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Environmental risk evaluation report: Isodecyl diphenyl phosphate (CAS no. 29761-21-5)

ea/br/e/sci/v1

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

Published by:
Environment Agency, Rio House, Waterside Drive,
Aztec West, Almondsbury, Bristol, BS32 4UD
Tel: 01454 624400 Fax: 01454 624409
www.environment-agency.gov.uk

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Dissemination Status:
Publicly available

Keywords:
Aryl phosphates, flame retardant, UKCCRMP

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Product Code:
SCHO0809BQUF-E-P

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Steve Killeen

Steve Killeen

Head of Science

Executive summary

An environmental risk assessment has been carried out for isodecyl diphenyl phosphate (CAS no. 29761-21-5) on the basis of available information and using the methods of a European Technical Guidance Document. This substance is mainly used in Europe as a plasticizer/flame retardant in flexible PVC. It is also used in rubber, polyurethanes, textile coatings, paints and pigment dispersions.

Potential risks are identified for most or all areas of use for surface water (fresh and marine), sediment (fresh and marine) and soil compartments, for secondary poisoning in the terrestrial food chain, and for humans exposed through the environment.

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 will be sufficient to remove all of the risks identified.

The assessment could also be refined by performing toxicity tests. No testing on freshwater organisms is indicated. Testing on sediment and terrestrial organisms would allow the assessments for these compartments to be refined. In each case it is likely that three long term-studies would be required. The actual need for testing is closely linked with that for the other triaryl and alkyl/aryl phosphates considered as part of this project. A suggested testing strategy for the group as a whole is outlined in a separate overview document.

The risks to air from production and all uses are low. In addition, the risk to soil from production and to surface water and natural and agricultural soil from regional sources is also thought to be low. No risks were identified for marine food chains (with the exception of the production step). 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.

Isodecyl 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).

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

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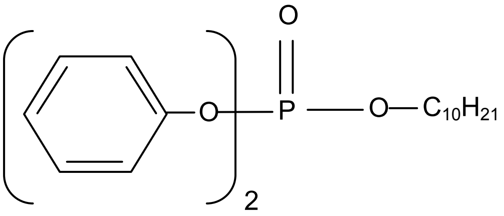
1 General substance information

1.1 Identification of the substance

This assessment considers the following commercial substance.

CAS No: 29761-21-5
EINECS No: 249-828-6
EINECS Name: Isodecyl diphenyl phosphate
Molecular formula: $C_{22}H_{31}O_4P$
Molecular weight: 390.5 g/mol
Structural formula[2]:



Other names, abbreviations, trade names and registered trademarks for this substance include the following.

IDDP
Phosflex 390®
Santicizer 148®

Some of the trade names and trademarks used in the literature may refer to older products no longer supplied to the EU, or products produced outside the EU.

The name isodecyl diphenyl phosphate is used in this assessment.

1.2 Purity/impurity, additives

1.2.1 Purity/impurities

A commercial isodecyl diphenyl phosphate was reported to contain significant amounts of triphenyl phosphate and di-isodecyl phenyl phosphate (Saeger *et al.* 1979). Cleveland *et al.* (1986) reported that the same commercial product consisted of 91 per cent isodecyl diphenyl phosphate and six per cent triphenyl phosphate. Ferro (2002) indicate that the current composition of a commercial product is above 90 per cent isodecyl diphenyl phosphate and less than 5 per cent triphenyl phosphate.

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[2] The structure of the $C_{10}H_{21}$ group is not specified; there are likely to be a number of branched isomeric forms due to the method of production of the decanol used.

1.2.2 Additives

Additives are not thought to be present in 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)

The commercial products are clear, oily liquids at room temperature (Ferro 2002).

1.3.2 Melting point

The melting point (pour point) of a commercial isodecyl diphenyl phosphate is reported as below -50°C (IUCLID 2000, Ferro 2002, Muir 1984).

A melting/pour point of below -50°C is assumed in the assessment.

1.3.3 Boiling point

A commercial isodecyl diphenyl phosphate is reported to start to decompose at 245°C at 1,330 Pa and so the true boiling point cannot be determined (Ferro 2002). IUCLID (2000) and Boethling and Cooper (1985) give the boiling point as 245°C at 1,330 Pa.

A boiling point of above 245°C at atmospheric pressure is assumed in the assessment.

1.3.4 Density

Shankwalkar and Cruz (1994) reported a relative density of 1.09 at 20°C for a commercial isodecyl diphenyl phosphate. A similar relative density of 1.07 at 20°C has been given for a commercial isodecyl diphenyl phosphate (Ferro 2002, IUCLID 2000).

A relative density of 1.07-1.09 is used in the assessment.

1.3.5 Vapour pressure

The vapour pressure at ambient temperature is an important physico-chemical property for use in environmental risk assessment as 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 isodecyl diphenyl phosphate at temperatures around 20-25°C. However, information on the vapour pressures at elevated temperature (see above) is available.

The vapour pressure at elevated temperature is reported to be 13 Pa at 150°C, 66 Pa at 200°C and 1,716 Pa at 250°C for a commercial isodecyl diphenyl phosphate product

(Ferro 2002). Ferro (2002) also report a vapour pressure of 9 Pa at 28°C, 97 Pa at 104°C and 2,990 Pa at 205°C for the same product on their Material Safety Data Sheet. There are considerable differences between the two sets of figures reported.

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

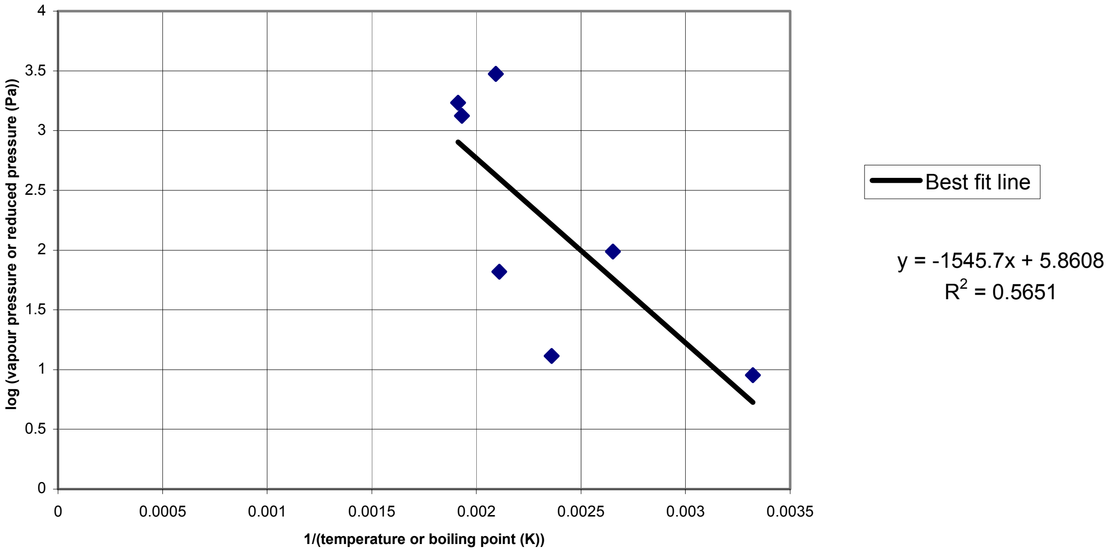
$$\log(\text{vapour pressure}) = [\Delta H_v/2.3RT] + \text{constant}$$

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

Figure 1.1 shows a plot of log (vapour pressure (Pa)) against 1/(temperature (K)) for the available data. This gives a straight line plot with the following regression equation.

$$\log(\text{vapour pressure (Pa)}) = [-1545.7 \times 1/(\text{temperature (K)})] + 5.86$$

Figure 1.1 Plot of log (vapour pressure or reduced pressure (Pa)) against 1/(temperature or boiling point (K)).



The value of ΔH_v for isodecyl diphenyl phosphate can be estimated from the slope of the plot to be 29,557 J/mol. This value is lower than for several other aryl phosphate esters. The correlation in this case is poor and so there is considerable uncertainty in this analysis. The poor correlation could be due to decomposition during determination of the vapour pressure at elevated temperature (decomposition was noted in boiling point determinations under reduced pressure as reported in Section 1.3.3).

Using this equation the vapour pressure of isodecyl diphenyl phosphate at 20°C (293K) can be estimated as 3.8 Pa. The value for ΔH_v may vary with temperature and this could introduce further errors in extrapolation of the data obtained at elevated temperatures to ambient temperatures.

The actual data available for isodecyl diphenyl phosphate are not wholly consistent (as can be seen from the poor correlation in Figure 1.1). Annex B provides an alternative method for estimating the vapour pressure of isodecyl diphenyl phosphate at 20°C, using the whole dataset available for aryl phosphates in general. This gives an estimated vapour pressure of 3.6×10^{-5} Pa at around 20°C. This value is, as would be expected, lower than but consistent with the vapour pressure estimated for the structurally similar 2-ethylhexyl diphenyl phosphate (3.4×10^{-4} Pa at 20°C; see the risk evaluation report for that substance in this series).

A vapour pressure (at 25°C) of 4.7×10^{-8} mmHg (6.3×10^{-6} Pa) can be estimated for isodecyl 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 at 25°C of 1.6×10^{-5} mmHg (2.1×10^{-3} Pa) from the boiling point of isodecyl diphenyl phosphate (Grain method).

A vapour pressure of 3.6×10^{-5} Pa at 20°C is used in the assessment. The EUSES program estimates a vapour pressure of 5.08×10^{-4} Pa at 25°C from this value. However, there are relatively large uncertainties over the actual vapour pressure of isodecyl diphenyl phosphate at room temperature.

1.3.6 Water solubility

The Research Institute for Chromatography (RIC 2004) determined the solubility of a commercial isodecyl diphenyl phosphate using a slow stirring method. Distilled water was stirred in a large glass vessel with a coated stirrer bar, with the vessel isolated from the stirrer plate to avoid temperature effects. The stirring rate used, 100 rpm, was low enough to avoid the formation of a vortex. After the water was stirred for 24 hours, a drop of 4 µl of the substance (4.0 mg) was added to the water surface, where it formed a single drop. Water was sampled from the bottom of the vessel through a tap at 2, 5, 9 and 19 days after the addition of the substance, with three samples at each time. Samples were extracted with cyclohexene, and the cyclohexene layer analysed by GC-MS. The mean concentration after two days was 6.8 µg/l, and at five days was 11.2 µg/l. After this time, the concentrations reduced with time, and extra peaks were observed in the chromatograms, presumably indicating decomposition.

Saeger *et al.* (1979) determined the solubility of a commercial isodecyl diphenyl phosphate using a shake flask method. The substance used was a commercial product consisting of isodecyl diphenyl phosphate along with triphenyl phosphate and diisodecyl phenyl phosphate. In the experiment, 25 ml of the phosphate ester was added to 500 ml of purified water and shaken for 48 hours. The solution was then allowed to stand for one week in the dark before the aqueous phase was centrifuged at 20,000 g for one hour to remove droplets of undissolved substance. The aqueous phase was then extracted twice with methylene dichloride and the extracts were analysed for the commercial product by a gas chromatography method (the centrifugation/extraction/analysis steps were carried out in duplicate and gave a mean relative average deviation of 13 per cent). The solubility of the substance tested (as the commercial product) was determined to be 0.75 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 being elevated in solution compared with that in the commercial product. This indicates a preferential dissolution of the triphenyl phosphate component (water solubility of triphenyl phosphate itself was determined as 1.9 mg/l). As the solubility of 0.75 mg/l was based on the total concentration of all components of the commercial product, the actual solubility of the isodecyl diphenyl phosphate may be lower than indicated by this figure.

Ferro (2002) reports a water solubility of 0.03 mg/l at 22°C for a commercial isodecyl diphenyl phosphate. The same value is also reported in IUCLID (2000) for isodecyl diphenyl phosphate. This report indicates that the value is for the main component of the product (the isodecyl diphenyl phosphate component) and that the value was obtained by a shake flask method.

A water solubility of around 0.002 mg/l at 25°C can be estimated for isodecyl diphenyl phosphate using the Syracuse Research Corporation WSKOW version 1.30 software (the estimate is based on an estimated log K_{ow} of 7.28).

The commercial product contains a proportion of the more soluble triphenyl phosphate, and so the results have to be interpreted with care. The RIC (2004) study is considered to be the most appropriate from which to derive the solubility for the substance, and so a water solubility of 11 µg/l at room temperature is assumed in the assessment.

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

The octanol-water partition coefficient of a commercial isodecyl diphenyl phosphate has been determined using a shake flask method (Saeger *et al.* 1979). The substance used was a commercial product consisting of isodecyl diphenyl phosphate along with triphenyl phosphate and diisodecyl 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 273,000 (log K_{ow} = 5.44).

Renberg *et al.* (1980) determined the octanol-water partition coefficient for an isodecyl diphenyl phosphate (the same substance as used by Saeger *et al.* 1979 above) using a high performance thin layer chromatography (HPTLC) method. Two main components of the commercial product were evident using the method and the partition coefficients determined (log values) for these components were 3.31 and 5.72. The mean value obtained for all components was 5.42. The component giving rise to the log K_{ow} value of 3.31 was tentatively identified as triphenyl phosphate (the log K_{ow} value for triphenyl phosphate itself was determined as 3.15 using the HPTLC method). These measured values are in reasonable agreement with the values estimated above.

A log K_{ow} of 7.28 can be estimated for isodecyl diphenyl phosphate from its structure using the Syracuse Research Corporation Log K_{ow} (version 1.60) software.

A log K_{ow} of 5.44 is used in the risk assessment.

1.3.8 Hazardous physico-chemical properties

Ferro (2002) and IUCLID (2000) give the flash point (open cup) for a commercial isodecyl diphenyl phosphate as 240°C.

Ferro (2002) give the fire point as 260°C for a commercial isodecyl diphenyl phosphate.

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

1.3.9 Other relevant physico-chemical properties

Surface tension

The surface tension for a commercial isodecyl diphenyl phosphate is reported to be 0.0343 Nm at 20°C (Ferro 2002).

Henry's law constant

A Henry's law constant of 1.8 Pa m^3/mol at around 25°C can be estimated for isodecyl diphenyl phosphate based on the water solubility of 0.011 mg/l (see Section 1.3.6) and vapour pressure of 5.08×10^{-5} Pa at 25°C (see Section 1.3.5).

A Henry's law constant of 4.36×10^{-7} atm m^3/mol (0.044 Pa m^3/mol) at 25°C can be estimated for isodecyl diphenyl phosphate from chemical structure (bond contribution method) using Syracuse Research Corporation HENRYWIN (version 3.00) software.

A Henry's law constant of 1.8 Pa m^3/mol at 20°C is used in the risk assessment. This value is consistent with the vapour pressure and water solubility of isodecyl diphenyl phosphate, and is similar to the values obtained for 2-ethylhexyl diphenyl phosphate.

1.3.10 Summary of physico-chemical properties

The physico-chemical properties of isodecyl diphenyl phosphate are summarised in Table 1.1.

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

Property	Value
Melting point	<-50°C (pour point)
Boiling point (at atmospheric pressure)	>245°C (decomposes)
Relative density	1.07-1.09 at 20°C
Vapour pressure	3.6×10^{-5} Pa at 20°C
Water solubility	0.011 mg/l at room temperature
Octanol-water partition coefficient (log value)	5.44
Henry's law constant	1.8 Pa m^3/mol at 25°C

2 General information on exposure

2.1 Production

Only one company (Ferro) is known to produce and supply isodecyl diphenyl phosphate in Europe, and so information on the quantities produced and other market information is confidential. Production is carried out under a toll agreement by Solutia UK Limited, Newport, Gwent, UK. It is possible that other companies may supply this substance, but no further information is available for this report.

2.2 Use

2.2.1 General introduction

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

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

The alkyl diphenyl phosphate products were originally developed to improve low temperature flexibility in PVC over that obtained with triaryl phosphates. Alkyl diphenyl phosphates are slightly less efficient as flame retardants than the triaryl phosphates but generally result in lower smoke formation when PVC is burned (Weil 1993).

2.2.2 Uses of isodecyl diphenyl phosphate

The main use of isodecyl diphenyl phosphate is as a plasticizer/flame retardant in flexible PVC (Weil 1993). Information on the sales of isodecyl diphenyl phosphate into the EU has been provided by the relevant supplier companies for the year 2005 and this confirms that PVC is the main current use in the EU. The substance is also used in rubber, polyurethanes, textile coatings, paints and pigment dispersions.

3 Environmental exposure

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

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

3.1 Environmental fate and distribution

3.1.1 Degradation

Abiotic degradation

Atmospheric degradation

A rate constant for reaction of isodecyl diphenyl phosphate with atmospheric hydroxyl radicals of 4.2×10^{-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 9.2 hours.

Hydrolysis

No information appears to be available on the hydrolysis of isodecyl diphenyl phosphate. By comparison with other aryl phosphates, hydrolysis of isodecyl diphenyl phosphate would be expected to occur, particularly under alkaline and acidic conditions, but it is not currently possible to estimate the rate of this reaction in the environment for isodecyl diphenyl phosphate. Proposed testing under the US High Production Volume (HPV) chemicals initiative includes a hydrolysis study.

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

Photolysis

No information is available on the direct photolysis reactions of isodecyl diphenyl phosphate under environmentally relevant conditions.

