

## Comparison of migration from polyethersulphone baby bottles with that of polycarbonate baby bottles

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#### **Food Additives and Contaminants**



## Comparison of migration from polyethersulphone baby bottles with that of polycarbonate baby bottles

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Abstract:	This work presents two analytical methods developed for measuring three components of polyethersulphone (PES) and applying them to the migration testing of 30 baby bottles made of PES. The study also provides migration results under the same conditions for Bisphenol A (BPA) from 40 polycarbonate baby bottles using a well established method adapted to low concentrations. For PES bottles migration analysis of diphenyl sulphone (DPS), 4, 4'-dichlorodiphenyl sulphone (DCPS) and 4,4'-dihydroxydiphenyl sulphone (DHPS; also known as bisphenol S), was done using the two different analytical methods with detection limits around 0.1 – 0.3 $\mu$ g/kg, and therefore much below their respective legislative limits of migration of 50-3000 $\mu$ g/kg, respectively (EU, 2002). In parallel, 40 bottles made of polycarbonate were analysed for the migration of BPA using a method validated at EU level and modified to a lower detection limit of 0.1 $\mu$ g/kg. Migration tests were conducted into the simulant for milk 50% EtOH (EU, 2011) according to the test conditions from the guidelines on test conditions for articles in contact with foodstuffs (with a focus on kitchenware) prepared by the European Union Reference Laboratory and its Network of National Reference Laboratories. None of the 30 bottles made of PES released a very low amount of DPS of DCPS or DHPS and only 2 bottles released a very low amount of DPS of DCPS or DHPS and only 2 bottles released a very low amount of DPS of DCPS or DHPS and only 2 bottles released a very low amount of DPS of DCPS or DHPS and only 2 bottles released a very low amount of DPS of DCPS or	

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# Comparison of migration from polyethersulphone and polycarbonate baby bottles

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#### Abstract

 This work presents two analytical methods developed for measuring three components of polyethersulphone (PES) and applying them to the migration testing of 30 baby bottles made of PES. The study also provides migration results under the same conditions for bisphenol A (BPA) from 40 polycarbonate baby bottles using a well established method adapted to low concentrations. For PES bottles migration of diphenyl sulphone (DPS), 4, 4'-dichlorodiphenyl sulphone (DCPS) and 4,4'-dihydroxydiphenyl sulphone (DHPS; also known as bisphenol S), was carried out using two different analytical methods with detection limits around 0.1 - 0.3 $\mu$ g/kg, and therefore much below their respective legislative migration limits of 50-3000 µg/kg, respectively (EU, 2002). In parallel, 40 bottles made of polycarbonate were analysed for the migration of BPA using a method validated at EU level and modified to give a lower detection limit of 0.1µg/kg. Migration tests were conducted into the simulant for milk 50% EtOH (EU, 2011) according to the test conditions from the guidelines on test conditions for articles in contact with foodstuffs (with a focus on kitchenware) prepared by the EU Reference Laboratory and its network of National Reference Laboratories. None of the 30 bottles made of PES released any detectable amounts of DCPS or DHPS and only 2 bottles released a very low amount of DPS of around 1 µg/kg in the milk food simulant compared to a regulatory limit of 3000 µg/kg. For PC bottles, 32 bottles out of 40 (80 %) did not release BPA above the LOD of 0.1  $\mu$ g/kg (in any of the three migration tests performed on each bottle). The other 20 % of bottles exhibited only very minor migration, where the highest level in the first migration test was 1.83 µg/kg and most bottles did not release detectable BPA in the second and third test. Only one bottle with a migration level of 1.08  $\mu$ g/kg in the

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first test still showed a detectable level in the last migration test (i.e.  $0.42 \ \mu g/kg$ ). It is important to note that the legal limit was still 600  $\mu g/kg$  for polycarbonate bottles at the time of purchase (EU, 2002), preceding the precautionary ban taking effect from 1 June 2011 (EU 2011a; EU 2011b). This confirms results that the likelihood of migration of BPA is very low and remains in very minute amounts. The results also suggest the absence of release from PES bottles based on the set of bottles investigated.

