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Environmental risk evaluation report: Tertbutylphenyl diphenyl phosphate (CAS no. 56803-37-3)

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Steve Killeen

Head of Science

Executive summary

An environmental risk evaluation has been carried out for tertbutylphenyl diphenyl phosphate (CAS no. 56803-37-3) on the basis of available information and using the methods of a European Technical Guidance Document. The report also covers 'phenol, isobutylated, phosphate (3:1)' (CAS no. 68937-40-6). In Europe, this substance is mainly used as a flame retardant additive for PVC, polyurethane, textile coatings, lubricants and hydraulic fluids and as a base fluid for power generation fluids.

Potential risks are identified for use in plastics materials for some or all of the surface water (fresh and marine), sediment (fresh and marine) and soil compartments, and for lubricant, hydraulic and power generation fluids for marine sediment. Emission estimates are based on information from a number of generic sources, including emission scenario documents and other risk assessments, so they could be refined with more specific information for the substance itself. However some of the risk characterisation ratios are high and it is unlikely that such information alone will be sufficient to remove all of the identified risks.

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.

Risks to the air compartment and for secondary poisoning are low from production and all uses of tertbutylphenyl diphenyl phosphate. In addition, a low risk to surface water, soil and sediment is identified from regional sources. No risk characterisation could be carried out for waste water treatment plant but the risk for this endpoint is thought to be low for all scenarios considered. No assessment for humans exposed through the environment is possible due to the limited toxicity database.

Tertbutylphenyl diphenyl phosphate does not meet the criteria for a persistent, bioaccumulative and toxic (PBT) or very persistent and very bioaccumulative (vPvB) substance.

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).

Note: Late on in the publication process, the Environment Agency became aware of a formal review of this substance by the US Environmental Protection Agency (USEPA 2008). A brief comparison of the two reports has been made, and comments have been added where relevant.

[1] This document has recently been replaced by similar guidance for the REACH Regulation.

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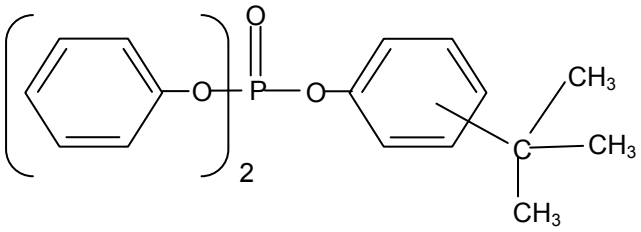
1 General substance information

1.1 Identification of the substance

This assessment considers the following commercial substances:

CAS No:	56803-37-3
EINECS No:	260-391-0
EINECS Name:	Tertbutylphenyl diphenyl phosphate
CAS No:	68937-40-6
EINECS No:	273-065-8
EINECS Name:	Phenol, isobutylated, phosphate (3:1)
Molecular formula:	$C_{22}H_{23}O_4P$
Molecular weight[2]:	382.40 g/mol
Structural formula[3]:	



CAS number 220352-35-2 (butylated triphenyl phosphate) is also used by European suppliers of this substance, although this is not listed on the European Inventory of Existing Commercial Chemical Substances (EINECS).

Other names, abbreviations, trade names and registered trade marks for this substance include the following[4]:

Durad 220B®
Fyrquel GT®
Phosflex 71B®
Santicizer 154®
TB220-H®
TB220-L®
TBDPP

[2] This is the value for the structure as presented. There are also components in the commercial products with two t-butyl groups (on the same or different phenyl groups), which have higher molecular weights.
[3] Structure is for one component. See Section 1.2.
[4] USEPA (2008) also mentions Phosflex 51B, Phosflex 61B and SYN-O-Ad 8485.

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

The name tertbutylphenyl diphenyl phosphate will be used in this assessment.

1.2 Purity/impurity, additives

1.2.1 Purity/impurities

The isomer distribution and the distribution of alkylation levels may vary between products from different manufacturers (Weil 1993).

Cleveland *et al.* (1986) reported that a commercial tertbutylphenyl diphenyl phosphate contained 15-20 per cent triphenyl phosphate with the remainder primarily consisting of isomers of tertbutylphenyl diphenyl phosphate (2-tertbutylphenyl diphenyl phosphate, 3-tertbutylphenyl diphenyl phosphate and 4-tertbutylphenyl diphenyl phosphate), along with di-tertbutylphenyl diphenyl phosphate isomers (2,6-, 2,4-, 2,5 and 3,5-ditertbutylphenyl diphenyl phosphate).

This mixed composition has implications for the interpretation of test results, and the report indicates where this has been taken into account in this assessment.

1.2.2 Additives

Additives are not thought to be present in the commercially supplied products, although some aryl phosphate ester products are sometimes supplied as blends with other (halogenated) flame retardants.

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)

One commercial tertbutylphenyl diphenyl phosphate is a colourless liquid at room temperature (Great Lakes Chemical Corporation 2002).

1.3.2 Melting point

Muir (1984) gives a melting point (pour point) of -21°C for commercial tertbutylphenyl diphenyl phosphate.

A melting point/pour point of -21°C is assumed in the assessment.

1.3.3 Boiling point

Wightman and Malalyandi (1983) determined the boiling points of pure isomers of tertbutylphenyl diphenyl phosphate at reduced pressure. The reported boiling points were 195°C at 0.2 mmHg (27 Pa) for *ortho*-tertbutylphenyl diphenyl phosphate, 200°C at 0.2 mmHg (27 Pa) for *meta*-tertbutylphenyl diphenyl phosphate and 190°C at 0.2 mmHg (27 Pa) for *para*-tertbutylphenyl diphenyl phosphate.

The boiling point of a commercial tertbutylphenyl diphenyl phosphate is above 300°C at 101,325 Pa (Great Lakes Chemical Corporation 2002). The decomposition temperature of the same product is also above 300°C.

IUCLID (2001) gives a boiling point of 260°C at 13.3 hPa (1,330 Pa) for another commercial product. Muir (1984) gives a similar boiling point of 261°C at 6 mmHg (800 Pa) for a commercial product. A boiling point of 420°C at 760 mmHg (101,325 Pa) is reported for commercial tertbutylphenyl diphenyl phosphate (Boethling and Cooper 1985).

A boiling point of 420°C at atmospheric pressure is assumed in the assessment[5].

1.3.4 Density

Shankwalkar and Cruz (1994) reported relative densities of 1.2, 1.17 and 1.15 at 20°C for three commercial tertbutylphenyl diphenyl phosphate products. The three products had phosphorus contents of 8.4 per cent, 8.2 per cent and 7.8 per cent, respectively.

Great Lakes Chemical Corporation (2002) gives a relative density of 1.17 at 20°C for a commercial tertbutylphenyl diphenyl phosphate product. The same value is reported in IUCLID (2001).

A relative density of 1.15-1.2 at 20°C is assumed in the assessment.

1.3.5 Vapour pressure

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

No reliable data appear to be available for tertbutylphenyl diphenyl phosphate at temperatures around 20-25°C. However, information on boiling points at reduced pressure (see Section 1.3.3) and vapour pressure at elevated temperatures are available for the commercial product and pure isomers of the substance.

IUCLID (2001) report a vapour pressure of 13 Pa at 155°C for a commercial tertbutylphenyl diphenyl phosphate product. Boethling and Cooper (1985) give a vapour pressure of 1.4×10^{-6} mmHg (1.9×10^{-4} Pa) at 30°C for a commercial tertbutylphenyl diphenyl phosphate product. Further vapour pressures for commercial products are reported as 1.35 mmHg (180 Pa) at 200°C and 10.2 mmHg (1,360 Pa) at 250°C (Muir 1984).

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:

[5] A further boiling point study has been carried out as part of the US HPV program. The reported boiling point is above 400°C using the OECD 103 method, as cited in USEPA (2008).

log (vapour pressure) = [ΔH_v/2.3RT] + 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

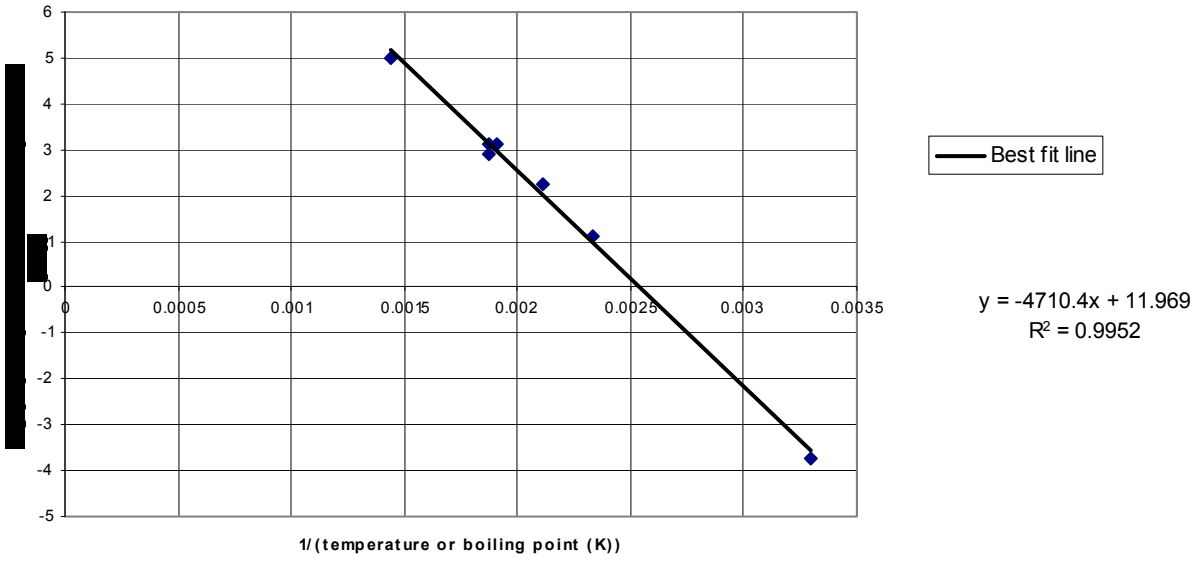
Figure 1.1 shows a plot of log (vapour pressure or reduced pressure (Pa)) against 1/(temperature or boiling point (K)) for the available measured data for commercial products. This gives a straight line plot corresponding to the following regression equation:

log (vapour pressure (Pa)) = [-4710.4 × 1/(temperature (K))] + 11.969

The value of ΔH_v for tertbutylphenyl diphenyl phosphate is estimated from the slope of the plot to be -90,073 J/mol.

Using this equation, the vapour pressure of tertbutylphenyl diphenyl phosphate is estimated as 7.8×10^{-5} Pa at 20°C, 1.5×10^{-4} Pa at 25°C, 6.8 Pa at 150°C and 102 Pa at 200°C. The value at 20°C is in reasonable agreement with the data reported by Dobry and Keller (1957) who estimated the vapour pressure at 20°C to be 1.6×10^{-4} Pa for a purified sample of tertbutylphenyl diphenyl phosphate, extrapolated from data obtained at elevated temperatures. The value of ΔH_v may vary with temperature and so could introduce further errors in extrapolation of the data obtained at elevated temperatures to ambient temperatures.

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



Assuming that the pure isomers of tertbutylphenyl diphenyl phosphates have the same value of ΔH_v as the commercial product, the following vapour pressures can be estimated for these isomers from their boiling points at reduced pressure reported in Section 1.3.3.

ortho-tertbutylphenyl diphenyl phosphate	2.6×10^{-5} Pa at 20°C
meta-tertbutylphenyl diphenyl phosphate	2.1×10^{-5} Pa at 20°C
para-tertbutylphenyl diphenyl phosphate	3.4×10^{-5} Pa at 20°C

A vapour pressure (at 25°C) of 2.61×10^{-8} mmHg (3.5×10^{-6} Pa) is estimated for tertbutylphenyl diphenyl phosphate from its structure using the Syracuse Research

Corporation MPBPWIN (version 1.28) software (modified Grain method). Boethling and Cooper (1985) estimated a vapour pressure of 4.6×10^{-7} mmHg (6.1×10^{-5} Pa) at 25°C from the boiling point of commercial tertbutylphenyl diphenyl phosphate (Grain method).

A vapour pressure of 7.8×10^{-5} Pa at 20°C and 1.5×10^{-4} Pa at 25°C based on the above analysis of the available data is used in this risk assessment[6].

1.3.6 Water solubility

Saeger *et al.* (1979) determined the solubility of a tertbutylphenyl diphenyl phosphate using a shake flask method. The substance used consisted of tertbutylphenyl diphenyl phosphate along with triphenyl phosphate and bis(tertbutylphenyl) 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 mixture) was determined to be 3.2 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 the solution indicating a preferential dissolution of the triphenyl phosphate component (water solubility of triphenyl phosphate itself was determined to be 1.9 mg/l). As the solubility of 3.2 mg/l was based on the total concentration of all components of the commercial product, the actual solubility of the tertbutylphenyl diphenyl phosphate isomer components will be lower than indicated by this figure.

IUCLID (2001) reports a water solubility of 0.04 μg/ml (0.04 mg/l) for tertbutylphenyl diphenyl phosphate obtained from an unpublished study conducted to the Organisation for Economic Cooperation and Development (OECD) 105 test guideline.

A water solubility of around 0.009 mg/l at 25°C was estimated for tertbutylphenyl diphenyl phosphate using the Syracuse Research Corporation WSKOW version 1.30 software (the estimate is based on an estimated log K_{ow} of 6.61).

Although the value of 3.2 mg/l has some uncertainties and is probably higher than the solubility of individual tertbutylphenyl diphenyl phosphate isomers, it was selected for use in this assessment as a representative value for the commercial substance. This is a different approach to that taken for 2-ethylhexyl diphenyl phosphate and isodecyl diphenyl phosphate, where the solubility of the specific substance was used rather than that of the commercial product. However, in the case of tertbutylphenyl diphenyl phosphate such specific information was not available.

[USEPA (2008) cites a water solubility value of 0.04 mg/l.]

[6] A further vapour pressure study was carried out under the US HPV program, with a reported vapour pressure of 1.08×10^{-3} Pa at 25°C using the OECD 104 method (cited in USEPA 2008). This value is around ten times higher than the one currently assumed here. The substance tested had a substantial amount of triphenyl phosphate present and the value determined was very similar to that of triphenyl phosphate (see the risk evaluation report of that substance). This result may not correctly reflect the vapour pressure of tertbutylphenyl diphenyl phosphate itself.

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

The octanol-water partition coefficient of a tertbutylphenyl diphenyl phosphate was determined using a shake flask method (Saeger *et al.* 1979). The substance used consisted of tertbutylphenyl diphenyl phosphate along with triphenyl phosphate and bis(tertbutylphenyl) 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 determined to be 133,000 (log K_{ow} = 5.12).

Renberg *et al.* (1980) determined the octanol-water partition coefficient for a tertbutylphenyl diphenyl phosphate (the same substance as used by Saeger *et al.* 1979 above) using a high performance thin layer chromatography (HPTLC) method. Three main components of the substance were evident using the method and the partition coefficients determined for these components were 3.23, 4.76 and 6.44 (as log values). The mean value obtained for all components was 5.79. 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 to be 3.15 using the HPTLC method). These measured values are in reasonable agreement with those estimated above.

Akzo Nobel (2003) determined the log K_{ow} of a commercial tertbutylphenyl diphenyl phosphate using the OECD 117 test guideline flask method. The log K_{ow} range determined for the various components of the product was 3.0 to 6.4.

A log K_{ow} of 6.61 can be estimated for tertbutylphenyl diphenyl phosphate from its structure using the Syracuse Research Corporation Log Kow (version 1.60) software.

A log K_{ow} of 5.12 as determined by Saeger *et al.* (1979) is used in the risk assessment as a representative value[7].

1.3.8 Hazardous physico-chemical properties

Great Lakes Chemical Corporation (2002) give a flash point of above 220°C for a commercial tertbutylphenyl diphenyl phosphate. IUCLID (2001) reports a flash point (closed cup) of 246°C for another commercial product.

An autoignition temperature of 560°C has been determined for a tertbutylphenyl diphenyl phosphate (Great Lakes Chemical Corporation 2002).

No information could be located for explosivity or oxidising properties of this substance.

1.3.9 Henry's law constant

A Henry's law constant of 1.03×10^{-7} atm m^3/mol (0.010 Pa m^3/mol) at 25°C can be estimated for tertbutylphenyl diphenyl phosphate from chemical structure (bond

[7] A further value has been determined under the US HPV program, with a reported log K_{ow} obtained using the OECD 107 method of 4.85 (cited by USEPA 2008). This is similar to the other values available.

contribution method) using the Syracuse Research Corporation HENRYWIN (version 3.00) software.

Muir *et al.* (1985) measured the Henry's law constant for ^{14}C-labelled tertbutylphenyl diphenyl phosphate using a gas sparging technique. The test was carried out at 25°C using a one-litre water column containing between 10 to 100 μg/l of the test substance. The column was sparged with nitrogen at a flow rate of 200 ml/min for up to 46 hours and the amount of test substance present in the gas was determined at various time intervals. A mean Henry's law constant of 2.18 Pa m^3/mol was determined from the slope of the first-order volatilisation curve. The actual purity of the substance used in this test was not given, but the substance was synthesised using ^{14}C-labelled phenol. As ^{14}C was used to determine the amounts of the test substance volatilised in this study, the presence of any ^{14}C impurity more volatile than the tertbutylphenyl diphenyl phosphate could have adversely affected the results of this test.

A further value for Henry's law constant can be estimated from the water solubility (3.2 mg/l at 25°C as used in the EUSES calculations) and vapour pressure of 7.8×10^{-5} Pa at 20°C or 1.5×10^{-4} Pa at 25°C. Using these data, a Henry's law constant of 0.009 Pa m^3/mol at 20°C and 0.018 Pa m^3/mol at 25°C is estimated.

A Henry's law constant of 0.009 Pa m^3/mol at 20°C and 0.018 Pa m^3/mol at 25°C is thus used in this assessment. These values are consistent with the available water solubility and vapour pressure data, but are somewhat lower than the value determined experimentally.

[USEPA (2008) cites a Henry's law constant of 8.9×10^{-7} atm m^3/mol (0.086 Pa m^3/mol), estimated using the EPISUITE software (although the actual method and temperature are not given). This is about ten times higher than the value used in this assessment, and may be related to the higher vapour pressure assumed in the US assessment.]

1.3.10 Summary of physico-chemical properties

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

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

Property	Value
Melting point	-21°C (pour point)
Boiling point (at atmospheric pressure)	420°C
Relative density	1.15-1.2 at 20°C
Vapour pressure	7.8×10^{-5} Pa at 20°C
	1.5×10^{-4} Pa at 25°C
Water solubility	0.04 to 3.2 mg/l at room temperature
	(3.2 mg/l at 25°C)
Octanol-water partition coefficient (log value)	5.12
Henry's law constant	0.009 Pa m^3/mol at 20°C
	0.018 Pa m^3/mol at 25°C

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

2 General information on exposure

2.1 Production

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 (see the confidential annex for some further details).

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. 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 reported to be used as non-flammable dispersing media for peroxide catalysts.

2.2.2 Uses of tertbutylphenyl diphenyl phosphate

Tertbutylphenyl diphenyl phosphate is reported to be a slightly less efficient plasticizer than tricresyl phosphate. It has been used as a flame retardant in engineering thermoplastics and as a fire-resistant hydraulic fluid (Weil 1993).

Information on the sales of tertbutylphenyl diphenyl phosphate in the EU was provided by the relevant supplier companies for the year 2005. The specific figures are confidential; however, major uses of the substance are in PVC, polyurethane and textile coatings, as an additive in lubricants and hydraulic fluids and as a base fluid for power generation 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)[8] and the methods laid down in Commission Regulation (EC) 1488/94[9] , which is supported by a technical guidance document or 'TGD' (EC 2003). The European Union System for the Evaluation of Substances (EUSES) computer program[10] (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 Environmental degradation

Abiotic degradation

Atmospheric photooxidation

A rate constant for reaction of tertbutyl phenyl diphenyl phosphate with atmospheric hydroxyl radicals of 1.6×10^{-11} cm^3/molecule s can be estimated from its structure using the Syracuse Research Corporation AOP (version 1.86) software. This program implements the method recommended in the TGD for estimating the rate constant.