Biodegradation

IUCLID (2000) reports the results of an unpublished OECD 301B Modified Sturm ready biodegradation test for isodecyl diphenyl phosphate. The test was reported to have used adapted activated sludge and so cannot be considered as a true ready biodegradation test. The substance was tested at a concentration of 20 mg/l and 63 per cent degradation (as determined by CO_2 evolution) was seen after 28 days incubation (the extent of degradation at various time points during the study was five per cent after five days, 13 per cent after seven days, 42 per cent after 14 days and 53 per cent after 20 days). Based on the results of this test, isodecyl diphenyl phosphate can be considered at least inherently biodegradable.

The results of another unpublished biodegradation test are reported in IUCLID (2000). This test again used adapted activated sludge and the concentration of the test substance used was 30 mg/l. The test was reported to be similar to the USEPA aerobic aquatic degradation test. The extent of degradation seen was 62 per cent after 28 days. Again, as adapted microorganisms were used, the results of this study show that the substance can be considered at least inherently biodegradable.

IUCLID (2000) also reports the results of an unpublished OECD 302A Modified SCAS inherent biodegradability test using an activated sludge inoculum. The substance was tested at 3 and 13 mg/l and removal rates of 45-75 per cent after 24 hours were reported to have been obtained. Based on these results, isodecyl diphenyl phosphate can again be considered to be at least inherently biodegradable. This is probably the same test as reported below by Saeger *et al.* (1979).

Saeger *et al.* (1979) determined the biodegradation of an isodecyl diphenyl phosphate (Santicizer 148) using various test systems. The substance used was a commercial product consisting of isodecyl diphenyl phosphate along with triphenyl phosphate and diisodecyl phenyl phosphate. The first test investigated the primary degradation of the test substance using a river die-away method. The water used in the test was settled Mississippi River water. The test substance (at a concentration of 1 mg/l) was added to the water and the test vessels (bottles) were sealed with a foil-lined cap and stored in the dark at room temperature. Sterile control solutions (containing the same concentration of test substance) and positive control solutions (containing linear alkyl benzene sulphonate) were also run. At various times during the study, a bottle was removed and the amount of the phosphate ester present was determined (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 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 24 weeks (at the lower concentration) or 15 weeks (at the higher concentration) and samples of the mixed liquor were removed at weekly intervals and the concentration of the phosphate ester present was determined. The results indicated an equilibrium removal rate of 54 ± 6 per cent at 3 mg/l and 20 ± 9 per cent at 13 mg/l in the test system. The higher test concentration was found to cause a significant decrease in the biomass present in the test system. To investigate the loss by volatilisation the off-gases were passed through a series of scrubbers. No significant loss by volatilisation (below 0.5 per cent per cycle) of the phosphate ester was seen.

The final part of the study investigated the ultimate mineralisation of the test substance using a degradation method based on the modified Sturm method. An acclimated bacterial seed was prepared by incubation of 100 ml of settled supernatant from a SCAS unit with 20 mg of one of eleven phosphate esters (including the test substance), 50 mg of yeast extract and 900 ml of standard biological oxygen demand (BOD) water for 14 days in the dark at room temperature. At the end of the incubation period a combined acclimated seed was prepared by mixing samples from each acclimation bottle and this was used as seed for the inherent biodegradation test. In the test 500 ml of the composite seed was added to 5,500 ml of BOD water and the substance was then added to the bottle (initial concentration 19.0 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 13 per cent after seven days, 63 per cent after 28 days and 68 per cent after 35 days. Therefore the substance can be considered as inherently biodegradable based on the results of this test.

A further, unpublished, river die-away study for isodecyl diphenyl phosphate has been reported in IUCLID (2000). This study used Mississippi River water and a test concentration of 0.767 mg/l. The results showed more than 93.5 per cent degradation as determined by parent compound analysis (less than 0.05 mg/l of isodecyl diphenyl phosphate was detectable after 21 days incubation). The half-life for degradation was around 11-12 days (the degradation seen at various time points during the study was 33 per cent after four days, 37 per cent after seven days, 48 per cent after 11 days and 65 per cent after 18 days). This may be the same study as reported above by Saeger *et al.* (1979).

Summary of degradation

Abiotic degradation

No information appears to be available on the hydrolysis of isodecyl diphenyl phosphate.

Based on the information available for other aryl phosphates (for example, see risk evaluation report for triphenyl phosphate in this series), significant hydrolysis of the substance would be expected to occur only under highly alkaline (pH 8-9 and above) or highly acidic conditions. The products of the initial hydrolysis would be expected to be either phenol and isodecyl phenyl phosphate or isodecanol and diphenyl phosphate. The diphenyl or alkyl phenyl phosphates would be expected to be more resistant to further hydrolysis than the parent compound.

It is not possible to estimate the likely rate of hydrolysis of isodecyl diphenyl phosphate in the environment, but the rate is expected to be slow except possibly at high or low environmental pHs. A hydrolysis rate of zero will therefore be used 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.

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

Atmospheric photo-oxidation of isodecyl diphenyl phosphate is predicted to occur with a half-life of around 9.2 hours. This reaction is taken into account in the risk assessment.

In summary, the abiotic rate constants and half-lives assumed in the assessment are as follows:

Hydrolysis	$khydr_{water} = 0\ d^{-1}$	half-life = infinite
Photolysis	$kphoto_{water} = 0\ d^{-1}$	half-life = infinite
Atmospheric photo-oxidation	$k_{OH} = 4.2\times10^{-11}\ cm^3$/molecule s	half-life = 9.2 h

Biodegradation

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

From the available standard biodegradation tests, isodecyl diphenyl phosphate can be considered as being at least inherently biodegradable (most of the tests have been carried out with acclimated microorganisms). The recommended biodegradation half-lives for sewage treatment, surface water and soil from the TGD are summarised below (inherently biodegradable (not clear if the specific criteria are fulfilled), based on a Kp_{soil} of 137 l/kg):

	Does not meet specific criteria	Meets specific criteria
STP	$k = 0\ h^{-1}$	$k = 0.1\ h^{-1}$
Surface water	$k = 0\ d^{-1}$	$k = 4.7\times10^{-3}\ d^{-1}$
Soil	$k = 2.3\times10^{-4}\ d^{-1}$	$k = 2.3\times10^{-4}\ d^{-1}$

There is evidence from river die-away studies that isodecyl diphenyl phosphate undergoes relatively rapid primary degradation (half-lives of the order of 10-21 days have been determined). Products from the primary degradation reaction are likely to be phenol and isodecanol, which could be expected to undergo further biodegradation. Therefore the above default biodegradation rate constants, assuming that the substance is inherently biodegradable (not meeting the criteria), may underestimate the actual degradation of this substance in the environment. Thus, the following default degradation rate constants (corresponding to inherently biodegradable, meeting specific criteria) are used in this assessment:

Sewage treatment plant	$k = 0.1\ h^{-1}$	half-life = 6.9 hours
Surface water	$k = 4.7\times10^{-3}\ d^{-1}$	half-life = 150 days
Sediment	$k = 2.3\times10^{-4}\ d^{-1}$	half-life = 3,000 days
Soil	$k = 2.3\times10^{-4}\ d^{-1}$	half-life = 3,000 days

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

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

3.1.2 Environmental partitioning

Adsorption

No experimental data are available for isodecyl diphenyl phosphate.

A K_{oc} value of 5.0×10^4 l/kg can be estimated for isodecyl diphenyl phosphate from its structure using the Syracuse Research Corporation PCKOC (version 1.63) software which employs a molecular connectivity index method.

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

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

Using this equation for isodecyl diphenyl phosphate (log K_{ow} of 5.44) results in an estimated K_{oc} value of 6,849 l/kg. Since this value is obtained using the method recommended in the Technical Guidance Document, it is used in the risk assessment. The resulting partition coefficients for soils and sediments calculated using the methods given in the Technical Guidance Document are shown below:

K_{oc}	6,849 l/kg		
Kp_{susp}	685 l/kg	$K_{susp\text{-}water}$	171 m^3/m^3
Kp_{sed}	342 l/kg	$K_{sed\text{-}water}$	171 m^3/m^3
Kp_{soil}	137 l/kg	$K_{soil\text{-}water}$	206 m^3/m^3

These values are used in the risk assessment.

Volatilisation

No studies on the volatilisation of isodecyl diphenyl phosphate appear to be available. The Henry's law constant estimated for isodecyl diphenyl phosphate is 1.8 Pa m^3/mol at 20°C. This indicates that volatilisation from water may be significant in some circumstances.

Fugacity modelling

The potential environmental distribution of isodecyl 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 Organisation for Economic Cooperation and Development (OECD) High Production Volume (HPV) programme. The model was run four times with a nominal release rate of 1,000 kg/hour initially entering the air, soil or water compartments in different proportions. The physico-chemical properties used and the results of the modelling exercise are shown in Table 3.1.

The results of the model show that only a very small amount of the isodecyl 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 generally remains in the soil, with only a small fraction distributing to the water and sediment compartment. When released to water, the substance is likely to distribute mainly to the sediment phase at steady state, but small fractions are also predicted to be found in the soil and water phases.

Table 3.1 Results of generic level III fugacity model for isodecyl diphenyl phosphate

Input data	Value				
Vapour pressure	3.6×10^{-5} Pa at 20°C				
Water solubility	0.011 mg/l				
Log K_{ow}	5.44				
Atmospheric half-life	9.2 hours				
Half-life in water	150 days				
Half-life in soil and sediment	3,000 days				
Emission rate	**Model results at steady state**				
	Amount in air	**Amount in soil**	**Amount in water**	**Amount in sediment**	**Overall residence time/persistence**
1,000 kg/hour to air 1,000 kg/hour to soil 1,000 kg/hour to water	8×10^{-3}%	92.9%	0.46%	6.6%	1,827 days
1,000 kg/hour to air 0 kg/hour to soil 0 kg/hour to water	0.047%	98.8%	0.077%	1.1%	823 days
0 kg/hour to air 1,000 kg/hour to soil 0 kg/hour to water	5×10^{-5}%	99.8%	0.01%	0.16%	4,250 days
0 kg/hour to air 0 kg/hour to soil 1,000 kg/hour to water	6×10^{-3}%	11.9%	5.8%	82.4%	420 days

The behaviour of isodecyl diphenyl phosphate during waste water treatment was estimated using the EUSES model. Using a degradation rate of 0.1 h^{-1} (see Section 3.1.1), a K_{oc} of 6,849 l/kg (see above) and a Henry's law constant of 1.8 Pa m^3/mol at 25°C (see Section 1.3.9), the following behaviour is predicted.

Degraded	23.1%
Adsorbed to sludge	40.1%
Volatilised to air	1.2%
To effluent	35.6%

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

3.1.3 Bioaccumulation and metabolism

Measured data

The uptake and accumulation of the commercial isodecyl diphenyl phosphate product by fathead minnows (*Pimephales promelas*) has been 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 91 per cent isodecyl diphenyl phosphate and six per cent triphenyl 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 isodecyl diphenyl phosphate and triphenyl phosphate. The concentrations of these two components in the water were also determined at fortnightly intervals. The results are summarised in Table 3.2. The paper reported that the mean BCF determined at 90 days in this study was 677 ± 159 l/kg for isodecyl diphenyl phosphate and 1,007 ± 224 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 less than seven days. Toxic effects were seen at various points during this study, particularly on growth at the higher concentrations, and so this adds some uncertainty to the BCF values determined.

Table 3.2 Bioconcentration of a commercial isodecyl diphenyl phosphate in fathead minnow

Mean measured concentration in water		Mean measured concentration in fish (mg/kg wet wt.)						BCF at 90 days (l/kg)	
(mg/l)		30 days		60 days		90 days			
TPP	IDDP	TPP	IDDP	TPP	IDDP	TPP	IDDP	TPP	IDDP
0.001	0.017	0.8	21	0.5	11	0.7	12	700	706
0.002	0.029	1	30	1	37	2	25	1,000	862
0.003	0.054	3	57	1	51	3	41	1,000	759
0.006	0.099	6	78	3	64	6	61	1,000	616
0.021	0.315	16	107	20	114	28	139	1,333	441
Control		0.2	25	<0.2	6	1	<3.5		

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

IUCLID (2000) reports the results of a further, unpublished bioconcentration study using isodecyl diphenyl phosphate with bluegill (*Lepomis macrochirus*). The test concentration used was 0.0169 mg/l and a whole fish BCF of 335 l/kg after 28 days at 21°C was obtained (the BCF for muscle alone was 160 l/kg). Elimination of the substance from the fish was reported to be rapid, with 90 per cent being eliminated within 14 days.

No data appear to be available for the uptake of isodecyl diphenyl phosphate 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 a earthworm BCF value is estimated using the following equation given in the TGD:

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

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

Using a log K_{ow} value of 5.44, the $BCF_{earthworm}$ is estimated as 3,305. This value is used in the assessment. The reliability of this estimate is unknown.

Summary of accumulation

Two bioconcentration studies are available for isodecyl diphenyl phosphate. The results from both studies are in reasonable agreement (335 l/kg with *Lepomis macrochirus* and 677 l/kg with *Pimephales promelas*). There are some uncertainties around the study with *Pimephales promelas* (significant effects on growth were seen at various times during the test as a result of the exposure to the higher concentrations) and so the value of 335 l/kg determined for *Lepomis macrochirus* will be considered in the risk assessment.

The log K_{ow} value of isodecyl diphenyl phosphate is 5.44. Using the methods recommended in the Technical Guidance Document, a BCF for fish of 8,395 l/kg can be estimated. This value is much higher than those determined experimentally.

A BCF of 335 l/kg is used in this risk assessment for isodecyl diphenyl phosphate. In addition to a BCF, the revised Technical Guidance Document also requires a biomagnification factor (BMF) to be taken into account. For isodecyl diphenyl phosphate, the default BMF would be 1 based on the BCF values determined above.

Using a log K_{ow} value of 5.44 and the methods recommended in the TGD, the $BCF_{earthworm}$ is estimated as 3,305.

3.2 Environmental releases

3.2.1 General discussion

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

The producers of isodecyl diphenyl phosphate provided information on the amounts used by representative large customers, and this was used in the local estimates of emissions from use. Some additional information on waste treatment and cleaning at a small number of user sites was also provided; this information did not contradict the assumptions made on the basis of the ESD.

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 3.4.

3.2.3 Releases from use (processing)

PVC

Emissions from the use in PVC were estimated using the methods outlined in the ESD on plastics additives (OECD 2004). 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 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. Emission factors in the ESD are derived from information on a model substance, di(2-ethylhexyl)phthalate (DEHP), and are modified according to the relative properties of this substance and the substance of interest. The main property affecting emissions is the vapour pressure of the substance. Isodecyl diphenyl phosphate has a similar vapour pressure to that of DEHP at processing temperatures, and is classed as of medium volatility according to the criteria in the ESD[6]. The ESD also uses the particle size or form of the substance in estimating possible releases from raw materials handling. Isodecyl diphenyl phosphate is a liquid (Section 0).

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

- Compounding (including raw materials handling): 0.005 per cent to air, 0.01- 0.015 per cent to waste water.
- Conversion: 0.005-0.025 per cent to air, 0.005-0.025 per cent to waste water.

For rubber, polyurethanes, and pigment dispersions, 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 (for pigment dispersions, conversion losses are assumed to be covered by those from the plastics into which they are included, so the conversion factor is zero).

Textile coating

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

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

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

Paints

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

3.2.4 Releases over lifetime of products

Isodecyl 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. Possible losses from PVC and other polymeric materials through leaching and volatilisation are considered in this section. A limited amount of information relevant to the release of isodecyl diphenyl phosphate is available and is included here. Estimates are based on the methods outlined in the Emission Scenario Document (OECD 2004) and also take into account approaches used in the risk assessment of other substances (for example, the risk assessment on medium-chain chlorinated paraffins that has been 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.

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

Leaching loss

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

Factors from the ESD on plastics additives are used in the assessment for emissions from PVC and rubber products, and textiles. Compared to the model substance DEHP in the ESD, isodecyl diphenyl phosphate is classed as a low solubility substance, and so the same factor as for DEHP is used: 0.05 per cent over the lifetime of the product. Some PVC products are used in areas where exposure to water is unlikely and for these leaching losses are set to zero. Other products are used in external areas where the potential for leaching is much greater. For these, a factor of up to four per cent over the lifetime of the product is used, depending on the product lifetime.

The polyurethanes in which isodecyl diphenyl phosphate is used are not considered likely to come into contact with water in the course of their normal use, so leaching emissions from this use are negligible.

Emission factors for paints are also based on the ESD, with leaching of 0.15 per cent per year (based on external use of the paints).

Volatile loss

The stability of, and volatile loss from, several commercial aryl and alkyl/aryl phosphate products has been studied using a combination of differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) under both a nitrogen atmosphere (Shankwalkar and Cruz 1994) and an oxygen atmosphere (Shankwalkar and Placek 1992). The results of the studies are summarised in Table 3.3.

