

A Multimedia Assessment of the Environmental Fate of Bisphenol A

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ABSTRACT

A comprehensive multimedia assessment of the environmental fate of bisphenol A (BPA) is presented. Components of the assessment include an evaluation of relevant partitioning and reactive properties, estimation of discharge quantities in the U.S. and the European Union (E.U.) resulting in conservative and realistic emission scenarios, and a review of monitoring data. Evaluative assessments of chemical fate using the Equilibrium Criterion (EQC) model are described from which it is concluded that the low volatility of BPA will result in negligible presence in the atmosphere. It is relatively rapidly degraded in the environment with half-lives in water and soil of about 4.5 days and less than 1 day in air, and with an overall half-life of 4.5 to 4.7 days, depending on the medium of release. The degradation rate in water is such that it may be transported some hundreds of kilometres in rivers, but long-range transport potential in air is negligible. Its low bioconcentration factor is consistent with rapid metabolism in fish (half-life less than 1 day). The estimated concentrations were generally consistent with the monitoring data, with the exception of sediment-water concentration ratios. Several hypotheses for the apparent nonequilibrium sediment-water partitioning are presented.

Key Words: bisphenol A, fate, exposure, multimedia, model, fugacity, assessment.

INTRODUCTION

Bisphenol A (BPA) (CAS 80-05-07) is the common name for 2,2-(4,4'-dihydroxydiphenyl) propane (Figure 1). Most (99.9%) of the BPA produced is used as an intermediate in the production of polycarbonate and epoxy resins, flame retardants, and other specialty products (Staples *et al.* 1998). A small fraction of this BPA can be

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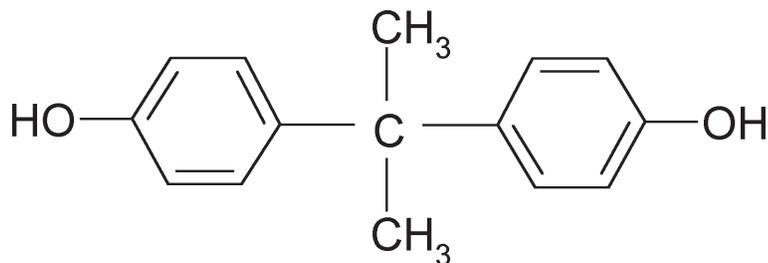


Figure 1. Structure of bisphenol A.

released to the environment during manufacturing, processing and use of products. Modern analytical methods, which permit detection at low levels, have shown the presence of BPA in some environmental samples. Concerns have recently been raised over the exposure of humans and wildlife to environmental levels of BPA, principally because it has been shown to have weak endocrine activity (Sohoni *et al.* 2001).

Given that there are potential releases to the environment and concerns over possible effects, it is desirable to establish a fuller and more quantitative understanding of the environmental sources and fate of BPA. Multimedia models are often employed to reconcile observed exposure concentrations with reported emission rates of chemicals to the environment. A satisfactory reconciliation has several benefits. It indicates that emissions are substantially or fully accounted for. It identifies the dominant fate processes (including degradation rates). It provides a method by which future changes in emission rates can be translated into a time course of exposure changes. In general, the availability of a verifiable mass balance model provides confidence that the fate of chemicals in the environment can be predicted, given sufficiently accurate data on chemical properties and emission rates. Recently, Mackay *et al.* (1996 a,b,c) outlined a five-stage strategy for assessing the fate and exposure of new and existing chemicals that incorporates the use of multimedia contaminant fate models. The strategy entails (1) chemical classification, (2) acquisition of environmental concentrations and discharge data, and (3) evaluative assessment of chemical fate, followed by (4) regional far-field, then (5) local near-field evaluations. This five-stage strategy has been used to assess the environmental fate of chlorobenzenes in Canada (MacLeod and Mackay 1999).

The Bisphenol A Environmental Working Group of the Society of the Plastics Industry is currently directing a research program to develop a more accurate assessment of the environmental exposure and ecotoxicity of BPA. Specifically, the objectives of this study are to:

- compile relevant chemical property and reactivity data;
- estimate emissions to the environment;
- review multimedia monitoring data;
- undertake evaluative modeling using the Equilibrium Criterion (EQC) model, including estimation of persistence and potential for long-range transport;

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- undertake regional modeling for European conditions, including a comparison with previous model results.

To achieve these objectives, the first four stages of the five-stage assessment strategy outlined by Mackay *et al.* (1996 a,b,c) are applied to BPA and the findings compared with a similar assessment that was undertaken recently using the EUSES (European Union System for the Evaluation of Substances) modeling framework (RIVM 1996).

STAGE 1 — CHEMICAL CLASSIFICATION

Physical-Chemical Properties and Partition Coefficients

Under ambient conditions, BPA is a solid (melting point 155°C) and is distributed as crystals, prills, or flakes. The physical-chemical properties of BPA have been reviewed by Staples *et al.* (1998) and Mackay *et al.* (2000). Values reported for each key property were evaluated and those selected are listed in Table 1.

Chemicals such as BPA that have measurable vapor pressures, aqueous solubilities and octanol-water partition coefficients (K_{OW}) are expected to partition to some extent to all available environmental phases.

BPA is a moderately hydrophobic compound (K_{OW} of $10^{3.4}$) that is fairly soluble in water (300 g/m^3). It will partition to organic phases such as soils and sediments, but an appreciable fraction of the compound will be present in the dissolved phase. Adsorption of BPA to four different soils has recently been investigated (Möndel 2001a) and adsorption constants (K_d) and organic carbon-water partition coefficients (K_{OC}) deduced. Experimental values of K_{OC} from this study ranged between 640 and 930. These measurements are consistent with methods that estimate K_{OC} from K_{OW} , *e.g.*, $K_{OC} = 0.35 * K_{OW}$ (Seth *et al.* 1999), which predicts a K_{OC} value of 880.

Table 1. Physical-chemical properties of bisphenol A at 25°C and associated uncertainty.

Parameter	Value	Confidence Factor ⁴
Molar mass	228.29 g/mol	—
Melting point	155°C	—
Water solubility	300 g/m ³	2
Vapor pressure	5.3 x 10 ⁻⁶ Pa	2
Log K_{OW}	3.40	1.1
Henry's law constant	4.03 x 10 ⁻⁶ Pa.m ³ /mol ¹	—
Log K_{AW}	-9.01 ²	—
Log K_{OA}	12.41 ³	—
pKa	9.59-11.30	—

¹ Calculated as the ratio of vapor pressure (Pa) and solubility in water (mol/m³): *i.e.*, $5.3 \times 10^{-6} \times 228/300$. ² Calculated from the Henry's law constant (H), *i.e.*, $K_{AW} = H/RT$, where R is the Gas Constant (J/mol/K) and T is the absolute temperature (K). ³ Calculated from the ratio K_{OW}/K_{AW} . ⁴ 95% confidence factors (Cf) were used as convenient expressions of variance where the standard deviation (σ) is equal to $0.5 \ln Cf$ (or $Cf = e^{2\sigma}$) for a lognormal distribution. A Cf of n implies that 95% of the data will be between n times and 1/n of the median value.

K_{AW} , the dimensionless air-water partition coefficient, is calculated as H/RT , where H is the Henry's law constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$), R is the gas constant ($\text{Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}$), and T is the absolute temperature (298 K). It is noteworthy that the air-water partition coefficient is very low, *i.e.*, 10^{-9} . The implication is that BPA is unlikely to evaporate from aqueous solution. For example, an aqueous solution containing a concentration of 16 ng/L (the median value contained in Table 5) will cause a corresponding concentration in air of about 16×10^{-9} ng/L or 16 fg/m³. This concentration is probably too low to be measured even using the most highly sophisticated, modern analytical techniques.

The dimensionless octanol-air partitioning coefficient (K_{OA}) is increasingly used to describe vapor-particle (Bidleman and Harner 2000), air-soil partitioning (Hippelein and McLachlan 1998), and vapor-plant partitioning (Kömp and McLachlan 1997). It was estimated as the ratio of K_{OW}/K_{AW} , although it is preferable to measure it directly, as has been done for a range of hydrophobic organic compounds (*e.g.*, Harner *et al.* 2000). The estimated octanol-air partition coefficient is 2.6×10^{12} . This very high value suggests that BPA in gaseous form will sorb strongly to solid surfaces, including soils, vegetation, and aerosols. It should be borne in mind that BPA will not often be present in its gaseous form in the environment because of its low vapor pressure.