Using an atmospheric hydroxyl radical concentration of 5×10^5 molecules/cm^3, a half-life for the reaction in air is estimated to be 24 hours.

[USEPA (2008) cites a photodegradation half-life of 24.5 hours.]

Hydrolysis

No information is available on the hydrolysis of tertbutylphenyl diphenyl phosphate[11].

[8] O.J. No L 084, 05/04/1993 p. 0001-0075.
[9] O.J. No L 161, 29/06/1994 p. 0003-0011.
[10] Available from the European Chemicals Bureau, http://ecb.jrc.ec.europa.eu/.
[11] An OECD 111 hydrolysis study was carried out for this substance under the US HPV program. Results of the study were not available in time for inclusion in this assessment, but USEPA (2008) gives the following hydrolysis half-life data:
At 25°C: 60 days at pH 4; 14 days at pH 7; 5.4 days at pH 9
At 15°C: above 100 days at pH 4; 28 days at pH 7; 15 days at pH 9
The USEPA assessment considers the rate of hydrolysis to be slow under neutral and alkaline conditions and negligible under acidic conditions.

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

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

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

For the phenyl group, σ equals zero 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 tertbutylphenyl is -0.1 (for the *ortho*-isomer) and -0.197 (for the *para*-isomer). Based on this value, the hydrolysis rate constant for the tertbutylphenyl group would be 0.18-0.25 l/mol s, giving a hydrolysis half-life of around 32 to 45 days for this group.

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 tertbutylphenyl 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. Note that alkaline hydrolysis would also occur at this pH, with a half-life estimated to be 320 to 450 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 in general 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.

Photodegradation

IUCLID (2001) reports the results from an unpublished aqueous photodegradation study using tertbutylphenyl diphenyl phosphate. The experiment was carried out using natural sunlight and both natural river water and purified water. The concentration of the test substance used was 10 mg/l and the exposure was to direct sunlight over 14 days. The average maximum and minimum temperatures over the period of the test were 28°C and 18°C respectively. Samples of water were analysed on days 2, 5, 9 and 14 of the exposure for the presence of the test substance. No significant loss of the test substance was seen over the 14-day test period and the results indicated that abiotic processes such as photodegradation and/or hydrolysis were not significant under the conditions of this test.

Biodegradation

The results from a standard ready biodegradability test are available (van Ginkel 2006). The method used was the closed bottle test (OECD 301D). The substance tested was a commercial product, containing 40 per cent tertbutyl phenyl diphenyl phosphate, 46 per cent triphenyl phosphate and the remainder higher butylated phosphates. The study is well reported and is considered valid. The test substance was degraded by 61 per cent at day 28, and the study concluded that the test substance was readily biodegradable. The result does not meet the 10-day window criterion. The presence of 46 per cent of triphenyl phosphate, a readily biodegradable substance (see the risk evaluation report for triphenyl phosphate) makes the interpretation of the result in terms of the degradability of tertbutylphenyl diphenyl phosphate itself more difficult. If mineralisation of triphenyl phosphate of 80 per cent is assumed, then a level of mineralisation of tertbutylphenyl diphenyl phosphate of 70 per cent is calculated assuming no degradation of the higher butylated components. Other assumptions on triphenyl phosphate mineralisation lead to estimates of 50 to 80 per cent mineralisation for tertbutylphenyl diphenyl phosphate. Overall, the test demonstrates ready biodegradability for tertbutylphenyl diphenyl phosphate, not meeting the 10-day window.

Saeger *et al.* (1979) determined the biodegradation of a tertbutylphenyl diphenyl phosphate using various test systems. The substance consisted of tertbutylphenyl diphenyl phosphate along with triphenyl phosphate and bis(tertbutylphenyl) 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 controls 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 (the gas chromatographic method used 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 almost complete degradation in around 10-21 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 or 13 mg/l per 24-hour cycle. The units were operated for a period of eight to nine weeks and samples of the mixed liquor were removed at weekly intervals and the concentration of the phosphate ester determined. The results indicated an equilibrium removal rate of greater than 93 per cent at 3 mg/l and 84 ± 3 per cent at 13 mg/l in the test system. To investigate loss by volatilisation, the off-gases were passed through a series of scrubbers. No significant loss by volatilisation (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[12] 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 19.8 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 43 per cent after seven days, 90 per cent after 28 days and 92 per cent after 48 days. Thus, as an acclimated inoculum appears to have been used in the test, the substance can be considered inherently biodegradable based on the results of this test. The authors considered the most likely pathway for biodegradation of aryl phosphates to be the initial hydrolysis of the phosphate ester to form orthophosphate and corresponding phenolic compounds or alcohols, which then themselves undergo further biodegradation.

Carson *et al.* (1990) also reported the results for the biodegradation of a mixture of triphenyl phosphate and tributylphenyl diphenyl phosphate (no information on purity) in microcosm and outdoor simulation tests (these results appear to be the same as those reported by Saeger *et al.* 1979). The microcosm tests were carried out using lake water and sediment collected from the littoral region of a spring-fed freshwater lake in 5- or 10-gallon aquaria. The sediment was screened (1.3 cm) and placed to a depth of 8 cm in the aquaria. Twenty-two litres of lake water were then added to the aquaria and the system was allowed to stabilise for six weeks. After this time, core chambers were created within the aquaria by inserting glass cylinders through the water column and sediment and the test substance was added to each chamber at a concentration of 75 or 675 μg/l. Sterile control chambers were created by adding formaldehyde to the chamber. The half-life for primary degradation in the system was 1 to 3 days.

The outdoor simulation test was carried out using the same mixture of triphenyl phosphate and tributyl phosphate (Carson *et al.* 1990). The tests were carried out in tanks (10 ft diameter and 2 ft deep) containing a 10-15 cm depth of Missouri River flood plain soil and 3,000 litres of well water. The tanks were constantly aerated and allowed to stabilise over a three- to four-month period. After this period, core chambers were created within the tanks as before (each core chamber contained a water volume of 9.5 l) and the test substance was added to the chambers at concentrations of 25, 75 or 675 μg/l. Sterile control chambers were also created by adding formaldehyde to the

[12] Akzo Nobel (2003) argued that the substance should be considered readily biodegradable on the basis of this test as it was unclear if the term “acclimated” used in the test referred to acclimation of the inocula to the test substance or acclimation of the inocula to laboratory conditions. Further details of this and another test (using the Monsanto Shake Flask Procedure) are reported in Monsanto (1976). For the shake flask test, an acclimated bacterial seed was used with reference to the method used by Gledhill (1975). This same procedure appears as USEPA Method 796.3100 Aerobic Aquatic Biodegradation, and this test guideline clearly shows that the acclimation procedure involves a two-week adaptation period whereby the inoculum is exposed to incremental concentrations of 4, 8 and 8 mg/l of the test substance on day zero, seven and 11 of the acclimation period. The level of mineralisation seen with tertbutylphenyl diphenyl phosphate in this shake flask test was 43 per cent after 28 days. It is likely that a similar acclimated inoculum was also used in the modified Sturm test. Hence the interpretation of the test in the main text is retained, that is, inherent biodegradability.

chamber. The experiment was run for 35 days. The half-life for primary degradation in this test system was determined to be 2 to 3 days.

Heitkamp *et al.* (1985) identified 28 fungi capable of metabolising tertbutylphenyl diphenyl phosphate. The main products formed were alkyl side chain-oxidised and aromatic ring-oxidised metabolites, with di- and monoaryl phosphates formed to a lesser extent.

The biodegradation of tertbutylphenyl diphenyl phosphate in microcosm systems was investigated by Heitkamp and Cerniglia (1986) and Heitkamp *et al.* (1986). The tertbutylphenyl diphenyl phosphate used in this study was isolated and purified from a commercial product using column chromatography and had a purity of above 99 per cent. This substance was mixed with ^{14}C-labelled tertbutylphenyl diphenyl phosphate (purity above 99 per cent). The microcosms used in the study consisted of 0.5 litre glass tanks containing 20 g of moist sediment and 180 ml of water from one of five different ecosystems. The ecosystems sampled were Arkansas River (sediment organic carbon content of 0.8 per cent with little or intermittent low-level exposure to chemicals), DeGray Reservoir (sediment organic carbon content of 3.2 per cent with little exposure to chemicals), Lake Chicot (sediment organic carbon content of 6.2 per cent with long-term exposure to significant concentrations of chemicals), Little Dixie Reservoir (sediment organic carbon content of 5.7 per cent with intermittent low-level exposure to chemicals) and Redfish Bay (estuarine environment, sediment organic carbon content of 3.5 per cent with intermittent low-level exposure to chemicals).

The biodegradation of tertbutylphenyl diphenyl phosphate was investigated by adding 0.1, 1 or 10 mg of the test substance to the microcosm (each concentration/microcosm combination was tested in duplicate) and incubating the system at 22°C for eight weeks. Sterile controls were also run to determine the rate of abiotic degradation of the test substance in the systems used. The amounts of CO_2 evolved (at weekly intervals), and the amounts of non-volatile and volatile metabolites and undegraded test substance (after eight weeks incubation), were determined. The results are summarised in Table 3.1. The concentration of the test substance was found to affect the rate of mineralisation in some of the systems tested. For the experiments using Lake Chicot and Little Dixie Reservoir sediment/water, a one-week lag period prior to $^{14}CO_2$-evolution was seen at all concentrations tested, but the highest rate of mineralisation after eight weeks was seen in both systems (37 and 14 per cent respectively) at the lowest test concentration (0.1 mg). The total amount mineralised was 50 per cent and 90 per cent lower in both systems at a concentration of 1 and 10 mg respectively. The experiments with Redfish Bay sediment showed a two-week lag phase prior to $^{14}CO_2$ evolution at a concentration of 0.1 mg and a five-week lag phase at 10 mg, but no difference was seen in the total amount mineralised after eight weeks at either concentration. The experiments with sediments from DeGray Reservoir and Arkansas River showed little or no lag period or difference in the total mineralisation seen at any concentration. Sterile controls showed that the abiotic degradation of the test substance under the conditions used was minimal.

The volatile metabolites identified in this experiment included phenol and tertbutyl phenol. The polar metabolites isolated from the sediment-water phases included phenol (the major metabolite found), tertbutyl phenol and diphenyl phosphate.

The effect of temperature and redox potential on the degradation of several phosphate esters, including tertbutylphenyl diphenyl phosphate, in two natural sediments was investigated by Muir *et al.* (1989). The triphenyl phosphate tested was ^{14}C-labelled (phenyl ring labelled) mixed with a purified non-labelled tertbutylphenyl diphenyl phosphate. The sediment samples used in the study were collected from a eutrophic farm pond and the Red River, Winnipeg (both samples were from agricultural areas remote from industry). The pond sediment consisted of 75 per cent clay, 24 per cent silt and one per cent sand and had an organic carbon content of 3.7 per cent and a pH of

7.6, and the river sediment consisted of 48 per cent clay, seven per cent sand and 43 per cent silt and had an organic carbon content of 2.3 per cent and a pH of 7.7.

Table 3.1 Biodegradation of ^{14}C-tertbutylphenyl diphenyl phosphate after eight weeks in sediment microcosms (as percentages)

Ecosystem	Total mineral-isation (%)	Volatile ^{14}C- meta-bolites (%)	Total extract-able ^{14}C-residues[a]	Identity of extractable ^{14}C-residues[a]		
				BPDP (%)	TPP (%)	Polar metabolites
Arkansas River	5.8-8.5	0.8	48.0 (6.1)[b]	64.7 (32.9)[b]	33.0 (11.0)[b]	2.3 (56.1)[b]
DeGray Reservoir	1.7	0.2	69.3 (17.8)[b]	100 (100)[b]		
Lake Chicot	Up to 37.2	0.9	25.2 (16.5)[b]	71.5 (31.8)[b]	27.0 (25.9)[b]	1.5 (42.3)[b]
Little Dixie Reservoir	13.6	0.2	68.8 (11.5)[b]	99.4 (96.9)[b]	0.6	(3.1)[b]
Redfish Bay	Up to 12.5	0.1	27.3 (6.2)[b]	90.5 (73.6)[b]	9.0 (16.3)[b]	0.5 (10.1)[b]

Source: Heitkamp *et al.* (1986).
Notes: [a]Values refer to methylene chloride extracts for combined water and sediment phase.
[b]Values in parentheses refer to methanol extracts of solid sediment phase alone.

The aerobic sediment experiments were carried out using loosely capped flasks (static test) or in respirometer flasks with air flowing through the system (1-2 ml/minute). The sediments incubated under anaerobic conditions (in respirometer flasks under a nitrogen flow (1-2 ml/minute)) were amended with one per cent by weight of microcrystalline cellulose to provide an additional source of carbon. The degradation experiments were carried out using around 10 g (dry weight) of sediment in dechlorinated water (sediment:water ratios of 1:10 (static test) or 1:20 (respirometer flask)). Each sediment sample was pre-incubated for 21 days at the intended experimental temperature prior to the addition of the test substance. The concentration tested was 0.1 mg/l (static test) or 0.05 mg/l (respirometer flasks) and the substance was added as 0.1 ml of a solution in acetone. All experiments were carried out in duplicate for up to 64 days and sterile controls were also run to investigate the abiotic degradation of tertbutylphenyl diphenyl phosphate under the conditions used. The aerobic experiments were incubated with a 16:8 hours light:dark photoperiod (using low intensity light) whereas the anaerobic experiments were incubated in darkness. The microbial biomass present in the test systems was between 9×10^6 and 32×10^6 colony forming units (CFU)/g in the experiments with river sediments. The microbial biomass present in the aerobic pond respirometer sediments was found to decline from 42×10^6 CFU/g to 0.3 CFU/g over the 64-day period. The total microbial biomass (aerobic and facultative anaerobic heterotrophs) present in the N_2-purged respirometer experiments was 5.3×10^6 CFU/g after 3 to 8 days and 24×10^6 after 30-40 days, but the number of strict anaerobes present was around eight to 40 times less, and so the incubations were not strictly anaerobic. The results of the experiments are summarised in Table 3.2.

Table 3.2 Effect of temperature and redox potential on degradation of ^{14}C-tertbutyl diphenyl phosphate in sediments

Test system	Sediment	Temp.	Time (days)	Amount of ^{14}C present (% of applied)							Estimated half-life[c] (days)
				Sediment – extractable[a]	Sediment – non-extract-able	Water – extract-able[b]	Water – non-extract-able	CO_2	Total	%of total as parent cpd.	
Aerobic static test system	Pond	25°C	0.25	95.5	2.0	0.9	n/a		98.4		4.2 ± 1.7
			64	47.6	15.3	0.8	5.0		68.7		
		10°C	0.25	73.2	2.4	0.5	1.3		77.4		5.5 ± 0.6
			64	63.3	5.8	0.2	2.2		71.5		
		2°C	0.25	78.8	3.6	1.0	n/a		83.4		16.1 ± 13.3
			6	68.6	3.4	0.8	n/a		72.8		
	River	25°C	0.25	99.1	2.6	0.8	2.3		104.7		8.4 ± 0.3
			40	75.4	9.0	0.0	8.7		93.1		
Aerobic respirometer	Pond	25°C	8	29.2	29.0	6.0	n/a	14.5	80.2	18.4	
			64	19.8	43.7	2.5	n/a	14.4	80.4	23.9	
	River	25°C	3	109.7	3.3	7.9	n/a	0.1	119.2	82.7	
			40	52.3	17.7	10.7	n/a	21.6	95.2	45.9	
Anaerobic respirometer	Pond	25°C	8	81.9	4.0	5.3	n/a	0.9	91.2	19.1	
			64	54.4	6.5	4.1	n/a	15.4	80.4	19.2	
	River	25°C	3	72.3	2.3	6.0	n/a	0.1	80.7	71.9	
			40	75.8	9.2	11.3	n/a	8.2	104.6	31.9	
Autoclaved sample (aerobic static test system)	Pond	25°C	64	70.2	4.4	1.1	3.2		78.9		

Source: Muir *et al.* (1989).

Notes: a) Extracted with aqueous methanol to recover undegraded phosphate ester and any diaryl phosphate degradation products.
b) Extracted with dichloromethane to recover undegraded phosphate ester.
c) Half-life estimated based on the data obtained over days 0-6 for pond sediment and days 0-10 for river sediment. The half-life refers to the disappearance of the parent compound from the sediment phase.

The results show extensive degradation of tertbutylphenyl diphenyl phosphate in the study. Initially, most of the tertbutylphenyl diphenyl phosphate added to the system adsorbed onto the sediment phase but by the end of the experiment the amount of extractable radioactivity associated with the sediment phase had decreased substantially. Detailed analysis of the sediment extracts indicated that the major portion of extractable radioactivity was as unchanged tertbutyl diphenyl phosphate, with low levels of degradation products, including triphenyl phosphate and diphenyl phosphate.

IUCLID (2001) reports the results of an unpublished biodegradation study with tertbutylphenyl diphenyl phosphate in naturally occurring river water. The test was carried out using a river die-away procedure with Mississippi River water at 24°C. The substance was tested in duplicate at both 50 μg/l and 500 μg/l over a 27-day period. The half-life for disappearance of the tertbutylphenyl diphenyl phosphate (primary biodegradation) was below 0.5 days at both concentrations. The half-life in autoclaved control samples was about 39 days, indicating that the degradation seen was due mainly to biotic processes. Experiments were also carried out using membrane-filtered river water in which biodegradation was still seen at a reasonably rapid rate.

Summary of environmental degradation

Abiotic degradation

The available information indicates that tertbutylphenyl diphenyl phosphate will hydrolyse only slowly at pHs typically found in the environment. Compared with the data available for other triaryl phosphates (for example, see risk evaluation report of triphenyl phosphate), the products from the reaction will be phenol and tertbutylphenyl phenyl phosphate or tertbutyl phenol and diphenyl phosphate. The diaryl phosphate products formed are likely to be more stable to hydrolysis than the parent compound. Since the rate of hydrolysis is predicted to be significant only at very high pHs and possibly low pHs, the rate of hydrolysis of tertbutylphenyl diphenyl 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.

The available information on photolysis indicates that tertbutylphenyl diphenyl phosphate is likely to be relatively stable to photodegradation in the environment. The rate of this reaction is assumed to be zero in this assessment.

Atmospheric photo-oxidation of tertbutylphenyl diphenyl phosphate is predicted to occur with a half-life of around 24 hours. 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.

Hydrolysis	$khydr_{water}$ = 0 d^{-1}	half-life = infinite
Photolysis	$kphoto_{water}$ = 0 d^{-1}	half-life = infinite
Atmospheric photooxidation	k_{OH} = 1.6×10^{-11} cm^3/molecule s	half-life = 24 h

Biodegradation

Several studies available have shown that tertbutylphenyl diphenyl phosphate is degraded rapidly in a range of test systems. One standard test shows ready biodegradability of a commercial substance; although it is likely that the triphenyl phosphate component contributes to the result, on balance, this study shows that

tertbutylphenyl diphenyl phosphate is readily biodegradable. There is a further standard ready biodegradation test available but the test was carried out using an acclimated inoculum. On the basis of the results of these tests, the substance is considered to be readily biodegradable, not meeting the 10-day window criterion.

The recommended biodegradation (mineralisation) rate constants and half-lives from the TGD (assuming it is inherently biodegradable (meeting specific criteria), with a Kp_{soil} of 95 l/kg) are summarised below.

Sewage treatment plant	$k = 0.3\ h^{-1}$	half-life = 2.3 hours
Surface water	$k = 0.014\ d^{-1}$	half-life = 50 days
Sediment	$k = 7.7\times10^{-3}\ d^{-1}$	half-life = 90 days
Soil	$k = 7.7\times10^{-3}\ d^{-1}$	half-life = 90 days

Results from several screening studies can be used to compare these data. River die-away studies have generally shown primary biodegradation rates of below 0.5 days to 10-21 days. Given that these half-lives represent primary degradation, and the studies have usually been carried out at room temperature, the default mineralisation half-life estimated above appears to be in reasonable agreement with the available data. [USEPA (2008) assumes a biodegradation half-life of below 0.5 days.]