Table 3.3 Thermal degradation temperature and weight loss of aryl and alkyl/aryl phosphates

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

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

The results under a nitrogen atmosphere show that the triaryl phosphates start to decompose at temperatures of around 310-350°C, whereas the alkyl diphenyl phosphates tested start to decompose at a temperature of around 260°C. The decomposition temperatures under an oxygen atmosphere are significantly lower. For all the substances tested, significant weight loss occurs 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. The factors from the ESD on plastics additives are used, as applied in the risk assessment of medium-chain chlorinated paraffins (ECB 2005) as appropriate. These are applied to articles from PVC, rubber, polyurethanes and to textiles. Volatile losses from products occur at ambient temperatures, and at these temperatures isodecyl 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 the use in thin films, where a higher value of 2 per cent over the lifetime is used for paints.

Waste in the environment

This considers the loss of substance in particles of plastic material from articles in use. The approach is the same as that used in the risk assessment for medium-chain chlorinated paraffins. For use in PVC, a loss of 0 to 3.125 per cent of the material over the lifetime of the products or articles is assumed, depending on the use of the products. A further two per cent loss on disposal at the end of the service life is also assumed. For textiles, losses of two per cent over the service life and two per cent on disposal are assumed. For rubber and polyurethanes, no waste generation during the lifetime is assumed, but two per cent loss on disposal is assumed. For paints, a loss of 2 to 5 per cent on disposal is assumed. As noted above, losses of pigment dispersions are taken as five per cent across the whole of service life and disposal. In the calculations, the substance in these particles is assumed to be available in the environment; this is likely to be an overestimate, but there are no actual data to indicate how much may be available.

Other sources of release

There is a small quantity of isodecyl diphenyl phosphate which is not allocated to one of the three use areas. It has been assumed that this amount is in fact used in these areas, but passes through a longer supply chain and hence its use is not known to the major producers and suppliers who provided the information. To deal with this, an overall emission factor was derived from the estimated releases from the quantity allocated to specific uses. This factor was applied to the unallocated tonnage, and the release divided between the different compartments in the same ratio as for the allocated tonnage. These releases appear in the summary table (Table 3.4) under miscellaneous uses.

3.2.5 Summary of environmental releases

The estimated environmental releases of isodecyl diphenyl phosphate are summarised in Table 3.4.

Table 3.4 Summary of estimated environmental releases of isodecyl 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			90			9,000 to surface water[b]				
PVC – 1	Raw materials handling and compounding		0.17							
	Conversion	0.42	0.42							
	Raw materials handling, compounding and conversion	0.42	0.59		c	c		c	c	
	In service losses				30	30		270	270	
	Waste in the environment[d]				3	756 to surface water	2,277	27.3	6,804 to surface water	20,494
PVC – 2	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0625	0.0625							
	Raw materials handling, compounding and conversion	0.075	0.10		c	c		c	c	
	In service losses				3.5	3.5		31.5	31.5	
	Waste in the environment[d]				0.14	34.8 to surface water	105	1.26	313 to surface water	944

Table 3.4 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	0.016	0.048							
	Conversion	0.08	0.08							
	Raw materials handling, compounding and conversion	0.096	0.128		c	c		c	c	
	In service losses				499	12		4,493	108	
	Waste in the environment[d]				0.48	119 to surface water	360	4.3	1,074 to surface water	3,236
PVC – 4	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0125	0.0125							
	Raw materials handling, compounding and conversion	0.025	0.05		c	c		c	c	
	In service losses				7.5			67.5		
	Waste in the environment[d]				0.06	14.9 to surface water	45	0.54	134 to surface water	405

Table 3.4 continued.

Life cycle stage		**Local (kg/day)**			**Regional (kg/year)**			**Continental (kg/year)**		
		Air	**Water**	**Soil**	**Air**	**Water**[a]	**Soil**	**Air**	**Water** [a]	**Soil**
PVC – 5	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0625	0.0625							
	Raw materials handling, compounding and conversion	0.075	0.10		c	c		c	c	
	In service losses[d]				6	360		54	3,240	
	Waste in the environment[d]				0.82	204 to surface water	615	7.39	1,839 to surface water	5,539
PVC – 6	Raw materials handling and compounding	0.0125	0.0375							
	Conversion	0.0125	0.0125							
	Raw materials handling, compounding and conversion	0.025	0.05		c	c		c	c	
	In service losses[d]				2.5	75		22.5	675	
	Waste in the environment[d]				2.74	683 to surface water	2,057	24.68	6,145 to surface water	18,509

Table 3.4 Continued.

Life cycle stage		**Local (kg/day)**			**Regional (kg/year)**			**Continental**		
		Air	**Water**	**Soil**	**Air**	**Water**[a]	**Soil**	**Air**	**Water** [a]	**Soil**
Rubber	Raw materials handling and compounding	0.025	0.075							
	Conversion	0.025	0.025							
	Raw materials handling, compounding and conversion	0.05	0.10		c	c		c	c	
	In service losses[d]				2.5	2.5		22.5	22.5	
	Waste in the environment[d]				0.1	24.9 to surface water	74.9	0.9	224 to surface water	674
Polyurethane	Raw materials handling and compounding	0.025	0.075							
	Conversion	0.025	0.025							
	Raw materials handling, compounding and conversion	0.05	0.10		c	c		c	c	
	In service losses[d]				4.75			42.75		
	Waste in the environment[d]				0.19	47.3 to surface water	142	1.71	425 to surface water	1,281

Table 3.4 continued.

Life cycle stage		Local (kg/day)			Regional (kg/year)			Continental (kg/year)		
		Air	Water	Soil	Air	Water[a]	Soil	Air	Water [a]	Soil
Textiles	Raw materials handling and compounding		0.02							
	Conversion	0.05	0.05							
	Raw materials handling, compounding and conversion	0.05	0.07		c	c		c	c	
	In service losses[d]				1.25	1.25		11.25	11.25	
	Waste in the environment[d]				0.09	22.7 to surface water	68.25	0.82	204 to surface water	614
Pigment dispersion	Raw materials handling and compounding	0.025	0.075							
	In service losses/waste in environment[d]				0.1	24.9 to surface water	75	0.9	224.1 to surface water	675

Table 3.4 continued.

Life cycle stage		**Local (kg/day)**			**Regional (kg/year)**			**Continental (kg/year**		
		Air	**Water**	**Soil**	**Air**	**Water**[a]	**Soil**	**Air**	**Water** [a]	**Soil**
Paints	Formulation	0.133	0.4							
	Processing		0.03		c	c		c	c	
	Losses during service life[d]				86	42 to surface water		774	378 to surface water	
	Waste remaining in the environment[d]				0.39	96.9 to surface water	292	3.5	872 to surface water	2,626
Miscellaneous					4.6	3.5 plus 13.4 to surface water	39.5	40.9	31.8 plus 120 to surface water	355
Total					872	1,2009	6,169	6,023	23,324	55,480

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

b) Emissions calculated from site-specific data, after wastewater 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 as waste in the environment and from service life in some uses 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 3.5.

Table 3.5 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.)
PVC – 1	Compounding	0.03	3.16	2.63	0.47
	Conversion	0.07	7.57	6.26	1.13
	Combined compounding and conversion	0.11	10.6	8.72	1.58
PVC – 2	Compounding	6.68×10^{-3}	0.83	0.71	0.12
	Conversion	0.01	1.27	1.07	0.19
	Combined compounding and conversion	0.02	1.93	1.62	0.29
PVC – 3	Compounding	8.55×10^{-3}	1.01	0.86	0.15
	Conversion	0.01	1.58	1.33	0.24
	Combined compounding and conversion	0.02	2.42	2.02	0.36
PVC – 4	Compounding	6.68×10^{-3}	0.83	0.71	0.12
	Conversion	2.23×10^{-3}	0.39	0.35	0.06
	Combined compounding and conversion	8.91×10^{-3}	1.05	0.89	0.16
PVC – 5	Compounding	6.68×10^{-3}	0.83	0.38	0.12
	Conversion	0.01	1.27	0.53	0.19
	Combined compounding and conversion	0.02	1.93	0.75	0.29
PVC – 6	Compounding	6.68×10^{-3}	0.83	0.17	0.12
	Conversion	2.23×10^{-3}	0.39	0.39	0.06
	Combined compounding and conversion	8.91×10^{-3}	1.05	0.89	0.16

Table 3.5 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.)
Rubber	Compounding	0.01	1.49	0.17	0.22
	Conversion	4.46×10^{-3}	0.61	0.61	0.09
	Combined compounding and conversion	0.02	1.93	1.62	0.29
Poly-urethane	Compounding	0.01	1.49	0.17	0.22
	Conversion	4.46×10^{-3}	0.61	0.61	0.09
	Combined compounding and conversion	0.02	1.93	1.62	0.29
Textiles/ fabric coating	Compounding	3.56×10^{-3}	0.52	0.17	0.08
	Conversion	8.91×10^{-3}	1.05	0.17	0.16
	Combined compounding and conversion	0.01	1.4	1.18	0.21
Pigment dispersions	Production of dispersions	0.01	1.49	1.25	0.22
Paints	Formulation	0.07	7.22	5.97	1.08
	Application	5.35×10^{-3}	0.70	0.17	0.10

Note that production is not included in this table since the production sites only discharge to the marine environment. The predicted regional concentrations are 0.17 μg/l for surface water and 0.042 mg/kg wet weight for sediment.

Predicted concentrations were also calculated for the marine environment using the EUSES program and are included in Table 3.6.

Table 3.6 Summary of predicted local concentrations for the marine compartment

Scenario		PEC$_{local}$		
		Marine water - emission episode (μg/l)	Marin water - annual average (μg/l)	Marine sediment (mg/kg wet wt.)
Production of isodecyl diphenyl phosphate		18.8[a]	5.4[a]	2.81
PVC – 1	Compounding	0.86	0.71	0.13
	Conversion	2.09	1.72	0.31
	Combined compounding and conversion	2.94	2.42	0.44
PVC – 2	Compounding	0.2	0.17	0.03
	Conversion	0.33	0.27	0.05
	Combined compounding and conversion	0.51	0.42	0.08

Table 3.6 continued.

Scenario		**PEC$_{local}$**		
		Marine water - emission episode (µg/l)	**Marin water - annual average (µg/l)**	**Marine sediment (mg/kg wet wt.)**
PVC – 3	Compounding	0.25	0.21	0.04
	Conversion	0.41	0.34	0.06
	Combined compounding and conversion	0.65	0.54	0.1
PVC – 4	Compounding	0.2	0.17	0.03
	Conversion	0.08	0.07	0.01
	Combined compounding and conversion	0.26	0.22	0.04
PVC – 5	Compounding	0.2	0.08	0.03
	Conversion	0.33	0.12	0.05
	Combined compounding and conversion	0.51	0.18	0.08
PVC – 6	Compounding	0.2	0.02	0.03
	Conversion	0.08	0.08	0.01
	Combined compounding and conversion	0.26	0.22	0.04
Rubber	Compounding	0.39	0.02	0.06
	Conversion	0.14	0.14	0.02
	Combined compounding and conversion	0.51	0.42	0.08
Poly-urethane	Compounding	0.39	0.02	0.06
	Conversion	0.14	0.14	0.02
	Combined compounding and conversion	0.51	0.42	0.08
Textiles/ fabric coating	Compounding	0.12	0.02	0.02
	Conversion	0.26	0.02	0.04
	Combined compounding and conversion	0.36	0.3	0.05
Pigment dispersions	Production of dispersions	0.39	0.32	0.06
Paints	Formulation	2.0	1.64	0.3
	Application	0.16	0.02	0.02

Notes: a) Calculation uses average dilution in receiving water. If minimum dilution at the site was used, the PEC would be a factor of 1.88 times higher. Similarly if maximum dilution at the site was used, the PEC would be a factor of 6.67 times lower.

Measured levels in water and sediment

Isodecyl diphenyl phosphate was monitored in England and Wales over the period November 2007 to April 2008 as part of the Environment Agency's Targeted Risk Based Monitoring (TRBM) initiative. Six samples were collected at approximately weekly intervals from 15 paired WWTP effluent/receiving water sites across all eight

Environment Agency Regions. The site selection criteria are not specified – it is likely that most are reasonably large WWTP with mixed industrial/household influent.

There were no positive detections of isodecyl diphenyl phosphate in any sample, at a detection limit of 0.05 µg/l.

Boethling and Cooper (1985) reported the results of an early 1980s survey of the levels of isodecyl 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 isodecyl diphenyl phosphate in sediment in the United States. The substance was not found (detection limit of the method was 0.03-0.2 mg/kg) in four samples from Saginaw River (industrialised area), three samples from Baltimore Harbour (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), but was present at below 0.13 mg/kg in one out of two samples from Detroit River (industrialised area). The report indicates that some interfering material was present in the sample and so it was not possible to determine precise concentrations.

There are insufficient data available to make a comparison between measured levels and predicted concentrations for the various scenarios considered. Predicted concentrations are used in the risk characterisation.

3.3.2 Terrestrial compartment

Calculation of PECs

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

Table 3.7 Summary of predicted local concentrations for the terrestrial compartment

Scenario		PEC_{local}			
		Annual average conc. in air (mg/m^3)	Agricultural soil – 30 day average (mg/kg wet wt.)	Agricultural soil – 180 day average (mg/kg wet wt.)	Groundwater under agricultural soil (µg/l)
Production of isodecyl diphenyl phosphate		1.92×10^{-7}	1.4×10^{-3a}	1.4×10^{-3a}	0.01^{a}
PVC – 1	Compounding	6.65×10^{-7}	0.87	0.85	7.02
	Conversion	9.62×10^{-5}	2.15	2.11	17.5
	Combined compounding and conversion	9.62×10^{-5}	3.02	2.96	24.5

Table 3.7 continued.

Scenario		**PEC$_{local}$**			
		Annual average conc. in air (mg/m^3)	**Agricultural soil – 30 day average (mg/kg wet wt.)**	**Agricultural soil – 180 day average (mg/kg wet wt.)**	**Groundwater under agricultural soil (μg/l)**
PVC – 2	Compounding	3.05×10^{-6}	0.19	0.19	1.56
	Conversion	1.45×10^{-5}	0.32	0.32	2.61
	Combined compounding and conversion	1.73×10^{-5}	0.51	0.50	4.16
PVC – 3	Compounding	3.85×10^{-6}	0.25	0.24	2.0
	Conversion	1.85×10^{-5}	0.41	0.40	3.34
	Combined compounding and conversion	2.21×10^{-5}	0.66	0.64	5.32
PVC – 4	Compounding	3.05×10^{-6}	0.19	0.19	1.56
	Conversion	3.05×10^{-6}	0.07	0.06	0.53
	Combined compounding and conversion	5.9×10^{-6}	0.26	0.25	2.08
PVC – 5	Compounding	1.33×10^{-6}	0.19	0.19	1.56
	Conversion	5.9×10^{-6}	0.32	0.31	2.6
	Combined compounding and conversion	7.05×10^{-6}	0.51	0.50	4.14
PVC – 6	Compounding	2.02×10^{-7}	0.19	0.19	1.56
	Conversion	3.67×10^{-6}	0.07	0.06	0.53
	Combined compounding and conversion	5.9×10^{-6}	0.26	0.25	2.08
Rubber	Compounding	2.11×10^{-7}	0.38	0.38	3.1
	Conversion	7.14×10^{-6}	0.13	0.13	1.05
	Combined compounding and conversion	1.16×10^{-5}	0.51	0.50	4.15
Polyurethane	Compounding	2.11×10^{-7}	0.38	0.38	3.1
	Conversion	7.14×10^{-6}	0.13	0.13	1.05
	Combined compounding and conversion	1.16×10^{-5}	0.51	0.50	4.15
Textiles/ fabric coating	Compounding	1.92×10^{-7}	0.10	0.10	0.84
	Conversion	2.3×10^{-7}	0.26	0.25	2.07
	Combined compounding and conversion	1.16×10^{-5}	0.36	0.35	2.91
Pigment dispersions	Production of dispersions	5.9×10^{-6}	0.38	0.38	3.11
Paints	Formulation	3.06×10^{-5}	2.04	2.0	16.5
	Application	1.92×10^{-7}	0.15	0.15	1.25

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

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

PEC$_{regional}$ = 9.7×10^{-4} mg/kg wet weight for agricultural soil

= 8.0×10^{-3} μg/l for pore water of agricultural soil
= 1.4×10^{-3} mg/kg wet weight for natural soil
= 0.08 mg/kg wet weight for industrial soil

No measured data appear to be available, so it is not possible to carry out a comparison between measured levels and predicted levels. Calculated PECs are therefore used in the risk characterisation.

3.3.3 Air compartment

Calculation of PECs

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

The predicted regional concentration in air is 1.9×10^{-7} mg/m^3.

No measured data appear to be available, so it is not possible to carry out a comparison of measured levels with predicted levels. Calculated PECs are therefore used in the risk characterisation.

3.3.4 Non-compartment specific exposure relevant for the food chain

Predicted concentrations in biota and food

Predicted concentrations of isodecyl diphenyl phosphate in fish and earthworms are shown in Table 3.8 along with predicted concentrations in marine fish and marine top predators. Predicted concentrations in food for human consumption are shown in Table 3.9. The concentrations have been calculated using EUSES 2.0.3.

Table 3.8 Summary of predicted local concentrations for secondary poisoning

Scenario		Predicted concentration			
		Fish (mg/kg)	Earthworms (mg/kg)	Marine fish (mg/kg)	Marine top predators (mg/kg)
Production of isodecyl diphenyl phosphate		n/a	0.03	0.91	0.19
PVC – 1	Compounding	0.47	10.5	0.12	0.03
	Conversion	1.08	26	0.29	0.06
	Combined compounding and conversion	1.49	36.5	0.41	0.09
PVC – 2	Compounding	0.15	2.34	0.03	0.01
	Conversion	0.21	3.9	0.05	0.01
	Combined compounding and conversion	0.3	6.21	0.07	0.02

Table 3.8 continued.

