compartment

4.2.1 Toxicity to plants

Chapleo and Allan (2002) determined the EC_{50}s for emergence and growth of three species of terrestrial plants of above 100 mg/kg dry weight (the highest concentration tested). The result was from an OECD 208 Terrestrial Plant Growth Test study with a commercial tris(isopropylphenyl) phosphate product (Durad 310M), that consisted of five per cent dodecyl phosphate, four per cent triphenyl phosphate, with the remainder made up of isopropylated triaryl phosphates. Soil used in the test was characterised as a loamy sand soil with an organic carbon content of 0.4 per cent and a pH of 5.6. The plants tested included wheat (*Triticum aestivum*), radish (*Raphanus sativus*) and mung bean (*Phaseolus aureus*) and the length of the test was 19, 18 and 19 days for the three species respectively (this represents 14 days after at least 50 per cent of the control seeds had emerged). The concentrations tested were 1, 10 and 100 mg/kg and no phytotoxic effects appear to have been seen at any concentration (although on re-analysis of raw data in the report, the growth of radish seedlings (as determined by dry weight) may have been slightly, but statistically significantly (p=0.05), reduced compared with the control population at the 100 mg/kg treatment level). Therefore the results of this test can be taken to show an EC_{50} of above 10-100 mg/kg dry weight depending on the species. Converting this to the standard soil in the TGD, with an organic carbon content of two per cent, gives an $EC_{50\ standard}$ of above 486 mg/kg dry weight.

4.2.2 Predicted no effect concentration (PNEC) for the terrestrial compartment

A 19-day EC_{50} of above 486 mg/kg has been calculated for isopropylated triphenyl phosphate with plants. According to the TGD, an assessment factor of 1,000 is appropriate for the result of this test. This gives a $PNEC_{soil}$ above 0.49 mg/kg dry weight. Using the default water content of soil given in the TGD, this value is equivalent to a $PNEC_{soil}$ above 0.43 mg/kg wet weight.

In the case where terrestrial toxicity data are available for plants only, the TGD indicates the assessment should also consider a PNEC derived from the equilibrium partitioning method, with the lowest PNEC taken forward to the risk characterisation.

$$\mathrm{PNEC}_{soil} = \frac{\mathrm{K}_{\mathrm{soil-water}}}{\mathrm{RHO}_{\mathrm{soil}}} \times \mathrm{PNEC}_{water} \times 1000$$

where $K_{soil\text{-}water}$ = soil-water partition coefficient, 176 m^3/m^3 for isopropylphenyl diphenyl phosphate or 433 m^3/m^3 for tris(isopropylphenyl) phosphate (see Section 3.1.2).

RHO_{soil} = bulk density of wet soil = 1,700 kg/m^3.

Using the $PNEC_{water}$ of 0.6 µg/l, the $PNEC_{soil}$ is estimated to be 0.062 mg/kg wet weight using the properties of isopropylphenyl diphenyl phosphate or 0.153 mg/kg wet weight

using the properties of tris(isopropylphenyl) phosphate. These values are used in the risk characterisation.

As the log K_{ow} of these substances 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 isopropylated triphenyl phosphates 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 isopropylated triphenyl phosphate contributing to atmospheric effects such as global warming and acid rain is 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

Two IUCLID files are available for the isopropylated triphenyl phosphates; one was published in 2000 which is not summarised to current standards (IUCLID 2000) and a later version was published in 2001 which contained fewer study summaries also of limited detail (IUCLID 2001).

The studies contained in these IUCLID files relate to a number of different commercial products and, while the trade names of these were generally included in the 2000 but not the 2001 version, only limited information on formulation and purity details are specified (see Table 4.7). Therefore, the commercial name of the test substance (but not purity) has been specified in this assessment wherever possible.

Table 4.7 Composition of some commercial preparations of isopropylated triaryl phosphate

Product	% Triphenyl phosphate	% Isopropylated triaryl phosphate
Reofos 35	35	65
Reofos 50	30	70
Reofos 65	20	80
Reofos 95	9	91
Reofos 120	7.5	92.5
Durad 300	5	95

Source: IUCLID (2000).

In the 2001 IUCLID, Klimisch codes are specified for each study discussed, providing an indication of reliability. However, no primary reports were available at the time of this review with which to confirm the conclusions on reliability. In a letter dated November 2001 (IUCLID 2001) from a sponsoring company to the USEPA regarding the US HPV program, there was a commitment to address a number of data gaps for genotoxicity, and reproductive and developmental toxicity. However, the results of such testing do not appear to have been published as yet.

A number of possible areas for clarification in the mammalian toxicity data base are listed in Appendix 1.

4.4.1 Toxicokinetics, metabolism and distribution

There are no data available on the absorption, distribution and metabolism of isopropylated triphenyl phosphates in experimental animals or humans.

Two *in vitro* studies investigated the absorption of Reolube HYD 46 and Reofos 50 through human skin (Scott 1985, Scott and Thompson 1985, cited in IUCLID 2000). Both studies appear to have been conducted using identical methods, although only one was conducted to GLP. In both studies, human epidermis was drawn over a receptor chamber containing 70 per cent ethanol in a glass diffusion cell. The test substance (Reolube HYD 46 or Reofos 50, concentrations not given) was placed in the donor chamber. After an exposure of 57 hours, the ethanol was analysed for the presence of test substance. Absorption rates for TPP and 2-IDPP were calculated at 0.67 ± 0.3 and 3.32 ± 0.12 µg/cm^2/h, respectively in the non-GLP compliant study, and 0.9 ± 0.13 and 0.54 ± 0.12 µg/cm^2/h respectively, in the GLP study. It is not clear to which test substance TPP and 2-IDPP refer, although TPP is likely to be triphenyl phosphate from the composition information in Table 1.1. It was reported that a steady state was achieved within one hour, but that the experimental design could give rise to greater absorption than might occur under normal dermal exposure scenarios.

4.4.2 Acute toxicity

Only data for experimental animals are available.

Oral

Several oral lethality studies are reported in IUCLID (IUCLID 2000) on various commercial preparations (Reofos 50, 65, 95, Durad 300). However, full study details are not presented and the majority were performed before 1985 and appear not to have been to GLP standards or international test guidelines. Thus, the quality of the studies cannot be determined with confidence. Nonetheless, the weight of evidence suggests that isopropylated triphenyl phosphates are not particularly acutely toxic to rats or Chinese hamsters.

In a number of studies conducted by the Food and Drug Research Laboratories Inc. (FDRL) in 1975 (Bailey 1975g, h, i, j, cited in IUCLID 2000, and FDRL 1975b, cited inIUCLID 2001), groups of rats (ten animals in total comprising, in the majority of cases, five of each sex) were given 20,000 mg/kg bodyweight of isopropylated triphenyl phosphates in the form of, for example, Reofos 50, 65, 95 or Durad 300 (method of oral administration not reported), followed by an observation period of 14 days. None of the rats given Reofos 95 or Durad 300 died but 4/5 females given Reofos 50 and 4/5 females given Reofos 65 died during the observation period; this suggests that female rats may be more susceptible to a single, high dose of these substances than males.

In another non-GLP compliant study by Ciba-Geigy (Kobel 1983c, cited in IUCLID 2000), there were no deaths in Chinese hamsters (five per sex) given 5,000 mg/kg bodyweight Reofos 50 during a 14-day observation period.

In two other studies conducted to GLP but not international test guidelines (Freeman 1990c, d, cited in IUCLID 2000), there were no deaths over a 14-day observation period in groups of rats (three per sex) given single oral doses of Reofos 50 or Durad

300 at 5,000 mg/kg bodyweight. However, clinical signs were noted in those rats given Reofos 50; these included tremor, oral discharge, ataxia, decreased locomotion, chromorhinorrhea, chromodacryorrhea and abdominogenital staining. Recovery was apparent by day 11; no further detail was reported. Abdominogenital staining and chromorhinorrhea were also reported for rats given Durad 300 during the first two days of the observation period; no further information was given. For these studies, the LD_{50} was calculated to be above 5,000 mg/kg bodyweight.

Inhalation

No data from reliable studies are available.

There are two studies of limited quality on the acute inhalation of isopropylated triphenyl phosphates (Bailey 1975e, f, cited in IUCLID 2000, and FDRL 1975a, cited in IUCLID 2001). In each study, rats (five per sex) were exposed to 200 mg/l aerosolised Reofos 65 or Reofos 50 gas/vapour for one hour, followed by a 14-day observation period. No other information on test material or study design was given. One female exposed to Reofos 65 died on day four and one female exposed to Reofos 50 died on day seven.No other animals died during the observation period, and no signs of toxicity were reported. Neither of these studies conforms to current test guidelines (which require an exposure period of four hours) and thus they are considered to be of only limited value.

Dermal

In a GLP-compliant study, Reofos 50 at 2,000 mg/kg was applied to the skin of Sprague-Dawley rats, three or five per sex) under an occlusive patch for 24 hours; it was not reported if shaving or abrasion of the test site was undertaken (Freeman 1990a, cited in IUCLID 2000, 2001). The test site was observed immediately after the 24-hour exposure period, and then daily for 14 days. Bodyweights were recorded on days one, three, senve and 14, and gross necropsies were performed on all animals. No animals died and no skin irritation was observed. There was no apparent effect on body weight and no gross pathology was noted. The LD_{50} was above 2,000 mg/kg bw.

In two non-GLP compliant studies conducted to OECD Guideline 402 by Ciba-Geigy (Kobel 1983a, b, cited in IUCLID 2000), test material - either Reofos 50 or Reolube HYD 46) - was applied at 2,000 mg/kg to either intact and/or shaved skin of two groups of rats (five per sex) and covered with an occlusive dressing for 24 hours. The test site was then cleaned with lukewarm water, and the rats observed for 14 days. No animals died in either study but signs of toxicity included dyspnea, ruffled fur, hunched posture, curved and ventral body position, sedation and erythema of the exposed skin of rats treated with Reolube HYD 46; neither the numbers affected nor the degree of severity were reported. Based on these studies, the LD_{50} was above 2,000 mg/kg.

In a GLP study not conducted to an established international test guideline (Freeman 1990b, cited in IUCLID 2000), Durad 300 was applied at 2,000 mg/kg to the intact skin of three rabbits, under occlusive conditions for 24 hours. It was not stated whether the substance was then rinsed from the skin after the exposure period, and no additional study details were given. No deaths or signs of toxicity or irritation were reported during the 14-day observation period. The LD_{50} was above 2,000 mg/kg bodyweight.

A number of other non-GLP compliant studies were reported in rabbits although the level of detail available is limited (Bailey 1975a, b, c, d, cited in IUCLID 2000). In these studies, Reofos 50, Reofos 65, Reofos 95 or Durad 300 was applied at 10,000 mg/kg bodyweight to the intact or abraded skin of groups of five rabbits for 24 hours, followed

by a 14-day observation period. IUCLID (2000) does not specify if semi-occluded or occluded conditions were used. None of the rabbits exposed to Reofos 50, Reofos 65 or Reofos 95 died, but no information on signs of toxicity are reported. No information on mortality among rabbits exposed to Durad 300 was given. Based on these studies, the LD_{50} for Reofos 50, Reofos 65 and Reofos 95 is above 10,000 mg/kg bodyweight.

Neurotoxicity

Oral

A number of single-dose studies have evaluated the neurotoxic potential of isopropylated triphenyl phosphates, but none have been conducted to international (OECD) guidelines and the level of reporting in the secondary sources used varies.

In a GLP-compliant rodent study (Krueger 1990, cited in IUCLID 2000), male Long-Evans rats (five/group) were given a single oral dose of 2,000 mg/kg bodyweight Reofos 65 after overnight fasting; controls received either saline (negative) or tri-*ortho*-cresyl phosphate (TOCP) (positive). Blood samples were taken before, and 24 hours after, dosing and analysed for plasma cholinesterase (ChE) activity. Rats were killed 44 hours after dosing and brains were removed and assayed for brain ChE and neuropathy target esterase (NTE) activities. Reduced plasma ChE activities were noted in the positive control (94 per cent) and treated animals (84 per cent), compared with the saline controls (100 per cent); it is not clear whether the differences achieved statistical significance. Significant inhibition of brain ChE (35 per cent) and NTE (50 per cent) activity was reported in treated animals, with values lower than those of the positive controls (69 per cent and 91 per cent, respectively). Reofos 50-treated animals did not show any clinical effects in contrast to TOCP-treated rats which showed lacrimation, tremor, staining and lowered body temperature.