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

Experiments investigating degradation in sediments have generally shown reasonably rapid primary degradation (half-lives of 1 to 3 days in some experiments have been seen), but one series of experiments using sediment microcosms found that the rate of mineralisation depended on the actual concentration of the test substance; mineralisation rates of 1.7 per cent up to 37 per cent over eight weeks were seen in these studies. The default mineralisation half-life of 90 days estimated above appears to be consistent with these data.

Given that the default degradation half-lives derived here appear to be in reasonable agreement with the available degradation data, these are used in the risk assessment for tertbutylphenyl diphenyl phosphate.

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} of 3.74×10^{4} l/kg can be estimated for tertbutylphenyl diphenyl phosphate from its structure using the Syracuse Research Corporation PCKOC version 1.63 software with a molecular connectivity index method. [This is the value for K_{oc} cited by USEPA 2008.]

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

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

Using this equation for tertbutylphenyl diphenyl phosphate (log K_{ow} of 5.12) results in an estimated K_{oc} of 4,773 l/kg. This value is used in this assessment as it is estimated using a more specific method for phosphates, although it has not been determined whether this particular substance falls within the applicability domain of the model.

The resulting partition coefficients for soils and sediment calculated from this K_{oc} value are summarised below.

K_{oc}	4,773 l/kg		
Kp_{susp}	477 l/kg	$K_{susp\text{-}water}$	120 m^3/m^3
Kp_{sed}	239 l/kg	$K_{sed\text{-}water}$	120 m^3/m^3
Kp_{soil}	95 l/kg	$K_{soil\text{-}water}$	143 m^3/m^3

These values are used as representative of the commercial substance. As the K_{ow} value of the individual components will vary, so will the K_{oc}. However, this variation is not expected to lead to significant differences in adsorption behaviour.

Volatilisation

Muir *et al.* (1985) investigated volatilisation from and distribution in an artificial pond (15-17 m^2 area and 0.5 m depth) over 360 days. The substance tested was ^{14}C-labelled tertbutylphenyl diphenyl phosphate which was added to give an initial water concentration of 50 μg/l. Air above the pond was sampled continuously for the first five days at heights of 5, 10 and 20 cm; the maximum concentration found was 197 ng/m^3 above the centre of the pond. The paper also estimated (using a two-resistance model) that the potential cumulative losses by volatilisation accounted for around 6 per cent of the total radioactivity added by day 21. The results of the study are shown in Table 3.3. The half-life of the substance in the water and sediment phase was estimated to be 0.44 and 39 days respectively based on parent compound analysis.

The Henry's law constant estimated for tertbutylphenyl diphenyl phosphate is 0.009 Pa m^3/mol at 20°C (see Section 1.3.9). This indicates that volatilisation from water is likely to be limited.

Table 3.3 Distribution of ^{14}C-labelled tertbutylphenyl diphenyl phosphate in an artificial pond

Time	Distribution (as percentage of initial amount applied)			
	Water	Sediment	Air[a]	Biota
1 hour	80.9	-		-
18 hours	24.0	61.5	3.7	1.8
7 days	11.4	36.0	5.3	0.5
21 days	3.7	34.7	6.2	<0.1
105 days	<2.0	28.7	-	<0.1
360 days	-	23.6	-	-

Source: Muir *et al.* (1985).
Notes: a) Values for air represent theoretical cumulative total using a two-resistance model.

Fugacity modelling

The potential environmental distribution of tertbutylphenyl diphenyl 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 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 3.4.

The results of the model show that only a small amount of the tertbutylphenyl diphenyl phosphate released to the environment will be in the air compartment at steady state. When the substance is released to air it distributes mainly to the soil compartment, presumably by atmospheric deposition. When it is released to soil, the substance remains almost entirely in the soil. When released to water, the substance is likely to distribute between the water and sediment phase at steady state.

The behaviour of tertbutylphenyl diphenyl phosphate during waste water treatment has also been estimated using the EUSES model. Using a degradation rate constant of 0.3 h^{-1} (see Section 3.1.1), a K_{oc} of 4,773 l/kg (see above) and a vapour pressure of 1.5×10^{-4} Pa at 25°C (see Section 1.3.5), the following behaviour is predicted:

Degraded	46.4%
Adsorbed to sludge	29.9%
Volatilised to air	0.01%
To effluent	23.7%

These values are used in PEC calculations. Given the composition of the substance, and uncertainties in K_{oc} and vapour pressure estimates, these are only indicative.

Table 3.4 Results of level III fugacity model for tertbutylphenyl phosphate

Input data	**Value**				
Vapour pressure	7.8×10^{-5} Pa at 20°C				
Water solubility	0.04 mg/l				
Henry's law constant	0.75 Pa m^3/mol at 20°C				
Log K_{ow}	5.12				
Atmospheric half-life	24.1 hours				
Half-life in water	150 days				
Half-life in soil/sediment	300 days				
Emission rate	**Model results at steady state**				
	Amount in air	**Amount in soil**	**Amount in water**	**Amount in sediment**	**Overall residence time**
1,000 kg/hour to air 1,000 kg/hour to soil 1,000 kg/hour to water	0.27%	79.4%	10.0%	10.4%	75 days
1,000 kg/hour to air 0 kg/hour to soil 0 kg/hour to water	1.2%	95.1%	1.8%	1.9%	53 days
0 kg/hour to air 1,000 kg/hour to soil 0 kg/hour to water	4×10^{-5}%	100%	0.015%	0.016%	130 days
0 kg/hour to air 0 kg/hour to soil 1,000 kg/hour to water	6×10^{-4}%	0.05%	49.0%	51.0%	44 days

3.1.3 Bioaccumulation and metabolism

Measured data

The uptake and accumulation of a commercial tertbutylphenyl diphenyl phosphate product (Fyrquel GT) 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 substance tested consisted of 15-20 per cent triphenyl phosphate, with the remainder being mainly isomers of tertbutylphenyl diphenyl phosphate, along with isomers of di-tertbutylphenyl diphenyl phosphate. 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 the tertbutylphenyl diphenyl phosphate and triphenyl phosphate components of the product. Concentrations of these two components in the water were also determined at fortnightly intervals. The results are summarised in Table 3.5. The paper reported that the mean bioconcentration factor (BCF) determined at 90 days in this study was 3,816 ± 1,088 l/kg for tertbutylphenyl diphenyl phosphate and 1,958 ± 382 l/kg for triphenyl phosphate. When placed in clean water, depuration of both components from the fish was found to be rapid, with half-lives of below 7 days. Toxic effects were seen in some of the treatments (particularly at the higher concentrations), including effects on growth, and so this adds some uncertainty to the BCF values estimated in this study.

Table 3.5 Bioconcentration of a commercial tertbutyl diphenyl phosphate in fathead minnow

Mean measured concentration in water (mg/l)		Mean measured concentration in fish (mg/kg wet wt.)						BCF at 90 days (l/kg)	
		30 days		60 days		90 days			
TPP	TBDP	TPP	TBDP	TPP	TBDP	TPP	TBDP	TPP	TBDP
0.005	0.017	1	14	4	2	8	75	1,600	4,412
0.010	0.030	1	23	7	52	16	136	1,600	4,533
0.022	0.071	1	36	22	110	42	322	1,909	4,535
0.042	0.152	18	163	60	222	93	548	2,214	3,605
0.111	0.385	54	652	246	512	274	769	2,468	1,997
Control		1	17	<0.2	<1	1	4		

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

Muir *et al.* (1983) investigated the bioconcentration of ^{14}C-labelled tertbutylphenyl diphenyl phosphate (radiochemical purity above 98 per cent; mixed with unlabelled triphenyl phosphate) by both rainbow trout (*Oncorhynchus mykiss*) and fathead minnows (*Pimephales promelas*). The fish (mean weight 0.75 g for rainbow trout (loading density 3.0 g/l) and 2.5 g for fathead minnows (loading density 7.2 g/l)) were exposed in glass aquaria containing 10 litres of dechlorinated, carbon-filtered tap water at 10°C. The fish were acclimated to the aquaria for 16 hours prior to the addition of the test substance at 5 μg/l or 50 μg/l (the test substance was added as a solution in acetone (0.05-0.4 ml added to each aquaria)). Fish (three at each sampling point) were removed from the aquaria at various times (1, 3, 6, 12 and 24 hours) during the exposure period for analysis of the concentration of radiolabel. At the end of the 24-hour exposure period, the remaining fish were removed and placed in a 40-litre tank

with a continuous flow of water and depurated for up to 432 hours (fish were sampled after 12, 24, 48, 96, 144, 240 and 432 hours of depuration). In addition, the concentration of radiolabel present in the water phase was determined during the exposure part of the experiment. In some cases, the concentrations of the test substance present were also determined by parent compound analysis (gas chromatography using an N-P detector).

During the exposure part of the test, the concentration of the test substance in water decreased with time as a result of uptake into the fish. This decrease was more marked for fathead minnows than for rainbow trout due to the higher loading used for fathead minnow. For trout, steady-state concentration was not reached within the 24-hour exposure period but the concentrations in fathead minnows generally reached a maximum, steady-state value within 12 hours of exposure. The kinetic data and the bioconcentration factors (BCF) determined from the data are summarised inTable 3.6. The authors also estimated BCF values of 778 ± 62 l/kg and 578 ± 18 l/kg for rainbow trout and fathead minnows respectively based on the estimated amount of untransformed tertbutylphenyl diphenyl phosphate present in the fish.

Table 3.6 Uptake and elimination of ^{14}C-labelled tertbutylphenyl diphenyl phosphate in rainbow trout and fathead minnow

Species	Exposure concentration (μg/l)		Uptake rate constant (initial rate method) (hour^{-1})[a]	Depuration rate constant (hour^{-1})[a]		Bioconcentration factor (BCF)		
	0 hours	24 hours		0-144 hour	0-432 hour	b	c	d
Rainbow trout	6.2	1.8	22.8 ± 13.5	0.0137 ±0.0053	0.0106 ±0.0036	2,298 ± 619	1,096 ± 55	1,335 ± 122
	55.0	14.8	29.3 ± 17.3	0.0113 ±0.0043	0.0111 ±0.0034			
Fathead minnow	3.9	0.8	17.7 ± 9.6	0.0088 ±0.0037	0.0078 ±0.0027	3,316 ± 500	785 ± 509	498 ± 184
	36.5	11.3	18.0 ± 10.0	0.0074 ±0.0033	0.0070 ±0.0039			

Source: Muir *et al.* (1983).

Notes: a) Uptake and depuration data calculated based on ^{14}C measurements.
b) BCF determined using initial rate method for uptake rate constant.
c) Bioconcentration factor determined using the method of Zitko (1980) to take account of the decrease in exposure concentration with time.
d) Bioconcentration factor determined using the BIOFAC computer program. The values calculated by this method are not considered reliable as the method requires the exposure concentration to remain constant during the test.

Muir *et al.* (1985) determined the uptake of ^{14}C-labelled tertbutylphenyl diphenyl phosphate by *Pimephales promelas* in an artificial pond. The pond was 15-17 m^2 in area, with a depth of 0.5 m, and the substance was added to the pond water to give an initial concentration of 50 μg/l. The maximum concentration of ^{14}C in the fish was determined eight hours after addition of the test substance to the pond and an approximate BCF of 528 l/kg was reported at this time. After this time, the concentration of the test substance in fish declined, reflecting the decline in concentration in the water phase in the experimental pond. The same study also investigated uptake of the test substance by invertebrate (*Chironomus tentans*) larvae. The larvae were found to accumulate ^{14}C via pore water or from the sediment itself, and the maximum concentration found in the organism was 2.72 mg/kg at day 14. The

authors estimated concentration factors (based on the measured concentration of the tertbutylphenyl diphenyl phosphate present in sediment) of 37 at day 49, with the factor generally below 10 over days 21 to 70. As the concentration of tertbutylphenyl phenyl phosphate was not adequately maintained in this study, the reported fish BCF and other concentration factors should be treated with caution.

There are no data available on the uptake of tertbutylphenyl phosphate by aquatic organisms from food.

Calculated data

For the terrestrial food chain, the TGD requires a BCF for earthworms. No experimental data are available for this endpoint and so an earthworm BCF value was 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 5.12, the $BCF_{earthworm}$ is estimated as 1,583 l/kg. This value is used in the assessment, though the reliability of this estimate is unknown.

Summary of accumulation

Several studies have shown that tertbutylphenyl phosphate can bioconcentrate in fish. The interpretation of the available data is not straightforward, as toxicity was seen in one study (Cleveland *et al.* 1986), particularly at the higher concentrations tested, and the exposure concentrations were not constant during the exposure period in two other studies (Muir *et al.* 1983 and Muir *et al.* 1985). The data obtained by Muir *et al*. (1983) was analysed by a method that allowed for the exposure concentration to decrease during the test. This leads to fish BCFs of the order of 785 to 1,096 l/kg based on ^{14}C-measurements and these values are considered to be the most reliable of the available data for tertbutylphenyl diphenyl phosphate. These values include contributions from any metabolites present, and the same authors estimate the BCF to be 578 to 778 l/kg based on the parent compound.

The available BCF data for triaryl phosphates as a whole are considered in Annex B. Using the analysis given in this Annex, a BCF of around 686 l/kg would appear to be appropriate for tertbutylphenyl diphenyl phosphate. This is very close to the values reported above by Muir *et al.* (1983) based on parent compound analysis and so the measured BCF value of 778 l/kg determined in this study is used in this risk assessment. [USEPA (2008) cites a fish BCF of 180, estimated using EPISUITE (the actual method is not given).]

In addition to a BCF, the TGD also requires a biomagnification factor (BMF) to be taken into account. For tertbutylphenyl diphenyl phosphate, the default BMF would be 1 based on the BCF values determined above. This value is used in the assessment.

For the terrestrial food chain, the TGD requires a BCF for earthworms. Using a log K_{ow} of 5.12, $BCF_{earthworm}$ is estimated to be 1,583 l/kg. The reliability of this estimate is unknown.

3.2 Environmental releases

3.2.1 General discussion

Releases from the production and use of tertbutylphenyl diphenyl 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) and the ESD on lubricants (OECD 2004b). In the absence of specific information on the substance, the ESDs 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, estimates from these sources will have a degree of uncertainty. The actual calculations are considered confidential as they are based on confidential production and use figures.

The producers of tertbutylphenyl diphenyl 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 3.8.

3.2.3 Releases from use (processing)

Emissions from use in polymers 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-diethylhexyl)phthalate (DEHP), and are modified according to the relative properties of this substance and the substance of interest. The main property affecting emissions is the vapour pressure of the substance. Tertbutylphenyl diphenyl phosphate has a similar vapour pressure to that of DEHP, and is classed as of medium volatility according to the criteria in the ESD[13]. The ESD also uses the particle size or form of the substance in estimating the possible releases from raw materials handling. Tertbutylphenyl diphenyl phosphate is a liquid

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

[13] 'Medium volatility' is used in comparison to DEHP which is considered of medium volatility. All phosphates assessed in this series have low vapour pressures for organic substances.

- Compounding: 0.025 per cent to air, 0.025 per cent to waste water.
- Conversion (including raw materials handling): 0.005-0.01 per cent to air, 0.011 per cent to waste water.

For polyurethanes, the emission factors are:

- Compounding (including raw materials handling): 0.005 per cent to air, 0.015 per cent to waste water.
- Conversion: 0.005 per cent to air, 0.005 per cent to waste water.

Textile coating produces PVC coatings on fabrics, and as such can be considered to be a plastics process. The ESD on plastics additives (OECD 2004a) provides the following emission factors for this use:

- Compounding (including raw materials handling): 0.01 per cent to water.
- Conversion: 0.125 per cent to air, 0.125 per cent to water.

Similarly, emissions from use of the substance in lubricants (assumed to be automotive lubricants) and hydraulic fluids from the blending step were estimated using methods outlined in the ESD on lubricants (OECD 2004b). Estimates were made for use as an additive in lubricants and hydraulic fluids and as a base fluid in power generation fluids. The estimated emissions to air from lubricant blending are very low. The emission factor for releases to water from blending is calculated as 1.75×10^{-5} kg/tonne lubricant for use as an additive and 8.2×10^{-4} kg/tonne lubricant for use as a base fluid.

3.2.4 Releases over the lifetime of products

Tertbutylphenyl diphenyl phosphate is used in products which are expected to have extended service lives (more than one year). These are therefore potentially important sources of emission.

Releases from the service life of lubricants were estimated using the methods in the ESD (OECD 2004b). For automotive lubricants, the emission factors are 6.9 per cent to surface water and 6.8 per cent to industrial soil. Use in hydraulic fluids of types HM and HV was assumed, leading to releases of eight per cent to soil and two per cent to water. Emissions from the use of power generation fluids are assumed to be negligible.

Possible losses from PVC and other materials through leaching and volatilisation are also considered in this section. A limited amount of information relevant to the release of tertbutylphenyl diphenyl phosphate is available, and was included here, but estimates are based on the methods outlined in the Emission Scenario Document (OECD 2004a) and also take into account 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.

Leaching loss

No information appears to be available on the leaching of tertbutylphenyl diphenyl phosphate from products.

The factors from the ESD on plastics additives are used in the assessment for emissions from PVC products. Compared to the model substance DEHP in the ESD,

tertbutylphenyl diphenyl phosphate is classed as a high solubility substance, and so the factor is increased by a factor of ten to account for this. The factor is 0.5 per cent over the lifetime of the product. The same factor is used for textile coatings.

Polyurethane articles are considered not to come into contact with water on a regular basis in their lifetime and so emissions to water from this use are negligible.

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 a nitrogen atmosphere (Shankwalkar and Cruz 1994) and an oxygen atmosphere (Shankwalkar and Placek 1992). The results of the studies are summarised in

Table 3.7.

Table 3.7 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
Isopropyl-phenyl diphenyl phosphate[a]	210-215°C	200-218°C	239-265°C	263-288°C	311-314°C	264-282°C	293-307°C
Tertbutyl-phenyl 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.

The results under a nitrogen atmosphere show that the triaryl phosphates start to decompose at temperatures of around 310-350°C, whereas alkyl diphenyl phosphates start to decompose at a temperature of around 260°C. 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.

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 (ECB 2005). These are applied to articles from PVC (including textiles) and polyurethane. Volatile losses from products occur at ambient temperatures, and at these temperatures tertbutylphenyl diphenyl phosphate is considered to have a similar vapour pressure to DEHP, the reference compound. The appropriate factor from the ESD is therefore that for medium volatility substances; or 0.05 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 4.5 per cent over the lifetime was used.

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 of medium-chain chlorinated paraffins (ECB 2005). For use in PVC, a loss of 0 to 3.125 per cent of the material over the lifetime of the products or articles is assumed, depending on the type of product. For textiles, a two per cent loss is assumed. In addition, a further two per cent loss on disposal at the end of the service life is assumed for PVC and textiles. For polyurethanes, no waste generation during the lifetime is assumed, but two per cent loss on disposal is assumed. 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 actual data to indicate how much may be available.

3.2.5 Summary of environmental releases

The estimated environmental releases of tertbutylphenyl diphenyl phosphate are summarised in Table 3.8.