#### Introduction

Newborns come in contact with different types of plastic utensils such as feeding bottles. Chemical substances such as monomers or additives might migrate from the plastic into the foodstuffs. Since infants have a lower body weight compared to adults, their exposure to the food in contact with the plastic material is higher and ensuring no health concerns is of highest importance. Recent years have shown new concerns regarding the safety of polycarbonate (PC) plastic baby bottles due to the monomer bisphenol A (BPA) used in its production. In 1993 Krishnan et al. reported that BPA exhibited estrogenic activity. Since small amounts of BPA may leach from polycarbonate material into foodstuff many studies have since then been conducted and reviewed on BPA release from baby bottles from mild to harsh conditions as well as ageing (Hoekstra and Simoneau, 2011; Biedermann-Brem et al, 2008; Brede et al, 2003; Ehlert et al, 2008; Food and Consumer Product Safety Authority, 2005, 2008; Kubwabo, et al, 2009; Maragou, et al, 2008; Mountfort et al, 1997; Santillana et al, 2011).

The European Commission had set a specific migration limit of 600  $\mu$ g/kg food for BPA (EU, 2002). However, as a precautionary measure, and following the publication of the EFSA scientific opinion (EFSA, 2010), the European Commission recently decided to ban the use of BPA for the manufacture of polycarbonate infant feeding bottles (EU 2011a, EU 2011b). The market is thus facing a phasing out of polycarbonate (PC) baby bottles as a consequence of the EU legislation effectively prohibiting the manufacture as of 1 March 2011 and their placing on the market as of 1<sup>st</sup> June 2011. As direct consequence, plastic substitutes have massively appeared on the EU market. Such materials include for example polypropylene (PP), silicone, polyamide (PA), a new co-polyester, and polyether sulphone (PES). In particular, PES has the interesting characteristics that its potential starting components are diphenyl sulphone (DPS), 4, 4'-dichlorodiphenyl sulphone (DCPS) and 4,4'-

dihydroxydiphenyl sulphone (DHPS) also known as bisphenol S (BPS). Recent studies demonstrated the likelihood that bisphenol S may have similar endocrine disrupting characteristics as BPA (Kuruto-Niwa et al, 2005; Grignard and Bremer, 2011). Since PES is one of the materials available on the European market to replace PC baby bottles, our study focused first on developing specific methods measuring three components (including BPS) migrating from PES. The methods were then applied to the migration testing of 30 PES baby bottles. In addition, 40 PC baby bottles were analysed for migration of BPA using a method validated at EU level (Bratinova et al, 2010). Considering the lack of data on migration from substitute baby bottles (Aschberger et al, 2010) and yet the structural similarities of some of components of PES with BPA, we felt it there was a strong need to evaluate the safety of a potential relevant replacement of PC with materials including in particular PES in some countries.

#### Materials and methods

#### Samples:

 40 PC baby bottles were analysed from 9 European countries (including one box of duplicates and two boxes of triplicates). Additionally, 30 PES baby bottles were analysed from 12 countries (including four boxes of duplicates one box of three baby bottles). The samples were purchased or obtained via the collaboration of our network of National Reference Laboratories for Food Contact Materials. These were collected and purchased in the period November 2009 –January 2011.

#### Chemicals:

Ultrapure water was prepared from a Milli-Q purification system (Millipore); Methanol and ethanol, HPLC grade quality  $\geq$  99.95%, and Ammonium acetate was purchased from Sigma Aldrich (Italy) with >99.9% quality. Standards of 4,4'-dichlorodiphenyl sulphone (DCPS) and 4,4'-dihydroxydiphenyl sulphone (DHPS) were obtained from Aldrich (Italy) and were of 98% quality. Diphenyl sulphone (DPS) was purchased from Riedel-de Haën with 99.4% quality. 2,2-bis(4-hydroxyphenyl)propane (Bisphenol A) was obtained from Aldrich with >99% quality.