In a single dose study conducted by Huntingdon Research Centre in 1980 to GLP (Roberts 1980b, cited in IUCLID 2000), domestic hens (ten/group) were given Reofos 50 orally at 2,000, 4,000, 6,000 or 8,000 mg/kg bodyweight. Controls (18 per group) were dosed with either corn oil (negative) or TOCP (positive); no further details of dosing regimen were given. Hens were monitored for signs of neurotoxicity for 21 days after dosing. Ataxia was noted in one out of 10 birds in the 2,000 mg/kg bodyweight dose group, four out of 10 in the 4,000 mg/kg bodyweight dose group, six out of 10 in the 6,000 mg/kg bodyweight dose group and three out of 10 in the 8,000 mg/kg bodyweight dose group. Histological examination of the spinal cord showed some swollen and severely degenerated nerve fibres in some animals from each dose (it is unclear if this was observed in either of the control groups) and it was reported that these changes did not always correlate with observed ataxia (no further details given).

In another GLP-compliant single-dose study conducted by Huntingdon Research Centre in 1980 (Study no. FCC7/79329, cited in IUCLID 2001), adult domestic hens (ten/group) were given Kronitex 100/Reofos 65 at 3,000, 5,000, 7,000 or 9,000 mg/kg bodyweight; control hens (18 per group) were given corn oil (negative) or 500 mg/kg bodyweight TOCP (positive). Hens were observed for 21 days for clinical signs, particularly ataxia. Body weights were measured on days one, seven, 14 and 21. Necropsy was performed on all birds on day 21, and the cervical, thoracic and lumbar regions of the spinal cord and sciatic nerve then examined histopathologically for evidence of neuropathy. Hens of the positive control and high-dose test groups showed marked bodyweight reductions (data were not presented). Transient ataxia was observed in some hens from the 3,000 and 5,000 mg/kg bodyweight groups (precise details not given) but symptoms were no longer apparent by the end of the observation period. One hen in the 7,000 mg/kg bodyweight-dose group showed signs of ataxia on day ten which became more pronounced by day 21, and another high-dose hen

showed signs of ataxia on day ten which became so severe that it was killed on day 15. Histopathologically, one hen from each of the 3,000 and 5,000 mg/kg bodyweight groups and two from the 9,000 mg/kg bodyweight group showed distinct neuropathological lesions, which in some cases were reported as “relatively severe”. However, neither the precise nature of the abnormalities nor any potential correlation with observed clinical signs were specified. Neither ataxia nor neuropathological lesions were noted in the negative control hens but 17 of the 18 hen positive controls developed ataxia and serious neuropathological lesions.

In a poorly reported study on Reofos 50, an ED_{50} in hens for delayed neurotoxicity of 3,928 mg/kg bodyweight (2,715-5,265 mg/kg bodyweight) was reported. However, no study details were reported (Bradley 1980, cited in IUCLID 2000).

The results of the available avian single dose oral neurotoxicity studies are summarised in Table 4.8.

Table 4.8 Summary of available single oral dose neurotoxicity studies in hens

Test material	Dose (g/kg bw)*	No. of hens	No. of hens showing ataxia	GLP status	Reference
Reofos 50	5, 8 or 12	2/group	0	No	Swallow 1981b
Reofos 50	2, 4, 6 or 8	10/group	1, 4, 6 and 3, respectively	Yes	Roberts 1980b
Reofos 50	0.5, 1 or 2	3/group	0	No	Cascieri 1977a
Reofos 50	4	20/group	14	No	Cascieri 1977a
Reofos 120	8 or 12	2/group	0	No	Swallow 1981a
Reofos 65	0.5, 1, 2 or 4	10/group	2 in 4 g/kg dose group	No	Cascieri 1977b
Reofos 65	3, 5, 7 or 9	10/group	0, 3 (transient), 1, 1	Yes	Roberts 1980c
Reofos 95	2.5, 5, 10 or 20	10/group	0, 0, 0 and 2, respectively	No	Cascieri 1977c
Reofos 95	20, 30, 40 or 50	10/group	1, (transient), 2, 2 and 2, respectively	No	Roberts 1980d
Durad 300	2, 4, 8 or 16	4/group or 10/group (high dose only)	0, 0, 0 and 3, respectively	No	Cascieri 1977d

Notes: * Hens observed for a 21-day period after dosing.

Inhalation

In a GLP-compliant study by Huntingdon Research Centre (1980), hens (ten/group) were exposed to isopropylated triphenyl phosphates (as Reofos 50) aerosol at achieved doses of 0.62, 2.40, 2.54 or 3.09 mg/l by inhalation for eight hours followed by a 21-day observation period (Roberts 1980a, cited in IUCLID 2000); no further details of study design were given and it not stated whether controls were included. Mild or moderate ataxia was observed in two out of 10 birds given 2.40 mg/l and four of the 10 birds given 3.09 mg/l, and histopathology showed neurodegenerative changes in animals from these dose groups. No effects were reported at the lowest dose of 0.62 mg/l. Information was not reported for the group given 2.54 mg/l. The no observed adverse effect level (NOAEL) in this study appears to be 0.62 mg/l, although the poor level of reporting makes assessment of study reliability difficult.

Summary of acute toxicity

No information is available from human studies.

No studies conducted to current guideline tests are available for acute oral toxicity. However, the data from a number of other studies of limited quality may be used to build a weight-of-evidence approach to establishing the acute toxic profile and determining an LD_{50}. For rats and Chinese hamsters given single oral doses of isopropylated triphenyl phosphates, LD_{50} values ranged from above 5,000 mg/kg bodyweight to above 20,000 mg/kg bodyweight, which are above the limit value of 2,000 mg/kg bodyweight applied in modern studies. This indicates a low level of toxicity when isopropylated triphenyl phosphates are administered in a single oral dose.

The acute toxicity of isopropylated triphenyl phosphates following dermal application to rabbits is low, with a LD_{50} of greater than 2,000 mg/kg bodyweight. In two non-GLP rat studies conducted to OECD guideline 402, Reofos 50 and Reolube HYD 46 at 2,000 mg/kg resulted in a number of signs of toxicity, including: dyspnea; ruffled fur; hunched posture; abnormally curved and ventral body position; and sedation; those given Reolube HYD 46 also showed erythmea.

There is one acute inhalation study in rodents available on isopropylated triphenyl phosphates, but the exposure period was only one hour rather than the current recommended duration of four hours. This is, therefore, not considered to be valid. A GLP-compliant inhalation neurotoxicity study in hens found that hens treated with Reofos 50 aerosol at doses of 2.40-3.09 mg/l for eight hours developed mild or moderate ataxia (two out of 10 birds given 2.40 mg/l, four out of 10 birds given 3.09 mg/l) and neurodegenerative changes. Available study details are, however, limited but since no effects were reported at the lowest dose employed, a NOAEL of 0.62 mg/l could be proposed.

At high oral doses of isopropylated triphenyl phosphates (above 2,000 mg/kg bodyweight), hens showed ataxia with, in some studies, associated neuropathological lesions. However, none of the acute neurotoxicity studies were conducted to international (OECD) guidelines and only limited details are available. Nonetheless, collectively the studies suggest single doses of isopropylated triphenyl phosphates may, at sufficient doses, result in neurotoxicity.

4.4.3 Irritation

Only experimental animal data are available.

Skin

In a study carried out by FMC Corporation to GLP but not international guidelines (Freeman 1990h, cited in IUCLID 2000, 2001), Reofos 50 was applied at 0.1 or 0.5 ml under semi-occlusive conditions to the shaved skin of three New Zealand rabbits for four hours. At the end of the exposure period, the skin was washed to remove the test substance and the test site scored for irritation using the Draize system, at 4.5, 24, 48 and 72 hours after removal of the test substance. The primary irritation score was zero, indicating that the substance was not a skin irritant. No further study details were given.

In another study conducted to OECD guideline 404 but not GLP standards (Swallow 1984c, cited in IUCLID 2000), 0.5 ml Reofos 50 was applied to the intact skin of three rabbits under an occlusive dressing for four hours. Irritation was scored at 30-60 minutes, and 24, 48 and 72 hours after removal of the dressing; no further details are reported. No signs of irritation were noted.

A study investigating the irritant potential of Reolube HYD 46 was conducted according to OECD guideline 404 but not GLP (Swallow 1984d, cited in IUCLID 2000). In this, 0.5 ml of test substance was applied to the intact skin of rabbits (two per sex) under an occluded patch. After 24 hours, the patches were removed (not specified if test sites were washed) and the test sites observed over a ten-day period. One rabbit showed slight erythema for up to 72 hours after removal of the patch but by day ten all rabbits were normal.

Several earlier non-GLP rabbit studies on Reofos 50, Reofos 95 and Durad 300 (Bailey 1975o, p, q, cited in IUCLID 2000) found the test materials to be non-irritant when applied for 24 hours to intact or abraded skin under semi-occlusive dressing, and it was reported that a GLP-compliant study on Durad 300 (Freeman 1990g, cited in IUCLID 2000) found no signs of irritancy applied at a dose of 0.5 ml for four hours under semiocclusive patch to three rabbits.

Eye

In a non-guideline study conducted under GLP (Freeman 1990e, cited in IUCLID 2000, 2001), 0.1 ml of Reofos 50 was applied to the conjunctival sac of the right eye of each of three New Zealand rabbits; eyelids were held closed for approximately one second after dosing; no information regarding controls was given. The eyes were scored for irritation using the Draize system at one, 24, 48 and 72 hours after dosing. At 24 hours, two treated eyes showed slight conjunctival redness but this disappeared by 48 hours. At 24, 48 and 72 hours the primary irritation index was 1.3, zero and zero, respectively.

In a similar, but poorly reported, GLP study, Durad 300 was found to not be irritating to the eyes of three rabbits (Freeman 1990f, cited in IUCLID 2000).

In another study conducted to OECD guideline 405 but not to GLP (Swallow 1984a, cited in IUCLID 2000), three out of four rabbits given Reofos 50 at 0.1 ml into the conjunctival sac were reported to show signs of conjunctival irritation. However, the time of appearance and severity were not reported although it was noted that signs had resolved by seven days. No further information was given in the study summary.

Reports of several other studies on Reofos 50, Reofos 65, Reofos 95 and Durad 300 that were non-GLP and not to international test guidelines (Bailey 1975k, l, m, n, cited in IUCLID 2000), reported the test substances not to be irritant after application of 0.1 ml of the test substance to one eye of each of nine rabbits. In three out of nine rabbits the test substance was rinsed from the eye four seconds after application. Observations were made at 24, 48, 72 hours and seven days. Reofos 65 was also found not to be irritant in three rabbits given the test substance in one eye, and observed for seven days (Benthe 1982, cited in IUCLID 2000).

In a study conducted to OECD guideline 405 but not GLP, application of 0.1 ml Reolube HYD 46 to one eye of rabbits (two per sex) resulted in slight/moderate redness in all treated eyes one hour after administration (Swallow 1984b, cited in IUCLID 2000). Irritation was recorded at one, 24, 48, 72 hours, seven and 10 days after dosing, but details were not reported. However, signs of irritation had resolved for all animals by day ten.

Summary of irritation

No information is available from human studies.

In a study conducted to OECD guideline 404 but non-GLP compliant and in another GLP, non-guideline study, Reofos 50 was found not to be irritant to the skin of rabbits.

In a non-GLP compliant study conducted to OECD guideline 404, the skin of one of four rabbits exposed to Reolube HYD 46 showed slight, transient erythema for up to 72 hours after the end of the exposure period.