Scenario		Predicted concentration			
		Fish (mg/kg)	Earthworms (mg/kg)	Marine fish (mg/kg)	Marine top predators (mg/kg)
PVC – 3	Compounding	0.17	2.99	0.04	0.01
	Conversion	0.25	4.98	0.06	0.02
	Combined compounding and conversion	0.37	7.94	0.09	0.02
PVC – 4	Compounding	0.15	2.34	0.03	0.01
	Conversion	0.09	0.80	0.01	6.93×10^{-3}
	Combined compounding and conversion	0.18	3.11	0.04	0.01
PVC – 5	Compounding	0.09	2.34	0.02	7.27×10^{-3}
	Conversion	0.12	3.88	0.02	8.63×10^{-3}
	Combined compounding and conversion	0.15	6.19	0.03	0.01
PVC – 6	Combined compounding and conversion	0.18	3.11	0.04	0.01
	Compounding	0.06	2.33	5.31×10^{-3}	5.24×10^{-3}
	Conversion	0.09	0.81	0.02	7.3×10^{-3}
Rubber	Compounding	0.06	4.64	5.4×10^{-3}	5.26×10^{-3}
	Conversion	0.13	1.58	0.03	9.37×10^{-3}
	Combined compounding and conversion	0.3	6.2	0.07	0.02
Poly-urethane	Compounding	0.06	4.64	5.4×10^{-3}	5.26×10^{-3}
	Conversion	0.13	1.58	0.03	9.37×10^{-3}
	Combined compounding and conversion	0.3	6.2	0.07	0.02
Textiles/ fabric coating	Compounding	0.06	1.26	5.27×10^{-3}	5.23×10^{-3}
	Conversion	0.06	3.1	5.34×10^{-3}	5.25×10^{-3}
	Combined compounding and conversion	0.23	4.36	0.05	0.01
Pigment dispersions	Production of dispersions	0.24	4.65	0.06	0.02
Paints	Formulation	1.03	24.7	0.28	0.06
	Application	0.06	1.87	5.29×10^{-3}	5.24×10^{-3}

Notes: a) Calculation uses average dilution in receiving water. If minimum dilution at the site was used, the PEC would be around 1.88 times higher. Similarly, if maximum dilution at the site was used, the PEC would be approximately 6.67 times lower.

b) Sewage sludge from the production site is not applied to land.

As no measured data are available, it is not possible to carry out a comparison of measured and predicted levels. Calculated PECs are therefore used in the risk characterisation.

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

Scenario		Predicted 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 isodecyl diphenyl phosphate		1.81[a]	0.02	1.4×10^{-4}	1.4×10^{-3}	5.8×10^{-4}	1.8×10^{-4}	0	3.2×10^{-3}
PVC – 1	Compounding	0.88	14.8	1.8×10^{-3}	7.0×10^{-3}	4.2×10^{-3}	1.3×10^{-3}	4.7×10^{-7}	0.08
	Conversion	2.1	36.7	0.07	0.02	0.04	0.01	9.6×10^{-5}	0.21
	Combined compounding and conversion	2.92	51.5	0.07	0.02	0.05	0.01	9.6×10^{-5}	0.29
PVC – 2	Compounding	0.24	3.29	2.5×10^{-3}	1.6×10^{-3}	1.9×10^{-3}	6.0×10^{-4}	2.9×10^{-6}	0.02
	Conversion	0.36	5.49	0.01	2.6×10^{-3}	6.3×10^{-3}	2.0×10^{-3}	1.4×10^{-5}	0.03
	Combined compounding and conversion	0.54	8.75	0.01	4.2×10^{-3}	8.1×10^{-3}	2.6×10^{-3}	1.7×10^{-5}	0.05
PVC – 3	Compounding	0.29	4.2	3.1×10^{-3}	2.0×10^{-3}	2.4×10^{-3}	7.6×10^{-4}	3.7×10^{-6}	0.02
	Conversion	0.44	7.02	0.01	3.3×10^{-3}	8.1×10^{-3}	2.5×10^{-3}	1.8×10^{-5}	0.04
	Combined compounding and conversion	0.68	11.2	0.02	5.3×10^{-3}	0.01	3.3×10^{-3}	2.2×10^{-5}	0.06
PVC – 4	Compounding	0.24	3.29	2.5×10^{-3}	1.6×10^{-3}	1.9×10^{-3}	6.0×10^{-4}	2.9×10^{-6}	0.02
	Conversion	0.12	1.12	2.3×10^{-3}	5.3×10^{-4}	1.3×10^{-3}	4.2×10^{-4}	2.9×10^{-6}	6.4×10^{-3}
	Combined compounding and conversion	0.3	4.38	4.6×10^{-3}	2.1×10^{-3}	3.2×10^{-3}	9.9×10^{-4}	5.7×10^{-6}	0.02
PVC – 5	Compounding	0.13	3.28	1.2×10^{-3}	1.6×10^{-3}	1.3×10^{-3}	4.2×10^{-4}	1.1×10^{-6}	0.02
	Conversion	0.18	5.46	4.7×10^{-3}	2.6×10^{-3}	3.4×10^{-3}	1.1×10^{-3}	5.7×10^{-6}	0.03
	Combined compounding and conversion	0.25	8.72	5.8×10^{-3}	4.1×10^{-3}	4.7×10^{-3}	1.5×10^{-3}	6.9×10^{-6}	0.05

Table 3.9 continued.

Scenario		**Predicted concentration**							
		Fish (mg/kg)	**Root crops (mg/ kg)**	**Leaf crops (mg/kg)**	**Drinking water (mg/l)**	**Meat (mg/kg)**	**Milk (mg/kg)**	**Air (mg/m^3)**	**Total daily human intake (mg/kg bw/day)**
PVC – 6	Compounding	0.06	3.28	4.3×10^{-4}	1.6×10^{-3}	9.5×10^{-4}	3.0×10^{-4}	9.5×10^{-9}	0.02
	Conversion	0.13	1.12	2.7×10^{-3}	5.3×10^{-4}	1.5×10^{-3}	4.8×10^{-4}	3.5×10^{-6}	6.4×10^{-3}
	Combined compounding and conversion	0.3	4.38	4.6×10^{-3}	2.1×10^{-3}	3.2×10^{-3}	9.9×10^{-4}	5.7×10^{-6}	0.02
Rubber	Compounding	0.06	6.53	7.2×10^{-4}	3.1×10^{-3}	1.8×10^{-3}	5.8×10^{-4}	1.9×10^{-8}	0.04
	Conversion	0.2	2.21	5.3×10^{-3}	1.1×10^{-3}	3.0×10^{-3}	9.4×10^{-4}	7.0×10^{-6}	0.01
	Combined compounding and conversion	0.54	8.73	9.0×10^{-3}	4.2×10^{-3}	6.2×10^{-3}	2.0×10^{-3}	1.1×10^{-5}	0.05
Poly-urethane	Compounding	0.06	6.53	7.2×10^{-4}	3.1×10^{-3}	1.8×10^{-3}	5.8×10^{-4}	1.9×10^{-8}	0.04
	Conversion	0.20	2.21	5.3×10^{-3}	1.1×10^{-3}	3.0×10^{-3}	9.4×10^{-4}	7.0×10^{-6}	0.01
	Combined compounding and conversion	0.54	8.73	9.0×10^{-3}	4.2×10^{-3}	6.2×10^{-3}	2.0×10^{-3}	1.1×10^{-5}	0.05
Textiles/ fabric coating	Compounding	0.06	1.76	2.9×10^{-4}	8.4×10^{-4}	5.4×10^{-4}	1.7×10^{-4}	1.9×10^{-10}	9.8×10^{-3}
	Conversion	0.06	4.36	5.4×10^{-4}	2.1×10^{-3}	1.3×10^{-3}	3.9×10^{-4}	3.8×10^{-8}	0.02
	Combined compounding and conversion	0.4	6.13	8.8×10^{-3}	2.9×10^{-3}	5.5×10^{-3}	1.8×10^{-3}	1.1×10^{-5}	0.03
Pigment dispersions	Production of dispersions	0.42	6.55	4.8×10^{-3}	3.1×10^{-3}	3.7×10^{-3}	1.2×10^{-3}	5.7×10^{-6}	0.04
Paints	Formulation	2.0	34.8	0.02	0.02	0.02	6.2×10^{-3}	3.0×10^{-5}	0.2
	Application	0.06	2.63	3.7×10^{-4}	1.3×10^{-3}	7.7×10^{-4}	2.4×10^{-4}	2.8×10^{-10}	0.01
Regional sources		0.06	0.02	1.4×10^{-4}	4.2×10^{-5}	8.3×10^{-5}	2.6×10^{-5}	1.9×10^{-7}	1.9×10^{-4}

Notes: a) Calculation uses average dilution in receiving water. If minimum dilution at the site was used, the concentration would be a factor of 1.88 times higher. Similarly, if maximum dilution at the site was used, the concentration would be approximately 6.67 times lower.

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

4.1 Aquatic compartment

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

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

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

One important property when considering the aquatic toxicity data is water solubility. The water solubility of isodecyl diphenyl phosphate is in the range 0.011-0.75 mg/l, and the value of 0.011 mg/l is used in this assessment. Several studies have been carried out at concentrations greater than this range of water solubility and, although this in itself does not necessarily invalidate the test (for example, co-solvents or solubility aids could have been used in the test to aid dispersion of the substance in the test media), this then introduces some uncertainty over the concentration to which the organisms were actually exposed in the test. In cases where it is clear that undissolved test substance was present in the test media, the tests have been marked as invalid.

A further complication arises in the interpretation of the test results, as some products containing significant amounts of triphenyl phosphate have been tested. This substance itself has been shown to be very toxic to aquatic organisms (see the risk evaluation report for triphenyl phosphate in this series) but it is impossible to determine if the effects seen in the tests with commercial isodecyl diphenyl phosphate products were due to the isodecyl diphenyl phosphate component, the triphenyl phosphate component or both.

4.1.1 Toxicity to fish

Short-term studies

Fresh-water fish

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

The acute toxicity of isodecyl diphenyl phosphate (no information on purity) to bluegill sunfish (*Lepomis macrochirus*) has been determined by Dawson *et al.* (1977). The test system used was a static system and the report indicates that gentle aeration was applied if the dissolved oxygen was being depleted during the test (no information is given as to whether or not this occurred in the test with isodecyl diphenyl phosphate). The 96-hour LC_{50} was 6,700 mg/l. Concentrations tested in this study are much greater than the water solubility of the substance, and the substance appears to have been added directly to the test vessel. It is therefore possible that the effects seen in this test were indirect effects resulting from undissolved test substance rather than a direct toxic effect of the substance itself and so the test is considered invalid.

Cleveland *et al.* (1986) determined the acute toxicity of a commercial isodecyl diphenyl phosphate product to rainbow trout (*Oncorhynchus mykiss*) and bluegill (*Lepomis macrochirus*). The substance tested consisted of 91 per cent isodecyl diphenyl phosphate and six per cent triphenyl phosphate. The tests were all carried out using a static test system using acetone as co-solvent. The 96-hour LC_{50} was determined as 26 mg/l for *O. mykiss* and 72 mg/l for *L. macrochirus*. Tests were also carried out to investigate the effects of varying the water hardness (in the range 40 to 320 mg/l as $CaCO_3$), pH (in the range 6.5 to 8.5) and temperature (in the range 7°C to 17°C for *O. mykiss* and 12°C to 22°C for *L. macrochirus*) on the toxicity. None of these parameters were found to have a significant affect on the 96-hour LC_{50} determined for either species. The report indicates that erratic mortalities were seen in the tests with *L. macrochirus* at the higher concentrations tested and so the LC_{50} value for this species is only approximate. These LC_{50} values are all above the water solubility for this substance, but it is not clear from the report if undissolved test substance was present.

Ferro (2002) reports the 96-hour LC_{50} from unpublished studies with a commercial isodecyl diphenyl phosphate as 18 mg/l for fathead minnow (*Pimephales promelas*) and 7.6 mg/l for rainbow trout (*Oncorhynchus mykiss*). These results are again above the water solubility of the substance.

IUCLID (2000) report 96-hour LC_{50}s of above100 mg/l and 10-100 mg/l from unpublished industry studies with bluegill (*Lepomis macrochirus*) and rainbow trout (*Oncorhynchus mykiss*) respectively. The report indicates that no toxicity was seen at concentrations in excess of the solubility of the substance.

A fish 96-hour LC_{50} and a 14-day LC_{50} of 0.85 mg/l and 0.53 mg/l respectively can be estimated for isodecyl diphenyl phosphate from the log K_{ow} value of 5.44 using the US EPA ECOSAR (version 0.99h) software.

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

Species	Test guideline	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End point	Control response	Effect conc.	Reference	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O					
Lepomis macrochirus		Loading was <1 g/l.	33-75 mm	Direct addition of the test substance.	1,000, 5,000 and 10,000 mg/l plus control.	N	Well water	23°C	55	7.6-7.9	Static		Mortality	1.3% Mortality overall.	96h-LC_{50} = 6,700 mg/l	Dawson *et al.* 1977	3
	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artificial water	22°C	38-46	7.2-7.6	Static		Mortality		96h-LC_{50} = 72 mg/l	Cleveland *et al.* 1986	2
		10		Acetone		N		19°C			Static		Mortality		96h-LC_{50} >100 mg/l	IUCLID 2002	4
Oncorhynchus mykiss	ASTM 1980			Acetone at ≤0.67 ml/l.	Logarithmic series plus control and solvent control.	N	Artificial water	12°C	38-46	7.2-7.6	Static		Mortality		96h-LC_{50} = 26 mg/l	Cleveland *et al.* 1986	2
	OECD 203					N							Mortality		96h-LC_{50} = 7.6 mg/l	Ferro 2002, IUCLID 2000	4
		10				N		12°C			Static		Mortality		96h-LC_{50} = 10-100 mg/l	IUCLID	4
Pimephales promelas	OECD 203					N							Mortality		96h-LC_{50} = 18 mg/l	Ferro 2002, IUCLID 2000	4

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.

Using the methods given in the TGD, a 96-hour LC_{50} of 0.23 mg/l can be estimated using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.44.

Marine fish

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

The acute toxicity of isodecyl phosphate (no information on purity) to tidewater silverside (*Menidia beryllina*) has been determined by Dawson *et al.* (1977). The test system used was a static system and continuous aeration was applied during the test. The 96-hour LC_{50} determined was 1,400 mg/l. Concentrations tested in this study are much greater than the water solubility of the substance, and the substance appears to have been added directly to the test vessel. It is therefore possible that the effects seen in this test were indirect effects of undissolved test substance rather than a direct toxic effect of the substance itself and so the test is considered invalid.

Long-term studies

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

A 90-day partial life-cycle toxicity study has been carried out for a commercial isodecyl diphenyl phosphate product using fathead minnows (*Pimephales promelas*) (Cleveland *et al.* 1986). The test substance consisted of 91 per cent isodecyl diphenyl phosphate and six per cent triphenyl phosphate. The study was carried out using a flow-through test system. The nominal concentrations of the test substance used were 0.05, 0.09, 0.19, 0.38 and 0.75 mg/l. Analyses of the water concentrations were carried out every two weeks during the experiment and these showed mean measured concentrations in the various exposure groups (expressed as the sum of the isodecyl diphenyl phosphate and the triphenyl phosphate components of the product) of 0.018, 0.031, 0.057, 0.105 and 0.336 mg/l respectively, corresponding to around 28 to 45 per cent of the nominal values. The survival of the fish was not statistically significantly different ($p=0.05$) in any treatment group compared with the control group. However, survival in the control group was relatively low (around 68 per cent survival at 30 days and 60 per cent survival at 60 and 90 days). Growth of the fish was found to be statistically significantly ($p=0.05$) reduced at 30 days compared to the control group at concentrations of 0.031, 0.105 and 0.336 mg/l but not at 0.018 or 0.057 mg/l. By day 60 the growth of the exposed fish was significantly reduced compared with the control group at a measured concentration of 0.336 mg/l only, and at day 90 the growth of the fish was significantly reduced compared with the control population at a mean measured concentration of 0.105 and 0.336 mg/l. Based on these data, the 30-day no observed effect concentration (NOEC) for growth is estimated to be around 0.018-0.057 mg/l, the 60-day NOEC for growth around 0.105 mg/l and the 90-day NOEC for growth around 0.057 mg/l. The relatively poor survival in the control population indicates that the conditions used in this particular test may not have been optimum for survival and growth.

A long-term no effect concentration of 0.032 mg/l is predicted with the US EPA ECOSAR program (v0.99h) which is similar to the above results.

No long-term toxicity data appear to be available for isodecyl diphenyl phosphate with marine fish.