The calibration curves were prepared on a 5 point basis (and 7 for UPLC-MS) for the range of concentration 0.3  $\mu$ g/L to 6  $\mu$ g/L in the food simulant 50% EtOH in water (v/v) for BPA, and 0.5  $\mu$ g/L to 5  $\mu$ g/L for the target analytes 4,4'-dihydroxydiphenyl sulphone (DHPS) and

 Diphenyl sulphone (DPS) in UPLC-MS. The regression coefficients were respectively 0.9997 for BPA, 0.9998 for DPS, 0.9994 for DHPS. In the case of HPLC DAD and HPLC FLD, the quantification was aimed at screening and therefore was performed semi quantitatively against the benchmark concentrations at the SMLs of these substances, i.e.  $50 \mu g/kg$  for 4,4'-dichlorodiphenyl sulphone (DCPS),  $50 \mu g/kg$  for 4,4'-dihydroxydiphenyl sulphone (DHPS) and  $3000 \mu g/kg$  (ie. 3 mg/kg) for Diphenyl sulphone (DPS).

#### Confirmation of materials of baby bottles

FT-IR was used to confirm the nature of the material of the baby bottles in the case of polycarbonate since it was not always stated. A Perkin Elmer FT-IR (Spectrum One) was applied using the attenuated total reflectance mode. ATR spectra were measured with a resolution of 4 cm<sup>-1</sup> in the range of 4000-650 cm<sup>-1</sup>, each generated from 4 scans. The polymer identification was achieved based on comparisons with reference spectra from our internal standard materials. In the case of PES, this identification was superfluous as the bottles were labelled, their colour (yellowish tint) recognisable and the presence of BPA could be immediately seen from any LC-MS spectrum running for the quantification of the other sulphone based compounds.

#### Migration tests

Since most manufacturers recommended sterilization of the baby bottle prior to use (specified on the leaflet) the bottles were sterilized. The common treatment was selected as boiling in water for 5 min. The bottles were then subjected to the conventional migration test for hot fill conditions i.e 2 hours at 70°C. The simulant used was as specified in the EU legislation 2007/19/EC for milk, i.e. 50% EtOH. This was identified as the worst case simulant for this study since for juices which would be modelled by acetic acid 3%, the age group of the infant would be older than the most sensitive population of newborn where the simulant for milk would apply.

The simulant was pre-heated to 70°C, and a volume corresponding to the specified volume to the baby bottles was added to the item. The test specimens were covered with a glass plate weighted to ensure absence of evaporation and placed in a convection oven for 2 hours at 70 °C. The loss of simulant was measured in preliminary tests and was shown not to exceed 3%. Calibration curves were done in the 50% EtOH simulant in order to take into account recoveries. After treatment the migration solution was transferred from the baby bottle into a

glass bottle with PTFE lined cap and left to cool down prior to analysis. An aliquot was then used in glass GC vial with PTFE lined cap for analysis. Since the sample was a repeated use article, a second and third migration tests were performed according to the repeated use conditions for food contact material (82/711/EEC as amended). The bottles were quickly rinsed with deionised water between two migration tests. In a first phase only the first migration was analyzed. However, all three migration solutions conducted from PC bottles were analyzed to confirm migration of BPA. Blank samples were also prepared from a portion of the simulant used for the migration tests.

#### Analysis of migration solutions:

 The concentrations of migrants in the simulant were determined by high performance liquid chromatography (HPLC) with diode array (DAD) and fluorescence (FLD) detection, as well as by UPLC-MS for PES bottles.