BPA has a pKa between 9.59 to 11.30 (Staples *et al.* 1998) and therefore will not appreciably ionize at environmental pH levels that are generally 7 and lower. It could ionize appreciably under industrial conditions of high pH, for example, during cleaning with alkaline solutions.

Environmental Degradation Rates

The environmental degradation processes of BPA in the environment have been reviewed by Staples *et al.* (1998), who concluded that aerobic biodegradation is the dominant loss process for BPA in all media except the atmosphere, where it is likely to be susceptible to rapid reaction with hydroxyl radicals. A recent river die-away study (Klečka *et al.* 2001) and a soil degradation study (Möndel 2001b) have helped provide guidance for assigning degradation half-lives to environmental media.

The photo-oxidation half-life for BPA in air, based on hydroxyl radical attack, was predicted to be in the range 0.74 to 7.4 h by using the Atmospheric Oxidation Program (AOP) (Staples *et al.* 1998; Meylan and Howard 1993), a structure-property based model.

River die-away studies that employed surface water collected from seven different rivers across the U.S. and Europe show that BPA was degraded with half-lives of 3 to 6 days (Klečka *et al.* 2001). Short half-lives were noted in river water regardless of geographic location, sampling site (upstream or downstream of wastewater outfalls), sediment addition, or test chemical concentration (0.05 to 5500 µg/L). This study represents the most comprehensive examination of the water degradation half-life.

Recent soil degradation experiments have shown rapid loss in four distinct soil types, with apparent half-lives for disappearance of the parent compound of less than 3 days (Möndel 2001b). Although a small fraction of metabolites was detected, these metabolites were also rapidly degraded. The predominant mechanism responsible for loss of BPA in soil was thought to be aerobic

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biodegradation, although some of the BPA may be incorporated into the soil organic matter, rendering it irrecoverable by extensive extraction. Whether the loss process is aerobic degradation or incorporation into the organic matter, it is improbable that the BPA will be bioavailable or available for transport (*e.g.*, leaching or revolatilization), so it is effectively lost from the biosphere.

Biodegradation of BPA in water slurries containing 10% sediment has shown that aerobic degradation half-lives are considerably shorter in the presence of sediment than with river water alone (Klečka *et al.* 2001). However, only suspended sediments and the top layer of bottom sediments in surface waters are likely to be aerobic. Buried sediments and bottom sediments in deep lakes will be completely anaerobic. In anaerobic sediments, BPA microbial degradation is expected to be much slower than in aerobic sediments, but the degradation rates are not currently known.

Table 2 shows the media half-lives used as input to a recent EUSES modeling exercise and the values that are recommended in this study. The estimate of the photo-oxidation half-life of 4.8 h used in EUSES was based on hydroxyl radical reaction using AOP and thus is consistent with the estimated half-life range reported by Staples *et al.* (1998) of 0.74 to 7.4 h. The midpoint of the AOP estimated half-life range for the air half-life was selected for this study, *i.e.*, 4 h. The water and soil half-lives of 15 and 30 days, respectively, are believed to be conservative, because the recent river and soil die-away studies report half-lives of 3 to 6 days. Thus, we recommend a shorter half-life for surface water and soil for use in fate models of 4.5 days, which is the midpoint reported in the river die-away studies and a little higher than measured in the soil studies (Table 2). Although aerobic degradation in sediments is expected to be rapid, anaerobic degradation is expected to be slow. Therefore, it was decided to take a conservative approach for bottom sediments and allocate the same half-life that was used in the EUSES modeling exercise of 300 days. It must be appreciated that these half-lives will vary depending on environmental conditions such as temperature and the nature and number of the microbial communities in soils, surface waters, and sediments. Because of this variability, a confidence factor of 5 has been ascribed to these input parameters in the mass balance modeling exercise.

Table 2. Estimated pseudo first-order degradation half-lives and associated uncertainty.

Media	Half-lives used in EUSES modeling	Half-lives recommended in this study	Confidence Factor ¹
Air	4.8 h (0.2 days)	4 h (0.17 days)	5
Water	360 h (15 days)	108 h (4.5 days)	5
Soil	720 h (30 days)	108 h (4.5 days)	5
Sediment	7200 h (300 days)	7200 h (300 days)	5

¹95% confidence factors (Cf) were used as convenient expressions of variance where the standard deviation (σ) is equal to $0.5 \ln Cf$ (or $Cf = e^{2\sigma}$) for a lognormal distribution. A Cf of n implies that 95% of the data will be between n times and 1/n of the median value.

STAGE 2 — ACQUISITION OF DISCHARGE DATA AND ENVIRONMENTAL CONCENTRATIONS

Environmental Releases

Total environmental releases and individual rates of discharge to air, water, and soil are required for regional mass balance modeling. Frequently, emission rates must be extrapolated from limited data sources, including national emissions inventories, monitoring from municipal treatment systems and landfills, *etc.* Neighboring natural and anthropogenic sources may contaminate air and water entering a region contributing what is termed “advective inflow.” The total release rate and mode of entry (*i.e.*, proportions to air, water, soil, *etc.*) of emissions by direct discharge and advective inflow from background air and water ultimately drive local environmental concentrations and thus exposure.

Worldwide production of BPA in 1996 was estimated to be 1.62×10^9 kg and was primarily produced in three regions: the U.S. (48%), Western Europe (32%), and Japan (20%) (SRI 1998). Some 65% of the BPA produced is used in polycarbonate resins, 28% is used in epoxy resins, and the remaining 7% is used for other applications, in other types of resins, and for the production of flame retardants.

BPA may be unintentionally released as fugitive dust from closed systems during processing, handling, and transportation. Because of the high temperatures used during manufacturing, BPA may be present in molten (liquid) form. The vapor pressure, which is very low at typical environmental temperatures (Table 1), may be significantly increased at these elevated temperatures and fugitive releases of gaseous BPA from manufacturing facilities are possible. The moderately high solubility of BPA in water suggests that wastewater and washing residue generated during manufacturing and processing may be the most likely sources to the environment. These wastewaters are normally treated prior to discharge to surface waters in onsite treatment plants or offsite in municipal sewage treatment plants. Fugitive gaseous emissions of BPA from products are believed to be negligible because the vast majority of BPA reacts to completion in the product during manufacture and BPA has a very low vapor pressure. As discussed earlier and unlike other organic chemicals such as benzene, BPA has an extremely low air water partition coefficient of 10^{-9} . As a result the rate of evaporation from water will be very low, thus discharges to water will tend to remain in water or partition to sediment. This is discussed later under the Level III analysis.

Total releases of BPA to the environment have been estimated separately for the U.S. and E.U. (Table 3). Releases have been estimated in the E.U. as part of the E.U. risk assessment and in the U.S. as part of the Toxics Release Inventory (TRI). These two sets of emission estimates have been reanalyzed and “best estimates” of emissions compiled for the two regions, as discussed in more detail below.

U.S. releases of BPA reported in the TRI include 85,300 kg of stack and fugitive emissions to air, 3500 kg directly to water, 1100 kg to water following 90% removal in offsite treatment plants, and an additional 10,000 kg to water assuming similar miscellaneous sources. These miscellaneous losses include losses from thermofax paper, migration from polymerization products and other losses from landfills, leaching from pipe linings, and other discarded materials that are not landfilled, and dust formation. U.S. emissions include large amounts of BPA released as fugitive stack

Table 3. E.U. and U.S. BPA release estimates (kg/year).

Medium of Release	A 85,300 (85%)	B 3,200 (18%)	C 2,140 (2.2%)	D 2,140 (10%)
Air				
Influent wastewater	11,100	11,100	154,200	18,900
Effluent wastewater	1,100	1,100	15,420	1,890
Direct to surface waters	13,500	13,500	77,800	17,000
Total to surface waters	14,600 (15%)	14,600 (82%)	93,220 (98%)	18,890 (90%)
Soil	0	0	0	0
Total	99,900	17,800	95,360	20,930

A, the U.S. TRI estimate includes high emissions to air estimated by using engineering emission factors rather than measurements. B, the U.S. "best-estimate" includes lower emissions to air estimated using E.U. data adjusted for the fraction of production. C, the E.U. risk assessment estimate, includes emissions to water based on default emission factors for several applications that are believed to be too high (see text). D, the E.U. "best estimate" has lower release to surface waters and is believed to be more realistic. Emissions from effluent wastewater include 90% BPA removal by treatment and those direct to surface water include other emissions estimated by Staples (2000). The treatment efficiency for removal of BPA from influent wastewater was estimated to be approximately 90% from an evaluation of monitoring data taken from both influent and effluent wastewaters at various treatment works (Belfroid *et al.* 1998; Lee and Peart, 2000; Furhacker, *et al.* 2000) and from estimation of removal efficiency using a Sewage Treatment Plant model (Clark *et al.* 1995).

emissions. Total releases in the E.U. are similar to the US, but are from different sources. Negligible amounts of BPA were released to air (2140 kg), 86,500 kg was assumed to be released to water from both direct and indirect sources and an additional 6,700 kg was assumed to be released to water from miscellaneous sources, based on the same assumptions as the US, proportional to production. Table 4 shows the breakdown of emissions to the entire E.U. as estimated in the E.U. risk assessment.