In two OECD guideline 405 studies, three out of four rabbits dosed in the eye with Reofos 50 showed conjunctival irritation which cleared by day seven while Reolube HYD 46 caused slight/moderate redness in all treated eyes by one hour after administration with resolution by day ten. In another GLP, non-guideline study, Reofos 50 caused slight, transient conjunctival redness in two out of three treated eyes of rabbits by 24 hours after administration with a primary irritation index of 1.3. Without further information regarding the Draize scores in these studies, it is not possible to fully assess the ocular irritant potential of isopropylated triphenyl phosphates.

4.4.4 Corrosivity

None of the studies available on skin and eye irritation suggest that isopropylated triphenyl phosphates has corrosive properties.

4.4.5 Sensitisation

Only data on experimental animals are available.

Skin

Two studies conducted to GLP and OECD guideline test 406 investigated the skin sensitisation potential of Reofos 50 and Reolube HYD 46 (Maurer 1983a, b, cited in IUCLID 2000). Guinea pigs (numbers not specified) were given intracutaneous injections of 0.1 per cent solution of the test substance in 20 per cent propylene glycol/80 per cent physiological saline every second day for a total of ten injections; controls were given vehicle alone. An adjuvant was added to the injection solution during the second and third weeks of treatment (no further information available). Fourteen days after the last induction treatment, an injection of 0.1 ml of 0.1 per cent test solution was given as a challenge into the skin of the left flank. Reactions were monitored for 24 hours after each injection in the first week, and following the challenge injection. Ten days after challenge, a sub-irritant dose (30 per cent of test substance in Vaseline) was applied to the skin under an occlusive dressing for 24 hours and reactions were recorded at 24 and 48 hours after removal of the dressing. Both test substances were reported not to cause sensitisation but no details were given.

Summary of sensitisation

Based on the limited information available from two GLP, OECD guideline 406 studies, isopropylated triphenyl phosphate does not appear to be a skin sensitizer.

No information on respiratory tract sensitisation is available.

4.4.6 Repeated-dose toxicity

Animal data

Several studies have investigated the effects of repeated exposure to isopropylated triphenyl phosphates via oral or dermal routes. However, in all cases reporting is limited and only the dermal exposure studies were performed according to OECD test guidelines and under GLP.

In a dietary study on Kronitex K-100 (purity not described; Foster D, Snell 1976, cited in IUCLID 2001), four groups of Sprague-Dawley rats (40 per sex) were given treated diets containing the test substance at 0.1, 0.5 or 1.0 per cent, for 28 days. A control group received the basal diet without test substance. Body weights were recorded at the start of the study and weekly thereafter, and food consumption was recorded weekly. Animals were observed daily for survival and clinical signs, and gross necropsies were performed at termination. Haematology (haemoglobin, haematocrit, erythrocyte count and total and differential leukocyte counts), blood chemistry (blood urea nitrogen (BUN), bilirubin, glutamic-pyruvic transaminase activity, glucose, cholesterol, lactic acid dehydrogenase activity, total protein and albumin levels) and urinalysis (pH, glucose, ketones, bilirubin and occult blood) was undertaken on five male and five female rats of unspecified groups. At necropsy, the following organs were collected and weighed; brain, thyroid, heart, liver, spleen, gonads and kidney. It is not specified if this was done on all animals but histopathological examination was conducted on the livers and kidneys of high-dose and control animals. Twelve rats died during the treatment period, four in each of the low- and mid-dose groups, three in the high-dose group, and one control. Bodyweight was reduced in high dose females and food consumption was lower in males and females of the mid- and high-dose groups; no further details were reported. The achieved intakes of test substance during the study were not provided. Abnormal haematological values were noted in high-dose animals and abnormal blood chemistry findings were noted in the mid- and high-dose. However, further details were not reported in the IUCLID. Urinalysis did not reveal any changes. At necropsy no treatment-related gross lesions were observed although liver-to-bodyweight ratios were increased in all treated groups; further details were not reported. Histopathological examination of the kidneys and livers of high-dose and control animals was reported to be unremarkable. The limited reporting makes it difficult to assess the importance of the various changes identified. However, based on the unspecified abnormalities in haematology and blood chemistry in high-, and mid- and high-dose, animals respectively, a NOAEL of 0.1 per cent was identified.

In a similar study, Kronitex 100 was again given in the diet at 0.1, 0.5, or 1.0 per cent to rats (ten/sex/group) for 28 days (Bailey1976, cited in IUCLID 2000); a control group received basal diet without test substance. No further methodological details were given in the IUCLID, except that microscopic examination was not undertaken. Mortality during the treatment period was equal among treated and control groups although actual numbers were not specified. Rats of the high-dose group had loose stools and showed lethargic behaviour. Bodyweight was reduced in high-dose females throughout the study, while food consumption was lower in males and females from the mid- and high-dose groups and red and white blood cell counts were slightly lower (presumably compared to controls) in high-dose animals; further results were not reported. Elevated liver-to-bodyweight ratios were noted in high-dose animals and BUN was elevated in all treatment groups. No statistical analysis of the data was noted and the authors of the IUCLID entry noted that the significance of the apparent changes in liver weight and BUN could not be evaluated, since no microscopic examination of the liver was performed. Given the poor level of reporting, this study is considered of limited usefulness.

In two briefly reported repeat dose studies conducted to OECD Guideline 410 and GLP (Kobel 1984a, b, cited in IUCLID 2000), Kronitex 50 (at 100, 500 or 2,000 mg/kg bodyweight) or Reolube HYD 46 (at 40, 200 or 1,000 mg/kg bodyweight) was applied to the shaved skin of rats (F3 hybrid of RII 1/Tif and RII 2/Tif or RAIF) (five/sex/group), for six hours per day, five days a week, for four weeks; vehicle (unspecified) alone was applied to the skin of controls. For Kronitex 50-treated animals, a slight but statistically significant ($p < 0.01$) decrease in plasma cholinesterase (ChE) activity was noted in mid- and high-dose females while the effect was slight and non-significant in the high-dose males. Erythrocyte ChE activity was also significantly ($p < 0.01$) depressed in high-dose males. Increased adrenal weights were noted in mid- and high-dose males (no further details). Histopathological examination revealed slight fatty change of the adrenal cortex in two of five males given 500 mg/kg bodyweight and three of five males given 2,000 mg/kg bodyweight Kronitex 50. Although the studies were reported to be conducted according to OECD guideline 410 “repeated dose dermal toxicity 21/28 day study”, no routine haematology or blood chemistry data were reported and the range of parameters investigated in the study is unclear. Based on the limited information provided, the NOAEL for Kronitex 50 was 100 mg/kg bodyweight. Female rats treated with Reolube HYD 46 at 1,000 mg/kg bw/day also showed a slight depression in plasma ChE activity, although it is not stated if this attained statistical significance. Lower absolute and relative testicular weights were noted in high-dose males (no further details given) while histopathology showed slight testicular tubular atrophy in control and treated rats (no further details). Slightly higher absolute and relative adrenal weights were noted in treated animals but this finding was reported not to correlate with any microscopic findings (no further details given). Based on the limited information available, a NOAEL of 200 mg/kg bodyweight was established for Reolube HYD 46.

Neurotoxicity

In a sub-acute study not conducted to GLP, six hens were given Reofos 50 at 5,000 mg/kg/day for five days and then observed for 21 days (Swallow 1982, cited in IUCLID 2000). Five of the six hens showed signs of ataxia, one dying on day 14 and another killed on day 16 because of severity of symptoms. Histopathology of the spinal cords of treated birds showed evidence of delayed organophosphate neurotoxicity (axonal degeneration). No further details were given.

In a GLP-compliant 28-day neurotoxicity study (Roberts 1985, cited in IUCLID 2000), hens (five per group) were given Reofos 50 at doses of 1.7, 5, 16, 49, 148, 444, 1,333 or 4,000 mg/kg/day. At the end of the 28-day dosing period, hens were killed without examination. No signs of ataxia were noted in hens given 1.7, 5, 16 or 49 mg/kg/day but 20 per cent of hens given 148 or 444 mg/kg/day, 40 per cent on 1,333 mg/kg/day, and all surviving hens (2/5) given 4,000 mg/kg/day, were reported to show signs of ataxia. The NOEL was therefore established as 49 mg/kg/day. The results of this study were used to select doses for the sub-chronic study described immediately below.

In a 91-day sub-chronic neurotoxicity study conducted to GLP, adult White Leghorn hens (20 per group) were given Reofos 50 at 10, 20, 90 or 270 mg/kg/day by oral gavage (Roberts 1985, cited in IUCLID 2000, and Huntingdon Research Centre study no. FCC 7/79329 1980, cited in IUCLID 2001). Control hens (20 per group) received daily oral doses of 1.5 or 7.5 mg/kg/day TOCP (positive) or corn oil (negative). Hens were observed daily for mortality and clinical signs, and bodyweight and food consumption were measured weekly. At the end of the treatment period, animals were killed and examined macroscopically. The brains, spinal cord and peripheral nerves (tibial and sciatic) of ten hens per group were fixed and examined microscopically. No signs suggestive of neurotoxicity were seen in the vehicle controls or those given the two lowest doses of Reofos 50. However, four hens given 90 mg/kg/day developed ataxia (of which two were killed during the treatment period) as did nine hens given 270 mg/kg/day (all of which were killed prior to the end of the study). Overall, deaths

occurred during the treatment period in all groups (vehicle control - two; positive control - four; 10 mg/kg/day - three; 20 mg/kg/day - three; 90 mg/kg/day - five; and 270 mg/kg/day - six). Body weight loss was noted in the 90 and 270 mg/kg/day groups and in positive controls (no further details). Histopathologically, degeneration of the spinal cord and peripheral nerves was observed in hens given 90 or 270 mg/kg/day; the finding correlated with the observations of ataxia, and the severity and incidence were dose-related (no further details). Significant degeneration of the spinal cord was also seen in the TOCP-treated hens (positive control) while two hens from the vehicle control group also showed significant degeneration at three levels of the spinal cord. The NOEL for neurotoxicity in this study was considered to be 20 mg/kg/day.

In a non-GLP compliant, repeat dose dermal exposure study not conducted to international guidelines, Reofos 65 at 50 mg/kg bw/day was applied to the combs of ten hens by pipette and spread evenly over the comb surface, five days a week, for four months (Cascieri and MacKellar 1977, cited in IUCLID 2000). A positive control group of ten hens received TOCP in the same way as the test substance. No information on the inclusion of a negative control was given. Blood samples were collected from the hens at the end of the treatment period for haematology and blood chemistry investigations and all birds were necropsied, with the brains removed for analysis for neurotoxic esterase activity. The spinal cords and peripheral nerves were subject to histopahtological examination for evidence of neuropathy. No signs of neurotoxicity were noted during the treatment period, and no haematological, blood biochemical or histological changes suggestive of toxicicty was noted in hens treated with the test substance. However, the positive control hens developed ataxia and nerve damage.

Human data

There are no valid human data available.

In an unpublished occupational exposure study of unknown quality (Reape 1989, cited in IUCLID 2000) conducted between July 1980 and December 1981 at an FMC Corporation plant producing aryl phosphates (particular chemicals unspecified), 60 exposed participants (52 males and eight females) and 53 unexposed controls (39 males and 14 females) were subject to clinical examination including nerve conduction velocity tests on four nerves. One group of workers (unspecified number and relationship to study groupings unclear) were noted to have worked in the facility prior to 1974. After this time, the aryl phosphate production system used was enclosed and the potential for worker contact and intensity of any exposure was reduced (no further details given). Air and surface samples were taken (not clear when or how often) for analysis of aryl phosphate levels as a measure of exposure. Aryl phosphates were reported to be present in “small quantities” on most surfaces tested and in air samples at concentrations of one ppb or less. Nerve conduction velocities were reported to be similar in control and exposed workers, and it was concluded that the effect of working with aryl phosphates in this plant was negligible. Given the limited study reporting and lack of data on exposure and other results, the findings are considered of limited value.