Table 3.8 Summary of estimated environmental release of tertbutylphenyl 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			0.4			56 to surface water[b]				
PVC – 1	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0625	0.0625							
	Raw materials handling, compounding and conversion	0.075	0.1		c	c				
	In service losses				1.95	19.5		17.55	176	
	Waste in the environment[d]				0.08	19.3 to surface water	58	0.70	174 to surface water	523
PVC – 2	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0625	0.0625							
	Raw materials handling, compounding and conversion	0.075	0.1		c	c				
	In service losses				52.8	6		475	54	
	Waste in the environment[d]				0.02	5.7 to surface water	17	0.21	51.4 to surface water	155

Table 3.8 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	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0625	0.0625							
	Raw materials handling, compounding and conversion	0.075	0.1		c	c				
	In service losses				1.15	322		10.35	2,898	
	Waste in the environment[d]				0.15	37.9 to surface water	114	1.37	341 to surface water	1,027
Textile/ fabric coating	Raw materials handling and compounding		0.02							
	Conversion	0.05	0.05							
	Raw materials handling, compounding and conversion	0.05	0.07		c	c				
	In service losses				0.95	9.5		8.55	85.5	
	Waste in the environment[d]				0.08	18.7 to surface water	56.3	0.68	168 to surface water	506

Table 3.8 continued

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	**Water**	**Soil**	**Air**	**Water[a]**	**Soil**	**Air**	**Water[a]**	**Soil**
Poly-urethane	Raw materials handling and compounding	0.025	0.075							
	Conversion	0.025	0.025							
	Raw materials handling, compounding and conversion	0.05	0.1		c	c				
	In service losses				25.5			230		
	Waste in the environment[d]				1.02	254 to surface water	764	9.2	2,284 to surface water	6,879
Lubricant additives	Blending	6.33×10^{-9}	6.65×10^{-4}		1.32×10^{-6}	0.14				
	In service losses[d]					326 to surface water	321		2,931 to surface water	2,889
Hydraulic fluids	Blending	4.68×10^{-9}	7.63×10^{-4}		3.46×10^{-7}	0.06		5.41×10^{-7}	0.09	
	In service losses[d]					98 to surface water	392		882 to surface water	3,528
Power generation fluid	Blending	0.0181	1.98×10^{-3}		0.457	0.05				
	In service losses[d]				negligible	negligible	negligible	negligible	negligible	negligible
Total					104	1,203	1,723	810	10,150	15,513

Notes:
a) Regional and continental emissions to water are split 80:20 between waste water treatment and direct discharge to surface water, except where noted.
b) Emissions calculated from site-specific data, after waste water treatment (sludges from production sites are incinerated, calculating the values after treatment allows this to be reflected in the emission estimates).
c) Values for individual steps are confidential, but are included in the total figure.
d) Releases from hydraulic fluids and as waste in the environment are assumed to go directly to surface water.

3.3 Environmental concentrations

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

Calculation of PECs

PECs for surface water and sediment were estimated with the EUSES 2.0.3 program using the data summarised in the previous sections as input. The concentrations predicted for water and sediment are shown in Table 3.9.

Table 3.9 Summary of predicted local concentrations for the aquatic compartment

Scenario		PEC_{local}			
		Microorganisms in sewage treatment plant (mg/l)	**Surface water - emission episode (μg/l)**	**Surface water - annual average (μg/l)**	**Sediment (mg/kg wet wt.)**
Production of tertbutylphenyl diphenyl phosphate		2.25×10^{-3}	0.08	0.07	7.88×10^{-3}
PVC – 1	Compounding	4.43×10^{-3}	0.46	0.38	0.05
	Conversion	7.39×10^{-3}	0.75	0.62	0.08
	Combined compounding and conversion	0.01	1.19	0.99	0.13
PVC – 2	Compounding	4.43×10^{-3}	0.46	0.18	0.05
	Conversion	7.39×10^{-3}	0.75	0.29	0.08
	Combined compounding and conversion	0.01	1.19	0.46	0.13
PVC – 3	Compounding	4.43×10^{-3}	0.46	0.02	0.05
	Conversion	7.39×10^{-3}	0.75	0.75	0.08
	Combined compounding and conversion	0.01	1.19	0.99	0.13
Poly-urethane	Compounding	8.87×10^{-3}	0.9	0.74	0.09
	Conversion	2.96×10^{-3}	0.31	0.26	0.03
	Combined compounding and conversion	0.01	1.19	9.85	0.13
Textile coating	Compounding	2.37×10^{-3}	0.25	0.02	0.03
	Conversion	5.91×10^{-3}	0.61	0.61	0.06
	Combined compounding and conversion	8.28×10^{-3}	0.84	0.70	0.09

Table 3.9 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 wt.)**
Lubricant additive	Blending of lubricant	7.86×10^{-5}	0.03	0.03	2.86×10^{-3}
Hydraulic fluids	Blending of fluid	9.02×10^{-5}	0.03	0.02	2.98×10^{-3}
Power generation fluid	Blending of fluid	2.34×10^{-4}	0.04	0.04	4.47×10^{-3}

The predicted regional concentrations are 0.02 μg/l for surface water and 2.1×10^{-3} mg/kg wet weight for sediment.

Predicted concentrations were also calculated for the marine environment using the EUSES program. These are included in Table 3.10. Note that production is not included in this table; the production sites do not discharge to the marine environment.

Measured levels in water and sediment

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

The limit of detection was 0.05 µg/l. The substance was only detected in the Davyhulme WWTP effluent (on five occasions, at concentrations up to 0.09 µg/l) and the associated Manchester Ship Canal (on one occasion, at a concentration of 0.07 µg/l). The Davyhulme WWTP serves an industrial complex which includes a production site. However, there could be other sources locally as well.

Boethling and Cooper (1985) reported the results of an early 1980s survey of the levels of tertbutylphenyl diphenyl phosphate in surface water in the United States. The substance was not found (detection limit of the method was 0.1 μg/l) in four samples from Saginaw River (industrialised area), four samples from Baltimore Harbour (industrialised area), three samples from Detroit River (industrialised area), four samples from Delaware River (industrialised area near to aryl phosphate manufacturer), seven samples from Kanawha River (industrialised area near to aryl phosphate manufacturer) and four samples from Eastern Lake Superior (remote area).

Boethling and Cooper (1985) also reported the results of an early 1980s survey of the levels of tertbutylphenyl diphenyl phosphate in sediment in the United States. The substance was not found in four samples from Saginaw River (industrialised area), three samples from Baltimore Harbour (industrialised area), two samples from Detroit River (industrialised area), two samples from Delaware River (industrialised area near to aryl phosphate manufacturer), six samples from Kanawha River (industrialised area near to aryl phosphate manufacturer) and two samples from Eastern Lake Superior (remote area). The detection limit of the method was 0.03 mg/kg.

There are insufficient monitoring data to compare with predicted levels in most of the scenarios. The predicted concentrations are used in the risk assessment.

Table 3.10 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 wt.)**
PVC – 1	Compounding	0.19	0.16	0.02
	Conversion	0.31	0.26	0.03
	Combined compounding and conversion	0.5	0.41	0.05
PVC – 2	Compounding	0.19	0.07	0.02
	Conversion	0.31	0.12	0.03
	Combined compounding and conversion	0.5	0.19	0.05
PVC – 3	Compounding	0.19	2.3×10^{-3}	0.02
	Conversion	0.31	0.31	0.03
	Combined compounding and conversion	0.5	0.41	0.05
Poly-urethane	Compounding	0.37	0.31	0.04
	Conversion	0.13	0.10	0.01
	Combined compounding and conversion	0.5	0.4	0.05
Textile coating	Compounding	0.10	2.07×10^{-3}	0.01
	Conversion	0.25	0.25	0.03
	Combined compounding and conversion	0.35	0.29	0.04
Lubricant additive	Blending of lubricant	5.1×10^{-3}	4.51×10^{-3}	5.33×10^{-4}
Hydraulic fluids	Blending of fluid	5.59×10^{-3}	2.38×10^{-3}	5.84×10^{-4}
Power generation fluid	Blending of fluid	0.01	9.88×10^{-3}	1.22×10^{-3}

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 3.11.

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

$PEC_{regional}$ = 4.69×10^{-6} mg/kg wet weight for agricultural soil
= 5.56×10^{-5} μg/l for pore water of agricultural soil

= 2.57×10^{-6} mg/kg wet weight for natural soil
= 1.76×10^{-3} mg/kg wet weight for industrial soil

As no measured data are available on the actual concentrations of tertbutylphenyl diphenyl phosphate in soil, predicted concentrations are used in the assessment.

Table 3.11 Summary of predicted local concentrations for the air and terrestrial compartments

Scenario		PEC_{local}			
		Annual average concentration in air (mg/m^3)	**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)**
Production of tertbutylphenyl diphenyl phosphate		1.33×10^{-8}	2.63×10^{-6a}	2.63×10^{-6a}	3.12×10^{-5a}
PVC – 1	Compounding	2.86×10^{-6}	0.02	0.01	0.14
	Conversion	1.43×10^{-5}	0.03	0.02	0.24
	Combined compounding and conversion	1.71×10^{-5}	0.05	0.03	0.38
PVC – 2	Compounding	1.3×10^{-6}	0.02	0.01	0.14
	Conversion	6.48×10^{-6}	0.03	0.02	0.24
	Combined compounding and conversion	7.77×10^{-6}	0.05	0.03	0.38
PVC – 3	Compounding	1.28×10^{-8}	0.02	0.01	0.14
	Conversion	1.74×10^{-5}	0.03	0.02	0.24
	Combined compounding and conversion	1.71×10^{-5}	0.05	0.03	0.38
Poly-urethane	Compounding	5.72×10^{-6}	0.04	0.02	0.29
	Conversion	5.72×10^{-6}	0.01	8.04×10^{-3}	0.1
	Combined compounding and conversion	1.14×10^{-5}	0.05	0.03	0.38
Textile coating	Compounding	3.28×10^{-9}	0.01	6.4×10^{-3}	0.08
	Conversion	1.39×10^{-5}	0.03	0.02	0.19
	Combined compounding and conversion	1.14×10^{-5}	0.04	0.02	0. 27
Lubricant additive	Blending of lubricant	3.29×10^{-9}	3.54×10^{-4}	2.15×10^{-4}	2.55×10^{-3}
Hydraulic fluids	Blending of fluid	3.28×10^{-9}	4.06×10^{-4}	2.47×10^{-4}	2.93×10^{-3}
Power generation fluid	Blending of fluid	4.14×10^{-6}	1.07×10^{-3}	6.6×10^{-4}	7.83×10^{-3}

Notes: a) Sludge from the production site is not applied to agricultural soil.

3.3.3 Air compartment

Calculation of PECs

The concentrations of tertbutylphenyl diphenyl phosphate in air were estimated using EUSES 2.0.3. The PECs calculated are summarised in Table 3.11.

The predicted regional concentration in air is 3.28×10^{-9} mg/m^3.

Measured levels

Sjödin *et al.* (2001) investigated the levels of tertbutylphenyl diphenyl 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). Duplicate samplers were used at each location investigated. Tertbutylphenyl diphenyl phosphate was found in air samples from the electronics equipment recycling facility at 0.2-1.9 ng/m^3 (mean 0.8 ng/m^3) in the dismantling hall and 15-19 ng/m^3 in the shredder room. Tertbutylphenyl diphenyl phosphate was found to be associated mainly with the particulate phase. No data were reported for the levels of tertbutylphenyl diphenyl phosphate present in air from the other locations sampled.

There are insufficient measured data to make a comparison with predicted levels. The predicted levels are used in the risk characterisation.

3.3.4 Non-compartment specific exposure relevant for the food chain

Predicted concentrations of tertbutylphenyl diphenyl phosphate in fish and earthworms are shown in Table 3.12. Predicted concentrations in prey species for marine food chains are also included. The predicted concentrations in human intake media are shown in Table 3.13. The concentrations were calculated using EUSES 2.0.3.

As there are no measured data on the actual concentrations of tertbutylphenyl diphenyl phosphate in biota, predicted concentrations are used in the assessment

Table 3.12 Summary of predicted local concentrations for secondary poisoning

Scenario		Predicted concentration			
		Fish (mg/kg)	**Earthworms (mg/kg)**	**Marine fish (mg/kg)**	**Marine top predators (mg/kg)**
Production of tertbutylphenyl diphenyl phosphate		0.04	6.2×10^{-5}	n/a	n/a
PVC – 1	Compounding	0.16	0.1	0.06	0.01
	Conversion	0.25	0.17	0.1	0.02
	Combined compounding and conversion	0.39	0.27	0.16	0.03
PVC – 2	Compounding	0.08	0.1	0.03	6.8×10^{-3}
	Conversion	0.12	0.17	0.05	0.01
	Combined compounding and conversion	0.19	0.27	0.07	0.02
PVC – 3	Compounding	0.2	0.1	1.6×10^{-3}	1.44×10^{-3}
	Conversion	0.3	0.17	0.12	0.03
	Combined compounding and conversion	0.39	0.27	0.16	0.03
Polyurethane	Compounding	0.3	0.2	0.12	0.03
	Conversion	0.11	0.07	0.04	9.34×10^{-3}
	Combined compounding and conversion	0.39	0.27	0.16	0.03
Textile coating	Compounding	0.02	0.05	1.51×10^{-3}	1.42×10^{-3}
	Conversion	0.24	0.14	0.1	0.02
	Combined compounding and conversion	0.28	0.19	0.11	0.02
Lubricant additive	Blending of lubricant	0.02	1.87×10^{-3}	2.45×10^{-3}	1.61×10^{-3}
Hydraulic fluids	Blending of fluid	0.02	2.13×10^{-3}	1.63×10^{-3}	1.44×10^{-3}
Power generation fluid	Blending of fluid	0.02	5.64×10^{-3}	4.54×10^{-3}	2.03×10^{-3}

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

Scenario		Concentration							
		Fish (mg/kg)	Root crops (mg/kg)	Leaf crops (mg/kg)	Drinking water (mg/l)	Meat (mg/kg)	Milk (mg/kg)	Air (mg/m^3)	Total daily human intake (mg/kg bw/day)
Production of tertbutylphenyl diphenyl phosphate		0.06	3.3×10^{-5}	6.6×10^{-5}	1.8×10^{-5}	1.8×10^{-5}	5.8×10^{-6}	1.0×10^{-8}	9.5×10^{-5}
PVC – 1	Compounding	0.3	0.15	0.01	1.4×10^{-4}	3.2×10^{-3}	1.0×10^{-3}	2.9×10^{-6}	1.6×10^{-3}
	Conversion	0.48	0.25	0.07	2.4×10^{-4}	0.02	5.1×10^{-3}	1.4×10^{-5}	3.5×10^{-3}
	Combined compounding and conversion	0.77	0.4	0.09	3.8×10^{-4}	0.02	6.1×10^{-3}	1.7×10^{-5}	5.1×10^{-3}
PVC – 2	Compounding	0.14	0.15	6.6×10^{-3}	1.4×10^{-4}	1.5×10^{-3}	4.7×10^{-4}	1.3×10^{-6}	1.2×10^{-3}
	Conversion	0.23	0.25	0.03	2.4×10^{-4}	7.3×10^{-3}	2.3×10^{-3}	6.5×10^{-6}	2.4×10^{-3}
	Combined compounding and conversion	0.36	0.4	0.04	3.8×10^{-4}	8.8×10^{-3}	2.8×10^{-3}	7.8×10^{-6}	3.5×10^{-3}
PVC – 3	Compounding	0.02	0.15	1.7×10^{-4}	1.4×10^{-4}	5.7×10^{-5}	1.8×10^{-5}	9.5×10^{-9}	8.5×10^{-4}
	Conversion	0.59	0.25	0.09	2.4×10^{-4}	0.02	6.1×10^{-3}	1.7×10^{-5}	4.0×10^{-3}
	Combined compounding and conversion	0.77	0.4	0.09	3.8×10^{-4}	0.02	6.1×10^{-3}	1.7×10^{-5}	5.1×10^{-3}
Polyurethane	Compounding	0.58	0.3	0.03	2.9×10^{-4}	6.5×10^{-3}	2.0×10^{-3}	5.7×10^{-6}	3.1×10^{-3}
	Conversion	0.2	0.1	0.03	9.5×10^{-5}	6.4×10^{-3}	2.0×10^{-3}	5.7×10^{-6}	1.4×10^{-3}
	Combined compounding and conversion	0.77	0.40	0.06	3.8×10^{-4}	0.01	4.0×10^{-3}	1.1×10^{-5}	4.5×10^{-3}
Textiles and coatings	Compounding	0.02	0.08	7.1×10^{-5}	7.6×10^{-5}	2.6×10^{-5}	8.3×10^{-6}	1.4×10^{-12}	4.7×10^{-4}
	Conversion	0.47	0.2	0.07	1.9×10^{-4}	0.02	4.9×10^{-3}	1.4×10^{-5}	3.2×10^{-3}
	Combined compounding and conversion	0.54	0.28	0.06	2.7×10^{-4}	0.01	4.1×10^{-3}	1.1×10^{-5}	3.5×10^{-3}
Lubricant additive	Blending of lubricant	0.02	2.7×10^{-3}	1.8×10^{-5}	6.5×10^{-6}	5.2×10^{-6}	1.6×10^{-6}	1.4×10^{-11}	4.8×10^{-5}
Hydraulic fluids	Blending of fluid	0.02	3.1×10^{-3}	1.8×10^{-5}	5.2×10^{-6}	5.0×10^{-6}	1.6×10^{-6}	3.1×10^{-12}	4.4×10^{-5}
Power generation fluid	Blending of fluid	0.03	8.2×10^{-3}	0.02	9.7×10^{-6}	4.6×10^{-3}	1.5×10^{-3}	4.1×10^{-6}	4.8×10^{-4}
Regional sources		0.02	5.8×10^{-5}	1.6×10^{-5}	4.9×10^{-6}	4.6×10^{-6}	1.4×10^{-6}	3.3×10^{-9}	2.6×10^{-5}

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

4.1 Aquatic compartment

The following sections review the available toxicity data for tertbutylphenyl diphenyl 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 to allow a decision to be made on the validity of the study.

For this report, toxicity data assigned a validity marking of one or two are considered of acceptable quality when deriving the predicted no effect concentration (PNEC).

A small number 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 were 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 tertbutylphenyl diphenyl phosphate is in the range 0.04-3.2 mg/l. Several studies have been carried out at concentrations greater than this water solubility and, although this in itself does not necessarily invalidate the test (for example, cosolvents or solubility aids could have been used to aid dispersion of the substance in the test media), this does introduce some uncertainty over the concentrations 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.

The final consideration with regards to the toxicity data is that data have generally been determined on commercial products. Some of these products may contain significant amounts of triphenyl phosphate, which is itself toxic to aquatic organisms (see the risk

evaluation report for triphenyl phosphate). In the tests reported, it is not possible to distinguish between the effects of triphenyl phosphate and tertbutylphenyl phosphate.

4.1.1 Toxicity to fish

Acute toxicity

Freshwater fish

The short-term toxicity of tertbutylphenyl diphenyl phosphate to freshwater fish is summarised in Table 4.1.

Cleveland *et al.* (1986) determined the acute toxicity of a commercial tertbutylphenyl diphenyl phosphate product to fathead minnow (*Pimephales promelas*), rainbow trout (*Oncorhynchus mykiss*), channel catfish (*Ictalurus punctatus*) and bluegill sunfish (*Lepomis macrochirus*). The substance tested consisted of 15 to 20 per cent triphenyl phosphate with the remainder consisting mainly of a mixture of isomers of tertbutylphenyl diphenyl phosphate, along with isomers of di-tertbutylphenyl diphenyl phosphate. The tests were all carried out using a static test system using acetone as co-solvent. The 96-hour LC_{50} was determined to be 2.3 mg/l for *P. promelas*, 2.0 mg/l for *O. mykiss*, 0.8 mg/l for *I. punctatus* and 3.1 mg/l for *L. macrochirus*. 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 to *O. mykiss* and *L. macrochirus*. None of these parameters were found to have a significant affect on the 96-hour LC_{50} determined for either species. The reported LC_{50} values are close to the upper limit of solubility of the test substance.

IUCLID (2001) reports the results of an unpublished acute flow-through toxicity test for tertbutylphenyl diphenyl phosphate using rainbow trout (*Oncorhynchus mykiss*). The 96-hour LC_{50} was determined to be 13.7 mg/l. The higher doses used in this study were reported to produce effects on the behaviour of exposed fish compared with the control fish. These effects included quiescence, irritation, erratic swimming and laboured respiration and these effects were found to increase in severity with increasing exposure concentration. The reported LC_{50} is well above the water solubility of the test substance.