It is inconceivable that the relative emissions to air and water for the E.U. and U.S. should be so markedly different because BPA is handled similarly in both regions. The reason for the large disparity is likely the use of default engineering estimates for reporting some environmental releases, which provide conservative, overestimates of emissions. For example, the U.S. emissions include large amounts of BPA released as fugitive stack emissions. These amounts are much higher than in the EU, which were largely based on measurements rather than engineering estimates or emission factors as done in the U.S. It is unlikely that there are high fugitive emissions of BPA because of its extremely low volatility. Therefore, a reasonable "best estimate" of emissions to the air in the U.S. is to assume that the releases are similar to those in the EU, on a fraction of production basis. In the EU, three categories of release, phenoplast cast resin production, thermal paper production and recycling, and PVC processing use as an inhibitor, were estimated using default engineering estimates, which may also be conservative estimates of the actual amounts released to the environment from these sites/applications. It is suggested that a "best estimate" would be if the actual releases to surface waters were 10% of the default assumptions. Compiled in Table 3 are emission data from the E.U. risk assessment, the U.S. TRI and the "best estimate" emissions made here for the U.S. and EU. The net result of the adjustments made for the "best estimate" emission scenarios is that the "best estimates" for the E.U. and U.S. have similar emissions to air and water and thus are more mutually consistent. The total emissions for the "best estimates" are also a factor of 4 to 5 lower than the default estimates.

Table 4. Releases to the E.U. environment as estimated in the E.U. risk assessment. The grand total is 227,000 kg/yr or 0.044% of E.U. production.

Process	Air (kg/yr)	Receiving Water (kg/yr)	Wastewater (kg/yr)
Bisphenol-A production	960	1,140	n/a
Polycarbonate production	180	260	n/a
Epoxy resin production	0	490	n/a
Phenoplast cast resin production	0	18,500	43,100
Thermal paper production	0	3190	n/a
Thermal paper recycling	0	21,000	49,100
PVC – Inhibitor during prod. process	0	24,900	58,100
PVC – Antioxidant during processing	250	320	750
PVC – Preparation of additive package	0	320	740
PVC – Use of additive package	250	320	750
PVC – Antioxidant in plasticiser	0	640	1,490
PVC – Plasticiser use	500	40	100
Miscellaneous	0	6,700	0
Total	2,140	71,100	154,200

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The approach used in the E.U. risk assessment for estimating environmental emissions to the EUSES “regional” modeling scenario, a subregion supposedly representative of the EU, was to assume that at least 10% of the emissions to the entire E.U. are released to the model subregion (BRE 2000). BPA is produced at six sites within the E.U. and the vast majority of emissions originate from either these six production sites or the 85 processing facilities in the E.U. If a production/processing site was identified with >10% of the entire E.U. emissions, then the emissions from this site were used for the EUSES “regional” modeling scenario. The estimated regional emissions to air and water are 15% and 12%, respectively, of the estimated continental emissions (*i.e.*, the emission to the entire EU). These regional emissions are proportionately high relative to the assumed surface area of the EUSES regional environment, 40,000 km², which is only 1.1% of the entire E.U. continental environment (3,560,000 km²) and thus provides a conservative assessment of exposure. Calculating emissions on a “per area” or “per capita” basis, as is sometimes done in risk assessments, is inappropriate because emissions largely occur near manufacturing or processing facilities.

Monitoring Data

In addition to compiling emissions information, a database tabulating observed environmental concentrations in all relevant environmental media has been prepared. The monitoring data were taken from publications in the open, peer-reviewed scientific literature that include Matsumoto and Genki (1982), Staples *et al.* (2000), Clark *et al.* (1991), Matsumoto *et al.* (1977), del Olomo *et al.* (1997), Hendriks *et al.* (1994), Matsumoto and Hanya (1980), Rudel *et al.* (1988), Yamamoto and Yasuhara (1999), and other published documents from Europe, the U.S., and Japan. A copy of the monitoring database containing all individual data points and references used is available as an Excel™ spreadsheet from the corresponding author.

A statistical summary of the water and sediment data was compiled (Table 5). Unfortunately, because many studies reported median concentrations and ranges, but did not report all the individual concentration data, it was not possible to derive statistics based on all the individual data points. Instead, it was decided to calculate the median and the 10th and 90th percentiles of the reported study medians. One-half of the reported method detection limit was used when only nondetect values were reported in a study.

The data compilation exercise revealed that although there are numerous measurements of BPA in European and Japanese surface water and sediment samples, there are no measurements of concentrations in ambient air and soil of acceptable quality in Europe and Japan, and very few measurements for any media in the rest of the world. The dominance of water and sediment data is not surprising because BPA is known to enter surface waters in the wastewater of manufacturing facilities. Surface waters and sediments are thus an obvious sampling medium as concentrations and exposures will be relatively high in these media. It is unfortunate, however, that soil and air have been totally neglected because this greatly reduces the capability of validating predicted concentrations and exposure. However, as previously discussed, atmospheric concentrations are likely to be too low to be measured even using the most sophisticated analytical techniques.

Table 5. Statistical summary of monitoring data.

Statistic	Europe	United States
Number of reported surface water concentrations	157	14
Median reported water concentration	16 ng/L	0.5 µg/L¹
10th percentile concentration	5.0 ng/L	0.5 µg/L¹
90th percentile concentration	75 ng/L	4.4 µg/L
Number of reported sediment concentrations	21	0
Median reported sediment concentration	42 µg/kg	-
10th percentile concentration	3.5 µg/kg	-
90th percentile concentration	180 µg/kg	-

¹ The median and 10th percentile U.S. surface water concentrations are actually _ of the detection limit of 1.0 µg/L reported for these analyses by Staples *et al.* (1999). European studies reported much lower detection limits (0.6-10 ng/L). It is therefore possible that analysis of U.S. surface waters using more sensitive analytical techniques would reveal lower water concentrations, more comparable to European levels.

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The monitoring data have been separated into two geographical regions, Europe and the US, where the best data on environmental concentrations and environmental release estimates exist. It is likely that the monitoring data are focused on locations where concentrations are suspected of being high, *i.e.*, close to point sources or disposal locations. As a consequence, the database may be biased toward overestimation of regional concentrations. A further positive bias may be introduced by the assumption of nondetect data points being equal to half the method detection limit.

The ratio of the average sediment and water concentration in Europe is approximately 42,000 ng/kg/16 ng/L or 2600 L/kg. This ratio is remarkably high, given that the sediment-water partition coefficient estimated from K_{OW} in the evaluative modeling suggests a much lower sediment-water partition coefficient of about 40 L/kg. This is discussed in the following section.

STAGE 3 — EVALUATIVE ASSESSMENT OF CHEMICAL FATE

EQC Model Description

Conducting evaluative assessments provides invaluable insights into the characteristics of chemical behavior in the environment. The aim is to establish the general features of chemical behavior, *i.e.*, into which media the chemical will tend to partition, the primary loss mechanisms, its tendency for intermedia transport, its tendency to bioaccumulate, its tendency to undergo long-range transport, and its environmental persistence. In this report we use the Equilibrium Criterion or EQC model that has been fully described elsewhere (Mackay *et al.* 1996a). Briefly, this model in the form of a computer program, deduces the fate of a chemical in Levels I, II, and III evaluative environments using principles described by Mackay (2001). The EQC evaluative environment is an area of 100,000 km², which is regarded as being representative of a jurisdictional region such as the U.S. State of Ohio, or the country of Greece.