A case report is available about a 48-year-old worker who had been exposed to hydraulic fluids, particularly on his hands and arms, during work for the previous two years (Jarvholm *et al*. 1986, cited in IUCLID 2000). The worker was reported to have developed weakness and paresthesia in his hands, and his nerve conduction velocities were said to be “reduced”. The study was unable to relate these symptoms to exposure to hydraulic fluid components. This report also presented another investigation in which electromyographs of four nerves were recorded for eight men with a history of exposure to hydraulic fluids; four showed a reduced number of motor unit potentials and some single potentials of increased duration and amplitude, when compared with eight controls (no information on the control subjects was reported).

Summary and discussion of repeated-dose toxicity

Limited reports of studies on oral or dermal exposure are available on the toxicity of isopropylated triphenyl phosphates arising from repeated exposure, with only the available dermal studies conducted to international test guidelines and GLP.

In a 28-day oral study where groups of rats were treated with Kronitex K-100 (0.1, 0.5, or 1.0 per cent), unspecified abnormal haematology and blood chemistry was noted in high- and mid/high-dose animals, respectively. Based on the findings, a NOAEL of 0.1 per cent is proposed.

In rats treated with Kronitex 50 for four weeks, slight fatty change of the adrenal cortex was noted for two of five males given 500 mg/kg bodyweight and three of five males given 2,000 mg/kg bodyweight. Based on these findings and other reports of decreases in plasma and erythrocyrte ChE activity, a NOAEL of 100 mg/kg bodyweight was established in male and female rats.

A non-GLP, non-guideline, repeat dermal exposure study reported no signs of neurotoxicity in hens treated with Reofos 65 at 50 mg/kg bw/day, five days a week for four months. However, other studies have identified neurotoxic effects following repeated exposure to isopropylated triphenyl phosphates. In a sub-acute non-GLP compliant study, five of six hens given Reofos 50 at 5,000 mg/kg/day for five days showed signs of ataxia and evidence of delayed organophosphate neurotoxicity (axonal degeneration) and, in a 91-day, GLP-compliant, sub-chronic study in which adult White Leghorn hens were given Reofos 50 at 10, 20, 90, or 270 mg/kg/day by oral gavage, birds from the two highest doses showed degeneration of the spinal cord and peripheral nerves, which correlated with signs of ataxia; both severity and incidence was dose-related. No clinical signs of neurotoxicity were reported in birds given the two lower doses, and the NOEL for neurotoxicity was established at 20 mg/kg/day.

4.4.7 Mutagenicity

Studies in vitro

Genetic mutations

A number of bacterial reverse mutation studies were conducted by Ciba-Geigy or Microbiological Associates between 1976 and 1983 (Arni 1978a, b, Deparade 1983, Auletta 1976, Kouri 1977, Rouri 1977, cited in IUCLID 2000); these were carried out before adoption of international test guidelines and only one study was GLP-compliant (Deparade 1983, cited in IUCLID 2000). However, the findings from these studies may be used to build a weight of evidence approach.

In summary, Reofos 50, Reofos 65, Reofos 95, Durad 300 and Reolube HYD 46 have been tested in up to five strains of *Salmonella typhimurium* (TA98, TA100, TA1535, TA1537 and TA1538), in the presence or absence of metabolic activation. Positive controls were included in some but not all studies. All compounds tested negative for mutagenicity although it was noted that Reolube HYD 46 precipitated at concentrations of 320 µg per 0.1 ml or above (IUCLID 2000).

A number of mammalian cell gene mutation studies conducted between 1981 and 1985, generally to GLP but not to international guidelines, are also available (IUCLID 2000). Several have investigated the potential for Reofos 50 (at 0.04 to 28 µg/ml) and Reolube HYD 46 (at 0.5 to 44 µg/ml) to induce transformed foci in Balb/3T3 mouse

embryo fibroblasts (Beilstein 1985a, b, Puri 1985, Sivak 1981, cited in IUCLID 2000). Both compounds tested negative in the presence or absence of metabolic activation.

In a further mammalian cell study conducted under GLP, the potential for isopropylated triphenyl phosphates to induce mutations at the thymidine kinase (TK) locus in cultured L5178Y mouse lymphoma cells was investigated (Kirby 1982, cited in IUCLID 2000). The study was conducted on Reofos 50 (at 0.0013 to 0.1 µl/ml) in the presence and absence of metabolic activation but no further details are available. In the absence of metabolic activation Reofos 50 was negative but, with metabolic activation, results were considered equivocal. Some evidence of a dose response was suggested although mutation frequencies were generally less than two-fold above background level for cultures exhibiting greater than ten per cent total growth. Detailed results were not reported and cytotoxicity was not discussed, limiting interpretation of this finding.

Cytogenetic effects

Two non-GLP studies have investigated the potential for isopropylated triphenyl phosphates to induce DNA damage and repair (Puri 1984 and Strasser 1987, cited in IUCLID 2000). The studies were not carried out to international guidelines and reporting of methodology is limited. Cultured rat hepatocytes were treated with Reofos 50 or Reolube HYD 46 (at 0.6, 3, 15 or 75 nl/ml) in dimethyl sulfoxide (DMSO) without metabolic activation, and the uptake of ^{3}H-thymidine by the cells visualised by autoradiograph. Neither test substance was found to cause unscheduled DNA repair.

Chromosomal effects

There is no available *in vitro* test information relating to chromosomal aberrations.

Studies in vivo

In a GLP-compliant dominant lethal assay (Valencia 1985, cited in IUCLID 2000) the potential of Reofos 50 to induce sex-linked recessive lethal mutations in male *Drosophila melanogaster* was investigated. Young adult male flies were treated with Reofos 50 (at 32.5, 75 or 150 mg/ml in a water-sucrose media) for three days before mating with Basc females. F_1 flies were grown and mated and the F_2 generation examined for the presence (non-lethal) or absence (lethal) of wild type males. Reofos 50 was found to be negative.

In a non-GLP, non-guideline study where the potential of Reolube HYD 46 to induce micronuclei was evaluated, NMRI female mice were given a single dose of 0.1, 0.5, 1.0, 10.0 or 50.0 g/kg bodyweight of test substance by oral gavage (Benthe 1988, cited in IUCLID 2000). Control animals received either arachidis oil (negative) or cyclophosphamide (positive). Bone marrow smears were prepared and examined for changes in the percentage of polychromatic (PCEs) and normochromatic (NCEs) erythrocytes. An increase in PCEs was observed at 10 and 50 g/kg bodyweight and the number of PCEs with micronuclei was increased in all groups; it is not clear whether this statement also relates to controls. This was attributed to inhibition of erythrocyte maturation (IUCLID 2000) and no chromosomal damage was induced.

Two studies investigated the potential for commercial isopropylated triphenyl phosphate compounds to induce sister chromatid exchanges (SCEs) in the Chinese hamster (Strasser 1983, 1984c, cited in IUCLID 2000). The studies were not to GLP or international guidelines. However, some study details are available. In these, male and female Chinese hamsters (four/sex/group) were given a single oral dose of Reolube HYD 46 or Reofos 50 (at 1,250, 2,500 or 5,000 mg/kg bodyweight in vehicle (arachidis oil for Reolube HYD 46, carboxymethylcellulose (CMC) for Reofos 50)). Colcemide was

administered two hours before sacrifice at 24 hours after dosing, and bone marrow slides were prepared. Neither substance was found to induce sister chromatid exchange (SCE).

A number of GLP-compliant studies have evaluated the potential for isopropylated triphenyl phosphates to induce somatic mutation in the Chinese hamster. In two studies conducted to OECD Guideline 475, Chinese hamsters (24 per sex) were given 5,000 mg/kg bodyweight of either Reofos 50 or Reolube HYD 46 (Strasser 1987a, b, cited in IUCLID 2000). Positive and negative controls were included, although details for these were not available. Animals were killed at three time points, 16, 24 and 48 hours after dosing, with bone marrow smears from the femur then examined for chromosomal aberrations. Neither test substances induced chromosomal damage (no further details).

Two earlier GLP but non-guideline studies on the same test substances reported positive results (Strasser 1984a, b, cited in IUCLID 2000). In these, hamsters (six or eight per sex per group) were dosed by oral gavage on two consecutive days with Reofos 50 (at 1,250, 2,500 or 5,000 mg/kg bodyweight in CMC) or Reolube HYD 46 (experiment 1: at 1,250, 2,500 or 5,000 mg/kg bodyweight; experiment 2: at 500, 822, 1,351, 2,221, 3,650 or 6,000 mg/kg bodyweight). Control groups were included in both studies but details of these are not available. Animals were killed 24 hours after the second dose and bone marrow smears prepared. Mid- and high-dose animals treated with Reofos 50 (2,500 or 5,000 mg/kg bodyweight) showed significantly increased frequencies of cells with chromosomal aberrations compared with control hamsters (further details not given). Animals treated in experiment 1 also had significantly increased frequencies of cells with aberrations at all treatment levels. In the second experiment on Reolube HYD 46, using a wider range of doses (500 to 6,000 mg/kg bodyweight), a significantly higher frequency of aberrations were noted in the high-dose group compared with controls (no further details).

Summary of mutagenicity

A number of genotoxicity test were conducted *in vitro* and *in vivo* on various commercial preparations of isopropylated triphenyl phosphate, a few of which gave positive or equivocal results. Reporting of study details in the 2000 IUCLID is limited, precluding detailed evaluation of the quality of the individual studies, particularly since Klimisch codes were not included in this IUCLID. Nevertheless, using a weight-of-evidence approach, overall the available information suggests that isopropylated triphenyl phosphate compounds may not be genotoxic. Reofos 50, Reofos 65, Reofos 95, Durad 300 and Reolube HYD 46 have all tested negative in bacterial reverse mutation assays, and Reofos 50 and Reolube HYD 46 did not transform cells or induce unscheduled DNA repair (although Reofos 50 gave some positive results including an apparent dose-response in the presence of metabolic activation in a TK mouse lymphoma assay).

In vivo Reofos 50 was negative in a dominant lethal assay in *D. melanogaster* and neither Reolube HYD 46 nor Reofos 50 induced SCEs in hamster bone marrow cells when tested *in vivo*. In a non-GLP study not to international guidelines, an increase in frequency of micronucleated PCEs was reported in mice treated with Reolube HYD 46 but this was attributed to inhibition of erythrocyte maturation rather than chromosomal damage. Furthermore, while positive and negative results were obtained in various somatic mutation assays for Reolube HYD 46 and Reofos 50, those studies performed according to OECD guidelines were negative. Overall, it is considered unlikely that isopropylated triphenyl phosphates are genotoxic.

4.4.8 Carcinogenicity

There are no experimental data on the carcinogenic potential of isopropylated triphenyl phosphates. However, an epidemiological study investigated cancer risk in employees of a plant in the USA (Shindell and Ulrich 1985, cited in IUCLID 2000). Mortality of the exposure group appeared unaffected, with cancer mortality slightly less than expected among white employees compared with the US population (no further details given) and no increases in mortality from specific cancers. However, information on the chemicals produced in the plant and employee exposure was not available, so this study was considered of limited value.

4.4.9 Toxicity to reproduction

There are no data available on the potential for isopropylated triphenyl phosphates to cause reproductive or developmental toxicity.

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

No experimental data are available on the potential for isopropylated triphenyl phosphates to cause reproductive or developmental toxicity. No experimental data are available for carcinogenicity, and the quality of the data on genetic toxicity could not be judged from the IUCLID files. The weight of evidence from the numerous *in vitro* and *in vivo* studies reported suggests that isopropylated triphenyl phosphates are not genotoxic. However, the data gap for reproductive toxicity is of more concern, due to the effects on fertility observed for some, but not all, aryl phosphates.

In a 28-day oral study where groups of rats were treated with Kronitex K-100 (0.1, 0.5, or 1.0 per cent), unspecified abnormal haematology and blood chemistry was noted in high- and mid/high dose animals, respectively. Based on the findings, a NOAEL of 0.1 per cent (1,000 ppm) is proposed.

In rats treated dermally with Kronitex 50 for four weeks, slight fatty change of the adrenal cortex was noted in two of the five males given 500 mg/kg bodyweight and three of five males given 2,000 mg/kg bodyweight. Based on these findings and other reports of decreases in plasma and erythrocyte ChE activity, a NOAEL of 100 mg/kg bodyweight was found in male and female rats.