#### HPLC for polycarbonate:

BPA was analysed from the migration solutions using an HPLC (Hewlett Packard 1100) coupled with fluorescence detector based on a validated method at EU level (Bratinova et al, 2010). Slights changes were further made to focus on very low calibration levels which do not necessarily correspond to those aimed at testing for compliance. The instrument was operated with a column Phenomenex (kinetex) C18, 150 x 3 mm x 2.6 µm, operated at a temperature of 30°C, using a flow rate of 0.27 ml/min and an injection volume of 20 µl. The fluorescence detector was operated with the excitation wavelength of  $\lambda_{exc} = 235$  nm and an emission wavelength of  $\lambda_{ems} = 317$  nm. The mobile phase was composed of methanol water in proportion (68:32) held for 10 minutes in isocratic conditions. The limit of limit of detection (LOD) was 0.1 µg/L and limit of quantification (LOQ) was 0.3 µg/L. The LOD was calculated based on a signal to noise ratio of 3, whereas the LOQ was based on 3 times the LOD.

#### HPLC for PES:

This method was applicable for all 3 components but was used specifically for the quantification of 4,4'-dichlorodiphenyl sulphone, whereas for the other two components the LC-MS method gave greater sensitivity and was used as primary analytical method. The migration solutions were analysed by HPLC (Hewlett Packard 1100) coupled with a Diode Array Detector and Fluorescence detector. The instrument operated with a column Halo C18,

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150 x 3 mm x 2.7µm operated at a temperature of 20°C, with a flow rate of 0.27 ml/min and an injection volume of 10 µl. The diode array detection was performed at a wavelength set at 260 nm, whereas the fluorescence detection was operated with an excitation wavelength of  $\lambda_{exc} = 260$  nm and an emission wavelength of  $\lambda_{ems} = 317$  nm. The mobile phase used was a gradient of methanol water (60:40) to 90:10 in 10 min., and held at 90:10 for 3 min. The LOD was 0.3 µg/kg and LOQ was 0.9 µg/kg. The LOD and LOQ were calculated as previously described.

#### UPLC-MS for PES:

This method was used for the analysis of diphenyl sulphone and 4,4'-dihydroxydiphenyl sulphone (Bisphenol S). The method was not adequate for 4,4'-dichlorodiphenyl sulphone. The migration solutions were analysed by UPLC-MS (Waters Xevo) coupled with an electrospray interface (ES+) in multiple reaction monitoring mode (MRM) using a column Waters Acuity BEH C18 (100 mm \* 2.1 mm \*  $1.7\mu$ m) operated at 30°C with a flow rate of 0.3 ml/min and an injection volume: 7.5 µl. The chromatographic conditions used a mobile phase of water ammonium acetate 1mM /methanol in proportion of (60:40) held for 0.3 min, followed by a gradient to 20:80 in 2.7 min., and held at the ratio of 20:80 for 0.5 min. The spectrometric conditions are summarised in table 1. The LOD was 0.1 µg/kg and LOQ was 0.3 µg/kg for both substances. The LOD and LOQ were calculated as previously described.

(Table 1 here please)

#### **Results and Discussion**

#### Bottles made of polycarbonate

In total, 40 bottles were subjected to migration testing in 50% EtOH simulant which was analysed to quantify the presence of BPA (Table 2). In 32 bottles (80 %) no BPA was found using an analytical method with a detection level of  $0.1\mu g/kg$  (in none of the three migration tests performed on each bottle). The remaining 8 bottles exhibited only very minor migration, where the highest level in the first migration was of 1.83  $\mu g/kg$  and most bottles did not release detectable BPA in the second and third round. Only one bottle with a migration level

of 1.08  $\mu$ g/kg in the first test still showed a detectable level in the last migration test (i.e. 0.42  $\mu$ g/kg). It is important to note that the legal limit was still 600  $\mu$ g/kg polycarbonate bottles at the time of purchase, preceding the precautionary ban taking place from 1 June 2011 (EU, 2011a; EU 2011b). This confirms results from a previous monitoring study carried out by the JRC in 2000 (Simoneau et al, 2000) and from the most recent studies and enforcement campaigns (Food and Consumer Product Safety Authority, 2008, Kubwabo et al, 2009, Santillana et al, 2011) that the likelihood of migration of BPA into the official simulant for milk 50% ethanol is very low and remains in very minute amounts. Bottles were also analysed for other compounds in a work currently in progress without showing any notable release (Simoneau et al, in preparation).