Level I Assessment: Equilibrium Partitioning

Level I EQC modeling of BPA indicates that under equilibrium conditions, the vast majority of the chemical will reside in either soil (67.9%) or surface water (30.5%), with more than 98% of BPA partitioning to these two media (Figure 2). The low vapor pressure of BPA results in small percentages partitioning to the air compartment (< 0.00003%). BPA is a moderately hydrophobic compound (K_{OW} of $10^{3.4}$) and is moderately soluble in water (300 g/m³), thus its estimated fugacity capacity or Z value in soil (Z_S : 1.23×10^7 mol/m³.Pa) is 50 times larger than in water (Z_W : 2.48×10^5 mol/m³.Pa), *i.e.*, the dimensionless soil-water partition coefficient or ratio of Z-values is 50. The water compartment in the EQC model has, however, a much larger volume (V_W : 2×10^{11} m³) than the soil compartment (V_S : 9×10^9 m³) and thus the total number of moles of BPA partitioning to water is still substantial. Similarly, although the bottom sediment has a larger fugacity capacity than the overlying water, the total amount partitioning to bottom sediments (1.5%) is small relative to water because the sediment compartment has a much smaller volume.

BPA partitioning to biota is not predicted to be high, even without consideration of metabolism in the organism, with the Level I model predicting an equilibrium fish/water partition coefficient or bioconcentration factor (BCF) of 125. Measured values

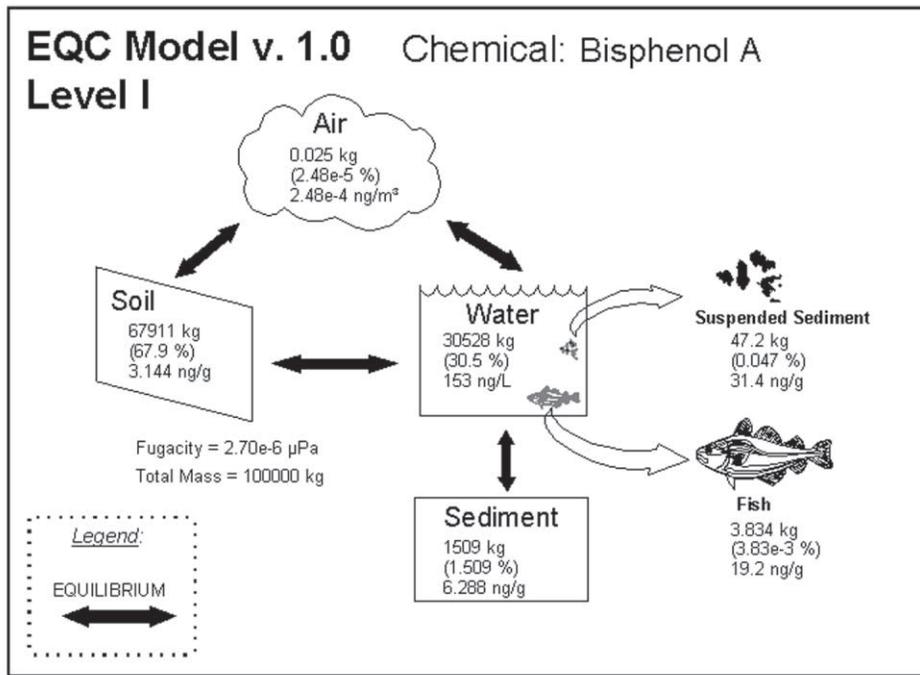


Figure 2. Level I EQC modeling diagram.

of BCF for fish, which include a reduction in concentration in the fish attributable to metabolism (using MITI test data, Tunkel *et al.*, 2000), are between 5 and 68.

There is consensus that when assessing the extent of bioaccumulation in fish, the preferred approach is to use (in decreasing order of preference) measured or observed BCF or bioaccumulation factor (BAF) data, then a BCF deduced from K_{OW} . The low measured values of BCF indicate the presence of rapid metabolism as shown by a simple screening level calculation. A typical respiratory uptake rate constant for a fish k_1 is 100 day⁻¹ (Mackay and Fraser 2000), thus the respiratory clearance rate constant k_2 is expected to be about 1 day⁻¹ based on K_{OW} , *i.e.*, k_2 is k_1/BCF . If an actual BCF of 20 is assumed, then because the actual BCF (including metabolism) is $k_1/(k_2 + k_M)$, then the metabolism rate constant k_M must be about 4 days⁻¹ and the half-life about 0.2 days. Thus, BPA is very rapidly metabolized in fish, a finding consistent with its rapid biodegradation in the environment.

The Level I model suggests equilibrium concentrations in sediment of 6.3 ng/g or 6300 ng/kg and in water of 153 ng/L, a ratio of 41 L/kg. This figure is a consequence of K_{OW} of 2512, implying a K_{OC} (organic carbon-water partition coefficient) of about 1000, which is consistent with recent K_{OC} measurements for soils (Möndel 2001a). Assuming 5% organic carbon in sediment suggests that K_p will be about 40 L/kg. The data in Table 5 show a median ratio of 42000 ng/kg to 16 ng/kg, *i.e.*, 2600 L/kg, a factor of 65 higher. It may not be appropriate to compare the median concentrations in water and sediments from a number of different studies. However, a recent study (Heemken *et al.* 2000) that measured concentrations of BPA in suspended sediments and water from the same river water samples reported measured K_{OC} values of 10^{4.5}, an order of magnitude higher than

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estimated from K_{OW} . The observed concentrations in sediment are much higher than expected. One unlikely explanation is that the fugacity of BPA in sediments is much higher than that in the water. There are reasons that indicate that a higher fugacity could exist by a factor of about 5 because of organic matter degradation releasing sorbed BPA, but a factor of 65 or higher is inconceivable. There may be several reasons for the apparent discrepancy in sediment partitioning. Given the difficulties in obtaining sediment samples, the reported concentrations may not be truly reflective of the environment, or they may be biased toward overestimation of sediment concentrations because they may contain a high proportion of data collected immediately downstream of wastewater outfalls. In addition to difficulties with sediment sampling, the lack of a validated method for sediment analysis may have led to inaccuracies in reported sediment concentrations. Alternatively, the reason may lie in the state or availability of the BPA in the sediment. In fugacity terms, the Z value for BPA in sediment is being underestimated by a factor of at least 10 and probably a factor of 50. There are several possible explanations

1. BPA binds to organic matter, mineral matter or black carbon (soot) in the sediment with unusual strength, *i.e.*, the actual sediment-water partition coefficient is much higher than is suggested by K_{OW} and K_{OC} . PAHs, for example, have been shown to sometimes bind to sediments more strongly than can be explained by K_{OW}/K_{OC} relationships (Accardi-Dey and Gshwend 2002).
2. BPA in the sediment is not present in free molecular form, but is present in another matrix. It is, however, released and measured during analysis, possibly because aggressive solvent extraction releases the compound from the matrix. BPA may have been strongly bound to the matrix when it was released to the environment and desorption to equilibrium partitioning conditions may be slow.
3. A third explanation is that BPA was discharged in the past in much greater quantities leading to "in place" contamination. This is unlikely to be the case because BPA is not persistent.

Carefully controlled laboratory sediment-water partitioning experiments are the only appropriate way to shed light on this issue.

Staples *et al.* (1998) have previously reported Level I modeling results for BPA with a distribution of 25% in the soil, 52% in the water, and 23% in the bottom sediments. The relatively higher partitioning to water and sediment was achieved by assuming different volume ratios of the media represented in the model world. For comparison, in the EQC model world the bottom sediment to soil to water to air volume ratios are 1 : 90 : 2000 : 1,000,000, whereas in the model world used by Staples *et al.* these volume ratios are 1 : 2 : 333 : 286,000. The volume ratios used by Staples *et al.* are biased to an assessment of fate in the aquatic environment, presumably because BPA is largely emitted to that medium. The EQC model world gives, in our opinion, a better representation of fate in the environment as a whole.

Level II Assessment: Initial Evaluation of Environmental Loss Processes

Level II EQC modeling requires the additional model inputs of environmental half-lives for each of the media: air, water, soil, and sediment (Table 2). Level II EQC modeling of BPA indicates that under equilibrium partitioning and steady state

conditions, the major loss routes for BPA will be reaction in water (29.6%) and soil (65.8%) and advection from the model world in water (4.6%) (Figure 3). The model predicts an overall residence time of 151 h (6.3 days) and reaction and advection residence time of 158 h (6.6 days) and 3272 h (136 days), respectively. Therefore, BPA is not predicted to be persistent in the environment and its overall persistence is dominated by reaction. The very low percentage (<0.0001%) predicted to be leaving the model world in advecting air indicates that the potential for atmospheric transport is very low. Transport potential in water is greater.