No neurotoxicity studies on mammals are available. Studies on hens gave a NOAEL of 20 mg/kg bodyweight day for neurotoxic effects. This result is not suitable for deriving a margin of safety for human health effects.

In view of the limited database and gaps in information for this substance, and uncertainty over the composition of the substances tested, it is not appropriate to derive a margin of safety at this time. A number of possible areas for clarification in the mammalian toxicity data base are listed in Appendix 1. In the risk characterisation section, the oral NOAEL value above is used to give an indication of the margin of exposure between the estimated doses for humans exposed via the environment.

4.4.11 PNEC for secondary poisoning

Although the study on neurotoxicity in hens is not considered suitable for use in the human health risk assessment, it is appropriate for the derivation of the PNEC for secondary poisoning. The NOAEL value is 20 mg/kg bw/day. A factor of 8.3 is used to

convert this to a NOEC value of 166 mg/kg in food. The study is a sub-chronic study of 91 days' duration. The TGD does not have a specific factor for such a study, suggesting 3,000 for an acute study and 30 for a chronic study. For the purpose of this assessment a factor of 90 is applied, in line with the factor for a sub-chronic mammalian study. The resulting PNEC is 1.8 mg/kg.

This value is considered to relate best to isopropylphenyl diphenyl phosphate. It is not possible to calculate a PNEC for secondary poisoning for tris(isopropylphenyl) phosphate due to the lack of available toxicity data. The aryl phosphates included in this series of assessments show a range of PNEC values for secondary poisoning, from 0.16 to 4.4 mg/kg (this excludes tetraphenyl resorcinol diphenyl since it has a somewhat different structure). There are examples of specific isomers with notably different toxicities (such as the tricresyl phosphate isomers). It is therefore considered inappropriate to read across from other substances to fill this data gap.

4.5 Hazard classification

4.5.1 Classification for human health

None of the CAS numbers identified in Section 1.1 appear on Annex 1 of Directive 67/548/EEC. According to the criteria of the European Union, isopropylated triphenyl phosphate need not be classified on the basis of its acute toxicity, irritancy to the skin or corrosive to the skin or eyes, skin sensitization potential or mutagenicity.

Based on the EU criteria for classification, isopropylated triphenyl phosphates[8] require classification (Xn R48 – harmful) for specific target organ systemic toxicity following repeated oral exposure, as a NOEL for neurotoxicity of 20 mg/kg/day was noted in a 91-day study.

There are inadequate data to characterise isopropylated triphenyl phosphates with regard to reproductive or developmental toxicity, or carcinogenic potential, and therefore recommendations for classification cannot be made. In view of the reports of ocular irritation in a number of studies, it would be advisable to examine in more detail the study methodology and results, particularly irritation scores and their time courses, to provide a firm conclusion about the chemical's potential to cause ocular irritancy.

A number of changes suggestive of liver, testes and adrenal toxicity were noted in some studies but the available information is inadequate to determine if isopropylated triphenyl phosphates should be classified in the EU for these organs with regard to systemic toxicity.

4.5.2 Classification for the environment

Isopropylated triphenyl phosphate is not itself currently classified as dangerous to the environment. However, the actual classification of commercial products is generally based on the triphenyl phosphate content of the product (Great Lakes Chemical Corporation 2003). For this purpose, a distinction is usually made between the isopropylated triphenyl phosphate products with lower degrees of alkylation (typically containing above 15 per cent triphenyl phosphate) and those products with higher degrees of alkylation (typically containing below 10 per cent triphenyl phosphate).

[8] The substance tested was Reofos 50, which is considered to have a lower degree of alkylation and hence to be more relevant for isopropylphenyl diphenyl phosphates.

The lower alkylated products that contain above 25 per cent triphenyl phosphate carry the following label:

N: Dangerous for the environment.
R50/53: Very toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment.

The lower alkylated products that contain between 15 and 25 per cent triphenyl phosphate carry the following label:

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

The higher alkylated products (containing below 10 per cent triphenyl phosphate) are not classified as dangerous to the environment based on the lack of toxicity seen for this type of product in acute tests with fish, *Daphnia* and algae using water accommodated fractions.

Proposed classification

The fish BCF is around 564 l/kg for isopropylphenyl diphenyl phosphate and 1,986 l/kg for tris(isopropylphenyl) phosphate (Section 3.1.3). Acute toxicity data are available for commercial products for fish, invertebrates and algae. The lowest results from the more reliable standard tests are a 96-hour LC_{50} of 0.65 mg/l for fish (*Oncorhynchus mykiss*), and a 48-hour LC_{50} of 0.25 mg/l for invertebrates (*Daphnia magna*). There is some uncertainty over the actual 96-hour IC_{50} for algae (one study is available that showed no effects at above 1,000 mg/l when tested as a water-accommodated fraction). Based on these data, the following classification would appear to be appropriate for the lower alkylated (such as isopropylphenyl diphenyl phosphate) products:

N: Dangerous for the environment.
R50/53: Very toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment.

As discussed above, the currently applied classifications for isopropylated triphenyl phosphates appear to be based upon the triphenyl phosphate content. However, it is not clear from the available toxicity tests whether the acute toxicity seen is a result of the triphenyl phosphate present, or rather the isopropylated triphenyl phosphate itself. This is an important consideration for the classification of these substances.

Available acute toxicity data for the higher alkylated products (such as tris(isopropylphenyl) phosphate) appear to show that this substance type exhibits no acute toxicity at concentrations up to the water solubility limit. However, these higher alkylated substances are not readily biodegradable (although they can be considered inherently biodegradable and may hydrolyse under certain conditions) and have fish BCF values above 100 (the estimated value in this report is 1,986 l/kg). Adverse effects over longer term exposure cannot currently be ruled out. On this basis, a classification of R53 could be considered for the higher alkylated substances.

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 4.9.

Table 4.9 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 in marine conditions.

Persistence: Isopropylphenyl diphenyl phosphate is readily biodegradable (Section 3.1.1), which is considered equivalent to a half-life of less than 40 days in freshwater. Hence the substance does not meet the P criterion. Tris(isopropylphenyl) phosphate is considered to be inherently biodegradable but it is not possible to determine if the specific criteria are met (Section 3.1.1). Hence the substance meets the first stage screening criteria for P and vP.

Bioconcentration: A value of 564 is selected from the available data in Section 3.1.3 for isopropylphenyl diphenyl phosphate. Hence this substance type does not meet the B criterion. A BCF of 1,986 is estimated for tris(isopropylphenyl) phosphate, and this narrowly fails to meet the B criterion. Other available data suggest that the BCF could be higher, and therefore tris(isopropylphenyl) phosphate is considered to meet the B criterion (although a fully valid test is not available).

Toxicity: The lowest NOEC value from the available tests is 0.006 mg/l for isopropylphenyl diphenyl phosphate, and this is read across to tris(isopropylphenyl) phosphate for the purposes of this assessment. Hence both substance types are considered to meet the T criterion. In addition, they may also be classifiable with R48, indicating chronic mammalian effects.

The overall conclusion is that isopropylphenyl diphenyl phosphate does not meet the P or B criteria, and so is not a PBT substance. Tris(isopropylphenyl) phosphate meets the P, B and T criteria (P on the basis of screening data only). It is therefore a candidate for further investigation. Testing on persistence to determine a relevant environmental half-life should be considered.

5 Risk characterisation

This section identifies the potential risks that isopropylated triphenyl 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 Aquatic compartment

5.1.1 Surface water

A PNEC for surface water was estimated as 0.6 μg/l for both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate. The resulting PEC/PNEC ratios are summarised in Table 5.1.

Table 5.1 Summary of risk characterisation ratios for surface water

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (μg/l)	PEC/PNEC	PEC (μg/l)	PEC/PNEC
Production of isopropylated triphenyl phosphate		3.39	**5.66**	1.33	**2.22**
Lubricant additive	Blending of lubricant	0.35	0.58	0.07	0.12
Hydraulic fluid	Blending of fluid	0.34	0.57	0.10	0.16
Power generation fluid	Blending of fluid			0.07	0.12
	Use at power station			negligible	negligible
Adhesives		negligible	negligible	negligible	negligible
Paints	Formulation	19.8	**32.9**	0.61	**1.01**
	Application	0.53	0.89	0.27	0.45

Table 5.1 continued.

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (μg/l)	PEC/PNEC	PEC (μg/l)	PEC/PNEC
Textile/ fabric coating	Compounding	1.01	**1.68**	0.74	**1.23**
	Application of coating	0.67	**1.12**	0.40	0.67
	Combined compounding and application of coating	1.34	**2.24**	1.08	**1.8**
PVC – 1[a]	Compounding	0.69	**1.16**	0.21	0.36
	Conversion	0.52	0.86	0.13	0.22
	Combined compounding and conversion	0.87	**1.45**	0.28	0.47
PVC – 2[a]	Compounding	0.64	**1.07**	1.14	**1.89**
	Conversion	0.48	0.79	0.16	0.27
	Combined compounding and conversion	0.78	**1.31**	1.21	**2.02**
PVC – 3[a]	Compounding	0.72	**1.19**	0.44	0.73
	Conversion	0.51	0.85	0.1	0.17
	Combined compounding and conversion	0.90	**1.49**	0.47	
PVC – 4[a]	Compounding	0.64	**1.07**		
	Conversion	0.37	0.61		
	Combined compounding and conversion	0.67	**1.12**		
PVC – 5[a]	Compounding	0.64	**1.07**		
	Conversion	0.37	0.61		
	Combined compounding and conversion	0.67	**1.12**		
PVC – 6[a]	Compounding	0.56	0.93		
	Conversion	0.44	0.73		
	Combined compounding and conversion	0.66	**1.1**		
PVC – 7[a]	Compounding	1.9	**3.17**		
	Conversion	1.06	**1.77**		
	Combined compounding and conversion	2.68	**4.47**		
Thermo-plastics and styrenics	Compounding	0.46	0.77		
	Conversion	0.35	0.58		
	Combined compounding and conversion	0.47	0.78		
Poly-urethane	Compounding	2.12	**3.54**	0.81	**1.35**
	Conversion	0.5	0.84	0.13	0.22
	Combined compounding and conversion	2.32	**3.87**	0.88	**1.46**

Table 5.1 continued.

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (μg/l)	PEC/PNEC	PEC (μg/l)	PEC/PNEC
Pigment dispersions	Production of dispersions	0.58	0.97	0.81	**1.35**
Regional sources		0.34	0.56	0.07	0.11

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate do not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

The preliminary worst case PEC/PNEC ratios for isopropylphenyl diphenyl phosphate are above one for production and use in some PVC scenarios, polyurethane, textiles and formulation of paints. Further information is needed on process emissions to refine the PECs for these scenarios. Many of the ratios are not very far above one, and so revision of the assessment through a re-evaluation of exposure may be possible. The PNEC is derived using an assessment factor of 10 and is not likely to be revised through further testing (although no valid algal NOEC is available, the result from such a test is unlikely to revise the PNEC).

The local risk from use of isopropylphenyl diphenyl phosphate in thermoplastics and styrenics, pigment dispersion, adhesives, lubricant additives and hydraulic fluid appears to be low, as does the risk from regional sources.

For tris(isopropylphenyl) phosphate, the preliminary worst case PEC/PNEC ratios are above one for production, formulation of paints, use in textiles, polyurethane, pigment dispersion and use in one PVC application. Again, most of these ratios are not very far above one, and so a re-evaluation of exposure (better information on process emissions) might remove the concern.

The local risk from use of tris(isopropylphenyl) phosphate in adhesives, lubricants, hydraulic fluids and power generation fluids, use in some PVC scenarios and during the application of paints appears to be low. The risk from regional sources also appears to be low.

For many uses, the regional concentration contributes significantly to the predicted local concentrations. This is particularly the case for the assessment of isopropylphenyl diphenyl phosphate. The main contributions to the regional emissions come from in-service losses and/or waste remaining in the environment from some PVC applications, paints, printed circuit boards, textiles and lubricant applications. A suitable monitoring programme might be able to establish a more reliable background concentration for use in the assessment. However, for a number of local scenarios (just under half), the PEC/PNEC ratios would still be above one if the regional contribution was ignored.