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

Species	Test guideline	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						Endpoint	Control response	Effect conc.	Ref.	Val.
							Media	Temp.	Sal.	pH	Static/ flow	D.O.					
Menidia beryllina		Loading <1 g/l.	40-100 mm	Direct addition of the test substance.	1,000, 2,000, 3,200 and 5,000 mg/l plus control.	N	Artificial seawater	20°C			Static		Mortality	3% Mortality overall.	96h-LC_{50} = 1,400 mg/l	Dawson *et al.* 1977	3

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

Table 4.3 Long-term toxicity of isodecyl diphenyl phosphate to freshwater fish

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control response	Effect conc.	Reference	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 0.05, 0.09, 0.19, 0.38 and 0.75 mg/l plus solvent control. Measured concs. were 28-45% of nominal.	M	Artificial water	25°C	40	7.2-7.4	Flow		Growth	Mean length at 30 days = 27.1 ± 3.3 mm.	30d-NOEC = 0.018-0.057 mg/l	Cleveland *et al.* 1986.	2
														Mean length at 60 days = 32.7 ± 2.7 mm.	60d-NOEC = 0.105 mg/l		
														Mean length at 90 days = 37.4 ± 3.4 mm.	90d-NOEC = 0.057 mg/l		
													Mortality	Mortality was 32% at day 30 and 40% at day 60 and day 90	30d-NOEC ≥0.336 mg/l 60d-NOEC ≥0.336 mg/l 90d-NOEC ≥0.336 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.

4.1.2 Toxicity to aquatic invertebrates

Short-term studies

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

Adams and Heidolph (1985) determined the acute toxicity of a commercial isodecyl diphenyl phosphate product to *Daphnia magna* using the ASTM E729 method. The 24-hour and 48-hour EC_{50} values determined were 0.79 mg/l and 0.48 mg/l respectively. These values are approaching the upper limit of the reported water solubility for the test substance.

EG and G Bionomics (1979a) report that a 48-hour EC_{50} of 0.22 mg/l was determined for isodecyl diphenyl phosphate as part of a 21-day *Daphnia magna* reproduction study. The value is based on nominal concentrations using a static procedure. The test report indicates that *Daphnids* were found to be trapped on the surface at concentrations of 0.22 mg/l and above and so it is not clear if the results from this test represent a true toxic effect or a physical effect (for example, caused by undissolved test substance adhering to the exposed *Daphnids*). However, the test report also notes that, during the 21-day reproduction study (carried out using a flow-through test system and measured concentrations), all animals exposed to a mean measured concentration of 49 µg/l were found to be dead/immobile within 48 hours of the start of the experiment. Based on these data, the 48-hour EC_{50} appears to be below 49 µg/l. Further details of the 21-day reproduction test are given in the next section.

Sanders *et al.* (1985) determined the acute toxicity of a commercial isodecyl diphenyl phosphate to *Daphnia magna*, midge (*Chironomus plumosus*) and an amphipod (*Gammarus pseudolimnaeus*). The tests were carried out using static test systems. The toxicity values obtained were a 48-hour EC_{50} of 18 mg/l for *D. magna*, a 48-hour EC_{50} of 1.2 mg/l for *C. plumosus* and a 96-hour LC_{50} of 4.4 mg/l for *G pseudolimnaeus*. These results are all above the reported water solubility of the substance.

Further, unpublished, invertebrate toxicity data are reported in IUCLID (2000). The values reported for isodecyl diphenyl phosphate include a 48-hour EC_{50} of 0.61 mg/l for midge (*Chironomus tentans*) and a 48-hour EC_{50} of 1.32 mg/l for the chironomid *Paratanytarsus parthenogentica.* The result for *P. parthenogentica* is above the upper limit for the water solubility of the substance.

Using the methods given in the TGD, a 48-hour EC_{50} of 0.56 mg/l can be estimated for *Daphnia magna* using the equation for polar narcosis (recommended for esters) and a log K_{ow} of 5.44. This is in good agreement with the available experimental data. The US EPA ECOSAR program (v0.99h) predicts a value of 0.23 mg/l for the same endpoint.

There are no short-term toxicity data for isodecyl diphenyl phosphate with marine invertebrates.

Table 4.4 Short-term toxicity of isodecyl diphenyl phosphate to freshwater invertebrates

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Chironomus plumosus	USEPA 1975		4th instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	22°C	270	7.2-7.4	Static		Immobil. mortality		96h-EC_{50} = 1.2 mg/l	Sanders *et al.* 1985	2
Chironomus tentans	USEPA 1975					N							Immobil. mortality		48h-EC_{50} = 0.61 mg/l	IUCLID 2000	4
Daphnia magna	ASTM E729		<24 h	Dimethyl formamide or acetone 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		24h-EC_{50} = 0.79 mg/l 48h-EC_{50} = 0.48 mg/l	Adams and Heidolph 1985	2
	USEPA 1975		<24 h	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-7.4	Static		Immobil. mortality		48h-EC_{50} = 18 mg/l	Sanders *et al.* 1985	2
	USEPA 1975	15 per treatment	<24 h	Dimethyl formamide (conc. not given)	28, 47, 78, 130, 220, 360 and 600 µg/l plus control and solvent control	N	Rec. well water	22°C	175	8.1	Static		Immobil. mortality	0% mortality	48h-EC_{50} = 0.22 mg/l	IUCLID 2000	2

Table 4.4 continued.

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Gammarus pseudolimnaeus	USEPA 1975		Early instar	Acetone at up to 0.1 ml/l	Control and solvent control run	N	Well water	18°C	270	7.2-7.4	Static		Mortality		96h-LC_{50} = 4.4 mg/l	Sanders *et al.* 1985	2
Paratanytarsus parthenogentica	USEPA 1975					N							Immobil./ mortality		48hEC_{50} = 1.32 mg/l	IUCLID 2000	4

Notes: N = Nominal concentration.
Temp. = Temperature.
M = Measured concentration.
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.

Long-term studies

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

Adams and Heidolph (1985) determined the toxicity of a commercial isodecyl diphenyl phosphate product to *Daphnia magna* in a flow-through 21-day reproduction study. The 21-day NOEC values were determined to be 0.008 mg/l based on survival and 0.004 mg/l based on reproduction.

EG and G Bionomics (1979a) carried out a 21-day *Daphnia magna* reproduction study with isodecyl diphenyl phosphate. The nominal concentrations used in the test were 9.4, 19, 38, 75 and 150 µg/l. The corresponding mean measured concentration (based on two replicate samples collected at weekly intervals) were below 4.0, below 4.5, 7.6, 20 and 49 µg/l respectively (the detection limit of the method used was around 4 µg/l). All *Daphnia* exposed to a mean concentration of 49 µg/l died during the first 48 hours of the experiment, and the survival of the *Daphnia* exposed to a mean measured concentration of 20 µg/l was statistically significantly ($p=0.05$) reduced compared with both the control and solvent control populations. The survival of *Daphnia* exposed to a mean measured concentration of 7.6 µg/l was reduced compared to the control and solvent control populations, but this reduction was never statistically significant. Thus the 21-day NOEC based on survival was 7.6 µg/l. The cumulative number of offspring per female was found to be reduced compared to the control and solvent control populations at concentrations of 7.6 µg/l and 20 µg/l. These reductions were statistically significant at all time points at 20 µg/l, but were only statistically significant for the 7.6 µg/l treatment group on test days 8, 9 and 11 when compared with the solvent control group and days 11 to 17 when compared with the control group. No statistically significant effects were seen at the lower concentrations tested. The 21-day NOEC based on reproduction was therefore the nominal concentration of 19 µg/l. The actual mean measured concentration in this exposure could not be determined (below the detection limit of the method used) but the exposure concentration in this treatment group was estimated as 3.8 µg/l assuming that the actual concentration was around 20 per cent of the nominal concentrations (based on the fact that the mean measured concentration in the nominal 38 µg/l treatment was 20 per cent of the nominal value (7.6 µg/l)). Thus the 21-day NOEC based on reproduction was 3.8 µg/l, which is very similar to the value obtained by Adams and Heidolph (1984) above (it is possible that these are in fact the same study).

Sanders *et al.* (1985) investigated the effects of a commercial isodecyl diphenyl phosphate on survival and reproduction of *Daphnia magna* over 21 days. The test was carried out using a flow-through system with nominal exposure concentrations. Survival of the adults at 21 days was statistically significantly ($p=0.05$) reduced from that of the control population at concentrations of 0.010 mg/l and above, and the 21-day NOEC for survival was 0.003 mg/l. For the reproduction endpoint, the mean number of offspring/adult was found to be statistically significantly reduced ($p=0.05$) at all concentrations tested and so the NOEC for this endpoint was below 0.003 mg/l. However, survival of adults in the control population at 21 days was only 75 per cent (the current OECD 202 reproduction test guidelines recommends that adult survival in the controls should be at least 80 per cent), and so the actual results from this study are considered less reliable than those from other studies.

No long-term toxicity data are available for isodecyl diphenyl phosphate with marine invertebrates.

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

Species	Test guide-line	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Daphnia magna	USEPA 1975	20 per replicate, four replicates per treatment	<24 h	Acetone or dimethyl formamide 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$_{50}$ = 0.015 mg/l 14d-EC$_{50}$ = 0.014 mg/l 21d-EC$_{50}$ = 0.014 mg/l	Adams and Heidolph 1985	2
													Survival		21d-NOEC = 0.008 mg/l		
													Repro.		21d-NOEC = 0.004 mg/l		
		10 per replicate, two replicates per treatment			3, 10, 40 and 80 µg/l plus control	N	Well water	18°C	270	7.2-7.4	Flow		Survival	75% survival	21d-NOEC = 0.01 mg/l	Sanders *et al.* 1985	3
													Repro.	Mean offspring /adult = 411	21-NOEC <0.003 mg/l		

Table 4.5 continued.

Species	Test guideline	Number of animals/ treatment	Age/ size	Cosolvent	Concs. tested	N or M	Test conditions						End-point	Control resp.	Effect conc.	Ref.	Val.
							Media	Temp.	Hard.	pH	Static/ flow	D.O.					
Daphnia magna	USEPA, 1975	20 per replicate, four replicates per treatment	<24 h	Dimethyl formamide at up to 41 µl/l.	5 concs. plus control and solvent control. Nominal concs. were 150, 75, 38, 19 and 9.4 µg/l. The respective mean measured concs. were 49, 20, 7.6 <4.5 and <4.0 µg/l.	M	Recon. well water	23°C	168-170 mg/l	8.1-8.3	Flow	7.6-7.8	Survival	91% survival in control; 94% survival in solvent control	21d-NOEC = 0.0076 mg/l	EG and G Bionomics 1979a	2
													Repro.	Mean offspring /adult ~70 for control and solvent control (read from graph)	21d-NOEC = 0.0038 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.

4.1.3 Toxicity to algae

The toxicity of isodecyl diphenyl phosphate to freshwater algae is summarised in Table 4.6.

The effect of isodecyl diphenyl phosphate exposure on *in vivo* chlorophyll A production in *Selenastrum capricornutum*[7] has been determined (EG and G Bionomics 1979b). The amounts of chlorophyll A present were determined after 24, 48, 72 and 96 hours by fluorometric measurements. The 72-hour and 96-hour EC_{50}s based on this endpoint were reported to be 154 and 71 mg/l respectively. In addition to the chlorophyll A measurements, the total cell numbers (biomass) present were determined after 96 hours exposure. The 96-hour EC_{50} based on biomass was determined to be 79 mg/l. Note that these values are based on nominal concentrations well above the reported water solubility of the test substance, and the toxicity values obtained had quite large 95 per cent confidence limits (for example, 4 to 6,608 mg/l and 8 to 624 mg/l for the 72-hour and 96-hour EC_{50} based on chlorophyll A respectively and 8 to 744 mg/l for the 96-hour EC_{50} based on biomass).

The raw data from the EG and G Bionomics (1979b) study were reanalysed to determine if an EC_{50} based on growth rate could be derived (according to the Technical Guidance Document this is the preferred endpoint from an algal toxicity test). The actual cell numbers were determined only at the end of the experiment and so an analysis of growth rate based on the cell numbers could not be made. However, the chlorophyll A measurements were taken at several time points during the experiment and when these data were analysed (assuming the chlorophyll A measurements were proportional to the total cell numbers present) in terms of the average specific growth rate, the 72-hour EC_{50} was 320 mg/l (the highest concentration tested).

Sanders *et al.* (1985) determined the toxicity of a commercial isodecyl diphenyl phosphate product to *Selenastrum capricornutum* over 14 days. The growth of the alga was determined by dry weight measurements. The concentrations tested were 0.1, 1.0, 10 and 100 mg/l and statistically significant ($p=0.05$) reductions in cell growth (dry weight) were seen at concentrations of 1.0 mg/l. Thus, the NOEC was 0.1 mg/l. However, the length of this study (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 result from this test is uncertain.

The USEPA ECOSAR program (v0.99h) predicts a 96-hour EC_{50} value of 0.077 mg/l and a long-term no effect concentration of 0.064 mg/l for green algae.

No data are available on the toxicity of isodecyl diphenyl phosphate to marine algae.

4.1.4 Toxicity to microorganisms

There are no specific test results on toxicity to microorganisms for isodecyl diphenyl phosphate. However, one of the biodegradation studies described in Section 3.1.1 can be used in this context. Sager *et al.* (1979) reported a decrease in biomass at 13 mg/l in a semi-continuous activated sludge test, with no decrease reported at 3 mg/l. Degradation of isodecyl diphenyl phosphate was lower at the higher concentration.

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[7] Now called *Pseudokirchneriella subcapitata*.

Table 4.6 Toxicity of isodecyl diphenyl phosphate to freshwater algae

Species	Test guide-line	Initial inoculum conc.	Cosolvent	Concs. tested	N or M	Test conditions				Endpoint	Control resp.	Effect conc.	Reference	Val.
						Media	Temp.	Hard.	pH					
Selenastrum capricornutum				0.1, 1.0, 10 and 100 mg/l plus control. Each run in triplicate.	N	Well water	24°C	270	7.2-7.4	Biomass (dry weight)		14d-NOEC = 0.1 mg/l (Santicizer 148)	Sanders *et al.* 1985	3
	USEPA 1971	2×10^4 cells/ml	Dimethyl formamide at up to 0.05 ml in each 125 ml flask (~0.4 ml/l)	10, 32, 56, 100 and 320 mg/l plus control and solvent control. Each run in triplicate.	N		24°C		7.2-7.4	Chlorophyll A		72h-EC_{50} = 154 mg/l 96h-EC_{50} = 71 mg/l	EG and G Bionomics 1979b	2
										Biomass		96h-EC_{50} = 79 mg/l	EG and G Bionomics 1979b	2

Notes: N = Nominal concentration.

M_f = Measured concentration in filtered (0.45 μm) solution.

M_u = Measured concentration in unfiltered solution.

M = Measured concentration (not clear if solution was filtered or unfiltered).

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.

In contrast, two biodegradation tests using adapted activated sludge reported high levels of degradation of isodecyl diphenyl phosphate at 20 mg/l and 30 mg/l. It is not possible to reconcile these results; as a conservative approach, a NOEC of 3 mg/l will be used in the assessment as a preliminary screening value.

4.1.5 Toxicity to sediment organisms

No data are available on the toxicity of isodecyl 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 (lowest LC_{50} = 7.6 mg/l), invertebrates (lowest EC_{50} = 0.22 mg/l for *Daphnia magna*) and algae (lowest EC_{50} = 71 mg/l). Given that the water solubility of the test substance is reported to be 0.0011 to 0.75 mg/l, the fish and algal results are difficult to interpret in terms of whether the substance is acutely toxic at concentrations below its solubility limit. The data do, however, indicate that invertebrates (*Daphnia magna*) are the most sensitive species tested.

Long-term toxicity data are available for fish and *Daphnia.* The 90-day NOEC for growth with *Pimephales promelas* was 0.057 mg/l. However the survival was relatively poor in the control population in this test, and the test was not equivalent to a current fish early life stage test as it did not investigate hatching success. Annex B considers the long-term fish data available for triaryl and trialkyl/aryl phosphates as a whole. Based on the analysis of the long-term NOECs from both growth studies and fish early life stage studies, the expected fish NOEC of isodecyl diphenyl phosphate would be around 0.016 mg/l. The 21-day NOEC for *Daphnia magna* from the more reliable reproduction study available is 0.004 mg/l. Although no reliable NOEC is available for algae, it is clear from the data available (and the analysis carried out in Annex B) that it would be higher than the NOEC found for *Daphnia magna.* ECOSAR also predicts a higher NOEC for algae.

Despite the uncertainties over the available long-term fish data, it can be concluded that *Daphnia magna* are likely to be the most sensitive species for derivation of the PNEC for this substance. Therefore, it is proposed that an assessment factor of 10 is applied to the *Daphnia magna* NOEC to give a $PNEC_{water}$ of 0.4 µg/l.

There are no valid data available on marine species. A PNEC of 0.04 µg/l can be calculated using the freshwater data as above with an assessment factor of 100.

Microorganisms

A NOEC of 3 mg/l was selected in Section 4.1.4, for a semi-continuous activated sludge unit operated over 24 weeks and using domestic sludge. For an activated sludge simulation test, the TGD indicates an assessment factor down to one depending on expert judgement. As there are two other degradation studies showing high degradation at higher concentrations, an assessment factor of one is used here, hence the $PNEC_{microorganisms}$ is 3 mg/l.

Sediment

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

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

where $K_{\text{susp-water}}$ = suspended sediment-water partition coefficient = 171 m^3/m^3 (see Section 3.1.2).