#### Bottles made of polyethersulphone

 Migration of diphenyl sulphone and 4,4'-dihydroxydiphenyl sulphone (bisphenol S) from PES baby bottles was specifically measured by UPLC-MS. 4,4'-dichlorodiphenyl sulphone was not visible with this method and was therefore analysed in parallel by HPLC-FLD. 2 out of 30 bottles indicated low presence of diphenyl sulphone (1.45 and 1.73  $\mu$ g/kg). Migration of Bisphenol S and 4,4'-dichlorodiphenyl sulphone was below the limit of detection (0.1 and 0.3  $\mu$ g/kg respectively). Figure 1 illustrates the chromatograms obtained by UPLC-MS of the quantification for one PES baby bottles with the highest quantifiable diphenyl sulphone and dihydroxydiphenyl sulphone (BPS) at a level of 1  $\mu$ g/L, as well as of a standard of BPA also at a level of 1 $\mu$ g/L. The results are summarised in Table 2.

The data obtained thus showed that the migration of all 30 bottles remained much below their migration limits of 3000  $\mu$ g/kg for diphenyl sulphone and 50  $\mu$ g/kg for bisphenol S and 4,4'- dichlorodiphenyl sulphone after the first migration test. All the analyzed baby bottles made of PES were therefore compliant with the European regulations concerning the migration of bisphenol S, diphenyl sulphone and 4,4'-dichlorodiphenyl sulphone.

#### Conclusion

The results on BPA release confirmed results that the likelihood of migration of BPA is very low. There is no data to our knowledge published in the literature on migration from PES baby bottles. Therefore this initial method development indicates that it is possible to identify and quantify the potential monomers from PES using HPLC-DAD and FLD and UPLC-MS.

 The sensitivity was much greater for UPLC MS as expected but the 4,4'-dichlorodiphenyl sulphone was not visible. The HPLC method was adequate for the purpose of targeted screening and can also include BPA together with the 3 analytes in one run.

The subsequent survey conducted on PES bottles suggests that with regard to migration, no issue was found so far for bottles made of PES for the release of 4,4'-dihydroxydiphenyl sulphone (bisphenol S), diphenyl sylphone, and 4,4'-dichlorodiphenyl sulphone using the food contact materials worst-case state-of-the-art protocols as reviewed in particular in the guidelines on testing conditions for articles in contact with foodstuffs (with a focus on kitchenware) (Simoneau, 2009).

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Table 1: Spectrometric conditions used in LC-MS for the quantification of diphenyl sulphone and 4,4'-dihydroxydiphenyl sulphone (bisphenol S) from 50% ethanol migration solutions..

Compound	Parent ion	Daughter ion	Cone voltage	Collision voltage
Diphenyl sulfone	219	77	26	18
Diphenyl sulfone	219	145	26	8
4,4'-dihydroxydiphenyl sulphone (bisphenol S)	251	93	32	25
4,4'-dihydroxydiphenyl sulphone (bisphenol S)	251	157	32	16