Akzo Nobel (2003) indicates that, in addition to the value of 13.7 mg/l discussed above, 96-hour LC_{50}s in the range 2.4-5.4 mg/l have been determined for tertbutylphenyl diphenyl phosphate with *Oncorhynchus mykiss*.

A further 96-hour LC_{50} of 5.4 mg/l was determined for a tertbutylphenyl diphenyl phosphate (Fyrquel GT) with *Oncorhynchus mykiss* (Union Carbide 1978). The test report indicates that the test substance formed an oily film on the surface of the water for all concentrations tested and, as the result was based on nominal concentrations, the result is considered to be invalid as undissolved test material appeared to be present. This may be one of the results mentioned by Akzo Nobel (2003).[14]

[14] USEPA 2008 has only cited the *Oncorhynchus mykiss* 96-hour LC_{50} of 13.7 mg/l.

Table 4.1 Short-term toxicity of tertbutylphenyl diphenyl phosphate to freshwater fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. Tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
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		96-h LC_{50} = 0.8 mg/l	Cleve-land *et al.* 1986	2
Lepomis macrochirus	ASTM 1980			Acetone at ≤0.67 mg/l.	Logarithmic series plus control and solvent control.	N	Artificial water	22°C	38-46	7.2-7.6	Static		Mortality		96-h LC_{50} = 3.1 mg/l	Cleve-land *et al.* 1986	2
Oncorhynchus mykiss	ASTM 1980			Acetone at ≤0.67 mg/l.	Logarithmic series plus control and solvent control.	N	Artificial water	12°C	38-46	7.2-7.6	Static		Mortality		96-h LC_{50} = 2.0 mg/l	Cleve-land *et al.* 1986	2
	USEPA 1975	10			1.3, 2.5, 5.0, 10 and 20 mg/l plus control	N					Flow		Mortality		96-h LC_{50} = 13.7 mg/l	IUCLID 2001	4
	USEPA 1975	10, loading 8.16 g/l	110 mm	Acetone	3.2, 5.6, 10, 18 and 32 mg/l plus control and solvent control	N	Well water	10°C	360	7.5-8.1	Static	7.1-10.2 mg/l	Mortality	0% Mortality	96-h LC_{50} = 5.4 mg/l	Union Carbide 1978	3
													Mortality		96-h LC_{50} = 2.4-5.4 mg/l	Akzo Nobel 2003	4/3

Table 4.1 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. Tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Pimephales promelas	ASTM, 1980			Acetone at ≤0.67 mg/l.	Logarithmic series plus control and solvent control.	N	Artificial water	22°C	38-46	7.2-7.6	Static		Mortality		96-h LC_{50} = 2.3 mg/l	Cleve-land *et al.* 1986	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.

A fish 96-hour LC_{50} and a 14-day LC_{50} of 1.24 and 0.98 mg/l respectively were estimated for triphenyl phosphate from the log K_{ow} value of 5.12 using the USEPA ECOSAR (version 0.99h) software. Using the methods given in the TGD, a 96-hour LC_{50} of 0.48 mg/l was estimated using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.12. This value is in reasonable agreement with the values obtained with the more sensitive species tested.

Marine fish

The short-term toxicity of tertbutylphenyl diphenyl phosphate to marine fish is summarised in Table 4.2.

The toxicity of two different commercial tertbutylated triphenyl phosphate products was investigated with sheepshead minnow (*Cyprinodon variegatus*) using a semi-static method (48-hour renewal) (Springborn Laboratories 1996a and 1996b). Compositions of the two products were not given but both were reported to be a "mixture of butylated triphenyl phosphates". The 96-hour LC_{50} was determined to be above 1 mg/l - no mortalities were seen at 1 mg/l, the highest nominal concentration that could be tested (Springborn Laboratories 1996a) or above 1.3 mg/l - no mortalities were seen at 1.3 mg/l, the highest mean measured concentration that could be tested (Springborn Laboratories 1996b). Water in the exposure tanks and solvent control tanks (but not the control tanks) was observed to be cloudy throughout the test. This was thought to be a result of increased microbial activity resulting from the presence of a carbon source (acetone) in the tanks. As no differences in mortality and behaviour were seen between the solvent control and control populations, this cloudiness was not thought to affect the results of the study.

Actual concentrations of the test substance in the tanks were determined at various times during the test (at time zero, just before and after renewal and at 96 hours). The samples for analysis were collected by pipette from the approximate mid-point of the vessels. The mean measured concentrations in the Springborn Laboratories (1996b) test were all close to the nominal values, and the results were based on the mean measured values. The mean measured values from the Springborn Laboratories (1996a) test were found to be more variable (ranging from 24 to 100 per cent of the nominal) and implied that the solubility of the substance in the test media may have been exceeded (the mean measured concentrations were 0.13, 0.13, 0.25, 0.31 and 0.27 mg/l for the nominal treatments 0.13 mg/l, 0.22 mg/l, 0.36 mg/l, 0.60 mg/l and 1.0 mg/l; these measured data are consistent with a solubility of around 0.3 mg/l in the media). The results of these tests are best interpreted in terms of the products showing no acute toxicity up to their respective solubility limits.

Chronic toxicity

The long-term toxicity of tertbutylphenyl diphenyl phosphate to freshwater fish is summarised in Table 4.3.

A 90-day partial life-cycle toxicity study was carried out for a commercial tertbutylphenyl diphenyl phosphate product using fathead minnows (*Pimephales promelas*) (Cleveland *et al.* 1986). The substance tested consisted of 15 to 20 per cent triphenyl phosphate, with the remainder being mainly isomers of tertbutylphenyl diphenyl phosphate, along with isomers of di-tertbutylphenyl diphenyl phosphate. 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, 0.5 and 1.0 mg/l. Analyses of the water concentrations were carried out every two weeks during the experiment and these showed that the mean measured concentrations in the various exposure groups

Table 4.2 Short-term toxicity of tertbutylphenyl diphenyl phosphate to marine fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. Tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Sal.	pH	Static/ flow	D.O.					
Cyprinodon variegates	OECD 203	10, loading 0.23 g/l	0.34 g	Acetone at 0.1 ml/l	0.13, 0.22, 0.36, 0.60 and 1.0 mg/l (nominal) plus control and solvent control	N	Natural sea-water	22°C	31‰	7.4-7.9	Semi-static	4.0-7.6	Mortality	0% Mortality	96-h LC_{50} ≥ 1 mg/l	Springborn Labs 1996a	2
	OECD 203	10, loading 0.23 g/l	0.34 g	Acetone at 0.1 ml/l	0.19, 0.33, 0.38,0.83 and 1.3 mg/l (mean measured) plus control and solvent control	M	Natural sea-water	22°C	31‰	7.4-7.9	Semi-static	4.5-7.6	Mortality	0% Mortality	96-h LC_{50} ≥ 1.3 mg/l	Springborn Labs 1996b	1

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 4.3 Long-term toxicity of tertbutylphenyl diphenyl phosphate to freshwater fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. Tested	N or M	Test conditions						End-point	Control response	Effect conc.	Ref.	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 after 30 days.	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 were 33 to 50 per cent of nominal.	M	Artificial water	25°C	40	7.2-7.4	Flow		Growth	Mean length at 30 days = 27.2±2.3 mm.	30-d NOEC= 0.194 mg/l	Cleve-land *et al*. 1986.	2
														Mean length at 60 days = 31.9±2.4 mm.	60-d NOEC = 0.194 mg/l		
														Mean length at 90 days = 36.1±3.1 mm.	90-d NOEC = 0.194 mg/l		
													Mortality	Mortality was 18% at day 30 and 20% at day 60 and day 90	30-d NOEC = 0.093 mg/l 60-d NOEC =0.093 mg/l 90-d NOEC = 0.093 mg/l		

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.

(expressed as the sum of the tertbutylphenyl diphenyl phosphate and the triphenyl phosphate components of the product) were 0.022, 0.040, 0.093, 0.194 and 0.496 mg/l respectively, corresponding to around 33-50 per cent of the nominal values (only the main components of the commercial product were analysed and so actual concentrations may be slightly higher than indicated by the measured data).

Survival of the fish was found to be statistically significantly (p=0.01) reduced at concentrations of 0.194 mg/l and 0.496 mg/l at day 30, day 60 and day 90 compared with the control group. Therefore, the no observed effect concentration (NOEC) for this endpoint was determined to be 0.093 mg/l based on the measured concentration.

Growth of the fish was found to be statistically significantly (p=0.01) reduced at day 30, 60 and 90 in the highest exposure group (0.496 μg/l) when compared to the control group. No statistically significant (p=0.05) reductions in growth were seen at any other exposure concentrations (growth at some concentrations was significantly higher than in the control group). Therefore, the NOEC for growth was 0.194 mg/l based on the measured concentrations.

The same results expressed as maximal acceptable toxicant concentrations (MATCs) (this is the geometric mean of the no observed effect concentration (NOEC) and lowest observed effect concentration (LOEC)) are given in Mayer *et al.* (1986).

The USEPA ECOSAR program (v0.99h) predicts a long-term no effect concentration of 0.058 mg/l for fish, which is similar to the result for survival.

No long-term toxicity data for the substance with marine fish are available.

4.1.2 Toxicity to aquatic invertebrates

Acute toxicity

Freshwater invertebrates

The short-term toxicity of tertbutylphenyl diphenyl phosphate to freshwater aquatic invertebrates is summarised in Table 4.4.

Ziegenfuss *et al.* (1986) determined the acute toxicity of tertbutylphenyl diphenyl phosphate (purity not given) to 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 0.30 mg/l for *D. magna* and 0.15 mg/l for *C. tentans.*

Adams and Heidolph (1985) determined the acute toxicity of three commercial tertbutylphenyl diphenyl phosphate products to *Daphnia magna* using the ASTM E729 method. The substances tested were TB220-L (tertbutylphenyl diphenyl phosphate with less than 1 per cent triphenyl phosphate), TB220-H (tertbutylphenyl phosphate with 18 per cent triphenyl phosphate) and Santicizer 154 (a mixture of tertbutylphenyl diphenyl phosphate, di-tertbutylphenyl phenyl phosphate and triphenyl phosphate). The 48-hour EC_{50} values determined were 1.1 mg/l for TB220-L, 0.25 mg/l for TB220-H and 0.30 mg/l for Santiciser 154.

Sanders *et al.* (1985) determined the acute toxicity of two commercial tertbutylphenyl diphenyl phosphate products (Fyrquel GT and Santiciser 154: purities not given) to *Daphnia magna*, midge (*Chironomus plumosus*) and an amphipod (*Gammaris pseudolimnaeus*). The tests were carried out using static test systems. Toxicity results for Fyrquel GT were a 48-hour EC_{50} of 2.9 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 1.4 mg/l with *G. pseudolimnaeus*.

Table 4.4 Short-term toxicity of tertbutylphenyl 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 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		48-h EC_{50} = 1.8 mg/l	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		48-h EC_{50} = 2.8 mg/l	Sanders *et al.* 1985	2
Chironomus tentans	ASTM 1980		2nd instar (10-14 day)				Well water				Static		Immobil. mortality		48-h LC_{50} = 0.15 mg/l	Ziegen-fuss *et al.* 1986	2
Daphnia magna	ASTM 1980		<24 h			N	Well water				Static		Immobil. mortality		48-h LC_{50} = 0.30 mg/l	Ziegen-fuss *et al.* 1986	2
	ASTM E729		<24h	Dimethyl formamide or acetone at up to 1.0 ml/l		N		20-23°C	120-250	7.0-8.5	Static	6.0-9.3 mg/l	Immobil. mortality		48-h EC_{50} = 1.1 mg/l	Adams and Heidolph 1985	2
	ASTM E729		<24h	Dimethyl formamide or acetone at up to 1.0 ml/l		N		20-23°C	120-250	7.0-8.5	Static	6.0-9.3 mg/l	Immobil. mortality		48-h EC_{50} = 0.25 mg/l	Adams and Heidolph 1985	2
	ASTM E729		<24h	Dimethyl formamide or acetone at up to 1.0 ml/l		N		20-23°C	120-250	7.0-8.5	Static	6.0-9.3 mg/l	Immobil. mortality		48-h EC_{50} = 0.30 mg/l	Adams and Heidolph 1985	2

Table 4.4 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. Tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Daphnia magna (continued)	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		48-h EC_{50} = 2.9 mg/l	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		48-h EC_{50} = 5.0 mg/l	Sanders *et al.* 1985	2
Gammarus pseudolimnaeus	USEPA 1975		Early instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-8.4	Static		Mortality		96-h LC_{50} = 1.4 mg/l	Sanders *et al.* 1985	2
	USEPA 1975		Early instar	Acetone at up to 0.1 ml/l	Control and solvent control	N	Well water	18°C	270	7.2-8.4	Static		Mortality		96-h LC_{50} = 1.9 mg/l	Sanders *et al.* 1985	2

Notes: N = Nominal concentration.
M = Measured concentration.
D.O. = Dissolved oxygen (given as mg O_2/l or per cent saturation).
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.

The equivalent toxicity values obtained using Santiciser 154 were a 48-hour EC_{50} of 5.0 mg/l with *D. magna*, a 48-hour EC_{50} of 2.8 mg/l with *C. plumosus* and a 96-hour LC_{50} of 1.9 mg/l with *G. pseudolimnaeus*. The values obtained are close to the water solubility of the test substance.

Using the methods given in the TGD, a 48-hour EC_{50} of 0.84 mg/l can be estimated for *Daphnia magna* using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.12. This is in good agreement with available experimental data. USEPA ECOSAR program (v0.99h) predicts a value of 0.44 mg/l for the same endpoint.

Marine invertebrates

The short-term toxicity of tertbutylphenyl diphenyl phosphate to marine invertebrates is summarised in Table 4.5.

Acute toxicity tests using two different tertbutylated triphenyl phosphates with mysid shrimp (*Mysidopsis bahia*[15]) have been reported (Springborn Laboratories 1996c and 1996d). The compositions of the two products were not given but both were reported to be a "mixture of butylated triphenyl phosphates". The tests were both static tests using nominal concentrations of 0.13, 0.22, 0.36, 0.60 and 1.0 mg/l. Analytical monitoring of the concentrations in the test solution at time zero and again at 96 hours indicated that the respective mean measured concentrations were variable at 0.093, 0.090, 19, 0.5 and 0.23 mg/l in the first test (the value of 19 mg/l was dominated by the concentration measured at time zero (39 mg/l) – the concentration measured after 96 hours in this exposure was 0.076 mg/l (Springborn Laboratories 1996c)) and 0.048, 0.15, 0.11, 0.23 and 0.24 mg/l in the second test (Springborn Laboratories 1996d).

In the first test, despite the variable measured levels, a good nominal dose-response was seen (the percentage immobilisation was 100 per cent at 1 mg/l, 95 per cent at 0.60 mg/l, 40 per cent at 0.36 mg/l and zero at the lower nominal test concentrations). The report also indicates no visible signs of undissolved test substance at any concentration during the test. Thus, results were expressed based on the nominal concentrations and the 96-hour LC_{50} was determined to be 0.39 mg/l in this study (Springborn Laboratories 1996c).

The mean measured concentrations found in the second test were 0.048, 0.15, 0.11, 0.23 and 0.24 mg/l for the five nominal treatment levels respectively. The pattern of measured levels seen is consistent with a solubility of around 0.24 mg/l in the test medium. The test report indicates no visible signs of undissolved test substance at any concentration during the test. No treatment-related mortality was seen (mortality was only five per cent in the highest treatment group) and so the 96-hour EC_{50} was determined to be above 1 mg/l based on nominal concentrations. The results from this test are best interpreted as the products showing essentially no acute toxicity at the limit of their solubility.

Chronic toxicity

The long-term toxicity of tertbutylphenyl diphenyl phosphate to freshwater invertebrates is summarised in Table 4.6.

[15] Now called *Americamysis bahia*.

Table 4.5 Short-term toxicity of tertbutylphenyl 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 resp.	Effect conc.	Reference	Val.
							Media	Temp.	Sal.	pH	Static/ flow	D.O.					
Mysidopsis bahia	OECD 202	10 per replicate, two replicates per treatment	<24 hours	Acetone at 0.1 ml/l	0.13, 0.22, 0.36, 0.60 and 1.0 mg/l (nominal) plus control and solvent control	N	Natural sea-water	24-25°C	24‰	7.5-7.9	Static	4.6-7.7 mg/l	Immobil. mortality	0% Mortality	96-h EC_{50} = 0.39 mg/l	Springborn Labs 1996c	2
	OECD 202	10 per replicate, two replicates per treatment	<24 hours	Acetone at 0.1 ml/l	0.13, 0.22, 0.36, 0.60 and 1.0 mg/l (nominal) plus control and solvent control	N	Natural sea-water	24-25°C	24‰	7.5-8.0	Static	4.7-7.7 mg/l	Immobil. mortality	0% Mortality	96-h EC_{50} ≥ 1 mg/l	Springborn Labs 1996d	2

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

Adams and Heidolph (1985) determined the toxicity of three commercial tertbutylphenyl diphenyl phosphate products to *Daphnia magna* using a flow-through 21-day reproduction study. The substances tested were TB220-L (tertbutylphenyl diphenyl phosphate with less than 1 per cent triphenyl phosphate), TB220-H (tertbutylphenyl phosphate with 18 per cent triphenyl phosphate) and Santicizer 154 (a mixture of tertbutylphenyl diphenyl phosphate, di-tertbutylphenyl phenyl phosphate and triphenyl phosphate) and the concentrations in the test were verified by measurement. The 21-day NOEC values were determined to be 0.03 mg/l for TB220-L, 0.03 mg/l for TB220-H and 0.04 mg/l for Santicizer 154 based on survival and 0.015 mg/l for TB220-L, above 0.026 for TB220-H and 0.04 mg/l for Santicizer 154 based on reproduction.

IUCLID (2001) reports the results of an unpublished 21-day toxicity test using tertbutylphenyl diphenyl phosphate with *Daphnia magna*. The NOECs determined in this study were 0.04 mg/l based on survival and reproduction, which are similar to those obtained in the study above.

Sanders *et al.* (1985) investigated the effects of two commercial tertbutylphenyl diphenyl phosphate products (Fyrquel GT and Santicizer 154, 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 at 21 days were below 0.032 mg/l for Fyrquel GT and 0.01 mg/l for Santicizer 154. The 21-day NOECs based on reproduction were 0.032 mg/l for Fyrquel GT and 0.010 mg/l for Santicizer 154 (statistically significant (p=0.05) effects on reproduction were seen with Fyrquel GT at 0.032 mg/l on day 14 of the study but no statistically significant effects were seen on reproduction at this concentration by day 21 of the study).

Sanders *et al.* (1985) also investigated the effects of the commercial product Fyrquel GT on the survival and growth of amphipods (*Gammarus pseudolimnaeus*) over 90 days using a flow-through system. The NOEC for survival was determined to be 0.011 mg/l and no statistically significant effect (p=0.05) on growth (mean length) was determined at any concentration tested (NOEC above 0.056 mg/l).

A final study carried out by Sanders *et al.* (1985) investigated the effects of the same commercial product (Fyrquel GT) on the emergence of midges (*Chironomus plumosus*) over 30 days using a flow-though system. In this test, 100 first-instar larvae were placed in a test chamber (10 × 20 × 10 cm) containing 1 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 NOEC, based on the percentage emergence after 30 days, was determined to be 36 μg/l.

There are no long-term toxicity data available for tertbutylphenyl diphenyl phosphate with marine invertebrates.

4.1.3 Toxicity to algae

The toxicity of tertbutylphenyl diphenyl phosphate to freshwater algae is summarised in Table 4.7.