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

Using a $PNEC_{water}$ of 0.4 µg/l, $PNEC_{sed}$ can be estimated as 0.059 mg/kg wet weight.

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

For the marine assessment, the marine water PNEC is used in the same way to derive a PNEC of 0.0059 mg/kg wet weight. An additional factor of 10 is applied to the PEC/PNEC ratios in this case as well.

4.2 Terrestrial compartment

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

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

where $K_{\text{soil-water}}$ = soil-water partition coefficient = 206 m^3/m^3 (see Section 3.1.2).

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

Using a $PNEC_{water}$ of 0.4 µg/l, $PNEC_{soil}$ can be estimated as 0.048 mg/kg wet weight.

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

4.3 Atmosphere

No information is available on the toxicity of isodecyl diphenyl phosphate to plants and other organisms exposed via air. The very 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 very low. This means that the possibility of isodecyl diphenyl phosphate contributing to atmospheric effects such as global warming and acid rain is likely to be very small. In addition, as the substance does not contain halogen atoms, it will not contribute to ozone depletion.

4.4 Mammalian toxicity

4.4.1 Toxicokinetics, metabolism and distribution

There are no available *in vivo* or *in vitro* data on the absorption, distribution or elimination of isodecyl diphenyl phosphate in mammals, including humans.

4.4.2 Acute toxicity

Oral

An acute oral lethality study in the rat conducted by Monsanto plc is briefly described in IUCLID (2000), and a further paper that includes a rat acute toxicity experiment was published by Johannsen *et al.* (1977).

In the study reported by Monsanto plc, rats of an unspecified strain were administered undiluted isodecyl diphenyl phosphate. Few study details were reported although it is noted that the test material was administered undiluted to an unspecified number of dose groups, with the high dose group comprising three males and two females; the study was not conducted to GLP. The LD_{50} was found to be greater than 15,800 mg/kg bodyweight, but no signs of reaction to treatment or necropsy findings were reported (Monsanto 1971, cited in IUCLID 2000).

In a study reported by Johannsen *et al.* (1977), single doses of test material were administered by gastric intubation to groups of male and female Sprague-Dawley rats to a maximum dosage of 15.8 g/kg, with animals then being observed over a 14-day period. No further details of the study design were given and the LD_{50} was stated as being greater than 15.8 g/kg bodyweight.

It is unclear, given that both reports relate to work undertaken by Monsanto plc and report the same LD_{50} value, whether these two reports represent the same experiment.

Inhalation

There are two acute inhalation studies in rats of which one was conducted according to EPA TSCA guidelines and to GLP standards.

In the EPA TSCA compliant study by Monsanto plc conducted to GLP, one group of five male and five female rats (strain not specified) was exposed to an aerosol generated from test material heated to 125°C for four hours, and then observed for 14 days. The achieved concentration was 6.3 mg/l, with the particles generated having a median mass aerodynamic diameter of 2.5 µm (SD 2.4), and the average test chamber temperature was 25°C The LC50 was stated to be greater than 6.3 mg/l (Monsanto 1983a, cited in IUCLID 2000).

In another study by Monsanto, not conducted to GLP (Monsanto 1979b, cited in IUCLID 2000), rats of unspecified strain were exposed to air containing test material that had been heated to 163°C to generate a nominal test atmosphere of 2.2 mg/l for six hours. No further study details were reported but the LD_{50} was stated as greater than 2.2 mg/l.

Dermal

An acute dermal lethality study in the rabbit conducted by Monsanto plc is briefly described in IUCLID (2000), and a further published paper that includes a rat acute toxicity experiment was published by Johannsen *et al.* (1977).

In a study not conducted to GLP or to any stated guidelines, rabbits of an unspecified strain were exposed to undiluted test material. The LD_{50} was reported to be greater than 7,940 mg/kg bodyweight but no further information was presented (Monsanto 1971, cited in IUCLID 2000).

In the other study reported by Johannsen *et al.* (1977), undiluted test material was applied to the intact, clipped dorsal skin of New Zealand albino male and female rabbits under occluded conditions. After 24 hours, the test material was removed by washing and the animals were then held for a 14-day observation period after which they were killed and subject to a gross pathological examination. The LD_{50} was reported to be greater than 7.9 g/kg.

It is unclear, given that both the reports relate to work undertaken by Monsanto plc and report similar LD_{50} values, whether these two reports represent the same experiment.

Neurotoxicity

There are no data available on the acute neurotoxicity of isodecyl diphenyl phosphate.

Summary of acute toxicity

No information is available from human studies.

Of the available studies, only one acute inhalation study in rats has been conducted to GLP and test guidelines. However, limited information on a few other studies using the dermal or oral route is available. It is, however, uncertain if some of data reported in IUCLID (2000) relates to the same experiments as were reported in a paper by Johannsen *et al.* (1977). Despite this uncertainty, it is apparent that the LD_{50} by the oral route in the rat is greater than 15,800 mg/kg bodyweight while that for the dermal route in rabbits is greater than 7,940 mg/kg bodyweight. The inhalation LD_{50} in rats is also high at greater than 6.3 mg/l. These values are above the limit doses (2,000 mg/kg in oral and dermal routes, and 5 mg/l for the inhalation route) applied in modern studies, which indicate a low level of toxicity.

4.4.3 Irritation

Skin

The skin irritation potential of isodecyl diphenyl phosphate was investigated in a non-GLP compliant study stated as being conducted to a Draize design by Monsanto (Monsanto 1971, cited in IUCLID 2000). Three rabbits of unspecified strain were employed and the test material was applied undiluted to the intact skin for an unspecified period. No detailed methodology or results were reported although the test was reported as demonstrating slight irritation.

Eye

In a non-GLP compliant study stated as being conducted to a Draize design by Monsanto (Monsanto 1971, cited in IUCLID 2000), test material was applied undiluted to the eyes of three rabbits of unspecified strain. No detailed methodology or results were reported but it was reported that slight irritation of the eye was found.

Summary of irritation

No information is available from human studies.

Limited information is available on the irritant potential of isodecyl diphenyl phosphate to the skin and eye and this comes from a poorly reported secondary source. Nonetheless, given the reports that only slight irritation was observed for both skin and eye, the irritant potential of isodecyl diphenyl phosphate may be considered low.

4.4.4 Corrosivity

Although of limited quality, available studies that assessed skin or eye irritation suggest that isodecyl diphenyl phosphate has only limited irritancy potential and, therefore, it is unlikely that isodecyl diphenyl phosphate possesses corrosive properties.

4.4.5 Sensitisation

One poorly reported dermal study on human volunteers was identified but no experimental animal data are available.

In a patch test on an unspecified number of individuals of unknown atopic status, paper impregnated with isodecyl diphenyl phosphate was applied to the skin and covered by an occlusive dressing for 48 hours. After removal of the patch, the site was scored after 24 and 48 hours. A second patch was applied 15 days after the first application and again removed after a 48-hour exposure period with scoring conducted after 24 and 48 hours. No further methodological details were reported and the study was not conducted under GLP. Detailed results of the examinations of the exposure sites were not reported; however, the study was stated to have shown the chemical to not be sensitizing (Monsanto 1968, cited in IUCLID 2000).

4.4.6 Repeated-dose toxicity

Animal data

There are no data relating to repeated inhalation exposure to isodecyl diphenyl phosphate.

In a 28-day study, Sprague-Dawley rats (numbers not stated) were fed diets containing isodecyl diphenyl phosphate at 0, 33,100, 330, 1,000 or 10,000 ppm; the concentrations were calculated, using a stated conversion factor of 0.09, to be equivalent to achieved dosages of 0, 3, 9, 30, 90 and 900 mg/kg/day, respectively (TSCA, cited in IUCLID 2000). Other details of study methodology, such as extent and timing of clinical pathology or extent of pathology investigations, were not reported. A decrease in serum cholinesterase activity (degree not reported) was noted for rats given 1,000 or 10,000 ppm. A decrease in bodyweight was also noted for those given 10,000 ppm, together with a number of other treatment-related changes suggestive of liver toxicity. These comprised: increase in serum total cholesterol; decrease in serum gamma glutamyl transpeptidase activity; increase in liver weight (unclear if this is in terms of absolute and/or bodyweight-relative values); and centrilobular hypertrophy with cholangitis. For this study, the LOAEL, based on a decrease in serum cholinesterase activity of uncertain extent, was 100 ppm (90 mg/kg/day) with the NOAEL being 330 ppm (30 mg/kg/day).

In another 28-day study (Monsanto 1979a, cited in IUCLID 2000), groups of ten male and ten female Sprague-Dawley rats were fed diet containing isodecyl diphenyl phosphate at concentrations designed to achieve dosages of 0, 250, 500, 750 or 2,000 mg/kg bodyweight. Animals were observed twice daily for signs of toxicity or death. At the end of the treatment period, all animals were killed and subject to a gross pathological examination but neither organ weight analysis or histopathological examination were undertaken. No post-treatment recovery period was included in the study design. No other details of study methodology were reported and only limited information on the results was presented. Decrease in bodyweight was noted in animals receiving 750 mg/kg or above, and liver enlargement was apparent at necropsy in all groups receiving the test material. It was thus not possible to define a NOAEL and 250 mg/kg bodyweight was, therefore, considered to be the LOAEL.

In a 90-day study, groups of Sprague-Dawley rats (numbers per group not defined) were fed a diet containing isodecyl diphenyl phosphate at concentrations of 0, 140, 1400 and 7,000 ppm (equivalent to overall achieved dosages of 0, 9.3, 93.8 and 465 mg/kg bw/day, respectively, for males and 0, 11.1, 110 and 533 mg/kg bw/day for females), for 90 days. Details of the study methodology were not provided, although it is apparent from the summarised results that examinations undertaken (at undefined time points) included measurement of bodyweight, food consumption and blood chemistry and urinalysis, as well as organ weight analysis and pathological examination of at least the liver (Monsanto 1983b, cited in IUCLID 2000). Results comprised: a decrease in bodyweight in animals given 7,000 ppm; increased serum gamma glutamyl transpeptidase (GGT) activity in animals given 1,400 ppm or above; elevated serum bilirubin and cholesterol in animals given 7,000 ppm; elevated serum phosphorus and reduced serum glucose in animals of both sexes given 7,000 ppm and females given 1,400 ppm; and elevation of urinary bilirubin in males and females of all treated groups and urinary urobilinogen in males only of all treated groups. Hepatic weight (unclear if this is in terms of absolute and/or bodyweight-relative values) was also reported to be increased in rats given 1,400 ppm or above, while histopathological examination of the liver showed hypertrophy and/or hyperplasia in both males and females given 7,000 ppm and males given 1,400 ppm. The extent of these effects in terms of severity, number of animals affected or statistical significance, was not reported so, on the basis of the available information, it must be assumed that these changes (including the changes in urinary bilirubin and urobilinogen profiles in males given 140 ppm) were of potential toxicological significance. Thus it was not possible to define a NOAEL for the study and, on this basis, 140 ppm (equivalent to an achieved dose of 9.3 mg/kg bw/day in males and 11 mg/kg bw/day in females) was considered to be the LOAEL for this study.

Neurotoxicity

In a study of poorly reported design and unknown GLP status conducted by Monsanto 1975, cited in IUCLID 2000), birds (species, sex and number not reported) were given twice daily doses of 10 g/kg of an unspecified material (assumed to be isodecyl diphenyl phosphate but of unknown purity) for three days and again, over a further three-day period, starting on day 21. The total dose received was stated to be 120 g/kg; no mention is made of any negative and positive control groups. No details of the observation periods or examinations performed were reported and it is merely stated that no effects were found in the treated birds. The limited reporting precludes conclusions being drawn from this study.

Johannsen *et al.* (1977) reported that adult hens (strain unspecified) were given isodecyl diphenyl phosphate at 10 g/kg in undiluted dose or a corn oil solution twice daily by oral gavage, for three days. A further three-day dosing period to the same regimen was conducted from day 21, to give a total dose received of 120 g/kg. Hens were observed for signs of neurotoxicity and subject to histopathological examination; no treatment-related effects were reported in any of the hens treated with isodecyl diphenyl phosphate. Although it appears that no positive control was included in the study design, evidence of neurotoxicity was reported in this paper for a number of other aryl phosphates tested, suggesting that the test method was capable of detecting neurotoxic agents.

Given that both reports relate to work undertaken by Monsanto plc with apparent similarities in design, it is unclear whether they represent the same experiment.

Human data

No human data are available.

Summary and discussion of repeated- dose toxicity

There are two oral (feeding) studies in rats of 28 days duration, of which one showed clear evidence of liver toxicity at 10,000 ppm and a decrease in serum cholinesterase activity of unknown extent at 1,000 or 10,000 ppm (equivalent to 90 and 900 mg/kg/day). A NOAEL of 330 ppm (30 mg/kg/day) was established. Given the limited information available, the toxicological significance of the effect on serum cholinesterase is unknown,

The 90-day oral study in rats also demonstrated changes in some urine parameters and in blood chemistry and associated liver pathology, with effects extending in some instances to the lowest dose. It was concluded that, although subject to some uncertainty because of the limited nature of available information, these changes were of potential toxicological significance and suggestive of at least hepatic involvement, and, hence, it was not possible to define a NOAEL. On this basis, 140 ppm (equivalent to an achieved dose of 9.3 mg/kg bw/day in males and 11 mg/kg bw/day in females) was considered to be the LOAEL for this study.

In a study by Johannsen *et al.* (1977) on adult hens (strain unspecified) given a total dose of 120 g/kg over a 21-day period, no treatment-related effects were reported in any of the hens treated with isodecyl diphenyl phosphate. The composition of the test material used in the studies on birds is not, however, clearly defined. Although it appears that no positive control was included in the study design, evidence of neurotoxicity was reported in this paper for a number of other aryl phosphates tested suggesting that the test method was capable of detecting neurotoxic agents.

Given the uncertainties in studies that have investigated endpoints relevant to neurotoxicity, it is not possible to reach a conclusion on the neurotoxic potential of isodecyl diphenyl phosphate.

4.4.7 Mutagenicity

Studies in vitro

Genetic mutations

Three *in vitro* studies that investigate the potential of isodecyl diphenyl phosphate to induce genetic mutations are presented in IUCLID.

In an Ames test using *Salmonella* (species not specified but assumed to be *S. typhimurium*) of strains TA-1535, TA-1537, TA-1538, TA-98 and TA-100, cells were exposed to unspecified test material at concentrations of 0.01 to 10 µl/plate in the presence or absence of metabolic activation (Monsanto 1978a, cited in IUCLID 2000). The result was reported to be negative, though details of methods and results are not reported in detail. The study was not conducted to GLP or to international guidelines.

In a yeast mutation assay using an unspecified *Sacchromyces* species, cells were also exposed to unspecified test material at the same concentrations of 0.01 to 10 µl/plate, in the presence or absence of metabolic activation (Monsanto 1978b, cited in IUCLID 2000). The result was reported to be negative, though it is unclear if both mutagenic and clastogenic endpoints were assessed since methods and results are not reported in detail. The study was not conducted to GLP or to specific international guidelines.

Cells of the mouse lymphoma line L5178Y were exposed to unspecified test material at concentrations of 0.004 to 0.063 µl/plate in the presence or absence of metabolic activation (Monsanto 1978a, cited in IUCLID 2000). The result was again reported to be negative, though methods and results are not reported in detail. The study was not conducted to GLP or to international guidelines.

Zeiger *et al.* (1987) reported negative results for isodecyl diphenyl phosphate in mutation tests using *Salmonella typhimurium* strains TA-98 TA-100, TA-1535 and TA-1537 and/or TA-97 (obtained from Dr Bruce Ames of the University of California). Assays were undertaken in both the presence and absence of liver S-9 fraction (derived from Arochlor 1254-treated male Sprague-Dawley rats or Syrian hamsters) as part of a US National Toxicology Programme (NTP) validation exercise undertaken to compare test findings on 255 chemicals at a number of independent laboratories.

Chromosomal effects

The existence of *in vitro* data on chromosomal effects of isodecyl diphenyl phosphate is uncertain. It is reported that mouse lymphoma line L5178Y cells were exposed to unspecified test material at concentrations of 0.004 to 0.063 µl/plate in the presence or absence of metabolic activation (Monsanto 1978a, cited in IUCLID 2000). The result was reported only as “negative” but since methods, endpoints and results were not reported in detail, it is unclear if endpoints relevant to chromosomal effects were addressed.

Studies in vivo

No *in vivo* data are available for genetic mutations or chromosomal aberrations.

Summary of mutagenicity

Tests for gene mutation in Salmonella bacterial, mammalian and yeast cells did not reveal any signs of mutagenicity. The robustness of these studies could not, however, be verified due to the minimal level of reporting in IUCLID (2000).

It is unclear, from available information, if the mouse lymphoma line L5178Y assay assessed the clastogenic potential and/or mutagenic potential of isodecyl diphenyl phosphate. There are also no data regarding the potential mutagenic or clastogenic potential of isodecyl diphenyl phosphate *in vivo.*

4.4.8 Carcinogenicity

There are no data available on the carcinogenicity of isodecyl diphenyl phosphate.

Were the robustness of the mouse lymphoma study to be established as good and details of the histopathology findings in the repeated exposure studies to be made available, then it might be possible to assess the level of concern with regard to carcinogenicity on the basis of a lack of genotoxic potential and absence of proliferative lesions/cytotoxicity in the repeated exposure studies.