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

In addition to the uncertainties over the emission estimates, there is also uncertainty over the PNEC for tris(isopropylphenyl) phosphate since there are no reliable chronic toxicity data. Further testing (such as a 21-day *Daphnia magna* reproduction test) could indicate whether the current PNEC for this substance type is appropriate.

5.1.2 Waste water treatment

A PNEC for waste water treatment of above one mg/l was derived for isopropylated triphenyl phosphate. The resulting preliminary worst case PEC/PNEC ratios are summarised in Table 5.2.

The worst case PEC/PNEC ratios indicate a low risk to waste water treatment plants from production and use of both isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate. However, the PNEC is actually a limit value based on a test where no effects are seen, and so the true PNEC will be higher than this value.

Table 5.2 Risk characterisation ratios for waste water treatment processes

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/l)	PEC/PNEC	PEC (mg/l)	PEC/PNEC
Production of isopropylated diphenyl phosphate		0.12	<0.12	0.05	<0.05
Lubricant additive	Blending of lubricant	8.93×10^{-5}	<0.01	5.29×10^{-5}	<0.01
Hydraulic fluid	Blending of fluid	4.92×10^{-5}	<0.01	3.19×10^{-4}	<0.01
Power generation fluid	Blending of fluid Use at power station			5.62×10^{-5} negligible	<0.01 negligible
Adhesives		negligible	negligible	negligible	negligible
Paints	Formulation Application	0.20 1.99×10^{-3}	<0.20 <0.01	5.51×10^{-3} 2.07×10^{-3}	<0.01 <0.01
Textile/ fabric coating	Compounding Application of coating Combined compounding and application of coating	6.76×10^{-3} 3.38×10^{-3} 0.01	<0.01 <0.01 <0.01	6.89×10^{-3} 3.44×10^{-3} 0.01	<0.01 <0.01 <0.01
Thermo-plastics and styrenics	Compounding Conversion Combined compounding and conversion	1.24×10^{-3} 1.13×10^{-4} 1.35×10^{-3}	<0.01 <0.01 <0.01		
PVC – 1[a]	Compounding Conversion Combined compounding and conversion	3.6×10^{-3} 1.8×10^{-3} 5.41×10^{-3}	<0.01 <0.01 <0.01	1.51×10^{-3} 6.89×10^{-3} 2.2×10^{-3}	<0.01 <0.01 <0.01
PVC – 2[a]	Compounding Conversion Combined compounding and conversion	3.1×10^{-3} 1.41×10^{-3} 4.51×10^{-3}	<0.01 <0.01 <0.01	0.01 1.01×10^{-3} 0.01	<0.01 <0.01
PVC – 3[a]	Compounding Conversion Combined compounding and conversion	3.83×10^{-3} 1.77×10^{-3} 5.63×10^{-3}	<0.01 <0.01 <0.01	3.79×10^{-3} 3.44×10^{-4} 4.13×10^{-3}	<0.01 <0.01 <0.01

Table 5.2 continued.

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/l)	PEC/PNEC	PEC (mg/l)	PEC/PNEC
PVC – 4[a]	Compounding	3.1×10^{-3}	<0.01		
	Conversion	2.82×10^{-4}	<0.01		
	Combined compounding and conversion	3.38×10^{-3}	<0.01		
PVC – 5[a]	Compounding	3.1×10^{-3}	<0.01		
	Conversion	2.82×10^{-4}	<0.01		
	Combined compounding and conversion	3.38×10^{-3}	<0.01		
PVC – 6[a]	Compounding	2.25×10^{-3}	<0.01		
	Conversion	1.04×10^{-3}	<0.01		
	Combined compounding and conversion	3.27×10^{-3}	<0.01		
PVC – 7[a]	Compounding	0.02	<0.02		
	Conversion	7.32×10^{-3}	<0.01		
	Combined compounding and conversion	0.02	<0.02		
Poly-urethane	Compounding	0.02	<0.02	7.57×10^{-3}	<0.01
	Conversion	1.69×10^{-3}	<0.01	6.89×10^{-4}	<0.01
	Combined compounding and conversion	0.02	<0.02	8.26×10^{-3}	<0.01
Pigment dispersions	Production of dispersions	2.48×10^{-3}	<0.01	7.57×10^{-3}	<0.01

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate do not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

5.1.3 Sediment

The PNEC for sediment was estimated as 0.077 mg/kg wet weight for isopropylphenyl diphenyl phosphate and 0.188 mg/kg wet weight for tris(isopropylphenyl) phosphate. 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		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/kg wet wt.)	PEC/ PNEC	PEC (mg/kg wet wt.)	PEC/ PNEC
Production of isopropylated diphenyl phosphate		0.43	**56.6**	0.42	**22.2**
Lubricant additive	Blending of lubricant	0.04	**5.76**	0.02	**1.19**

Table 5.3 continued.

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/kg wet wt.)	PEC/ PNEC	PEC (mg/kg wet wt.)	PEC/ PNEC
Hydraulic fluid	Blending of fluid	0.04	**5.69**	0.03	**1.62**
Power generation fluid	Blending of fluid Use at power station			0.02 negligible	**1.19** negligible
Adhesives		negligible	negligible	negligible	negligible
Paints	Formulation Application	2.53 0.07	**329** **8.91**	0.19 0.08	**10.1** **4.47**
Textile/ fabric coating	Compounding Application of coating Combined compounding and application of coating	0.13 0.09 0.17	**16.8** **11.2** **22.4**	0.23 0.13 0.34	**12.3** **6.72** **18**
Thermo-plastics and styrenics	Compounding Conversion Combined compounding and conversion	0.06 0.04 0.06	**7.66** **5.8** **7.84**		
PVC – 1[a]	Compounding Conversion Combined compounding and conversion	0.09 0.07 0.11	**11.6** **8.59** **14.5**	0.07 0.04 0.09	**3.57** **2.23** **4.7**
PVC – 2[a]	Compounding Conversion Combined compounding and conversion	0.08 0.06 0.1	**10.7** **7.94** **13.1**	0.36 0.05 0.38	**18.9** **2.74** **20.2**
PVC – 3[a]	Compounding Conversion Combined compounding and conversion	0.09 0.07 0.11	**11.9** **8.53** **14.9**	0.14 0.03 0.15	**7.28** **1.66** **7.84**
PVC – 4[a]	Compounding Conversion Combined compounding and conversion	0.08 0.05 0.09	**10.7** **6.08** **11.2**		
PVC – 5[a]	Compounding Conversion Combined compounding and conversion	0.08 0.05 0.09	**10.7** **6.08** **11.2**		
PVC – 6[a]	Compounding Conversion Combined compounding and conversion	0.07 0.06 0.08	**9.33** **7.32** **11**		

Table 5.3 continued.

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/kg wet wt.)	PEC/ PNEC	PEC (mg/kg wet wt.)	PEC/ PNEC
PVC – 7[a]	Compounding	0.24	**31.7**		
	Conversion	0.14	**17.7**		
	Combined compounding and conversion	0.34	**44.7**		
Poly-urethane	Compounding	0.27	**35.4**	0.25	**13.5**
	Conversion	0.06	**8.4**	0.04	**2.23**
	Combined compounding and conversion	0.30	**38.7**	0.28	**14.6**
Pigment dispersions	Production of dispersions	0.07	**9.71**	0.25	**13.5**
Regional sources		0.06	**8.11**	0.04	**1.95**

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate do not necessarily correspond to those used for tris(isopropylphenyl) phosphate.

Estimated PEC/PNEC ratios are above one for production and all uses of isopropylated triphenyl phosphate (except adhesives and power generation fluids), and also from regional sources. The local risk from use in adhesives (both substances) and power generation fluids (tris(isopropylphenyl) phosphate only) appears to be low. Further information noted for the surface water compartment would also refine the sediment assessment. However, the extra factor of 10 used for sediment means that emission estimates would have to be reduced significantly to remove all concerns. The majority of scenarios would still show a risk without the extra factor of ten.

As for surface water, the local sediment concentrations predicted for many of the uses of isopropylated triphenyl phosphate (particularly for isopropylphenyl diphenyl phosphate) are dominated by the contribution from the regional water concentration. The main sources for the regional emissions are in-service losses and/or waste remaining in the environment from some PVC applications, paints, printed circuit boards, textiles and lubricant applications.

The sensitivity analysis in Annex C suggests that a faster hydrolysis rate than assumed in this assessment could have a significant effect on the local and regional sediment PECs for tris(isopropylphenyl) phosphate. It may therefore be possible to refine the PECs by carrying out further testing[9] to investigate the actual degradation (mineralization) half-life in sediment under relevant environmental conditions.

The PNEC for sediment is based on the equilibrium partitioning approach. As noted above, the PNEC on which this is based is not likely to be revised. Toxicity data for sediment organisms would allow a sediment PNEC to be derived directly, and remove the need for the additional factor. It is likely that three long-term tests on sediment organisms would be required.

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

5.2 Terrestrial compartment

The PNEC for soil is estimated as 0.062 mg/kg wet weight for isopropylphenyl diphenyl phosphate and 0.153 mg/kg wet weight for tris(isopropylphenyl) phosphate. The resulting risk characterisation ratios, increased by a factor of 10 to take into account the possibility of direct ingestion of sediment-bound substance, are given in Table 5.4.

For isopropylphenyl diphenyl phosphate, the PEC/PNEC ratios are above one for use in paints, textiles, thermoplastics and styrenics, PVC, polyurethane and pigment dispersions. A risk from regional sources (industrial soil) has also been identified. The risk to the terrestrial compartment from production, use in lubricants, hydraulic fluids, adhesives, and from regional sources (agricultural and natural soil) is low.

Table 5.4 Summary of risk characterisation ratios for the terrestrial compartment

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/kg wet wt.)	PEC/ PNEC	PEC (mg/kg wet wt.)	PEC/ PNEC
Production of isopropylated diphenyl phosphate		1.73×10^{-4}[b]	0.03	8.56×10^{-5}[b]	<0.01
Lubricant additive	Blending of lubricant	2.03×10^{-3}	0.33	2.85×10^{-3}	0.19
Hydraulic fluid	Blending of fluid	1.19×10^{-3}	0.19	0.02	**1.11**
Power generation fluid	Blending of fluid Use at power station			4.06×10^{-3} negligible	0.27 negligible
Adhesives		negligible	negligible	negligible	negligible
Paints	Formulation Application	4.11 0.04	**663** **6.75**	0.29 0.11	**19.1** **7.14**
Textile/fabric coating	Compounding Application of coating Combined compounding and application of coating	0.14 0.07 0.21	**22.8** **11.5** **34.3**	0.36 0.18 0.55	**23.8** **11.9** **35.7**
Thermo-plastics and styrenics	Compounding Conversion Combined compounding and conversion	0.03 2.55×10^{-3} 0.03	**4.2** 0.41 **4.59**		
PVC – 1[a]	Compounding Conversion Combined compounding and conversion	0.08 0.04 0.11	**12.2** **6.17** **18.3**	0.08 0.04 0.12	**5.24** **2.39** **7.63**
PVC – 2[a]	Compounding Conversion Combined compounding and conversion	0.06 0.03 0.09	**10.5** **4.78** **15.2**	0.58 0.05 0.62	**37.8** **3.51** **40.5**

Table 5.4 continued.