Table 4.6 Long-term toxicity of tertbutylphenyl 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 resp.	Effect conc.	Reference	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 and 718 µg/l plus control	N	Well water	22°C	270	7.2-7.4	Flow		Emerge.	92% emerged at day 30	30-d NOEC = 0.036 mg/l	Sanders *et al*. 1985	2
Daphnia magna	USEPA 1976	20 per replicate, four replicates per treatment	<24 h	Acetone or dimethyl form-amide at up to 0.1 ml/l.	5 concs. Plus control and solvent control.	M		21-23°C	160-180 mg/l	8.0-8.5	Flow	7.5-8.0	Survival and repro.		7d-EC_{50} = 0.038 mg/l 14d-EC_{50} = 0.034 mg/l 21d-EC_{50} = 0.028	Adams and Heidolph 1985	2
													Survival		21-d NOEC = 0.03 mg/l		
													Repro.		21-d NOEC = 0.015 mg/l		
	USEPA, 1976	20 per replicate, four replicates per treatment	<24 h	Acetone or dimethyl form-amide at up to 0.1 ml/l.	5 concs. Plus control and solvent control.	M		21-23°C	160-180 mg/l	8.0-8.5	Flow	7.5-8.0	Survival and repro.		7d-EC_{50} = 0.042 mg/l 14d-EC_{50} = 0.038 mg/l 21d-EC_{50} = 0.023	Adams and Heidolph 1985	2
													Survival		21-d NOEC = 0.03 mg/l		
													Repro.		21-d NOEC > 0.026 mg/l		

Table 4.6 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. Tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Daphnia magna (continued)	USEPA 1976	20 per replicate, four replicates per treatment	<24 h	Acetone or dimethyl form-amide at up to 0.1 ml/l.	5 concs. plus control and solvent control.	M		21-23°C	160-180 mg/l	8.0-8.5	Flow	7.5-8.0 mg/l	Survival and repro.		7d-EC_{50} = 0.19 mg/l 14d-EC_{50} = 0.22 mg/l 21d-EC_{50} = 0.27 mg/l	Adams and Heidolph 1985	2
													Survival		21-d NOEC = 0.04 mg/l		
													Repro.		21-d NOEC = 0.04 mg/l		
					<2, 5, 8, 16, 40 and 100 µg/l plus control	M					Flow		Survival		NOEC = 0.040 mg/l	IUCLID 2001	4
													Repro.		NOEC = 0.040 mg/l		
		10 per replicate, two replicates per treatment	<24 h		32, 96, 256 and 352 µg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	80% survival	21-d NOEC <0.032 mg/l	Sanders *et al*. 1985	2
													Repro.	Mean offspring/ adult = 232	21-d NOEC = 0.032 mg/l		
		10 per replicate, two replicates per treatment	<24 h		4, 10, 30, 50, 100 and 190 µg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	95% survival	21-d NOEC = 0.010 mg/l	Sanders *et al*. 1985	2
													Repro.	Mean offspring/ adult = 330	21-d NOEC = 0.010 mg/l		

Table 4.6 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Co-solvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Gammarus pseudolim-naeus		10 per replicate, four replicates per treatment	5-10 day old		4.5, 6.7, 11, 26 and 56 µg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival Growth	80% Survival Mean length 9.0 mm	90-d NOEC = 0.011 mg/l 90-d NOEC >0.056 mg/l	Sanders *et al*. 1985	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.

Table 4.7 Toxicity of tertbutylphenyl diphenyl phosphate to freshwater algae

Species	Test guide-line	Initial inoculum conc.	Co-solvent	Concentrations tested	N or M	Test conditions				Endpoint	Control response	Effect concentration	Reference	Val.
						Media	Temp.	Hard.	pH					
Selenastrum capricornutum										Biomass		96-h EC_{50} = 2.6 mg/l	IUCLID 2001	4
										Chlorophyll A		96-h EC_{50} = 3.0 mg/l		
			Acetone at up to 0.1 ml/l	0.1, 1.0, 10 and 100 mg/l plus control and solvent control. Each run in triplicate	N	Well water	24°C	270	7.2-7.4	Dry weight		14-d NOEC = 1.0 mg/l 14d-LOEC = 10 mg/l	Sanders *et al.* 1985	3

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

IUCLID (2001) reports the results of an unpublished acute toxicity test using tertbutylphenyl diphenyl phosphate with *Selenastrum capricornutum*[16]. The 96-hour EC_{50} was determined to be 3.0 mg/l based on chlorophyll A measurements and 2.6 mg/l based on total biomass (cell numbers). These values are very close to the water solubility of the test substance.

Sanders *et al.* (1985) determined the toxicity of a commercial tertbutylphenyl diphenyl phosphate product (Fyrquel GT, composition not given) to *Selenastrum capricornutum* over 14 days. The growth of the algae 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 a concentration of 10 mg/l and above. Thus, the NOEC from this study is 1 mg/l. However, the length of this test (14 days rather than the normal 72 hours for an algal growth study) and the fact that widely spaced test concentrations were used means that the results from this test are uncertain.

The USEPA ECOSAR program (v0.99h) predicts a 96-hour EC_{50} value of 0.11 mg/l and a long-term no effect concentration of 0.091 mg/l for green algae.

There are no toxicity data available for tertbutylphenyl diphenyl phosphate with marine algae.

4.1.4 Toxicity to microorganisms

There appear to be no toxicity data available for tertbutylphenyl diphenyl phosphate with microorganisms.

4.1.5 Toxicity to sediment organisms

There are no data available on the toxicity of tertbutylphenyl diphenyl phosphate to 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 0.8 mg/l for fish (*Ictalurus punctatus*), a 48-hour LC_{50} of 0.15 mg/l for invertebrates (*Chironomus tentans*) and a 96-hour LC_{50} of 2.6 mg/l for algae (*Selenastrum capricornutum*).

Long-term data are also available for fish and invertebrates. The lowest NOECs obtained from the more reliable studies were a 90-day NOEC of 0.093 mg/l for fish (*Pimephales promelas*) in a fry growth study and a 21-day NOEC of 0.010 mg/l in a *Daphnia magna* reproduction test. No reliable NOEC is available for algae, and the available long-term data for fish covers 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 NOEC for tertbutyl diphenyl phosphate would be around 0.016 mg/l, which indicates the substance would be expected to be slightly less toxic to fish than

[16] *Selenastrum capricornutum* is now called *Pseudokirchneriella subcapitata*.

was found for *Daphnia*. In addition, the analysis given in Annex B indicates that the long-term NOEC of algae would also be expected to be higher than found for both fish and *Daphnia*. The ECOSAR predicted no-effect concentration for algae is 0.091 mg/l.

On this basis, we derive a $PNEC_{water}$ of 1 μg/l by applying an assessment factor of 10 to the available long-term NOEC for *Daphnia magna.*

There are limited data available on marine species, and these do not show any clear difference in sensitivity from the freshwater results. A PNEC of 0.1 μg/l can be calculated using the long-term freshwater data and an assessment factor of 100.

Microorganisms

It is not currently possible to estimate a PNEC for tertbutylphenyl phosphate for waste water treatment processes.

Sediment

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

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

where $K_{susp\text{-}water}$ = suspended sediment-water partition coefficient = 120 m^3/m^3 (see Section 3.1.2).
RHO_{susp} = bulk density of suspended sediment = 1,150 kg/m^3.

Using the $PNEC_{water}$ of 1 μg/l, the $PNEC_{sed}$ can be estimated as 0.104 mg/kg wet weight. This value is used in the provisional risk characterisation.

As the log K_{ow} of this substance is above five, the TGD recommends that 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 PNEC for marine sediments is derived in the same way from the marine water PNEC, and is 0.01 mg/kg wet weight. An additional factor of ten is applied to the PEC/PNEC ratios.

4.2 Terrestrial compartment

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

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

where $K_{soil\text{-}water}$ = soil-water partition coefficient = 143 m^3/m^3 (see Section 3.1.2).
RHO_{soil} = bulk density of wet soil = 1,700 kg/m^3.

Using the $PNEC_{water}$ of 1 μg/l, $PNEC_{soil}$ can be estimated as 0.084 mg/kg wet weight.

As the log K_{ow} of this substance is above five, the TGD recommends that 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 tertbutylphenyl diphenyl phosphate to plants and other organisms exposed via air. The low vapour pressure of the substance means that volatilisation to the atmosphere is likely to be limited and the resulting concentrations are likely to be low. The possibility of tertbutylphenyl diphenyl phosphate contributing to atmospheric effects such as global warming and acid rain is thus likely to be small. In addition, as the substance does not contain halogen atoms, it will not contribute to ozone depletion.

4.4 Mammalian toxicity

Tertbutylphenyl diphenyl phosphate (CAS No 56803-37-3) was assessed under the US Environmental Protection Agency's (EPA) High Production Volume (HPV) Challenge Programme in 2004. Therefore, many of the data used in this assessment were taken from the Robust Summary Dossier prepared under this programme. An IUCLID file from 2001 is also available although the majority of the data in this dossier is also contained within the USEPA dossier. Both dossiers briefly report the details of studies and are somewhat lacking in detail, making it difficult to fully assess the quality of the studies and the importance of some of the results. However, the 2001 IUCLID includes Klimisch codes for each study which give an indication of their reliability.

The majority of studies carried out in the late 1970s and early 1980s were conducted on Phosflex 51B, while more recent studies have been conducted on other commercial preparations, such as Durad 220B and Phosflex 61B. It is unclear how these commercial products differ in composition, although the IUCLID (2001) and USEPA (2004) dossiers describe the compositions of these substances as 75-80 per cent w/w tertbutylphenyl diphenyl phosphate (CAS 56803-37-3) with 20-25 per cent w/w triphenyl phosphate (CAS 115-86-6).

4.4.1 Toxicokinetics, metabolism and distribution

There are no data on the absorption, distribution and metabolism of tertbutylphenyl diphenyl phosphate in mammals, including humans.

4.4.2 Acute toxicity

Only data on experimental animals are available.

Oral

One acute oral study is available. The study was conducted in 1979 and does not fully conform to Good Laboratory Practice (GLP) or current OECD guidelines but was carried out according to the USEPA OTS 798.1175 guideline method for acute oral toxicity. In this limit test conducted by Stauffer Chemical Company (1979a, cited in USEPA 2004, IUCLID 2001), male and female Sprague-Dawley rats (five per sex) were

fasted for 24 hours then given a single dose by oral gavage of 5,000 mg/kg bodyweight Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate CAS no. 115-86-6) in corn oil. No details were given on the inclusion of a control group. Animals were observed daily for 14 days for clinical signs of toxicity and mortality, after which all animals were necropsied and organs examined for gross lesions. Signs of toxicity included depression (no further details given), diarrhoea and stains on the fur and around the nose; these had resolved by day six. No deaths or gross abnormalities at necropsy were reported. The LD_{50} was therefore considered to be greater than 5,000 mg/kg bodyweight.

Inhalation

A single study is available on acute inhalation. This was carried out by Stauffer Chemical Company (1979b, cited in USEPA 2004, IUCLID 2001) in 1979 according to USEPA OPPTS 870.1300 guidelines for acute inhalation toxicity. The study was not conducted to GLP. Male and female Sprague-Dawley rats (ten per sex) were exposed for four hours to Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate CAS no. 115-86-6) aerosol at 3.1 mg/l (the highest attainable concentration). No details were given on the inclusion of a control group. Aerosol samples collected from the breathing zone of the treated rats during exposure were measured to determine achieved concentration using gas-liquid chromatography with a flame ionization detector. The particle size, determined using a cascade impactor, ranged from 2.5-2.8 µm. Animal body weights were recorded on days 3, 7 and 14, and all animals were necropsied at the end of the observation period. No mortality or effect on bodyweight was reported. Ruffled fur was the only clinical sign of toxicity observed and at necropsy reddened lungs in one female and whitish lung in another female were reported; presumably these animals were from the treated group, although this was not stated. Based on the lack of mortality, the LC_{50} was greater than 3.1 mg/l, although it should be noted that this concentration is low.

Dermal

One study on acute dermal toxicity is available, which was conducted in 1979 according to the EPA OTS 798.1100 guideline method. The study was not conducted to GLP. In this limit test study by Stauffer Chemical Company (1979, cited in USEPA 2004, IUCLID 2001), 2,000 mg/kg undiluted Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) was applied to the closely clipped and abraded skin of one side of New Zealand White male and female rabbits (five per sex); the other side was left intact. Further details on the inclusion of controls or exposure conditions (occlusive or semi-occlusive) were not given. Following treatment, animals were observed daily for 14 days for signs of toxicity. Necropsies on all animals were carried out on day 15 and internal organs were examined for gross lesions. One of the animals died; the day on which this occurred was not reported. The remaining nine animals demonstrated mild depression (no other details given) and slight diarrhoea but showed full recovery before the end of the observation period. No treatment-related lesions were reported at necropsy. The acute dermal LD_{50} was greater then 2,000 mg/kg bodyweight.

Neurotoxicity

Two studies investigated the neurotoxicological effects of acute exposure to tertbutylphenyl diphenyl phosphate in hens. In one of the studies conducted by Stauffer

Chemical Company (1980, cited in USEPA 2004, IUCLID 2001) to the EPA OTS Guideline for Acute Neurotoxicity Testing – 1978 (USEPA 2004), a group of four White Leghorn hens were given a single dose by oral gavage of 11.7 g/kg bodyweight Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20 to 25 per cent w/w triphenyl phosphate CAS no. 115-86-6). Control hens (four per group) were given a single dose by oral gavage of vehicle (corn oil 10 ml/kg bodyweight) or tri-*ortho*-cresyl phosphate (TOCP, 45 mg/kg bodyweight). Animals were sacrificed 24 hours after dosing and analysed for plasma cholinesterase (ChE) activity and brain neurotoxic esterase activity (NTE). Tertbutylphenyl diphenyl phosphate-treated hens had lower plasma ChE activity (56 per cent) compared to vehicle controls; 47 per cent inhibition was observed in the positive control hens. No effect on NTE activity was observed in tertbutylphenyl diphenyl phosphate-treated animals while positive control animals showed 64 per cent inhibition of NTE activity.

The second study, which investigated acute delayed neurotoxicity, was also conducted by Stauffer Chemical Company (1980, cited in USEPA 2004, IUCLID 2001) to EPA OTS Guideline for Acute Neurotoxicity Testing – 1978 (USEPA 2004). A group of 15 adult White Leghorn hens received 11.7 g/kg bodyweight Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate CAS no. 115-86-6) by oral gavage on the first day of the study and another dose of the same amount 21 days later. Two other groups of 12 hens acted as positive and negative control groups, and were given doses of either 500 mg/kg bodyweight TOCP on day one and day 21, or vehicle (10 ml/kg bodyweight corn oil), respectively. Animals were observed daily for clinical signs of neurotoxicity and at weekly intervals for locomotor impairment. All animals were killed using sodium phenobarbital infused with neutral buffered formalin three weeks after administration of the second dose. The brain, spinal cord and sciatic nerves were examined histopathologically. No mortality was observed in the tertbutylphenyl diphenyl phosphate-treated group but animals showed mild body weight loss (no further details). Surviving positive control animals (nine of 12) showed severe body weight loss and the body weights of untreated control animals were unaffected. Clinical signs, gait and changes in central and peripheral nerves were similar in tertbutylphenyl diphenyl phosphate-treated animals and vehicle control animals. Positive control animals showed evidence of motor impairment and degenerative nerve lesions; no such effects were observed in animals treated with 11.7 g/kg bodyweight tertbutylphenyl diphenyl phosphate.

A study which evaluated the acute delayed neurotoxic potential of another commercial product Durad 220B (contains tertbutylphenyl diphenyl phosphate and triphenyl phosphate (CAS no. 115-86-6); exact quantities not known; Great Lakes Chemical Corporation 2001), is also available (Kotkoskie *et al*. 1992, cited in USEPA 2004, IUCLID 2001). Groups of nine hens received a single dose of either Durad 220B (2 g/kg bodyweight), tap water (1.7 g/kg bodyweight) or TOCP (500 mg/kg bodyweight). Three hens per group were sacrificed 48 hours after dosing and measured for brain and spinal NTE activity and brain ChE activity. The remaining hens were sacrificed 21 days after treatment, at which time the brain, spinal cord and peripheral nerves were removed and examined histopathologically. No effects on any of the parameters measured were observed in Durad 220B-treated hens. This contrasted with TOCP-treated animals which showed clinical signs of neurotoxicity and degenerative axonal changes. Base on these findings, Durad 220B is not considered a neurotoxicant when administered at a single dose of 2 g/mg bodyweight.

Summary of acute toxicity

No data are available on studies conducted in humans.

Individual studies were identified that addressed acute toxicity by each of the oral, inhalation and dermal exposure routes. All three studies were carried out in 1979, according to EPA guidelines, but were not conducted to GLP or current OECD guidelines. The limited data indicate an LD_{50} of above 5,000 mg/kg bodyweight for oral administration in rats, which is above the limit dose of 2,000 mg/kg bodyweight applied in more recent studies conducted to OECD guidelines.

The single study available for acute inhalation of tertbutylphenyl diphenyl phosphate was carried out at a single low exposure concentration. The LC_{50} for inhalation was above 3.1 mg/l for four hours in rats.

The toxicity of tertbutylphenyl diphenyl phosphate following dermal exposure appears to be low, with an LD_{50} of above 2,000 mg/kg bodyweight in rabbits (IUCLID 2001).

The studies that examined the acute neurotoxic potential of tertbutylphenyl diphenyl phosphate found inhibition of plasma ChE activity 24 hours after exposure in animals given a single dose (11.7 g/kg bodyweight) of tertbutylphenyl diphenyl phosphate, but no effect on brain NTE activity. Furthermore, no clinical signs of neurotoxicity or degenerative nerve tissue were observed in hens given a further dose (11.7 g/kg bodyweight) 21 days after the initial dosing occasion. Another study on a related commercial compound Durad 220B (which contains tertbutylphenyl diphenyl phosphate and triphenyl phosphate) showed no effects on any of the parameters measured in treated hens. These findings suggest that acute exposure to tertbutylphenyl diphenyl phosphate is unlikely to elicit neurotoxicity.

4.4.3 Irritation

Only experimental animal data are available for irritation.

Skin

A single study conducted in 1979 is available on skin irritation.

The study was conducted by Stauffer Chemical Company (1979, cited in USEPA 2004, IUCLID 2001) according the EPA OTS 798.4470 guidelines but was not GLP-compliant. In this study on six young adult New Zealand rabbits, 0.5 ml undiluted Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) was applied to shaved skin, half of which had been abraded 24 hours prior to exposure. The site was then wrapped under an occlusive patch for 24 hours. After the exposure period, the patches were removed and the substance was removed (no further details given). The animals were observed for signs of skin irritation after 24, 48 and 72 hours with the extent of response scored using the Draize system. Mild to moderate erythema was observed 24 hours after treatment; the number of rabbits with erythema was not reported. At 48 hours after treatment, mild erythema was present in four of the individual animals, but at 72 hours no irritation was present. No observations of oedema were made. The primary irritation score was 0.5, indicating that tertbutylphenyl diphenyl phosphate is mildly irritating to the skin.

Eye

One study for eye irritation is available.

This study was conducted in 1979 according to EPA OTS 798.4500 guidelines (Stauffer Chemical Company 1979, cited in USEPA 2004, IUCLID 2001). Nine rabbits were given a dose of 0.1 ml undiluted Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) in the everted lower left eyelid. The upper and lower eyelids were held together for one second, then after 30 seconds the treated eyes of three of the rabbits were washed with water for approximately one minute. The treated eyes of the remaining six rabbits were not rinsed. The untreated right eye of each rabbit served as a within animal control. Eyes were examined for signs of irritation using the Draize scoring system after 24, 48, 72 and 96 hours and seven days. At 24 hours after exposure, mild redness of the conjunctiva was observed in one rabbit with a washed eye and one rabbit with an unwashed eye. Both eyes had cleared by the 48 hour observation time point. Another rabbit with an unwashed eye had mild redness of the conjunctiva at 48 hours, but not at 72 and 96 hours and seven days, all eyes were clear of signs of irritation. The average irritation scores at 24 and 48 hours were 0.44 and 0.22 respectively, thus tertbutylphenyl diphenyl phosphate was described as slightly irritating to the eyes.