Level III Assessment: Nonequilibrium, Steady State

Level III modeling is useful in determining how the media into which the chemical is released affects the overall environmental fate. Level III fugacity calculations allow nonequilibrium conditions to exist between connected media at steady state and illustrate important transport and transformation processes. They are considered to be the most environmentally realistic calculation that can be undertaken with the EQC model. The tendency of chemicals to migrate between media can be assessed by modeling emissions to each individual medium and calculating the amount present at steady state. Table 6 contains the amount of chemical present in each medium of the EQC model environment, and the chemical persistence at steady state for individual emissions of 1000 kg/h to the air, water, and soil compartments, as well as for simultaneous emissions of 1000 kg/h to each compartment (illustrated in Figure 4).

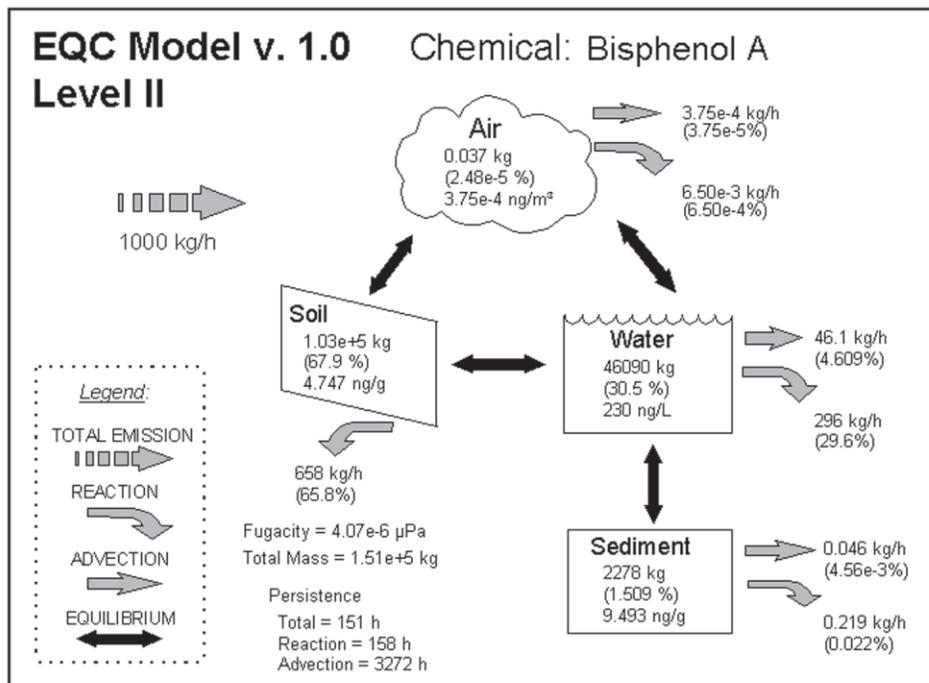


Figure 3. Level II EQC modeling diagram.

Multimedia Assessment of Bisphenol A

Table 6. EQC Level III results: chemical amounts in each medium based on single and multiple emissions.

Emission medium	Amount at steady state (kg) (percent in brackets)				Residence time (d) (without advection in brackets)
	Air	Water	Soil	Sediment	
Air	35 (<0.1)	13 600 (8.8)	139 000 (90.7)	741 (0.5)	6.4 (6.5)
Water	< 0.1 (<0.1)	135 000 (94.8)	< 0.1 (<0.1)	7 354 (5.2)	5.9 (6.7)
Soil	< 0.1 (<0.1)	212 (0.1)	156 000 (99.9)	12 (<0.1)	6.5 (6.5)
All three	35 (<0.1)	149 000 (32.9)	295 000 (65.3)	8 107 (1.8)	6.3 (6.6)

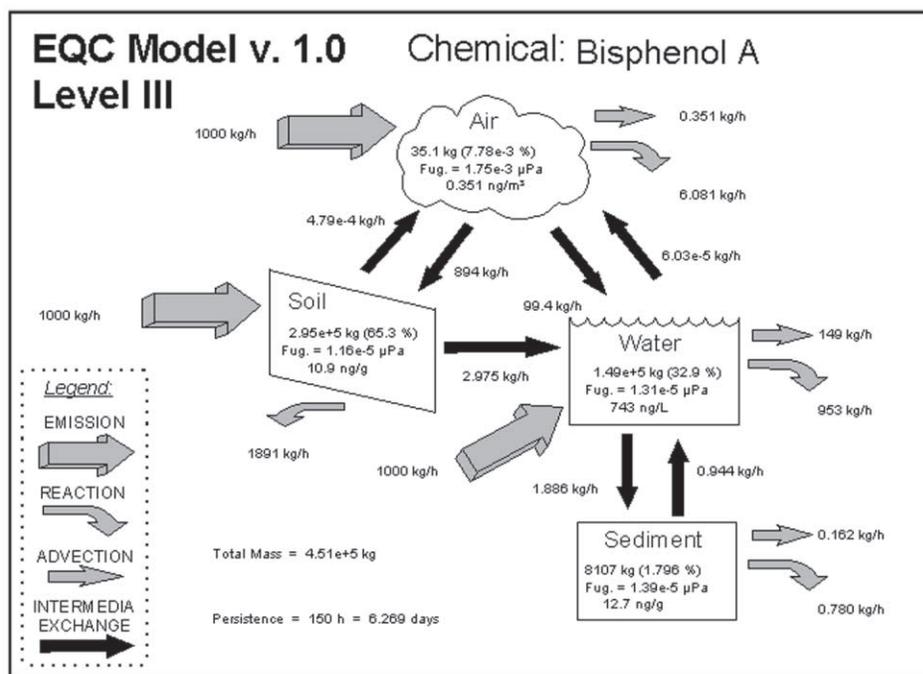


Figure 4. Level III EQC modeling diagram (1000 kg/h released simultaneously to air, water and soil).

If the emission is to air, the chemical partitions to atmospheric aerosols and deposits to soil and water. The soil compartment will accumulate a larger percentage of BPA because the soil compartment in EQC has a larger surface area to receive atmospheric deposition. If the emission is to water or soil, the model predicts that the BPA will remain in the compartment where it is emitted, although there is some transfer to bottom sediments when the emission is to water. The relative amounts emitted to different environmental media therefore have a large effect on environmental fate and exposure, thus it is essential that emission rates to the various media should be accurately quantified for meaningful risk analysis to be undertaken.

Assessing Environmental Persistence

Single media half-life criteria are used by regulators worldwide to assess whether a chemical is persistent in the environment (Rodan *et al.* 1999). For example, the single media half-life criteria used by Environment Canada to assess persistence are 2 days, 6 months, 6 months, and 1 year for air, water, soil, and sediments, respectively (Gouin *et al.* 2000). Criteria adopted by the United Nations Environment Program for international action on persistent organic pollutants (UNEP 2000) are 2 days, 2 months, 6 months, and 6 months for air, water, soil and sediments, respectively. If a chemical is estimated to have a half-life in any one of these media that exceeds these criteria, then that chemical is considered to be persistent. Clearly, BPA is not persistent in the environment when assessed against these criteria (see Table 2).

It has been proposed recently by Webster *et al.* (1998) that persistence in the environment should be operationally defined as the overall residence time at steady state in a multimedia environment. A simple Level III multimedia mass balance model is usually used for this calculation in which only irreversible losses are considered. Irreversible losses consist primarily of chemical transformation of parent compound, but also include unidirectional transport to deep ocean layers, sediments and groundwater as well as the upper atmosphere. The "persistence estimation" model used in this study is essentially the same as EQC, but it is set to mimic a closed system, from which no advective losses in air or water occur.

Data in Table 6 show that the mode of entry to the environment does not greatly affect the overall residence time in the environment. This is because aerobic biodegradation is rapid and of the same approximate rate in soil and water, the two primary media of accumulation. The estimated overall residence time with no advection is between 6.5 and 6.7 days. When advection is included in the calculation the overall residence time is similar, indicating that the majority of BPA emitted will remain in the model region and degrade there. A pseudo-first-order half-life for removal of BPA from the environment can be estimated as $\ln 2$ (0.693) multiplied by the residence time. The overall half-life for removal of BPA from the environment by reaction is therefore between 4.5 and 4.7 days and 97% will be removed from the environment in 5 half-lives or in about 23 days, assuming first-order loss kinetics. The overall residence time for removal of BPA from the environment by reaction only is between 6.5 and 6.8 days.

Gouin *et al.* (2000) suggested that a criterion for determining if a chemical is persistent based on overall persistence predicted by a multimedia model could be 1400 to 2000 h or 58 to 83 days. Clearly, BPA is also not persistent when assessed against this criterion for overall persistence.