4.4.9 Toxicity to reproduction

Fertility and reproductive performance

There is no information available on the effects of isodecyl diphenyl phosphate on fertility and reproductive performance. Information on any potential toxic changes of the reproductive organs in the repeat dose studies would be useful in deciding on the appropriate level of concern.

Developmental toxicity

In a teratogenicity study conducted to EPA TSCA guidelines and GLP (Monsanto 1980, cited in IUCLID 2000), female Sprague-Dawley rats (group size unspecified) were dosed with undiluted test material at 300, 1,000 or 3,000 mg/kg bw/day by oral gavage, on days six to 15 of gestation. A control group was also included but no other methodological information was provided. A dose-related decrease in maternal bodyweight was reported at 1,000 mg/kg//day or above, with the maternal NOAEL therefore being established as 300 mg/kg bw/day. The NOAEL for developmental effects was reported to be 3,000 mg/kg bw/day although the endpoints considered were not specified.

In a teratogenicity study (Robinson *et al.* 1986), groups of 25 mated Charles River COBS CD rats were dosed with undiluted material at dosages of 300, 1,000 and 3,000 mg/kg/d on gestation days six to 19. The tested material was Santicizer 148, of stated composition 90 per cent isodecyl diphenyl phosphate, five per cent di-isodecyl phenyl phosphate and five per cent triphenyl phosphate. Controls were dosed with distilled water at volumes equivalent to those received by high-dose animals. Rats were observed daily throughout the study and bodyweight was recorded on gestation days 0, 6, 9, 12, 16 and 20. Animals were killed by carbon dioxide inhalation on gestation day 20 and the foetuses delivered by caesarean section. Numbers of live, dead and resorbed foetuses, total implantations and corpora lutea were noted. The abdominal and thoracic cavities of the mothers were examined for gross change and tissues preserved for possible future examination; uteri from apparently non-pregnant rats were retained for subsequent detailed examination to confirm their status. All foetuses were weighed, externally sexed and examined for external alterations (including palate and eyes). One half of the foetuses were fixed in Bouin's solution and subject to step serial section examination using the technique of Wilson (1965). Remaining foetuses were fixed and subjected, after processing, to skeletal examination. Some signs of treatment-related effects were noted in rats given Santicizer 148; these included staining around the mouth, nose and forelimbs (particularly in those given 300 mg/kg bw/day, hair loss in those given 1,000 mg/kg bw/day or above, and matting or staining of the anogenital fur in those given 3,000 mg/kg bw/day. However, bodyweight was not affected by treatment and there were no other overt signs suggestive of toxicity in the dams. There was a slight, but not statistically significant, increase in percentage resorptions at 3,000 mg/kg bw/day, but no effect on numbers of live and dead foetuses, foetal sex ratio or foetal bodyweight. The incidences of malformations and variations were not considered to have been affected by treatment. Thus, while a maternal NOAEL was not established in this study, the effects observed were not such as to suggest overt toxicity had occurred. The NOAEL for developmental effects was 3,000 mg/kg bw/day.

Robinson *et al*. (1983) have also published a short abstract reporting the findings of a teratogenicity study on Charles River CD rats. In this study, groups of 25 mated females were given isodecyl diphenyl phosphate (as a commercial product) by oral gavage at 300, 100 or 3,000 mg/kg/day on days 6 to 15 of gestation and were then killed on day 20; all foetuses were examined externally prior to half going for visceral and half for skeletal examination. No effect on maternal bodyweight was found for any treated group. The mean numbers of viable foetuses, post-implantation losses, total implantations and numbers of corpora lutea were similar in treated groups to controls. Mean foetal weight and sex distribution was also unaffected by treatment, and no dose-related trends in malformations were reported. This paper thus established a NOAEL of 3,000 mg/kg bw/day for maternal and developmental endpoints.

While some differences in reporting of methodology and results can be discerned, there are many similarities between the study reports in the three sources. Given that, in each case, the work arose from the same organisation (Monsanto plc), it is uncertain whether these publications relate to the same experiments.

Summary of toxicity to reproduction

No information is available on the reproductive toxicity of isodecyl diphenyl phosphate or relating to post-natal developmental effects. A number of papers have, however, been identified that report on the teratogenic potential of this compound in the rat. While there is some question as to whether these relate to the same or different experiments, there is no evidence from any of the papers of any developmental effects at doses of up to 3,000 mg/kg bw/day.

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

There are no studies available on carcinogenicity or effects on fertility, but limited information on potential teratogenicity suggests no adverse developmental effects at up to 3,000 mg/kg bw/day. The extent of investigation of chromosomal effects is uncertain and the neurotoxic potential of this chemical is not well characterised.

Two 28-day and one 90-day repeat dose study in the rat were identified as suitable for consideration in the risk assessment for humans exposed through the environment. Of these, the 90-day study was selected as the most sensitive. In this study (Monsanto report 1983b, cited in IUCLID 2000), a NOAEL for isodecyl diphenyl phosphate was not identified because of effects on urinary chemistry at the lowest dose tested. The lowest dose of 140 ppm (equivalent to an achieved dose of 9.3 mg/kg bw/day in males and 11 mg/kg bw/day in females) was therefore considered to be the LOAEL.

A margin of safety of at least 800-fold is considered necessary to provide reassurance against effects on human health. This involves applying a factor of two to extrapolate from the LOAEL to a NOAEL (not a factor of 10 due to the minor nature of the changes seen), together with uncertainty factors for interspecies variation (10), intraspecies variation (10), extrapolation from sub-chronic to chronic (2) and a factor of two to account for weaknesses in the overall database.

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

4.4.11 Derivation of PNEC for secondary poisoning

A dietary LOAEL of 140 ppm (140 mg/kg diet; equivalent to 9.3 mg/kg bw/day in males, and 11 mg/kg bw/day in females) was established based on a 90-day dietary exposure study in rats. It was not possible to determine a NOAEL since increased levels of urinary bilirubin were observed in all treated groups. However, while this does not meet the criteria defined by the TGD for an adequate toxicological study, the change on which the LOAEL is based is considered to be minimal and of uncertain toxicological significance.

On this basis a ‘provisional’ PNEC estimate might be derived for information only, by applying an uncertainty factor of 3, rather than a more conservative value of 10, to this value to extrapolate from a LOAEL to a NOAEL. A NOAEL of 30 mg/kg bw/day was established for decreased serum cholinesterase in a 28-day study in rats.

TGD recommends an assessment factor of 90 for extrapolation of a 90-day mammalian toxicity test, and this is deemed the most appropriate assessment factor here.

Based on these values, a ‘provisional’ $\text{PNEC}_{\text{oral}}$ of (140/3)/90 = 0.52 mg/kg can be calculated.

No avian toxicology data appropriate for calculation of a $\text{PNEC}_{\text{oral}}$ were identified for isodecyl diphenyl phosphate.

4.5 Hazard classification

4.5.1 Classification for human health

The substance is currently not classified with respect to human health on Annex 1 of Directive 67/548/EEC. According to the criteria of the European Union (EU), isodecyl diphenyl phosphate does not need to be classified on the basis of its acute toxicity, corrosiveness to the skin or eye, skin-sensitizing potential or developmental toxicity. There are no data to address effects via or during lactation. Therefore, it is not possible to make recommendations regarding classification for such effects.

The data are inadequate to classify isodecyl dipheny phosphate in terms of its irritant potential, repeat dose toxicity, mutagenicity, carcinogenicity or reproductive toxicity.

4.5.2 Classification for the environment

The substance is currently not classified as dangerous to the environment.

The BCF in fish for isodecyl diphenyl phosphate is around 335 l/kg. Acute toxicity data are available for fish (lowest LC_{50} = 7.6 mg/l), invertebrates (lowest EC_{50} = 0.22 mg/l for *Daphnia magna*) and algae (lowest EC_{50} = 71 mg/l). Given that the water solubility of the test substance is reported to be 0.011 to 0.75 mg/l, the fish and algal results are difficult to interpret in terms of whether the substance is acutely toxic at concentrations below its solubility limit. In the case of the lowest invertebrate result, *Daphnia* were noted to be trapped at the surface in this test, which could invalidate the result. However, there is another short term test with a 48-hour EC_{50} of 0.48 mg/l, within the solubility range. In addition, in the 21-day *Daphnia* study, the organisms exposed to 49 µg/l in a flow through system all died within 48 hours. The combination of these data supports an EC_{50} value lower than 1 mg/l. Based on these results for *Daphnia magna* and the BCF of 335 l/kg, the following classification could be considered.

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 4.7.

Table 4.7 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: isodecyl diphenyl phosphate is considered to be inherently biodegradable but it is not possible to determine if the specific criteria are met (Section 3.1.1). Hence the substance meets the first stage screening criteria for P and vP.

Bioconcentration: a value of 335 is selected from the available data in Section 0. Hence the substance does not meet the B criterion.

Toxicity: the lowest NOEC value from the available tests is 0.004 mg/l. The substance meets the T criterion.

To conclude, the substance meets two of the criteria based partly on screening data, but clearly fails to meet the B criterion, and so is not considered to be PBT.

5 Risk characterisation

This section identifies the potential risks that isodecyl 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 Aquatic compartment

5.1.1 Surface water

The PNEC for surface water was estimated as 0.4 µg/l. The resulting worst case risk characterisation ratios are summarised in

Table 5.1.

The PEC/PNEC ratios are greater than one for the uses of isodecyl diphenyl phosphate in different forms of PVC, use in polyurethane, rubber, textiles, pigment dispersions and paints. Only two conversion-only scenarios do not show a risk. Further information is needed on process emissions to refine the PECs for these scenarios. Information received from three users of isodecyl diphenyl phosphate appears to confirm the possible emission routes to water, but with no information on possible levels. The PNEC is derived using an assessment factor of 10 and is not likely to be revised through further testing (although no valid algal NOEC is available, the result from such a test is unlikely to revise the PNEC).

The risk to surface water from regional sources appears to be low based on the approach taken.

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.

Table 5.1 Summary of risk characterisation ratios for surface water

Scenario		PEC (μg/l)	Risk characterisation ratio
PVC – 1	Compounding	3.16	**7.91**
	Conversion	7.57	**18.9**
	Combined compounding and conversion	10.6	**26.4**
PVC – 2	Compounding	0.83	**2.07**
	Conversion	1.27	**3.17**
	Combined compounding and conversion	1.93	**4.82**
PVC – 3	Compounding	1.01	**2.53**
	Conversion	1.58	**3.94**
	Combined compounding and conversion	2.42	**6.06**
PVC – 4	Compounding	0.83	**2.07**
	Conversion	0.39	0.97
	Combined compounding and conversion	1.05	**2.62**
PVC – 5	Compounding	0.83	**2.07**
	Conversion	1.27	**3.17**
	Combined compounding and conversion	1.93	**4.82**
PVC – 6	Compounding	0.83	**2.07**
	Conversion	0.39	0.97
	Combined compounding and conversion	1.05	**2.62**
Rubber	Compounding	1.49	**3.72**
	Conversion	0.61	**1.52**
	Combined compounding and conversion	1.93	**4.82**
Polyurethane	Compounding	1.49	**3.72**
	Conversion	0.61	**1.52**
	Combined compounding and conversion	1.93	**4.82**
Textiles/fabric coating	Compounding	0.52	**1.3**
	Conversion	1.05	**2.62**
	Combined compounding and conversion	1.4	**3.5**
Pigment dispersions	Production of dispersions	1.49	**3.72**
Paints	Formulation	7.22	**18.1**
	Application	0.70	**1.74**
Regional sources		0.17	0.42

5.1.2 Waste water treatment

The PNEC for waste water treatment processes is estimated at 3 mg/l. The resulting PEC/PNEC ratios are summarised in Table 5.2.

Table 5.2 Summary of risk characterisation ratios for WWTP

Scenario		PEC (μg/l)	Risk characterisation ratio
PVC – 1	Compounding	0.03	0.01
	Conversion	0.07	0.03
	Combined compounding and conversion	0.11	0.04
PVC – 2	Compounding	6.68×10^{-3}	<0.01
	Conversion	0.01	<0.01
	Combined compounding and conversion	0.02	<0.01
PVC – 3	Compounding	8.55×10^{-3}	<0.01
	Conversion	0.01	<0.01
	Combined compounding and conversion	0.02	<0.01
PVC – 4	Compounding	6.68×10^{-3}	<0.01
	Conversion	2.23×10^{-3}	<0.01
	Combined compounding and conversion	8.91×10^{-3}	<0.01
PVC – 5	Compounding	6.68×10^{-3}	<0.01
	Conversion	0.01	<0.01
	Combined compounding and conversion	0.02	<0.01
PVC – 6	Compounding	6.68×10^{-3}	<0.01
	Conversion	2.23×10^{-3}	<0.01
	Combined compounding and conversion	8.91×10^{-3}	<0.01
Rubber	Compounding	0.01	<0.01
	Conversion	4.46×10^{-3}	<0.01
	Combined compounding and conversion	0.02	<0.01
Polyurethane	Compounding	0.01	<0.01
	Conversion	4.46×10^{-3}	<0.01
	Combined compounding and conversion	0.02	<0.01
Textiles/fabric coating	Compounding	3.56×10^{-3}	<0.01
	Conversion	8.91×10^{-3}	<0.01
	Combined compounding and conversion	0.01	<0.01
Pigment dispersions	Production of dispersions	0.01	<0.01
Paints	Formulation	0.07	0.02
	Application	5.35×10^{-3}	<0.01

Based on the risk characterisation ratios, the risk to waste water treatment plants from use of isodecyl diphenyl phosphate is low.

5.1.3 Sediment

The PNEC for sediment was estimated to be 0.059 mg/kg wet weight. The resulting PEC/PNEC ratios, increased by a factor of 10 to take into account the possibility of direct ingestion of sediment-bound substance, are summarised in Table 5.3.

PEC/PNEC ratios are greater than one for all scenarios considered, including the regional scenario. Further information noted for the surface water compartment would also refine the sediment assessment. However, the extra factor of 10 used for sediment means that emission estimates would have to be reduced greatly to remove all of the concerns. All scenarios would still show a risk without the extra factor of ten (with the exception of two conversion-only scenarios and the regional concentration).

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[8] to investigate the actual degradation (mineralization) half-life in sediment under relevant environmental conditions.

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

5.2 Terrestrial compartment

The PNEC for soil is estimated tp be 0.048 mg/kg wet weight. The resulting PEC/PNEC ratios, increased by a factor of 10 to take into account the possibility of direct ingestion of sediment-bound substance, are summarised in Table 5.4.

PEC/PNEC ratios are greater than one for all local scenarios considered and also for industrial soil at the regional level. 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 greatly to remove all of the concerns The PEC/PNEC would still be greater than one for many of the scenarios without the extra factor of 10.

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

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

The risk to soil from production sites and to agricultural and natural soil from regional sources appears to be low based on the approach taken.

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

Table 5.3 Summary of risk characterisation ratios for sediment

Scenario		PEC (mg/kg wet wt)	Risk characterisation ratio
PVC – 1	Compounding	0.47	**79.1**
	Conversion	1.13	**189**
	Combined compounding and conversion	1.58	**264**
PVC – 2	Compounding	0.12	**20.7**
	Conversion	0.19	**31.7**
	Combined compounding and conversion	0.29	**48.2**
PVC – 3	Compounding	0.15	**25.3**
	Conversion	0.24	**39.4**
	Combined compounding and conversion	0.36	**60.6**
PVC – 4	Compounding	0.12	**20.7**
	Conversion	0.06	**9.66**
	Combined compounding and conversion	0.16	**26.2**
PVC – 5	Compounding	0.12	**20.7**
	Conversion	0.19	**31.7**
	Combined compounding and conversion	0.29	**48.2**
PVC – 6	Compounding	0.12	**20.7**
	Conversion	0.06	**9.66**
	Combined compounding and conversion	0.16	**26.2**
Rubber	Compounding	0.22	**37.2**
	Conversion	0.09	**15.2**
	Combined compounding and conversion	0.29	**48.2**
Polyurethane	Compounding	0.22	**37.2**
	Conversion	0.09	**15.2**
	Combined compounding and conversion	0.29	**48.2**
Textiles/fabric coating	Compounding	0.08	**13**
	Conversion	0.16	**26.2**
	Combined compounding and conversion	0.21	**35**
Pigment dispersions	Production of dispersions	0.22	**37.2**
Paints	Formulation	1.08	**181**
	Application	0.10	**17.4**
Regional sources		0.04	**7.06**

Table 5.4 Summary of risk characterisation ratios for the terrestrial compartment

Scenario		PEC (mg/kg wet wt)	Risk characterisation ratio
Production of isodecyl diphenyl phosphate		1.4×10^{-3}	0.29
PVC – 1	Compounding	0.87	**179**
	Conversion	2.15	**445**
	Combined compounding and conversion	3.02	**623**
PVC – 2	Compounding	0.19	**39.8**
	Conversion	0.32	**66.4**
	Combined compounding and conversion	0.51	**106**
PVC – 3	Compounding	0.25	**50.8**
	Conversion	0.41	**85**
	Combined compounding and conversion	0.66	**135**
PVC – 4	Compounding	0.19	**39.8**
	Conversion	0.07	**13.5**
	Combined compounding and conversion	0.26	**53**
PVC – 5	Compounding	0.19	**39.7**
	Conversion	0.32	**66.1**
	Combined compounding and conversion	0.51	**106**
PVC – 6	Compounding	0.19	**39.7**
	Conversion	0.07	**13.5**
	Combined compounding and conversion	0.26	**53**
Rubber	Compounding	0.38	**79**
	Conversion	0.13	**26.8**
	Combined compounding and conversion	0.51	**106**
Polyurethane	Compounding	0.38	**79**
	Conversion	0.13	**26.8**
	Combined compounding and conversion	0.51	**106**
Textiles/fabric coating	Compounding	0.10	**21.3**
	Conversion	0.26	**52.8**
	Combined compounding and conversion	0.36	**74.2**
Pigment dispersions	Production of dispersions	0.38	**79.3**
Paints	Formulation	2.04	**421**
	Application	0.15	**31.8**
Regional sources	Agricultural soil	9.66×10^{-4}	0.2
	Natural soil	1.4×10^{-3}	0.29
	Industrial soil	0.08	**16.67**

5.3 Atmosphere

No information is available on the toxicity of isodecyl 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 (below 2×10^{-4} mg/m^3). The possibility of isodecyl 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

A PNEC for secondary poisoning of 0.52 mg/kg food was derived for isodecyl diphenyl phosphate. The resulting PEC/PNEC ratios are shown in Table 5.5.