Summary of irritation

No information is available from human studies. The two available studies on the irritant properties of tertbutylphenyl diphenyl phosphate suggest that the substance is mildly irritating to the skin and eyes. In both cases, irritation was reversed after several days.

4.4.4 Corrosivity

The available studies on skin and eye irritation suggest that tertbutylphenyl diphenyl phosphate does not have corrosive potential.

4.4.5 Sensitisation

No data are available on sensitisation.

4.4.6 Repeated-dose toxicity

Animal data

One sub-chronic study is available on general toxicity from repeated exposure, conducted by Stauffer Chemical Company in 1981 to GLP and to EPA OTS 798.2650 guidelines (Freudenthal *et al*. 2001). In the study, four groups of male and female Sprague-Dawley rats (20/sex/group) were fed 0, 100, 400 or 1,600 ppm Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) in their diet, for 90 days. In the low-, mid-, and high-dose groups mean daily consumption of Phosflex 51B was 6.6, 26.7 and 107.5 mg/kg/day, respectively, by males and 7.7, 30.0, and 124.8 mg/kg/day, respectively, by females. During the study, bodyweight, food consumption, haematology, clinical chemistry and cholinesterase (plasma and erythrocyte activity) were measured. Brain cholinesterase activity was measured at termination. At the end of the study period, all animals were subject to a gross necropsy with tissues taken for histopathological examination. Treatment did not result in any gross or microscopic

lesions or abnormalities, although effects on organ weights were observed in the highest treatment group. These changes included significant increases in absolute (15.3 ± 1.2 g) and relative (3.1 ± 0.2 per cent) mean weights of livers from high dose males compared with the control group (13.0 ± 1.6 g and 2.5 ± 0.2 per cent, respectively), mean relative liver weights of high dose females (3.0 ± 0.2 per cent; control: 2.6 ± 0.3 per cent), mean relative kidney weights of high dose males (0.66 ± 0.04 per cent; control: 0.62 ± 0.05 per cent) and mean absolute (0.078 ± 0.013 g; control: 0.068 ± 0.011 g) and relative weights (0.028 ± 0.004 per cent; control: 0.025 ± 0.003 per cent) of adrenal glands from high dose females; no corresponding histopathological changes were observed. At day 45, a significant increase in platelet count was observed in mid-dose females (data not presented), but levels had returned to within the control range by the end of the study. At study termination, mid-dose males had a significantly lower leukocyte count than controls (10.1 ± 2.2 10^3/mm^3; controls 13.0 ± 1.8 10^3/mm^3). No other haematological changes were reported. Some changes in clinical chemistry parameters were reported, with decreased serum phosphorous and total bilirubin in all treated males being noted at day 45. At study termination, total bilirubin had returned to normal while serum phosphorous was increased in high-dose males but within the control range in mid- and low-dose males.

The authors suggested that the increase in serum phosphorous levels at termination might be attributable to metabolic decomposition of Phosflex 51B. At termination, a significant increase in total serum protein and significant decreases in lactate dehydrogenase and glutamic oxaloacetic transaminase activities were observed in high-dose males. Mid- and high-dose females showed a significant increase in serum phosphorous and calcium and a significantly low lactate dehydrogenase actvity. No significant clinical chemistry changes were observed in the low-dose animals. An increase in urinary protein was reported in mid- and high-dose male and female animals at day 45 but levels had returned to control levels by study termination. The authors considered these changes not to be of biological significance since no clear dose-responses were observed. Changes in cholinesterase activity were also reported in treated animals. At day 45, significant decreases in plasma cholinesterase activity were observed in mid- and high-dose males (24 per cent and 37 per cent, respectively) and in plasma and erythrocyte cholinesterase activities (both by 41 per cent), in high-dose females. At study termination, plasma cholinesterase levels in mid- and high-dose males had returned to control levels but activity in high-dose females remained significantly depressed (33 per cent). Furthermore, erythrocyte cholinesterase activity was decreased in mid-dose males only and brain cholinesterase activity was significantly depressed in low-dose males only. Based on the inconsistent nature of the cholinesterase results, the authors concluded that the data were not biologically relevant and not related to treatment with Phosflex 51B. Based on the organ weight effects observed at the highest dose of tertbutylphenyl diphenyl phosphate, the NOEC for this study is 26.7 mg/kg bodyweight/day in male rats or 30.0 mg/kg bodyweight/day in female rats (equivalent to 400 ppm).

Neurotoxicity

A sub-chronic neurotoxicity study was conducted on adult White Leghorn hens to assess the neurotoxic potential of various jet engine lubricants containing phosphate ester additives (Daughtrey *et al*. 1996). One of the lubricants tested contained jet engine turbo oil (a mixture of hydrocarbon polyol esters and ‘minor amounts of additives’; no further details given) and three per cent tertbutylphenyl diphenyl phosphate (100 per cent mixture of butyl and triphenyl phosphates). The study was not carried out to GLP or international guidelines such as OECD Test Guidelines which require protection with atropine to allow higher doses of cholinesterase inhibition to be tolerated, but nonetheless appears to be well-conducted and reported. In the study, groups of hens (17 to 20 pergroup) were given either lubricating oil containing three per cent tertbutylphenyl diphenyl phosphate (1 g/kg bodyweight), TOCP in corn oil

(7.5 mg/kg bodyweight) or saline, by oral gavage, five days a week, for 13 weeks. Animals in the TOCP positive control group were given an additional single dose of 500 mg TOCP/kg 12 days before the end of the study to induce signs of organophosphate-induced delayed neurotoxicity. The dose level of lubricant oil chosen was based on the limit dose specified in the EPA Test Guidelines for Delayed Neurotoxicity of Organophosphorous Substances (USEPA 1991, cited in Daughtrey *et al*. 1996). Hens were assessed daily for obvious behavioural and physical changes and mobility. Hens were also assessed twice each week specifically for signs of ataxia and once a week hens were weighed and the treatment dosing adjusted accordingly. Four hens from each group were assessed for acetyl cholinesterase (AChE) and NTE activity in the brain and spinal cord after six and 13 weeks. All remaining hens were sacrificed after 13 weeks, at which time the brain, spinal cord and sciatic and tibial nerves were removed for histological examination. After six weeks, AChE and NTE activities were no different in lubricant/tertbutylphenyl diphenyl phosphate-treated hens compared with saline controls. After 13 weeks, brain and spinal cord NTE activity was significantly reduced (by 32 per cent and 27 per cent, respectively) in lubricant/BTP-treated hens compared with saline controls; no effects were observed on AChE activity. Histological examination did not reveal any lesions characteristic of organophosphate-induced delayed neurotoxicity, as were seen in the positive control animals. The authors concluded that the lubricating oil containing three per cent tertbutylphenyl diphenyl phosphate had low neurotoxic potential. However, the depression in NTE activity after 13 weeks indicates that there is potential for one of the oil components to produce delayed neurotoxicity at non-cholinergic doses in humans.

Human data

No human data are available.

Summary and discussion of repeated- dose toxicity

One sub-chronic study assessed the general toxicity from repeated exposure to tertbutylphenyl diphenyl phosphate. In this study, male and female animals fed the highest dose of 1,600 ppm showed significant increases in absolute and/or relative weights of livers, kidney and adrenal glands, although no histopathological changes were observed in any of these organs. Changes in some haematological (platelet and leukocyte counts), clinical chemical parameters (serum phosphorous, total bilirubin, total serum protein, lactate dehydrogenase, calcium, glutamic oxaloacetic transaminase and urinary protein) and cholinesterase activity were noted in some treatment groups. However, the authors did not consider these to be biologically relevant.

In another, well-conducted study, the neurotoxic effects of repeated exposure to lubricant oil containing three per cent tertbutylphenyl diphenyl phosphate at a single dose level (1 g/kg bodyweight) were assessed. After 13 weeks, brain and spinal cord NTE activity was significantly reduced compared with saline controls but no histopathological changes were observed in the nervous system suggestive of organophosphate-induced delayed neurotoxicity. This study is considered of limited usefulness as the test compound is not adequately described and it is unclear if the observed changes could be attributable to tertbutylphenyl diphenyl phosphate.

While the data are limited, the two available studies suggest that tertbutylphenyl diphenyl phosphate exhibits low general toxicity. The NOEL for repeated exposure to tertbutylphenyl diphenyl phosphate via the diet is 26.7 mg/kg bodyweight/day in male rats or 30.0 mg/kg bodyweight/day in female rats (equivalent to 400 ppm).

4.4.7 Mutagenicity

Studies in vitro

Genetic mutations

Two EPA OTS guideline studies investigated the mutagenicity of tertbutylphenyl diphenyl phosphate *in vitro*. However, the studies were not conducted to GLP and the summaries are lacking in detail which makes it difficult to assess the quality of the methodologies employed.

A bacterial reverse mutation assay (Ames test) was conducted in 1979 by Litton Bionetics, Inc. (cited in USEPA 2004, IUCLID 2001) according to EPA OTS 798.5265 guidelines. In the study, Salmonella typhimurium strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538 were exposed to 0.005, 0.01, 0.1, 5.0 or 10.0 µg/plate of Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6), with and without a metabolic activation system (further details not given). Positive controls were included in the study although no details of these were reported. A solvent (DMSO) control and a negative control were also included. No details regarding the number of replicates or repeat studies performed were reported. The positive controls were reported to increase the number of revertants per plate, confirming that the assay was sensitive to mutagenic chemicals (USEPA 2004, IUCLID 2001). Tertbutylphenyl diphenyl phosphate was cytotoxic to bacteria at 0.1 µg per plate or above, but was not mutagenic to any of the bacterial strains at any of the concentrations tested with or without metabolic activation.

In a mammalian cell gene mutation study conducted by Litton Bionetics, Inc. (1979b, cited in USEPA 2004, IUCLID 2001) to EPA OTS 798.5300 guidelines, mouse lymphoma L5178Y cells were treated with Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) to evaluate the ability of the compound to induce mutations of the thymidine kinase (TK) locus. Cultured cells were treated with various concentrations of Phosflex 51B (0.975, 15.6, 31.3, 62.5 or 125 nl/ml) in the presence or absence of a rat liver metabolic activation system (no further information given). The concentration range was chosen based on results of a preliminary cytotoxicity test, although the results of this test were not given. Tertbutylphenyl diphenyl phosphate was cytotoxic at 15.6 nl/ml. Positive, negative and solvent (DMSO) controls were included in the study, and positive controls induced a significant increase in mutations of the TK gene, confirming that the assay was sensitive (USEPA 2004 and IUCLID 2001). Tertbutylphenyl diphenyl phosphate was not mutagenic in this assay. No further details of the methodology or results were given in the study summary.

Chromosomal effects

The potential for tertbutylphenyl diphenyl phosphate (Phosflex 51B, 75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) to induce chromosomal aberrations and/or sister chromatid exchanges was investigated in a mouse lymphoma L5178Y cytogenetic assay, conducted by Litton Bionetics, Inc. (1979c, cited in USEPA 2004, IUCLID 2001) according to EPA OTS 798.5900 guidelines. The study summary contains insufficient details on the methodology to be able to determine the quality of the study and full results were not presented. The study was not carried out to GLP. The treatment range (0.625, 1.25, 2.50, 5.0, 10.0 or 20 nl/ml) was chosen based on a preliminary cytotoxicity assay, although the results of this test were not given. Negative, solvent (DMSO) and positive controls were included. Positive controls induced a significant increase in cytogenetic

mutations. Phosflex 51B induced cytotoxicity at 2.5 nl/ml, but did not demonstrate genotoxic activity at any of the concentrations tested with or without a rat liver metabolic activation system. No further details were given in the study summary.

Studies in vivo

No data are available on *in vivo* genotoxicity.

Summary of mutagenicity

Tertbutylphenyl diphenyl phosphate did not induce mutations in two *in vitro* mutagenicity studies, a bacterial reverse gene mutation assay and a mouse lymphoma gene mutation assay, and did not induce chromosomal aberrations or sister chromosome exchanges in mouse lymphoma L5178Y cells.

There are no data on the genotoxicity and mutagenicity of tertbutylphenyl diphenyl phosphate *in vivo*.

Given the absence of any positive results *in vitro*, tertbutylphenyl diphenyl phosphate is not considered likely to be mutagenic *in vivo*.

4.4.8 Carcinogenicity

There are no data on the carcinogenic potential of tertbutylphenyl diphenyl phosphate.

4.4.9 Toxicity to reproduction

Fertility and reproductive toxicity

One recent study investigated the effects of tertbutylphenyl diphenyl phosphate on fertility and reproduction. The study was conducted to OECD 421 and EPA OPPTS 870.3550 test guidelines and to GLP (Experimur 2003, cited in USEPA 2004). Full details of the study methodology were not described in the study summary and it is thus difficult to assess the robustness of the study. Sprague-Dawley rats (12/sex/group) were given 0, 50, 250 or 1,000 mg/kg bw/day Phosflex 61B (Lot No. 00161K0103 T#129B, purity not stated) by oral gavage for two weeks prior to mating, during the two-week mating period and throughout gestation and lactation (for a total of approximately eight weeks). Parental food consumption, bodyweight, bodyweight gain, reproductive performance, organ weights, histopathology of reproductive organs, offspring bodyweights and survival, litter size and the presence of gross abnormalities were recorded. No changes in clinical signs of toxicity, food consumption, bodyweight, bodyweight gain or organ weights were observed, and no treatment-related histological changes were observed in the reproductive organs. There were no significant differences in litter size or in the number of live pups on postnatal days zero and four. The results were not described in any further detail. Based on the lack of parental and foetal toxicity, the no observed adverse effects level (NOAEL) for this study was greater than 1,000 mg/kg bw/day.

An additional continuous breeding study not conducted to GLP, has also been reported for a different test substance, a butylated triphenyl phosphate-based hydraulic fluid (CAS no. 115-86-6) reported to contain predominantly p-t-butylphenyl phenyl phosphates (84 per cent wt), with lesser amounts of triphenyl phosphate (13 per cent wt, Latendresse *et al*. 1994). The test substance was administered to male and female

F-344 rats at doses of 600, 1,000, or 1,700 mg butylated triphenyl phosphate/kg/day. Decreased fertility and the number of litters, prolonged oestrus cycle, and a decreased mating index were observed in mid and high-dose females. A significant decrease in bodyweight gain in both dose groups was apparent although this was not dose-related (bodyweight gain was lowest in the mid-dose group from about day ten through day 131). It has been suggested that systemic toxicity may have been the primary cause of the decreased fertility (USEPA 2004, IUCLID 2001). This study is described as invalid, based on unknown impurities present in the test compound and the possibility of incorrect dosing of animals (USEPA 2004, IUCLID 2001).

Developmental toxicity

In the OECD/EPA guideline study described above, no effects were observed on litter size or the number of live pups on postnatal days zero and four (Experimur 2003, cited in USEPA 2004). No further details were available.

In another study conducted to EPA OTS 798.4900 guidelines and GLP, pregnant female rats (30 per group) were given 0, 100, 400 or 1,000 mg/kg bw/day Phosflex 51B (75-80 per cent w/w tertbutylphenyl diphenyl phosphate, 20-25 per cent w/w triphenyl phosphate, CAS no. 115-86-6) by oral gavage from gestation day six to 20 (Stauffer Chemical Company 1981, cited in USEPA 2004, IUCLID 2001). Animals were observed daily for treatment-related effects, and bodyweights and food consumption were measured on days 0, 6, 9, 12, 16 and 21. Pregnant animals were sacrificed on day 21 and gross internal examination was conducted at necropsy. Livers and reproductive tracts were weighed. The uterus was examined for the number and distribution of foetuses and resorptions. Ovaries were examined and the number of corpora lutea counted. All foetuses were weighed, sexed and examined for external malformations. Foetuses were fixed and half of each litter was stained for skeletal examination and the other half for visceral examination. Food consumption was significantly reduced in the high-dose group, and five animals in this group had significantly reduced bodyweights between gestation days six and 16. However, the bodyweights were not significantly different from controls at termination.

A significant dose-related increase in absolute and relative liver weights was observed in all treatment groups, which was considered by the authors to be an adaptive response (enzyme induction) rather than due to toxicity of the compound, although no data were presented to support this conclusion. No gross treatment-related lesions were observed at necropsy and the livers were not examined histopathologically. No differences in uterine weights were observed and no treatment-related effects on the number of corpora lutea, implants, resorption sites or live foetuses per dam. Mean foetal weights were significantly lower (eight per cent) in the high-dose group, which was considered by the authors to be a result of reduced food consumption and bodyweights among treated dams. No effects on litter size or foetal weights were observed in the mid- and low-dose groups, and no significant increases in external soft tissue or skeletal anomalies were observed in any of the treated groups. In summary, the reduced bodyweights of dams and foetuses in the high-dose group appear to be a result of reduced food consumption in this group. The nature of the dose-related change in liver weight observed in dams and its toxicological significance or otherwise is not clearly established in the study summary. Furthermore, it is not known whether changes in liver weight were statistically different at the lowest dose. It is therefore not possible to propose a NOAEL for maternal toxicity. The NOAEL for developmental toxicity is, however, considered to be greater than the highest dose tested, 1,000 mg/kg bw/day.

Summary of toxicity to reproduction

A study conducted to OECD guideline 421 did not find any evidence of toxicity to fertility and reproduction of male and female rats during mating, gestation and lactation from exposure to tertbutylphenyl diphenyl phosphate, or any effects on litter size and the number of live pups at gestation day zero and four. In addition, there were no treatment-related effects on foetal development, except a reduction in mean foetal weights at 1,000 mg/kg bw/day, which was attributed to maternal toxicity in dams of this treatment group. A dose-related increase in liver weights was also observed in dams in all treatment groups, although the significance of these finding is uncertain. An earlier study not conducted to GLP identified possible changes in the reproductive capacity of rats at doses of tertbutylphenyl diphenyl phosphate of 1,000 or 1,700 mg/kg bw/day but these were considered to be secondary to systemic toxicity, rather than a direct effect on reproductive capacity per se.

Based on these findings, the NOAEL for fertility and development is considered to be above 1,000 mg/kg bw/day. The lowest observed adverse effect level (LOAEL) for maternal toxicity is 100 mg/kg bw/day based on increases in liver weight; a NOAEL could not be proposed. The NOEL for the repeat-dose oral feed study was 26.7 mg/kg bw/day in male rats or 30.0 mg/kg bw/day in female rats (equivalent to 400 ppm) based on changes in organ weights (including liver) among rats in the high-dose group (1,600 ppm). For the liver, the changes in weight had no histopathological correlate; it would be useful to have information on the magnitude of the changes.

4.4.10 NO(A)ELs and Margins of Safety (MOS) for the assessment of human exposure via the environment

There are data gaps for sensitisation potential, *in vivo* genotoxicity and carcinogenicity. Available data suggest that tertbutylphenyl diphenyl phosphate does not cause genotoxicity, neurotoxicity, or toxicity to reproduction. However, the currently available neurotoxicity tests were not carried out to OECD Test Guidelines (which require protection with atropine to allow higher doses of cholinesterase inhibition to be tolerated) and testing hens for the potential for delayed neuropathy in humans is generally considered to be unreliable for mixtures. Therefore, it is suggested that individual components should be tested for their relative potency as inhibitors of AChE and NTE in hen and mammalian (preferably human) enzymes.

A valid three-month oral feeding study in rats (Freudenthal *et al*. 2001) could be selected as the key study because it gives the lowest NOEL of all the available valid studies. In this, Sprague-Dawley rats received tertbutylphenyl diphenyl phosphate in the diet at 0, 100, 400 or 1,600 ppm (corresponding doses in mg/kg bw/day not given). There were no effects on bodyweight. There were significant increases in absolute and relative (assumed to be relative to bodyweight) weights of the liver in high-dose male rats, relative weight of livers in high-dose females, relative kidney weight of high-dose males, and absolute and relative weight of adrenal glands in high-dose females; there were no corresponding histopathological changes in these organs, and no other treatment-related changes were seen in any of the treated animals. Based on the increased organ weights noted in male and female rats that received the high dose, the NOEL for repeated dietary exposure is 26.7 mg/kg bw/day in male rats or 30.0 mg/kg bw/day in female rats (equivalent to 400 ppm).