Assessing Long-Range Transport Potential

Another important criterion that is used to prioritize organic compounds for regulation is the potential for long-range transport (LRT). There are two main factors that control a chemical's LRT potential: (1) persistence and (2) "stickiness" (*i.e.*, the propensity for a chemical to partition to the terrestrial surface if transported in air, or its propensity to partition to sediment if transported in water). TaPL3, a modification of the EQC model (Beyer *et al.* 2000), has been used to calculate a characteristic travel distance of BPA in air and water. In TaPL3 advection is again "turned off" and the characteristic transport distance (km) is calculated as the product of overall residence time (h), the velocity of the mobile medium (km/h) being considered, and the fraction of chemical in that medium. The TaPL3 calculated travel distances in air and water for BPA are 0.51 km and 561 km, respectively. The travel distance in air is very low compared to calculated atmospheric travel distances of 130,000 km for hexachlorobenzene, 13,000 km for technical lindane, 7600 km for tetrachlorobiphenyl, and 750 km for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin.

If emitted to air, the calculations suggest that BPA is expected to remain relatively close to point sources. The low transport potential of BPA in air is a reflection of both its high "stickiness" and relatively high reaction rate. If emitted to water, however, BPA may travel many hundreds of kilometres downstream of point sources. This has been confirmed in a study that measured concentrations at sampling sites in the Elbe River, its tributaries and in the North Sea estuary of the Elbe (Heemken *et al.* 2001), although it is acknowledged that multiple discharges likely exist along the waterway.

Based on the modeling calculations, it is unlikely that without point sources, BPA would be detected in the surface waters or sediments of river basins or lakes or in natural vegetation or soils. The only possible explanations if BPA were to be detected in areas remote from obvious point sources are therefore:

1. Laboratory contamination of samples. Some migration of residual levels of BPA present in polycarbonate plastics and epoxy resins has been shown, albeit at low levels.
2. Misidentification of BPA during analysis. Although this seems unlikely with modern methods of analysis that use mass spectrometry for confirmation, identification should not be based on presence of parent ion alone.
3. Natural sources of BPA. There is presently no evidence to support this explanation.
4. Formation as a breakdown product of a more persistent organic contaminant. No such pathway is known.
5. Diffuse sources from polymers containing unreacted BPA. There are limited monomeric uses for BPA such as in the production of thermal papers and in polyvinylchloride production and processing (BRE 2000). The presence of BPA in landfill leachates has been attributed to migration from waste plastics (Yamamoto and Yasuhara 1999).

STAGE 4 — REGIONAL FAR FIELD ASSESSMENT

Regional Mass Balance Models

The main objective of a regional fate assessment is to input reliable discharge data for a region into the model and obtain predicted regional average environmental concentrations for each media, which can be used in exposure and/or risk assessments. Regional models can be partially validated by comparing available data on ambient environmental concentrations with model predictions. It is expected that agreement between model predictions and environmental concentration data will be approximate, *i.e.*, a factor of 2 or 3 rather than, for example, plus or minus 20%. This level of accuracy, however, is often adequate to determine if concentrations are significant. In risk assessment applications, toxicity data are rarely more accurate than the above ranges.

Several models have been developed for assessing the regional chemical fate in the environment on a regional scale, for example, ChemCAN (Mackay *et al.* 1991), SimpleBox (van de Meent 1993), CalTOX (McKone 1993), and HAZCHEM (ECETOC 1994). A key factor in selection of a model for exposure and/or risk estimation is its reliability and consistency with other independent models. It is important that different fate models provide similar assessments. In 1995 an expert panel reported on a systematic evaluation of the strengths and weaknesses of regional contaminant fate models, and presented an intercomparison of available models (Cowan *et al.* 1995). Excellent agreement was achieved between ChemCAN 4.0, SimpleBox 1.0, and other models for two representative chemicals by harmonizing numerous input parameters describing environmental properties and kinetic processes. This exercise demonstrated the fundamental similarity of these models, but the expert panel identified the need for additional model comparison and validation exercises as critical research topics to facilitate improvement in performance of models. Cowan *et al.* (1995) recommended that comparisons be made between measured and predicted concentrations for several data sets, for a larger number of chemicals, and that this should be done by groups of experts acting independently and using different models. Kawamoto *et al.* (2001) have essentially done this by comparing SimpleBox 1.0 and ChemCAN 4.0 for 68 chemicals on two spatial scales in Japan.

ChemCAN Modeling

The ChemCAN v4.0 model used in this study treats four bulk compartments, *i.e.*, air, surface water, bottom sediments, and surface soil. Full details of the ChemCAN model are not given here, but can be found in Mackay *et al.* (1991).

Because the majority of the monitoring data have been collected in Europe, it was decided to focus model evaluation on the European environment using only reported environmental concentrations and emissions from the EU. Furthermore, this allows a direct comparison of the ChemCAN modeling results with predictions by using the EUSES model, recently produced as part of an E.U. risk assessment of BPA (BRE 2000). For the regional- and continental-scale risk assessments, EUSES uses the SimpleBox v1.0 model to predict environmental concentrations (PECs) in air, water, soil, and sediment, and compare these concentrations to predicted no effect concentrations (PNECs) for various test organisms. In this study, the results of this E.U. modeling exercise are compared with results from the ChemCAN model. For this comparison, the ChemCAN model was calibrated to the default region used for EUSES regional chemical risk assessments by inputting the regional characteristics contained in Table 7. "Calibration"

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Table 7. Environmental parameters input to ChemCAN 4.0 to achieve calibration with the regional risk assessment conducted with EUSES by BRE (2000).

Parameter	Median Value	Unit	Confidence Factor ¹
Total area of region	4 x 10 ¹⁰	m ²	–
Water surface area	1.2 x 10 ⁹	m ²	5
Water depth	3	m	3
Air mixing height	1000	m	3
Soil mixing depth	0.05	m	3
Sediment mixing depth	0.03	m	3
Rain scavenging ratio	20,000	–	3
Volume fraction of particles in air	2 x 10 ⁻¹¹	–	3
Volume fraction of particles in water	1.5 x 10 ⁻⁵	–	3
Volume fraction fish in water	10 ⁻⁶	–	3
Volume fraction of air in soil	0.2	–	1.5
Volume fraction of water in soil	0.2	–	1.5
Volume fraction of soil solids	0.6	–	1.5
Volume fraction of sediment pore water	0.8	–	1.5
Volume fraction of sediment solids	0.2	–	1.5
Organic carbon fraction of particles in water	0.1	–	3
Organic carbon fraction of soil solids	0.02	–	3
Organic carbon fraction of sediment solids	0.05	–	3
Advection residence time of air	0.684	days	3
Advection residence time of water	40.1	days	3
Emission to air	2,812	kg/year	10
Emission to water	13,356	kg/year	10
Emission to soil	2,995	kg/year	10
Background inflow air concentration	0.28	pg/m ³	3
Background inflow water concentration	20	ng/L	3
Water and aquatic biota density	1000	kg/m ³	1.5
Soil solids, sediment solids, atmospheric aerosol and water particle density	2400	kg/m ³	1.5

¹ 95% confidence factors (Cf) were used as convenient expressions of variance where the standard deviation (σ) is equal to $0.5 \ln Cf$ (or $Cf = e^{2\sigma}$) for a lognormal distribution. A Cf of n implies that 95% of the data will be between n times and $1/n$ of the median value.

implies that the parameters used to describe the environmental characteristics of the air, water, soil, and sediment compartment were set to the same values and the emissions and advective inflows used were the same in both models. The parameters and equations used to describe environmental partitioning and transport processes in the two models have not been harmonized. However, with a few notable exceptions (*e.g.*, gas-particle partitioning and sediment deposition velocity) these processes are described similarly in both models. A notable difference between ChemCAN and EUSES is that ChemCAN treats only one soil compartment, whereas EUSES treats three soil compartments, *i.e.*, natural soil, arable soil, and industrial soil.

Environmental characteristics of the ChemCAN model region used in this study are given in Table 7. Mass transfer coefficients are listed in Table 8. A notable difference

Table 8. Mass transfer coefficients used in ChemCAN to achieve partial calibration with the regional risk assessment conducted with EUSES.

Mass Transfer Coefficient (MTC)	Median Value (m/h)	Confidence Factor ²
Air side air-water MTC	5.0	3
Water side air-water MTC	0.05	3
Rain rate	1 x 10 ⁻⁴	3
Aerosol deposition	10.8	3
Soil-air phase diffusion MTC	0.02	3
Soil water phase diffusion MTC	1 x 10 ⁻⁵	3
Soil air boundary layer MTC	5.0	3
Sediment-water MTC	1.0 x 10 ⁻⁴	3
Sediment deposition	5.0 x 10 ⁻⁶	3
Sediment resuspension	2.0 x 10 ⁻⁶	3
Soil water runoff	5.0 x 10 ⁻⁵	3
Soil solids runoff	1.0 x 10 ⁻⁸	3
Sediment burial	Zero ¹	-
Diffusion to stratosphere	Zero ¹	-
Leaching from soil	Zero ¹	-

¹ These transport processes were set to zero because they are not included in SimpleBox.