Scenario		Isopropylphenyl diphenyl phosphate		Tris(isopropylphenyl) phosphate	
		PEC (mg/kg wet wt.)	PEC/ PNEC	PEC (mg/kg wet wt.)	PEC/ PNEC
PVC – 3[a]	Compounding	0.08	**12.9**	0.2	**13.1**
	Conversion	0.04	**6.05**	0.02	**1.2**
	Combined compounding and conversion	0.12	**19.1**	0.22	**14.3**
PVC – 4[a]	Compounding	0.06	**10.5**		
	Conversion	6.11×10^{-3}	0.99		
	Combined compounding and conversion	0.07	**11.4**		
PVC – 5[a]	Compounding	0.06	**10.5**		
	Conversion	6.11×10^{-3}	0.99		
	Combined compounding and conversion	0.07	**11.4**		
PVC – 6[a]	Compounding	0.05	**7.63**		
	Conversion	0.02	**3.56**		
	Combined compounding and conversion	0.07	**11.1**		
PVC – 7[a]	Compounding	0.33	**53.2**		
	Conversion	0.16	**25**		
	Combined compounding and conversion	0.50	**80.1**		
Polyurethane	Compounding	0.38	**60.8**	0.40	**26.2**
	Conversion	0.04	**5.78**	0.04	**2.39**
	Combined compounding and conversion	0.42	**67.7**	0.43	**28.6**
Pigment dispersions	Production of dispersions	0.05	**8.38**	0.40	**26.2**
Regional sources	Agricultural soil	2.21×10^{-3}	0.36	4.26×10^{-4}	0.03
	Natural soil	1.62×10^{-4}	0.03	6.3×10^{-5}	<0.01
	Industrial soil	0.13	**20.97**	0.08	**5.23**

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate do not necessarily correspond to those used for tris(isopropylphenyl) phosphate.
b) Sewage sludge from the production site is not spread onto agricultural land.

For tris(isopropylphenyl) phosphate, the PEC/PNEC ratios are above one for use in hydraulic fluids, paints, textiles, PVC, polyurethane and pigment dispersions. A risk from regional sources (industrial soil) has also been identified. The risk to the terrestrial compartment from production, use in lubricants, power generation, adhesives and regional sources (agricultural and natural soil) is low.

In both cases, further information on exposure identified for the aquatic compartment would also influence the risk ratios for soil. However, the extra factor of 10 used for the terrestrial assessment means that emission estimates would have to be reduced significantly to remove all concerns. The majority of scenarios would still show a risk without the extra factor of 10.

Like sediment, the sensitivity analysis in Annex C suggests that a faster hydrolysis rate than assumed in this assessment could have a significant effect on the local and regional soil PECs for tris(isopropylphenyl) phosphate. 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.

The PNEC for soil is based on the equilibrium partitioning approach. As noted above, the aquatic PNEC on which this is based is not likely to be revised. Toxicity data for terrestrial organisms would allow a soil PNEC to be derived directly, and remove the need for the additional factor. As for sediment, it is likely that three long-term tests would be required.

5.3 Atmosphere

No information is available on the toxicity of isopropylated triphenyl 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 resulting concentrations are likely to be low. The possibility of isopropylated triphenyl 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

The PNEC for secondary poisoning is estimated as 1.8 mg/kg food for isopropylphenyl diphenyl phosphate. The resulting preliminary worst case PEC/PNEC ratios are summarised in Table 5.5. No PNEC has been derived for tris(isopropylphenyl) phosphate as there are no suitable data.

For the fish food chain, only the formulation of paints indicates a risk. For the earthworm food chain, in addition to paint formulation the formulation (compounding) steps for textiles, polyurethanes and PVC 7 also show risks, either alone or in combination with the application or conversion step.

Again, further information is needed to refine the PECs for these scenarios in order to determine whether there is a risk of secondary poisoning. In addition, the estimated earthworm BCF is of uncertain validity, so this could be refined with a test if necessary.

The risk of secondary poisoning from production of isopropylphenyl diphenyl phosphate and use in lubricants, hydraulic fluids, adhesives and pigment dispersions is predicted to be low.

If the PNEC for isopropylphenyl diphenyl phosphate were used for tris(isopropylphenyl) phosphate, the PEC/PNEC ratios would be below one for all scenarios where the fish food chain was considered. Where the earthworm food chain was considered, the ratios would be above one for formulation and use of paints, all PVC applications, textiles, polyurethanes and pigment dispersions. No conclusions can be drawn for this substance at present.

Table 5.5 Summary of risk characterisation ratios for secondary poisoning

Scenario		Isopropylphenyl diphenyl phosphate				Tris(isopropylphenyl) phosphate			
		Fish food chain		Earthworm food chain		Fish food chain		Earthworm food chain	
		PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC
Production of isopropylated diphenyl phosphate		1.02	0.16	0.02[b]	0.46	1.34		0.01[b]	
Lubricant additive	Blending of lubricant	0.19	0.11	0.04	0.02	0.14		0.09	
Hydraulic fluid	Blending of fluid	0.19	0.11	0.03	0.02	0.13		0.46	
Power generation fluid	Blending of fluid Use at power station					0.14 negligible		0.12 negligible	
Adhesives		negligible		negligible		negligible		negligible	
Paints	Formulation	4.69	**2.64**	40.6	**22.8**	0.57		7.66	
	Application	0.24	0.13	0.44	0.25	0.16		2.87	
Textiles/fabric coating	Compounding	0.35	0.19	1.42	0.80	0.23		9.55	
	Application of coating	0.27	0.15	0.73	0.41	0.18		4.79	
	Combined compounding and application of coating	0.42	0.24	2.12	**1.19**	0.27		14.3	
Thermoplastics and styrenics	Compounding	0.19	0.11	0.28	0.16				
	Conversion	0.19	0.11	0.05	0.03				
	Combined compounding and conversion	0.22	0.12	0.3	0.17				

Table 5.5 continued.

Scenario		Isopropylphenyl diphenyl phosphate				Tris(isopropylphenyl) phosphate			
		Fish food chain		Earthworm food chain		Fish food chain		Earthworm food chain	
		PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC
PVC – 1[a]	Compounding	0.27	0.15	0.77	0.43	0.19		2.11	
	Conversion	0.23	0.13	0.4	0.23	0.16		0.97	
	Combined compounding and conversion	0.31	0.18	1.14	0.64	0.21		3.07	
PVC – 2[a]	Compounding	0.2	0.11	0.66	0.37	1.0		15.1	
	Conversion	0.19	0.11	0.32	0.18	0.21		1.42	
	Combined compounding and conversion	0.2	0.11	0.96	0.54	1.07			
PVC – 3[a]	Compounding	0.28	0.16	0.82	0.46	0.43		5.26	
	Conversion	0.23	0.13	0.39	0.22	0.16		0.49	
	Combined compounding and conversion	0.32	0.18	1.19	0.67	0.46			
PVC – 4[a]	Compounding	0.26	0.15	0.66	0.37				
	Conversion	0.2	0.11	0.08	0.05				
	Combined compounding and conversion	0.27	0.15	0.72	0.41				
PVC – 5[a]	Compounding	0.26	0.15	0.66	0.37				
	Conversion	0.2	0.11	0.08	0.05				
	Combined compounding and conversion	0.27	0.15	0.72	0.41				

Table 5.5 continued.

Scenario		Isopropylphenyl diphenyl phosphate				Tris(isopropylphenyl) phosphate			
		Fish food chain		Earthworm food chain		Fish food chain		Earthworm food chain	
		PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC
PVC – 6[a]	Compounding	0.24	0.14	0.49	0.28				
	Conversion	0.21	0.12	0.24	0.14				
	Combined compounding and conversion	0.27	0.15	0.7	0.40				
PVC – 7[a]	Compounding	0.55	0.31	3.28	**1.85**				
	Conversion	0.36	0.20	1.55	0.87				
	Combined compounding and conversion	0.73	0.41	4.93	**2.77**				
Polyurethane	Compounding	0.6	0.34	3.75	**2.11**	0.27		10.5	
	Conversion	0.23	0.13	0.38	0.21	0.14		0.97	
	Combined compounding and conversion	0.65	0.37	4.17	**2.34**	0.28		11.5	
Pigment dispersions	Production of dispersions	0.2	0.11	0.54	0.30	0.74		10.5	

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate do not necessarily correspond to those used for tris(isopropylphenyl) phosphate.
b) Sewage sludge from the production site is not spread onto agricultural land.

Table 5.6 Summary of risk characterisation ratios for the marine compartment

Scenario		PEC/PNEC ratio							
		Isopropyl phenyl diphenyl				Tris(isopropyl phenyl)			
		Local marine compart-ment	**Local marine sediment compart-ment**	**Fish-eating birds and mammals**	**Top predators**	**Local marine compart-ment**	**Local marine sediment compart-ment**	**Fish-eating birds and mammals[b]**	**Top predators[b]**
Lubricant additive	Blending of lubricant	0.58	**5.82**	0.01	<0.01	0.14	**1.38**		
Hydraulic fluid	Blending of fluid	0.55	**5.53**	<0.01	<0.01	0.3	**2.96**		
Power generation fluid	Blending of fluid Use at power station					0.14 negligible	**1.4** negligible		
Adhesives		negligible	negligible	negligible	negligible	negligible	negligible		
Paints	Formulation Application	**144** **1.98**	**1,440** **19.8**	**1.1** 0.02	0.24 0.01	**3.37** **1.33**	**33.7** **13.3**		
Thermoplastics and styrenics	Compounding Conversion Combined compounding and conversion	**1.43** 0.6 **1.51**	**14.3** **5.99** **15.1**	<0.01 0.01 0.02	<0.01 <0.01 0.01				
Textile/fabric coating	Compounding Application of coating Combined compounding and application of coating	**5.47** **2.99** **7.95**	**54.7** **29.9** **79.5**	0.05 0.03 0.07	0.02 0.01 0.02	**4.19** **2.15** **6.22**	**41.9** **21.5** **62.2**		
PVC – 1[a]	Compounding Conversion Combined compounding and conversion	**3.16** **1.84** **4.48**	**31.6** **18.4** **44.8**	0.03 0.02 0.04	0.01 0.01 0.02	**1** 0.51 **1.41**	**10** **5.14** **14.1**		

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Table 5.6 continued.

Scenario		PEC/PNEC ratio							
		Isopropyl phenyl diphenyl				Tris(isopropyl phenyl)			
		Local marine compart-ment	**Local marine sediment compart-ment**	**Fish-eating birds and mammals**	**Top predators**	**Local marine compart-ment**	**Local marine sediment compart-ment**	**Fish-eating birds and mammals[b]**	**Top predators[b]**
PVC – 2	Compounding	**2.79**	**27.9**	0.01	0.01	**6.57**	**65.7**		
	Conversion	**1.55**	**15.5**	0.01	0.01	0.7	**7.02**		
	Combined compounding and conversion	**3.82**	**38.2**	0.01	0.01	**7.04**	**70.4**		
PVC – 3	Compounding	**3.33**	**33.3**	0.03	0.01	**2.35**	**23.5**		
	Conversion	**1.81**	**18.1**	0.02	0.01	0.31	**3.1**		
	Combined compounding and conversion	**4.65**	**46.5**	0.04	0.02	**2.55**	**25.5**		
PVC – 4	Compounding	**2.79**	**27.9**	0.03	0.01				
	Conversion	0.72	**7.23**	0.01	0.01				
	Combined compounding and conversion	**2.99**	**29.9**	0.03	0.01				
PVC – 5	Compounding	**2.79**	**27.9**	0.03	0.01				
	Conversion	0.72	**7.23**	0.01	0.01				
	Combined compounding and conversion	**2.99**	**29.9**	0.03	0.01				
PVC – 6	Compounding	**2.17**	**21.7**	0.02	0.01				
	Conversion	**1.28**	**12.8**	0.02	0.01				
	Combined compounding and conversion	**2.91**	**29.1**	0.03	0.01				

Table 5.6 continued.

Scenario		PEC/PNEC ratio							
		Isopropyl phenyl diphenyl				Tris(isopropyl phenyl)			
		Local marine compart-ment	**Local marine sediment compart-ment**	**Fish-eating birds and mammals**	**Top predators**	**Local marine compart-ment**	**Local marine sediment compart-ment**	**Fish-eating birds and mammals[b]**	**Top predators[b]**
PVC – 7	Compounding	**12.1**	**121**	0.10	0.03				
	Conversion	**5.89**	**58.9**	0.05	0.02				
	Combined compounding and conversion	**17.9**	**179**	0.15	0.04				
Polyurethane	Compounding	**13.7**	**137**	0.11	0.03	**4.59**	**45.9**		
	Conversion	**1.76**	**17.6**	0.02	0.01	0.51	**5.14**		
	Combined compounding and conversion	**15.2**	**152**	0.13	0.03	**5**	**50**		
Pigment dispersion	Production of dispersions	**2.33**	**23.3**	0.02	0.01	**4.59**	**45.9**		

Notes: a) For confidentiality reasons, the numbering of the PVC scenarios for isopropylphenyl diphenyl phosphate does not necessarily correspond to those used for tris(isopropylphenyl) phosphate.
b) No PEC/PNEC ratios possible, as no PNEC derived.