In a reproductive/developmental screening test conducted to OECD TG 421, rats were dosed with tertbutylphenyl diphenyl phosphate by oral gavage for a total of approximately eight weeks (Experimur 2003, cited in USEPA 2004). This dosing period included a stated premating phase of two weeks, a mating period of two weeks, and then continued throughout gestation and lactation. No signs of toxicity were observed

in any of the animals, and the NOAEL was therefore the highest dose tested, 1,000 mg/kg bw/day. This good quality sub-chronic study is not used to derive the PNEC because a lower NOEL of only 400 ppm was established in the study conducted by Stauffer Chemical Company (1981, Freudenthal *et al*. 2001) in which animals were dosed for a longer period of three months.

In view of the limited database and gaps in information for this substance, and the uncertainty over the composition of the substances tested, it is not appropriate to derive a margin of safety here. A number of possible areas for clarification in the mammalian toxicity data base are included above. 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 Derivation of a PNEC for secondary poisoning

A NOEC of 400 ppm (400 mg/kg) diet has been established for changes in the weight of a number of organs in Sprague-Dawley rats, based on dietary exposure to dose levels of 100 to 1,600 ppm for three months. The TGD recommends an assessment factor of 90 for extrapolation of a mammalian toxicity test of 90 days duration.

This leads to a $PNEC_{oral}$ of 400/90 = 4.4 mg/kg.

No avian toxicity data relevant to the derivation of a $PNEC_{oral}$ were identified for tertbutylphenyl diphenyl phosphate.

4.5 Hazard classification

4.5.1 Classification for human health

Tertbutylphenyl diphenyl phosphate is not currently included on Annex I of Directive 67/548/EEC. According to the EU criteria, tertbutylphenyl diphenyl phosphate does not require classification on the basis of its acute toxicity, or skin and eye irritancy or corrosivity. There is, however, a lack of adequate data with which to assess skin-sensitizing potential or carcinogenicity.

The data do not suggest that tertbutylphenyl diphenyl phosphate should be classified, under EU criteria, for specific target organ systemic toxicity following repeated exposure, and should not be classified as mutagenic or toxic to reproduction.

4.5.2 Classification for the environment

Tertbutylphenyl diphenyl phosphate is currently not classified as dangerous to the environment; however, some suppliers provisionally classify the substance as dangerous to the environment and apply the following labels (IUCLID 2001):

N: Dangerous to the environment.
R50: Very toxic to aquatic organisms.

The BCF for tertbutylphenyl diphenyl phosphate is around 778 l/kg and the lowest acute toxicity values from the more reliable studies are a 96-hour LC_{50} of 0.8 mg/l for fish (*Ictalurus punctatus*), a 48-hour LC_{50} of 0.15 mg/l for invertebrates (*Chironomus tentans*) and a 96-hour LC_{50} of 2.6 mg/l for algae (*Selenastrum capricornutum*). Based on these data, the following classification would appear to be appropriate.

N: Dangerous for the environment.

R50/53: Very toxic to aquatic organisms; may cause long-term adverse effects in the aquatic environment.

4.6 PBT assessment

The criteria for persistence (P and vP), bioaccumulation potential (B and vB) and toxicity (T) included in the TGD are shown in Table 4.8.

Table 4.8 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: tertbutylphenyl diphenyl phosphate is considered to be readily biodegradable not meeting the 10-day window. Hence, the substance does not meet the first stage screening criteria for P or vP.

Bioconcentration: a fish BCF value of 778 has been selected for this assessment. Hence the substance does not meet the B criterion.

Toxicity: the lowest NOEC value from the available tests is 0.010 mg/l. This is on the borderline for the T criterion.

The overall conclusion is that the substance is not a PBT substance; it does not meet the P or B criteria.

5 Risk characterisation

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

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

5.1 Freshwater compartment

5.1.1 Surface water

A PNEC for surface water was estimated as 1 μg/l. The resulting PEC/PNEC ratios are summarised in Table 5.1.

Table 5.1 Summary of risk characterisation ratios for surface water

Scenario		PEC (μg/l)	PEC/PNEC
Production of tertbutylphenyl diphenyl phosphate		0.08	0.08
PVC – 1	Compounding	0.46	0.46
	Conversion	0.75	0.75
	Combined compounding and conversion	1.19	**1.19**
PVC – 2	Compounding	0.46	0.46
	Conversion	0.75	0.75
	Combined compounding and conversion	1.19	**1.19**
PVC – 3	Compounding	0.46	0.46
	Conversion	0.75	0.75
	Combined compounding and conversion	1.19	**1.19**
Polyurethane	Compounding	0.9	0.9
	Conversion	0.31	0.31
	Combined compounding and conversion	1.19	**1.19**

Table 5.1 continued.

Scenario		PEC (μg/l)	PEC/PNEC
Textiles	Compounding	0.25	0.25
	Conversion	0.61	0.61
	Combined compounding and conversion	0.84	0.84
Lubricant additive	Blending of fluid	0.03	0.03
Hydraulic fluids	Blending of fluid	0.03	0.03
Power generation fluid	Blending of fluid	0.04	0.04
Regional sources		0.02	0.02

The PEC/PNEC ratios are above one for some scenarios relating to the use of tertbutylphenyl diphenyl phosphate in PVC and polyurethane. Further information is needed on emissions from the processes to refine the PECs for these scenarios to determine whether there is a risk to surface water from these sources. Emission estimates are based on information for the industry area from the Emission Scenario Documents (ESD 2004a) or from other risk assessments, so could be revised with more specific information for the substance itself. The ratios are not very large and so revision of the exposure assessment may be enough to remove the risks. Although there is no long-term algal result available (and so a test could be carried out), this is unlikely to be significant for the assessment. 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.

The risks from production, use in textiles, blending of lubricant additives, hydraulic fluids, power generation fluids and regional sources appear to be low.

5.1.2 Waste water treatment

No PNEC for waste water treatment processes could be derived for tertbutylphenyl diphenyl phosphate and so no risk characterisation can be carried out. Based on the conclusions found for this endpoint in the risk assessments carried out for other triaryl phosphates as part of this project, the risks to waste water treatment processes from tertbutylphenyl diphenyl phosphate would be expected to be low.

5.1.3 Sediment

The PNEC for sediment was tentatively estimated as 0.104 mg/kg wet weight. 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 5.2.

Table 5.2 Summary of risk characterisation ratios for sediment

Scenario		PEC	PEC/PNEC
Production of tertbutylphenyl diphenyl phosphate		7.88×10^{-3}	0.75
PVC – 1	Compounding	0.05	**4.6**
	Conversion	0.08	**7.53**
	Combined compounding and conversion	0.13	**11.9**
PVC – 2	Compounding	0.05	**4.6**
	Conversion	0.08	**7.53**
	Combined compounding and conversion	0.13	**11.9**
PVC – 3	Compounding	0.05	**4.6**
	Conversion	0.08	**7.53**
	Combined compounding and conversion	0.13	**11.9**
Polyurethane	Compounding	0.09	**9**
	Conversion	0.03	**3.13**
	Combined compounding and conversion	0.13	**11.9**
Textiles	Compounding	0.03	**2.54**
	Conversion	0.06	**6.07**
	Combined compounding and conversion	0.09	**8.41**
Lubricant additives	Blending of fluid	2.86×10^{-3}	0.27
Hydraulic fluids	Blending of fluid	2.98×10^{-3}	0.29
Power generation fluids	Blending of fluid	4.47×10^{-3}	0.43
Regional sources		2.1×10^{-3}	0.2

The estimated PEC/PNEC ratios are above one for use of tertbutylphenyl diphenyl phosphate in PVC, polyurethane and textiles. Further information on exposures identified for the aquatic compartment would also have an influence on the risk ratios here. However, the extra factor of 10 used for sediment means that emission estimates would have to be reduced by at least one order of magnitude to remove all concerns.

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. It may therefore be possible to refine the PECs by carrying out further testing[17] to investigate the actual degradation (mineralization) half-life in sediment under relevant environmental conditions.

Toxicity data for sediment organisms would allow a PNEC to be derived directly, and would remove the need for the additional factor. It is likely that three long-term tests on sediment organisms would be required.

The risk to sediment from blending of lubricant additives, hydraulic fluids, power generation fluids and regional sources appears to be low.

[17] 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 tentatively estimated as 0.084 mg/kg wet weight. 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 5.3.

Table 5.3 Summary of risk characterisation ratios for the terrestrial compartment

Scenario		PEC (mg/kg wet wt.)	PEC/PNEC
Production of tertbutylphenyl diphenyl phosphate		negligible[a]	negligible[a]
PVC – 1	Compounding	0.02	**2.35**
	Conversion	0.03	**3.93**
	Combined compounding and conversion	0.05	**6.28**
PVC – 2	Compounding	0.02	**2.35**
	Conversion	0.03	**3.92**
	Combined compounding and conversion	0.05	**6.27**
PVC – 3	Compounding	0.02	**2.35**
	Conversion	0.03	**3.93**
	Combined compounding and conversion	0.05	**6.28**
Polyurethane	Compounding	0.04	**4.71**
	Conversion	0.01	**1.57**
	Combined compounding and conversion	0.05	**6.28**
Textiles	Compounding	0.01	**1.25**
	Conversion	0.03	**3.14**
	Combined compounding and conversion	0.04	**4.4**
Lubricant additive	Blending of fluid	3.54×10^{-4}	0.04
Hydraulic fluids	Blending of fluid	4.06×10^{-4}	0.05
Power generation fluids	Blending of fluid	1.07×10^{-3}	0.13
Regional sources	Agricultural soil	4.69×10^{-6}	<0.01
	Natural soil	2.57×10^{-6}	<0.01
	Industrial soil	1.76×10^{-3}	0.21

Notes: a) Sludge from the production site is not applied to agricultural land.

The estimated PEC/PNEC ratios are above one for use in PVC, textiles and use in polyurethane. Further information on exposures identified for the aquatic compartment would also have an influence on the risk ratios here. However, the extra factor of 10 used for soil means that emission estimates would have to be reduced by around one order of magnitude to remove all of the concerns.

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

Toxicity data for terrestrial organisms would allow a PNEC to be derived directly, and would remove the need for the additional factor. As for sediment, it is likely that three long-term tests would be required.

The risk to the terrestrial compartment from production of tertbutylphenyl diphenyl phosphate, blending of lubricant additives, hydraulic fluids, power generation fluids and regional sources appears to be low.

5.3 Atmosphere

No information is available on the toxicity of tertbutylphenyl diphenyl phosphate to terrestrial 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 tertbutylphenyl diphenyl 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 4.4 mg/kg food. The resulting risk characterisation ratios are summarised in Table 5.4.

The preliminary risk characterisation ratios indicate a low risk of secondary poisoning from the production and current uses of tertbutylphenyl diphenyl phosphate.

5.5 Risks to human health following environmental exposure

As noted in Section 4.4.10, the available data do not allow an acceptable margin of safety to be developed on which to base an assessment for humans exposed through the environment, and therefore no risk characterisation has been carried out. As an indication, based on the NOEL of 26.7 mg/kg bw/day which is considered the most suitable of the results in the database, the lowest margin of safety would be above 5,000, which may indicate a low risk.

5.6 Marine compartment

Although a PEC/PNEC approach can be applied to the marine environment, there are additional concerns which may not be adequately addressed using the above methods. Chief among these concerns is the possibility that hazardous substances may accumulate in parts of the marine environment. The effects of such accumulation are unpredictable in the long term, and once such accumulation has occurred it may be practically difficult to reverse. The properties which lead to substances behaving in this way also lead to greater uncertainty in estimating exposures and/or effect concentrations, and so make a quantitative risk assessment more difficult. In order to identify substances which are likely to behave in this way, criteria have been developed relating to the persistence, accumulation and toxicity of the substance. The first part of the marine assessment is therefore a comparison of the properties of the substance with these criteria. This is presented in Section 4.6.

Table 5.4 Summary of risk characterisation ratios for secondary poisoning

Scenario		Fish food chain		Earthworm food chain	
		PEC (mg/kg)	PEC/PNEC	PEC (mg/kg)	PEC/PNEC
Production of tertbutylphenyl diphenyl phosphate		0.04	<0.01	negligible[a]	<0.01
PVC – 1	Compounding	0.16	0.04	0.1	0.02
	Conversion	0.25	0.06	0.17	0.04
	Combined compounding and conversion	0.39	0.09	0.27	0.06
PVC – 2	Compounding	0.08	0.02	0.1	0.02
	Conversion	0.12	0.03	0.17	0.04
	Combined compounding and conversion	0.19	0.04	0.27	0.06
PVC – 3	Compounding	0.02	<0.01	0.1	0.02
	Conversion	0.3	0.07	0.17	0.04
	Combined compounding and conversion	0.39	0.09	0.27	0.06
Polyurethane	Compounding	0.3	0.07	0.2	0.05
	Conversion	0.11	0.02	0.07	0.02
	Combined compounding and conversion	0.39	0.09	0.27	0.06
Textiles	Compounding	0.02	<0.01	0.05	0.01
	Conversion	0.24	0.05	0.14	0.03
	Combined compounding and conversion	0.28	0.06	0.19	0.04
Lubricant additives	Blending of fluid	0.02	<0.01	1.87×10^{-3}	<0.01
Hydraulic fluid	Blending of fluid	0.02	<0.01	2.13×10^{-3}	<0.01
Power generation fluid	Blending of fluid	0.02	<0.01	5.64×10^{-3}	<0.01

Notes: a) Sludge from the production site is not applied to agricultural soil.

PEC values for the marine assessment are presented in Sections 3.3.1 and 3.3.4. PNECs for marine aquatic species are included in Section 4.1.6. The PNEC for secondary poisoning for the marine environment is the same as that for freshwater fish and terrestrial food chains (Section 4.4.11). The resulting PEC/PNEC ratios are presented in Table 5.5.

The production step is not included in these calculations as the known production sites do not discharge to the marine environment.

RCRs above one are indicated for marine waters and marine sediments for use in PVC, polyurethane and textiles. Further information on emissions from the processes indicated for the freshwater environment would also help to refine these results. More specifically for the marine assessment, information on whether any of these processes avoid discharging to the marine environment, or do so only after effluent treatment (the calculations above assume a direct discharge to the marine environment without waste water treatment) would be useful.

Table 5.5 Summary of risk characterisation ratios for the marine compartment

Scenario		PEC/PNEC ratio			
		Local marine compartment	**Local marine sediment compartment**	**Fish-eating birds and mammals**	**Top predators**
PVC – 1	Compounding	**9.4**	**94**	0.01	<0.01
	Conversion	**15.6**	**156**	0.02	<0.01
	Combined compounding and conversion	**24.9**	**249**	0.04	<0.01
PVC – 2	Compounding	**9.4**	**94**	<0.01	<0.01
	Conversion	**15.6**	**156**	0.01	<0.01
	Combined compounding and conversion	**24.9**	**249**	0.02	<0.01
PVC – 3	Compounding	**9.4**	**94**	<0.01	<0.01
	Conversion	**15.6**	**156**	0.03	<0.01
	Combined compounding and conversion	**24.9**	**249**	0.04	<0.01
Poly-urethane	Compounding	**18.7**	**187**	0.03	<0.01
	Conversion	**6.3**	**63**	<0.01	<0.01
	Combined compounding and conversion	**24.9**	**249**	0.04	<0.01
Textiles	Compounding	**5.05**	**50.5**	<0.01	<0.01
	Conversion	**12.5**	**125**	0.02	<0.01
	Combined compounding and conversion	**17.5**	**175**	0.03	<0.01
Lubricant additive	Blending of fluid	0.26	**2.55**	<0.01	<0.01
Hydraulic fluids	Blending of fluid	0.28	**2.79**	<0.01	<0.01
Power generation fluids	Blending of fluid	0.58	**5.81**	<0.01	<0.01

Testing on freshwater organisms might also affect the marine PNEC, although as noted in Section 3.3.1 such testing is not necessary for the freshwater assessment. Testing on sediment organisms would be of more value for the sediment assessment. There is also the possibility of testing on marine species, which would allow the assessment factor to be reduced.

No risks are found for use in lubricant additives, hydraulic fluids and power generation fluids. The regional concentrations in marine waters and sediments also do not indicate a risk. There is no risk to marine food chains for any scenario.

The size of the 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

Tertbutylphenyl diphenyl phosphate can enter the environment from its production and use, and from the use of articles made from materials containing the substance. Based on the available information, potential risks are identified for all of the life cycle steps for one or more of this assessment's protection goals. The overall conclusions are summarised in Table 6.1 in a simplified form. In particular, the different steps in the use of 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 tertbutylphenyl diphenyl phosphate

Life cycle stage	Surface water	Sediment	WWTP	Air	Soil	Aquatic food chain	Terrestrial food chain	Marine water	Marine sediment
Production	-	-	-	-	-	-	-	-	-
PVC	✸	✸	-	-	✸	-	-	✸	✸
Polyurethane	✸	✸	-	-	✸	-	-	✸	✸
Textile/fabric coating	-	✸	-	-	✸	-	-	✸	✸
Lubricants	-	-	-	-	-	-	-	-	✸
Hydraulic fluids	-	-	-	-	-	-	-	-	✸
Power generation fluids	-	-	-	-	-	-	-	-	✸
Regional	-	-	-	-	-	-	-	-	-

No risk assessment for humans exposed via the environment is currently possible.

The approach taken to estimate releases to the environment underlying the PECs is based on the best *available* information. The estimates take into account information supplied by companies on amounts used by customers. The emission estimates themselves are largely based on information for the particular industry areas, as included in Emission Scenario Documents, but not on information on tertbutylphenyl diphenyl phosphate specifically. The conclusions could therefore be reassessed following additional work, in particular:

- Collation of further site and industry-specific information on releases of tertbutylphenyl diphenyl phosphate from use in the different types of materials indicated. This work could include:
    - An improved description of practices at sites using tertbutylphenyl diphenyl 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). Further environmental monitoring for tertbutylphenyl diphenyl 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). The sites are different from those used in

the previous monitoring exercise. 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.
- Studies on the fate of the substance in WWTP (municipal and industrial).
- Further testing to investigate the actual degradation (mineralization) half-life in sediment and soil under relevant environmental conditions.

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

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8 Glossary of terms

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

9 Abbreviations

Acronym	Description
ASTM	American Society for Testing and Materials
B	Bioaccumulative
BCF	Bioconcentration factor
BMF	Biomagnifaction factor
BOD	Biochemical oxygen demand
bw	Bodyweight
CAS	Chemical Abstract Services
CMR	Carcinogenic, mutagenic and toxic to reproduction
DEHP	Di(2-ethylhexyl)phthalate
DSC	Differential scanning calorimetry
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 1.000 tonnes per year)
IUCLID	International Uniform Chemical Information Database: contains non-validated tonnage, use pattern, property and hazard information for chemicals, submitted by industry under the Existing Substances Regulation (ESR)
K_{oc}	Organic carbon normalised distribution coefficient
K_{ow}	Octanol-water partition coefficient
Kp	Solids-water partition coefficient
$L(E)C_{50}$	Median lethal (effect) concentration
LD_{50}	Median lethal dose

Acronym	Description
LL_{50}	Median lethal loading
LO(A)EL	Lowest observed (adverse) effect level
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
RCR	Risk characterisation ratio
SCAS	Semi-continuous activated sludge unit
TBDPP	Terbutylphenyl diphenyl phosphate
TGA	Thermogravimetric analysis
TGD	Technical Guidance Document
TPP	Triphenyl phosphate
USEPA	Environmental Protection Agency, USA
vB	Very bioaccumulative
vP	Very persistent
vPvB	Very persistent and very bioaccumulative
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.

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