² 95% confidence factors (Cf) were used as convenient expressions of variance where the standard deviation (σ) is equal to $0.5 \ln Cf$ (or $Cf = e^{2\sigma}$) for a lognormal distribution. A Cf of n implies that 95% of the data will be between n times and 1/n of the median value.

between the model region described in Table 7 and the EQC model world is the assumed percentage of surface area covered by water. The EUSES region has a surface water area of 3%, which is chosen to be representative of an area drained by rivers, and not containing large lakes. The EQC model has a large water surface area of 10%, which is chosen to account for the effect of large lakes and coastal waters on chemical fate.

Uncertainty Analysis

In addition to choosing single 'preferred' values for the model input parameters, a range of values has been selected to give a more realistic expression of uncertainty in the output. Uncertainty and sensitivity analysis of the model output to all model input parameters (most of which are listed in Tables 1, 2, 7, and 8) were conducted by simultaneously varying them using Crystal Ball 4.0* (Decisioneering, Colorado, USA). Lognormal distributions were assumed for all input variables in order to reduce skewness and were parameterized by the mean and standard deviation of the corresponding normal distribution on a log scale. Ninety-five percent confidence factors (Cf) were used as convenient expressions of variance where the standard deviation (σ) is equal to $0.5 \ln Cf$ (or $Cf = e^{2\sigma}$) for a lognormal distribution. A confidence factor of n implies that 95% of the data will be between n times and 1/n of the mean and the value of n is chosen to reflect both environmental variability and parameter uncertainty. Assigning a confidence factor is a subjective process

requiring expert judgment. MacLeod *et al.* (2002) provide a detailed analysis of the application of uncertainty analysis to multimedia models. They have attempted to assign confidence factors for all the input variables in multimedia models and their work was used as the starting point for assigning confidence factors in this study.

Input variables were sampled from their 95% confidence factors shown in these tables for 1000 simulations. With this many simulations, the standard error of estimate for the mean was always less than 5% of the standard deviation, which was considered adequate. The sensitivity of the model output was later evaluated in terms of contribution of individual input variables to variance in model output.

Reconciling Model Predictions with Monitoring Data

Compared in Table 9 and Figure 5 are observed European environmental concentrations for surface waters and sediments and PECs from three separate simulations, as follows:

- A. EUSES predicted regional environmental concentrations from BRE (2000)
- B. ChemCAN 4.0 predicted environmental concentrations, using the same chemical inputs as in the EUSES regional simulation from BRE (2000)
- C. ChemCAN 4.0 predicted environmental concentrations using the “best estimate” of chemical properties and emission estimates from this study

The following model inputs were used for modeling scenario “B”: physical-chemical parameters listed in Table 1, “EUSES” half-lives listed in Table 2, and environmental parameters listed in Tables 7 and 8. For modeling scenario “C”, the same inputs were used as for scenario “B” with the exception of emissions and half-lives. The half-lives recommended in this study and listed in Table 2 and the “best estimate” emissions for the E.U. listed in Table 3 were used. It was decided to assume that 15% and 12% of the total E.U. emissions to air ($0.15 \times 2140 = 321$ kg/yr) and water ($0.12 \times 18,890 = 2267$ kg/yr), respectively, occurred within the model region, as was done in the E.U. risk assessment.

Median and 10th and 90th percentiles were included for observed concentrations and the ChemCAN PECs in Table 9 and Figure 5. The results for modeling scenarios “A” and “B” show that for a common set of input parameters, model predictions from EUSES and ChemCAN compare favorably. The slight differences between the descriptions of partitioning and transport processes between the two models makes little difference to the predicted concentrations of BPA in air, water, sediments, and soil and are within model uncertainty. Agreement between model predictions and water monitoring data is best for scenario “C”, but predicted sediment concentrations are lower than observed levels in this modeling scenario, even if model uncertainty is accounted for. These results suggest, as previously discussed, that partitioning to bottom sediments is nonequilibrium in nature and thus is unlikely to be well predicted by fate models.

A steady state mass balance diagram for model scenario “C” is given in Figure 6. The diagram shows that BPA rapidly deposits from air to soil, and that the water/sediment exchange is important. The higher proportion in the sediment compartment in the regional model compared to EQC is due to the higher sedimentation/resuspension velocities. The regional model has sedimentation/resuspension ve-

Table 9. Various model predictions and monitoring data.

Medium	A	B	C	Median observed concentrations
Air (total)	0.27 pg/m ³	0.18 pg/m ³ (0.03–.0)	0.02 pg/m ³ (0.004–0.11)	–
Water (total)	130 ng/L	140 ng/L (26–940)	14 ng/L (3.0–82)	16 ng/L
Soil	0.10 µg/kg dry	0.30 µg/kg dry (0.05–1.5)	0.0023 µg/kg dry (0.0004–0.02)	–
Sediments	4.8 µg/kg dry	12 µg/kg dry (1.7–120)	2.0 µg/kg dry (0.24–22)	42 µg/kg dry

A is the EUSES/SimpleBox PECs from the E.U. risk assessment (BRE, 2000). The soil PEC is for “natural soil.” B is the ChemCAN PECs using the same model inputs used in the EUSES modeling. Only one soil type is treated in ChemCAN. The 10th and 90th percentiles representing model uncertainty are given in brackets. C is the median ChemCAN PECs using the “best estimate” model inputs and associated uncertainty suggested in this study. The 10th and 90th percentiles representing model uncertainty are given in brackets.

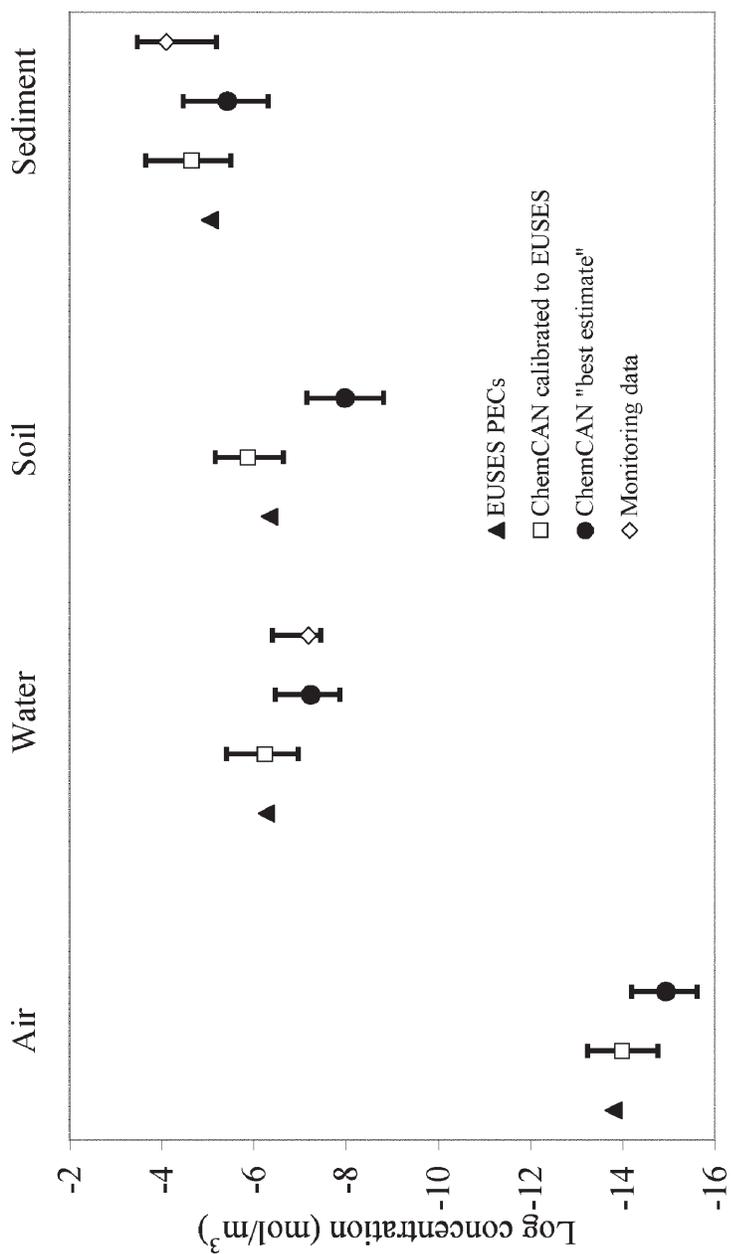


Figure 5. Comparison between monitoring data and predicted environmental concentrations from different modeling scenarios.