5.5 Risks to human health following environmental exposure

As noted in Section 4.4.10, the available data do not allow a suitable acceptable margin of exposure to be developed on which to base an assessment for humans exposed through the environment, and therefore no risk characterisation was carried out. As an indication, based on the NOAEL of 1,000 ppm which is considered the most suitable of the results in the database, the lowest margin of exposure would be 150, which may indicate potential risks. This part of the assessment should be revisited following work to address the questions in Appendix 1.

5.6 Marine assessment

Although a PEC/PNEC approach can be applied to the marine environment, there are additional concerns which may not be adequately addressed using the methods 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. 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 4.6.

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 3.3.4. The PNEC for secondary poisoning for the marine environment is the same as that for the freshwater fish and terrestrial food chains (Section 4.1.6). The resulting PEC/PNEC ratios for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate are shown in Table 5.6.

PEC/PNEC ratios indicate risks to marine waters and sediments for all scenarios for isopropylphenyl diphenyl phosphate, and for the majority of scenarios for tris(isopropylphenyl) phosphate (the exceptions being blending of hydraulic fluids and lubricants, for marine waters). For the marine secondary poisoning assessment, the PEC/PNEC ratios for isopropylphenyl diphenyl phosphate indicate a risk only from the formulation of paints for fish-eating marine birds and mammals.

Further information on emissions from these processes indicated for the freshwater environment would help to refine these results. More specifically for the marine assessment, information would be useful on whether any of these processes avoid discharging to the marine environment, or if they do so only after effluent treatment (the calculations assume a direct discharge to the marine environment without treatment).

Testing on freshwater organisms is not essential for the freshwater assessment (with the possible exception of tris(isopropylphenyl) phosphate), whereas toxicity testing with sediment organisms would be valuable. There is also the possibility of testing marine species, which would allow the assessment factor to be reduced.

The size of some PEC/PNEC ratios suggests that no one part of the further information requirements would be sufficient on its own to reduce the ratios to below one.

6 Conclusions

Isopropylated triphenyl phosphate can enter the environment from production and use, and from the use of articles made from materials containing it. Based on the available information, potential risks are identified for all of the life cycle steps for one or more of the protection goals. The overall conclusions are summarised in Table 6.1 for isopropylphenyl diphenyl phosphate and in Table 6.2 for tris(isopropylphenyl) phosphate in a simplified form. In particular, the different steps within the use in each material have been combined here, and risks are indicated for PVC provided at least one of the different uses shows a risk for the specific protection goal. Section 5 should be consulted for the detailed results.

Table 6.1 Summarised potential environmental risks identified for isopropylphenyl diphenyl phosphate

Life cycle stage	Surface water	Sediment	WWTP	Air	Soil	Aquatic food chain	Terrestrial food chain	Marine water	Marine sediment
Production	✸	✸	-	-	-	-	-	-	-
Lubricants	-	✸	-	-	-	-		✸	✸
Hydraulic fluids	-	✸	-	-	-	-		✸	✸
Adhesives	-	-	-	-	-	-		-	-
Paints	✸	✸	-	-	✸	✸	✸	✸	✸
Textile/fabric coating	✸	✸	-	-	✸	-	✸	✸	✸
PVC	✸	✸	-	-	✸	-	✸[a]	✸	✸
Thermoplastics/styrenics	-	✸	-	-	✸	-	-	✸	✸
Polyurethane	✸	✸	-	-	✸	-	✸	✸	✸
Pigment dispersions	-	✸	-	-	✸	-	-	✸	✸
Regional	-	✸	-	-	-	-	-	-	-

Note: a) for one PVC use

For isopropylphenyl diphenyl phosphate, there are no risks for marine food chain exposure, with the exception of paint formulation. It is not possible at present to assess marine food chain exposure for tris(isopropylphenyl) phosphate. No risk assessment for humans exposed via the environment is currently possible for either substance.

Some monitoring data on tricresyl phosphate show elevated levels near to sources of release; however, these cannot be related to current activities in Europe.

Table 6.2 Summarised potential environmental risks identified for tris(isopropylphenyl) phosphate

Life cycle stage	Surface water	Sediment	WWTP	Air	Soil	Marine water	Marine sediment
Production	✸	✸	-	-	-	-	-
Lubricants	-	✸	-	-	-	-	✸
Hydraulic fluids	-	✸	-	-	✸	-	✸
Power generation fluids	-	✸	-	-	-	-	✸
Adhesives	-	-	-	-	-	-	✸
Paints	✸	✸	-	-	✸	✸	✸
Textile/fabric coating	✸	✸	-	-	✸	✸	✸
PVC	✸[a]	✸	-	-	✸	✸	✸
Polyurethane	✸	✸	-	-	✸	✸	✸
Pigment dispersions	✸	✸	-	-	✸	✸	✸
Regional	-	✸	-	-	-	-	-

Note: a) for one PVC use

In particular, tris(isopropylphenyl) phosphate meets the screening PBT criteria on the basis of available data. Testing on persistence to determine a relevant environmental half-life should be considered for this substance before any revision of other parts of the assessment is carried out.

The potential PEC/PNEC risks identified could be reassessed following additional work, in particular:

- Collation of further site and industry-specific information on releases of isopropylated triphenyl phosphate from use in the different types of materials indicated. This work could include:
  - An improved description of practices at sites using isopropylated triphenyl 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 water, sediments and WWTP sludge). Environmental monitoring for isopropylphenyl diphenyl phosphate and tris(isopropylphenyl) phosphate is taking place in England and Wales, at one WWTP per Environment Agency region, in both final effluent and associated receiving waters (6 samples at 4 week intervals). Sampling is expected to take place from September 2008 until March 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, and possible further aquatic toxicity testing for tris(isopropylphenyl) phosphate.
- Studies on the fate of the substance in WWTP (municipal and industrial).

- Further testing to investigate the actual degradation (mineralization) half-life of tris(isopropylphenyl) phosphate in sediment and soil under relevant environmental conditions.
- Clarification of some aspects of the mammalian toxicity data (see Appendix 1).
- The earthworm BCF value could also be refined with a test if necessary.

The possible risks identified for production sites could also be addressed by some aspects of the work above, but as there are limited numbers of production sites these are considered to be better addressed by local control authorities.

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 List of abbreviations

Acronym	Description
ASTM	American Society for Testing and Materials
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
DEHP	Di(2-ethylhexyl)phthalate
DOC	Dissolved organic carbon
DSC	Differential scanning calorimetry
dw	Dry weight
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)
HPTLC	High performance thin layer chromatography
HPV	High Production Volume (supply above 1000 tonnes per year)
IPDP	Isopropylphenyl diphenyl phosphate
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
LOEC	Lowest observed effect concentration
log K_{ow}	Log of the octanol-water partition coefficient (K_{ow})
NO(A)EL	No observed (adverse) effect level
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
ppm	Parts per million
PVC	Polyvinyl chloride
(Q)SAR	(Quantitative) Structure-Activity Relationship
SCAS	Semi-continuous activated sludge unit
TGA	Thermogravimetric analysis
TGD	Technical Guidance Document
TPP	Triphenyl phosphate
ThOD	Theoretical oxygen demand
USEPA	Environmental Protection Agency, USA
vB	Very bioaccumulative
vP	Very persistent
vPvB	Very persistent and very bioaccumulative
WAF	Water-accommodated fraction
w/w	Weight per weight ratio
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 cooperation.

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.

Appendix 1 Points for clarification on the mammalian toxicity data

The following points summarise uncertainties in the mammalian dataset (Section 4.4), and may lead to revision of the assessment of risks for humans exposed via the environment, and of the classification, if addressed.

- In the *in vitro* toxicokinetic studies by Imperial Chemical Industries plc (Study nos Scott 1985, Scott and Thompson 1985, cited in IUCLID 2000) on Reolube HYD 46 and Reofos 50 it is not clear to which test substance TPP and 2-IDPP refer.
- The study by FMC Corporation (Freeman1990a, cited in IUCLID 2000, 2001) is reported somewhat differently in the two IUCLID files. It would be helpful to clarify the study details or to obtain the original report. Particular areas are the identity of the test material, number of animals per group, occasions when observations and bodyweights were recorded and whether necropsy was performed on all animals.
- In FMC Corporation study (Freeman 1990b, cited in IUCLID 2000), it would help to confirm if the substance was rinsed from the skin at the test site after the exposure period and what serial observations were conducted. In addition, it is not clear if necropsy was conducted on all animals and if there were any findings from this.
- For the study by Mobil Environmental and Health Science Laboratory (Krueger 1990, cited in IUCLID 2000), the exact test material studied is not clear as there is apparent conflict between the study title in the reference citation and study details.
- In the single-dose study by Huntingdon Research Centre (Roberts 1980b, cited in IUCLID 2000), it is not clear if the histological changes in the spinal cord of test animals were also detected in any positive or negative controls. Data to justify the statement that the pathological changes observed did not correlate with in-life clinical observations would be useful.
- In a Huntingdon Research Centre study (Roberts 1980c, cited in IUCLID 2001), the description of the test article is unclear as it refers to Kronitex 100/Reofos 65. In addition, with regard to signs of ataxia reported, it would be useful to have details of the nature, degree and duration of effect and the animals/group affected. There are also inconsistencies between the IUCLID files as to the numbers showing histopathological changes.
- In a Huntingdon Research Centre study (Roberts 1980a) in which hens were exposed to TIPPP (as Reofos 50) it is not clear if any control group (positive or negative) was included.
- In the study by FMC Corporation (Freeman 1990h, cited in IUCLID 2000, 2001), the volume and dilution of Reofos 50 applied to the test groups are not clear.
- The reporting of findings from studies on Reofos 50, Reofos 65, Reofos 95 and Durad 300 in FDRL (Bailey 1975a-q, cited in IUCLID 2000) is unclear as to which test materials elicited what responses, in particular in relation to numbers affected, severity of any effect and time course for resolution.

- Details of the numbers affected, recorded Draize scores and time course of the effects noted in the two available OECD guideline 405 studies (Swallow 1984a, b, cited in IUCLID 2000) would be useful.
- A number of points relating to the dietary study on Kronitex K-100 (Foster D. Snell, 1976, cited in IUCLID 2001 need to be clarified. These include: the number of animals per sex per group used; how many animals in each of the study groups were subject to haematological and clinical chemistry investigations and when during the study these were undertaken; the parameters affected, levels of statistical significance attained and biological significance inferred for the various haematological and blood chemistry changes briefly mentioned as having occurred in the treated groups; an explanation as to why the effect on liver weight noted in all treated groups should be discounted when establishing a NOAEL for the study.
- The study on Kronitex 100 by FDRL (Bailey 1976 cited in IUCLID 2000) is poorly reported in the available data sources. Any additional information would be useful, in particular on the changes in liver weight noted and the biological significance of this and the changes in BUN also mentioned.
- For the two OECD Guideline 410 studies reported by Ciba-Geigy (Kobel 1984a, b cited in IUCLID 2000), it is not clear if shaving of the skin was conducted. There is also uncertinaty over the nature of any control group(s) included in the study and the vehicle used. Further information on changes in testes weight (such as numbers affected per group, magnitude of effect and any pathological correlates), together with similar information on the changes in the adrenal gland reported, would be useful.
- For the study on Reolube HYD 46 by the University of Hamburg (Benthe 1988, cited in IUCLID 2000) the date of the study (1975 or 1988) and nature of the test material investigated are not clear. Also, the number of PCEs with micronuclei was stated to be increased in all groups, but it is unclear whether this statement also relates to the controls. Information to support the contention that the changes seen related to inhibition of erythrocyte maturation would be useful.

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