The PEC/PNEC ratios are greater than one for uses of isodecyl diphenyl phosphate in different forms of PVC and in formulation of paint, when the fish food chain is considered. In addition, PEC/PNEC ratios greater than one are also obtained for all scenarios for the earthworm food chain. Further information is needed on process emissions to refine the PECs for these scenarios.

Table 5.5 Summary of risk characterisation ratios for secondary poisoning

Scenario		Fish food chain		Earthworm food chain	
		PEC (mg/kg)	Risk characterisation ratio	PEC (mg/kg)	Risk characterisation ratio
Production of isodecyl diphenyl phosphate		n/a[a]	-	0.03[b]	0.06
PVC – 1	Compounding	0.47	0.9	10.5	**20.2**
	Conversion	1.08	**2.07**	26.0	**50.2**
	Combined compounding and conversion	1.49	**2.87**	36.5	**70.4**
PVC – 2	Compounding	0.15	0.28	2.34	**4.51**
	Conversion	0.21	0.4	3.9	**7.52**
	Combined compounding and conversion	0.3	0.58	6.21	**12**
PVC – 3	Compounding	0.17	0.33	2.99	**5.76**
	Conversion	0.25	0.48	4.98	**9.61**
	Combined compounding and conversion	0.37	0.71	7.94	**15.3**
PVC – 4	Compounding	0.15	0.28	2.34	**4.51**
	Conversion	0.09	0.17	0.80	**1.55**
	Combined compounding and conversion	0.18	0.34	3.11	**6.01**

Table 5.5 continued.

Scenario		Fish food chain		Earthworm food chain	
		PEC (mg/kg)	Risk characterisation ratio	PEC (mg/kg)	Risk characterisation ratio
PVC – 5	Compounding	0.09	0.18	2.34	**4.51**
	Conversion	0.12	0.22	3.88	**7.49**
	Combined compounding and conversion	0.15	0.3	6.19	**11.9**
PVC – 6	Compounding	0.06	0.11	2.33	**4.5**
	Conversion	0.09	0.18	0.81	**1.55**
	Combined compounding and conversion	0.18	0.34	3.11	**6.01**
Rubber	Compounding	0.06	0.11	4.64	**8.94**
	Conversion	0.13	0.25	1.58	**3.05**
	Combined compounding and conversion	0.3	0.58	6.2	**12**
Polyurethane	Compounding	0.06	0.11	4.64	**8.94**
	Conversion	0.13	0.25	1.58	**3.05**
	Combined compounding and conversion	0.3	0.58	6.2	**12**
Textiles/ fabric coating	Compounding	0.06	0.11	1.26	**2.43**
	Conversion	0.06	0.11	3.1	**5.98**
	Combined compounding and conversion	0.23	0.44	4.36	**8.4**
Pigment dispersion	Production of dispersions	0.24	0.46	4.65	**8.97**
Paints	Formulation	1.03	**1.98**	24.7	**47.6**
	Application	0.06	0.11	1.87	**3.61**

Notes: a) Production sites do not discharge to freshwater.
b) Sewage sludge from the production site is not applied to land.

The significance of the toxicological endpoint on which the PNEC is based might be questionable. A more detailed consideration of other endpoints might allow the consequences of this to be established. In addition, the estimated earthworm BCF value is of uncertain validity, so this could be refined with a test if necessary.

5.5 Risk characterisation for human exposure via the environment

A dietary LOAEL of 9.3 mg/kg bw/day in male rats was identified in Section 4.4.10 as the most appropriate value for use in this assessment. A margin of safety of 800 is considered necessary to provide sufficient reassurance against effects on human health with this result (see Section 4.4.10). The estimated human exposures via the environment were calculated in Section 3.3.4 and are included in

Table 5.6 together with the resulting margins of safety.

Table 5.6 Margin of exposure between daily human doses and the LOAEL (9.3 mg/kg bw/day)

Scenario		**Total daily human intake (mg/kg bw/day)**	**Margin of exposure**
Production of isodecyl diphenyl phosphate		3.2×10^{-3}	2,906
PVC – 1	Compounding	0.08	**116**
	Conversion	0.21	**44**
	Combined compounding and conversion	0.29	**32**
PVC – 2	Compounding	0.02	**465**
	Conversion	0.03	**310**
	Combined compounding and conversion	0.05	**186**
PVC – 3	Compounding	0.02	**465**
	Conversion	0.04	**232**
	Combined compounding and conversion	0.06	**155**
PVC – 4	Compounding	0.02	**465**
	Conversion	6.4×10^{-3}	1,543
	Combined compounding and conversion	0.02	**465**
PVC – 5	Compounding	0.02	**465**
	Conversion	0.03	**310**
	Combined compounding and conversion	0.05	**186**
PVC – 6	Compounding	0.02	**465**
	Conversion	6.4×10^{-3}	1543
	Combined compounding and conversion	0.02	**465**
Rubber	Compounding	0.04	**232**
	Conversion	0.01	930
	Combined compounding and conversion	0.05	**186**
Polyurethane	Compounding	0.04	**232**
	Conversion	0.01	930
	Combined compounding and conversion	0.05	**186**
Textiles/ fabric coating	Compounding	9.8×10^{-3}	949
	Conversion	0.02	**465**
	Combined compounding and conversion	0.03	**310**
Pigment dispersions	Production of dispersions	0.04	**232**
Paints	Formulation	0.2	**47**
	Application	0.01	930
Regional sources		1.9×10^{-4}	49,000

Risks are indicated for the majority of the scenarios, the exceptions being production, two conversion-only scenarios for PVC, conversion-only scenarios for rubber and polyurethane, the compounding step for textile/fabric coating, and application of paints. There is no concern for exposure at the regional level.

The assessment could be refined by improving the estimates for total daily human dose. This could involve:

- better release information and/or monitoring data at locations close to sources of release;
- measurements of the uptake of isodecyl diphenyl phosphate into plants to replace the current estimated values. The root crop contribution to the total dose is greater than 95 per cent in all of the scenarios showing a risk (and in almost all of the others).

5.6 Marine risk assessment

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

PEC values for the marine assessment are presented in Sections 3.3.1 and 3.3.4. These have been calculated using EUSES. 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 the freshwater fish and terrestrial food chains (Section 4.4.11). The resulting PEC/PNEC ratios are in Table 5.7.

Table 5.7 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**
Production of isodecyl diphenyl phosphate		**470**	**4,700**[a]	**1.75**	0.36
PVC – 1	Compounding	**21.4**	**214**	0.23	0.05
	Conversion	**52.4**	**524**	0.56	0.12
	Combined compounding and conversion	**73.4**	**734**	0.79	0.17
PVC – 2	Compounding	**5.03**	**50.3**	0.06	0.02
	Conversion	**8.12**	**81.2**	0.09	0.03
	Combined compounding and conversion	**12.8**	**128**	0.14	0.03
PVC – 3	Compounding	**6.33**	**63.3**	0.07	0.02
	Conversion	**10.3**	**103**	0.12	0.03
	Combined compounding and conversion	**16.2**	**162**	0.18	0.04

Table 5.7 continued.

Scenario		**PEC/PNEC ratio**			
		Local marine compartment	**Local marine sediment compartment**	**Fish-eating birds and mammals**	**Top predators**
PVC – 4	Compounding	**5.03**	**50.3**	0.06	0.02
	Conversion	**1.94**	**19.4**	0.03	0.01
	Combined compounding and conversion	**6.58**	**65.8**	0.08	0.02
PVC – 5	Compounding	**5.03**	**50.3**	0.03	0.01
	Conversion	**8.12**	**81.2**	0.04	0.02
	Combined compounding and conversion	**12.8**	**128**	0.06	0.02
PVC – 6	Compounding	**5.03**	**50.3**	0.01	0.01
	Conversion	**1.94**	**19.4**	0.03	0.01
	Combined compounding and conversion	**6.58**	**65.8**	0.08	0.02
Rubber	Compounding	**9.67**	**96.7**	0.01	0.01
	Conversion	**3.48**	**34.8**	0.05	0.02
	Combined compounding and conversion	**12.8**	**128**	0.14	0.04
Poly-urethane	Compounding	**9.67**	**96.7**	0.01	0.01
	Conversion	**3.48**	**34.8**	0.05	0.02
	Combined compounding and conversion	**12.8**	**128**	0.14	0.04
Textiles and fabric coating	Compounding	**2.86**	**28.6**	0.01	0.01
	Conversion	**6.58**	**65.8**	0.01	0.01
	Combined compounding and conversion	**9.05**	**90.5**	0.10	0.03
Pigment disp.	Production of dispersions	**9.67**	**96.7**	0.11	0.03
Paints	Formulation	**49.9**	**499**	0.54	0.12
	Application	**4.1**	**41**	0.01	0.01

Notes: a) Calculation uses average dilution in receiving water. If minimum dilution at the site was used, the PEC/PNEC would be a factor of 1.88 times higher. Similarly, if maximum dilution at the site was used, the PEC/PNEC would be 6.67 times lower.

Risks are indicated for all scenarios for marine waters and marine sediments. The regional concentration in marine waters does not indicate a risk. However, a risk is indicated for marine sediments for the regional scenario.

Further information on emissions from these 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 if they only do so after effluent treatment (the calculations above assume a direct discharge to the marine environment without waste water treatment) would be useful.

Testing on freshwater organisms is not indicated for the freshwater assessment. Testing on freshwater sediment organisms would have implications for the marine sediment assessment. There is also the possibility of testing on marine species, which would allow the assessment factor to be reduced.

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.

Risks for marine food chains are indicated for production of isodecyl diphenyl phosphate when fish-eating birds are considered. The PEC/PNEC ratios are less than one for all other scenarios for predatory organisms.

6 Conclusions

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

Life cycle stage	Surface water	Sediment	WWTP	Air	Soil	Aquatic food chain	Terrestrial food chain	Marine water	Marine sediment
Production	-	-	-	-	-	-		✸	✸
PVC	✸[a]	✸[a]	-	-	✸	✸[b]	✸[a]	✸[a]	✸[a]
Rubber	✸	✸	-	-	✸	-	✸	✸	✸
Polyurethane	✸	✸	-	-	✸	-	✸	✸	✸
Textile/fabric coating	✸	✸	-	-	✸	-	✸	✸	✸
Pigment dispersions	✸	✸	-	-	✸	-	✸	✸	✸
Paints	✸	✸	-	-	✸	-	✸	✸	✸
Regional	-	✸	-	-	-	-	-	-	-

Notes: a) Risks for all PVC uses.
b) Risks for only one PVC use.

There are also risks for humans exposed via environment from the majority of the life cycle stages. There are no risks for marine food chain exposure for any life cycle stage except production.

Limited monitoring data are available for isodecyl diphenyl phosphate and these cannot be related to specific current activities.

Potential risks identified here could be reassessed following further work, in particular:

- Collation of further site and industry-specific information on releases of isodecyl diphenyl phosphate from use in the different types of materials indicated. This work could include:
    - Improved description of practices at sites using isodecyl 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, sediment and WWTP sludge). Further environmental monitoring for isodecyl 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 testing and a long-term fish test.
- 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.
- Studies on uptake of isodecyl diphenyl phosphate into plants from soil.
- Clarification of some aspects of the mammalian toxicity data (see Appendix 1)

The significance of the toxicological endpoint on which the secondary poisoning PNEC is based might be questionable. A more detailed consideration of other endpoints might allow the consequences of this to be established. The earthworm BCF value could also be refined with a test if necessary.

A possible risk to marine organisms is identified for production. This conclusion could be refined through further testing as indicated above, but it is more appropriate for the local control authority to consider this outcome[9].

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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[9] More recent data suggest that current emissions are lower than assumed for this report. In addition, a biological WWTP is being installed, which should have a significant effect on emissions when it becomes operational later in 2009. Further details are provided in the confidential appendix.

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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 micro-organisms.
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 micro-organisms.

9 List of abbreviations

Acronym	**Description**
ASTM	American Society for Testing and Materials
B	Bioaccumulative
BCF	Bioconcentration factor
BMF	Biomagnification factor
BOD	Biochemical oxygen demand
bw	Bodyweight
CAS	Chemical Abstract Services
CMR	Carcinogenic, mutagenic and toxic to reproduction
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 18 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)
HPV	High Production Volume (supply above 1,000 tonnes/year)
IDDPP	Isodecyl diphenyl phosphate
IUCLID	International Uniform Chemical Information Database: contains non-validated tonnage, use pattern, property and hazard information for chemicals, submitted by industry under the Existing Substances Regulation (ESR)
K_{oc}	Organic carbon normalised distribution coefficient
K_{ow}	Octanol-water partition coefficient
Kp	Solids-water partition coefficient
$L(E)C_{50}$	Median lethal (effect) concentration
LD_{50}	Median lethal dose
LL_{50}	Median lethal loading
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
NTP	US National Toxicological Programme
OECD	Organisation for Economic Co-operation 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+]
PNEC	Predicted no effect concentration
ppm	Parts per million
STP	Sewage treatment plant
TGD	Technical Guidance Document
TPP	Tetrapropenylphenol
TSCA	Toxic Substances Control Act, USA
US EPA	Environmental Protection Agency, USA
vB	Very bioaccumulative
vP	Very persistent
vPvB	Very persistent and very bioaccumulative
wt	Weight
wwt	Wet weight
WWTP	Waste water treatment plant

10 Data collection and peer review process

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

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

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

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

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

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

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

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

Appendix 1 Points for clarification on mammalian toxicity data

The following points summarise uncertainties in the mammalian dataset (Section 4.4), and may lead to revision of the assessment of human exposure via the environment.

- In the source documents used to prepare this report, the precise nature of the test materials employed is poorly described (whether the substance comprises only one isomer or a mixture of several). Clarification of this issue would enable more robust conclusions to be reached for the various endpoints considered.
- Although no experiments were reported for toxicokinetics, metabolism and distribution, it would be helpful if industry could provide predictions based upon the physicochemical characteristics of the substance.
- With regard to available acute oral toxicity data, it would be useful to confirm if the Monsanto experiment included in the IUCLID (Monsanto 1971, cited in IUCLID 2000) is the same as that reported by Johannsen *et al.* (1977).
- Similarly, it would be useful to confirm if the acute dermal lethality study in the rabbit conducted by Monsanto plc that is briefly described in IUCLID (2000) is the same experiment as that reported in the paper by Johannsen *et al.* (1977).
- In view of the report in the secondary source that suggests only slight irritant potential may exist, it would be advisable to examine in more detail the irritation scores and timescale over which effects were observed in these experiments (Monsanto 1971, cited in IUCLID), since this may permit a firm conclusion to be reached as to the chemical's potential to cause dermal and ocular irritancy
- With regard to repeat dose study reports, the secondary reporting of Monsanto, 1984, TSCA Submission 878213951) states for the group given 10,000 ppm, that there were "decreased serum cholinesterase" and "serum cholinesterase decrease"; it would help to clarify if this represents an erroneous duplication or if one of these entries should refer to some other parameter.
- Given the response noted in rats on a 28-day study and uncertainties with regard to composition of the test material investigated and methods used in the avian neurotoxicity studies identified, it may be appropriate to consider further testing *in vitro* to inform on the neurotoxic potential of this compound.
- For a 28-day study (Monsanto 1979a, cited in IUCLID 2000), it would be useful to clarify if the decrease in bodyweight reported in animals receiving 750 mg/kg or above was in terms of absolute bodyweight or if this was a reduction in bodyweight gain. For this study, it would also be helpful to confirm if the liver enlargement noted in treated groups was in terms of absolute or bodyweight relative values, visual observations or some other metric and if this showed dose relationship and was statistically significant. Also, information on the endpoints assessed in the 28-and 90-day repeat dose studies by Monsanto, in particular with regard to findings for reproductive organs, would be helpful.
- It would be useful to confirm the actual test material used in Monsanto 1980, cited in IUCLID (2000)
- The Monsanto Report (1980, cited in IUCLID 2000) and the paper by Robinson *et al.* (1986) and the short abstract also published by Robinson *et al*. have many similarities. It would be useful to confirm if these relate to the same experiment.

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