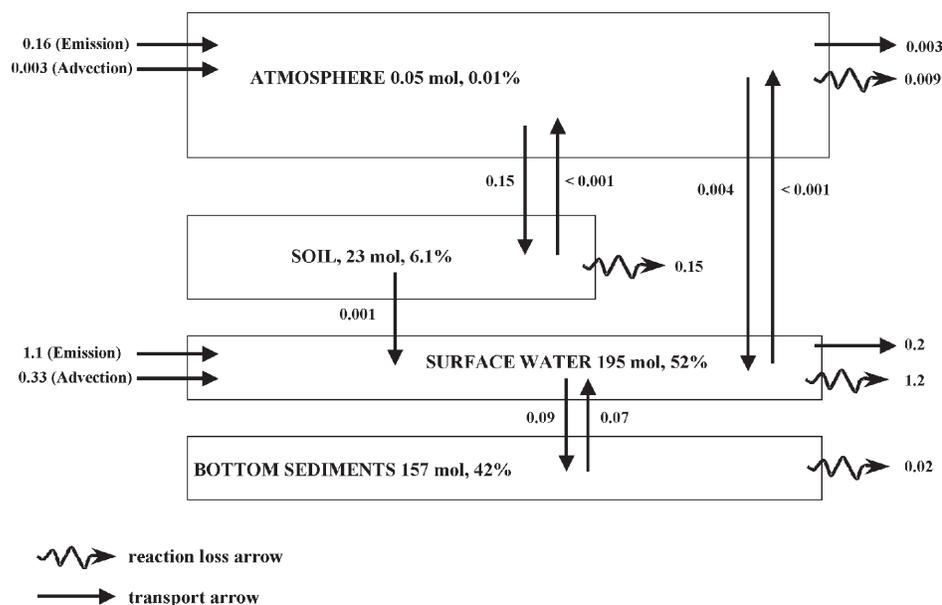


Figure 6. ChemCAN steady state mass balance for BPA (all fluxes in mol/h).

locities representative of riverine systems, whereas EQC is reflective of lacustrine systems. Volatilization from soils and surface waters is negligible. The majority of BPA discharged to the model region is degraded in surface waters (75%) and soils (9.4%), although 13% of the total discharged is transported out the model region in advecting water. The model predicts that when total emissions of BPA to the environment are 3249 kg/year the total inventory in the environment is 86 kg. As a result the residence time is $86/3249$ or 0.03 years or about 10 days. It is noteworthy that this residence time is slightly longer than that calculated with the EQC model, reflective of the higher percentage of BPA in the sediment compartment where degradation is relatively slow. Mathematically, the residence time is a "characteristic time" describing BPA dynamics in the system. A dynamic model of BPA under initial conditions of zero concentrations, followed by sustained constant emissions would display an approach to a steady state that would be essentially 97% complete after five characteristic times or 0.13 years or 48 days. Similarly, if BPA emissions were stopped entirely the system would clear of BPA almost entirely in 48 days. The implication is that because BPA has been in use for many years, it must have reached a steady state condition in the environment, thus the use of a steady state model is justified for regional mass balance calculations. The fact that water concentrations have been reconciled successfully with emissions is further support for this assertion.

The water concentration used by BRE (2000) in the draft E.U. risk assessment to estimate risk is an order of magnitude higher than both the observed and predicted levels reported in this study. Because there are already safety factors built in to the risk assessment process, it may be appropriate to use a lower water concentration in future risk calculations.

CONCLUSIONS

Chemical Properties

The physical-chemical properties selected for use in this study are in agreement with those used in the E.U. draft risk assessment. We are confident that the selected values used in this study and in the recent E.U. draft risk assessment represent the most up-to-date measurements and are of sufficient accuracy for assessment purposes.

Environmental Degradation Rates

Aerobic biodegradation is the dominant loss process for BPA in all media except the atmosphere, where it is likely to be susceptible to rapid reaction with hydroxyl radicals. Recent river- and soil-die-away studies have provided strong evidence for aerobic biodegradation half-lives of less than 1 week in surface waters and soils. Similarly rapid aerobic biodegradation is thought likely to occur in surface benthic sediments, but anaerobic biodegradation in deeper sediments is thought to be a slow removal process. These recent die-away studies in surface waters and soils provide the best estimates of environmental half-lives of BPA, although it must be appreciated that environmental half-lives will vary depending on environmental conditions such as temperature and the condition of the microbial community.

Environmental Fate Including Persistence and Long-Range Transport

Environmental releases of BPA are mainly to surface waters. Taken together with the low vapor pressure of the compound leads to surface water being the principal environmental medium of concern. Using a water degradation half-life of 4.5 days in modeling calculations (the mid-point from the study by Klečka *et al.* 2001), rather than the half-life of 15 days used in the E.U. draft risk assessment, tends to lower predicted water concentrations by more than a factor of two. Using the 4.5-day half-life, it is estimated that it will take about 23 days (five half-lives) for 97% of BPA discharged into receiving waters to be degraded. Thus, BPA is clearly nonpersistent when compared with current half-life criteria that are generally measured in months.

Based on the results of a long-range transport model (TaPL3), BPA may be transported some hundreds of kilometers downstream from a point source discharge as it is being degraded. This estimated travel distance is based on the distance water in a river will flow in the time it takes the BPA in the river to be degraded to 50% of its initial concentration, *i.e.*, 4.5 days. This distance assumes a typical but fast river flow velocity of 1 m/s or 3.6 km/h. The estimated transport distance of BPA in air is much shorter (< 100 km) because its low vapor pressure results in rapid deposition from the atmosphere to the terrestrial surface, and it is rapidly degraded in the atmosphere. Based on these results it is expected that BPA will only be detected in rivers downstream from point sources, although it may be detected a long distance downstream of a source. If there is no point source upstream it is improbable that BPA will be detected. Should BPA be detected in areas with no obvious point sources, a likely explanation is the release of small quantities from landfill leachate or municipal or industrial effluents containing BPA as a result of contact with products such as recycled paper, polymers and resins. The potential for laboratory contamination of samples and the possibility for mis-identification of

BPA should also be investigated. Further, the possibility of natural sources cannot be ruled-out and could be investigated by analysis of samples from pristine regions.

ChemCAN and EUSES Model Comparison

A detailed comparison of the results of the ChemCAN 4.0 and EUSES models shows good agreement between the models with only slight differences attributable to different partitioning and transport expressions. The models are thus similar, but they will of course give quite different results if emission or chemical property input data differ.

Reconciliation between Model Predicted Concentrations and Monitoring Data

The reconciliation between observed and predicted environmental concentrations was not as complete as desired because there is a lack of soil and air concentrations available for model calibration. Because BPA is primarily emitted to surface waters, it is unlikely to be detected in air and natural soils at high levels and thus there is little incentive to undertake these measurements. However, for a thorough analysis of risks to humans and wildlife, these measurements should be undertaken.

It is encouraging that the predicted concentration in water (which is a primary environmental concern) of 14 ng/L using the “best case” discharge scenario compared favorably with the median observed concentration of 16 ng/L. This suggests that the “best case” discharge scenario provides the best estimate of discharges to European surface waters.

Sediment-water partitioning was poorly described by the model, and reasons for this apparent discrepancy have been presented earlier in the paper. Sediment-water partitioning experiments would help to determine the correct explanation for the apparent nonequilibrium sediment-water partitioning.

The successful reconciliation of the concentrations in water indicates that all sources are fully accounted for and there are no substantial unknown sources. The absolute levels of the modeled and monitored concentrations are low, *i.e.*, in the region of 10 ng/L or 1 part in 10^{11} in water and for sediments 10 $\mu\text{g}/\text{kg}$ or 1 part in 10^8 , and it is expected that the “available” quantity in sediments is even lower.

SUMMARY

Overall, because BPA is a widely used high production volume chemical, it is not surprising that it will be detected in the environment, especially in the vicinity of sources and usually at low concentrations. Fortunately, the expected and monitored concentrations are low, bioaccumulation is not an issue, and the substance is degraded fairly rapidly. The rate of degradation is sufficient to alleviate concerns about persistence, but it is slow enough that BPA will be detectable in water and sediments in regions within a flow time on the order of a week from sources.

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