 Compound
 Parent
 Daughter
 Cone
 Collision

 Siphenyl sulfone
 219
 77
 26
 18

 Jiphenyl sulfone
 219
 145
 26
 8

 .4'-dihydroxydiphenyl sulphone (bisphenol S)
 251
 93
 32
 25

 .4'-dihydroxydiphenyl sulphone (bisphenol S)
 251
 157
 32
 16

#### Table 2: Migration from polycarbonate baby bottles analysed by HPLC

Sample code	Volume of bottle (ml)	first migration (µg/kg)	second migration (μg/kg)	third migration (μg/kg)
CH002	250	n.d.	n.d.	n.d.
CH003	240	n.d.	n.d.	n.d.
DE001	110	n.d.	n.d.	n.d.
ES001	240	< LOQ	n.d.	n.d.
FIN002	120	0.32	n.d.	n.d.
FIN003	250	n.d.	n.d.	n.d.
FIN004	260	n.d.	n.d.	n.d.
FIN005	250	n.d.	n.d.	n.d.
FIN006	200	n.d.	n.d.	n.d.
FIN007	300	n.d.	n.d.	n.d.
FIN008	200	n.d.	n.d.	n.d.
FIN009	250	0.33	n.d.	n.d.
FIN010	280	n.d.	n.d.	n.d.
FR004	120	n.d.	n.d.	n.d.
FR005	250	n.d.	n.d.	n.d.
FR006	300	n.d.	n.d.	n.d.
FR007	260	n.d.	n.d.	n.d.
FR008	240	n.d.	n.d.	n.d.
FR009	260	n.d.	n.d.	n.d.
IT001	125	< LOQ	n.d.	n.d.
IT005	300	n.d.	n.d.	n.d.
IT016	130	n.d.	n.d.	n.d.
IT017	130	n.d.	n.d.	n.d.
IT019	150	n.d.	n.d.	n.d.
IT020	100	1.08	0.54	0.42
IT021A	150	n.d.	n.d.	n.d.
IT021B	150	n.d.	n.d.	n.d.
IT022	100	n.d.	n.d.	n.d.
LT001	250	n.d.	n.d.	n.d.
LT002	125	n.d.	n.d.	n.d.
LT003	125	0.44	n.d.	n.d.
LT004	120	n.d.	n.d.	n.d.
LT005	180	0.45	n.d.	n.d.
NL001A	125	n.d.	n.d.	n.d.
NL001B	125	n.d.	n.d.	n.d. 💧
NL001C	125	n.d.	n.d.	n.d.
NL002A	250	n.d.	n.d.	n.d.
NL002B	250	1.83	n.d.	n.d.
NL002C	250	n.d.	n.d.	n.d.
SW002	250	n.d.	n.d.	n.d.

Note: n.d.: non detectable; < LOQ is used for values in between n.d. and LOQ.

Volumo		UPLC-N	AS	HPLC	
Sample code	of bottle	first migration		first migration	
	(ml)	diphenyl sulphone	Bisphenol S	4,4'-dichlorodiphenyl sulphone	
DE002	170	(µg/kg)	(µg/kg)	(µg/Kg)	
BE002	170	n.d.	n.d.	n.d.	
DE007	170	n.d.	n.d.	n.d.	
BG007	150	n.d.	n d	n.d.	
DE007	330	n.u.	n.d.	n d	
DE012 DK001	125	n.d.	n.d.	n.d.	
ES006A	300	n.d.	n.d.	n.d.	
ES006B	300	n.d.	n.d.	n.d.	
FR003	260	n.d.	n.d.	n.d.	
FR019	250	n.d.	n.d.	n.d.	
IT003	300	n.d.	n.d.	n.d.	
IT004	150	n.d.	n.d.	n.d.	
IT007	140	1.45	n.d.	n.d.	
IT008	150	n.d.	n.d.	n.d.	
IT013A	125	n.d.	n.d.	n.d.	
IT013B	125	n.d.	n.d.	n.d.	
IT014	140	1.73	n.d.	n.d.	
IT015A	150	n.d.	n.d.	n.d.	
IT015B	150	n.d.	n.d.	n.d.	
IT018A	280	n.d.	n.d.	n.d.	
IT018B	280	n.d.	n.d.	n.d.	
IT018D	280	n.d.	n.d.	n.d.	
LT010	250	n.d.	n.d.	n.d.	
MT007A	160	n.d.	n.d.	n.d.	
MT007B	160	n.d.	n.d.	n.d.	
PL004	125	n.d.	n.d.	n.d.	
UK006	260	n.d.	n.d.	n.d.	
USA003	160	n.d.	n.d.	n.d.	
USA008	125	n.d.	n.d.	n.d.	
USA008	125	n.d.	n.d.	n.d.	

#### Table 3: Migration from PES baby bottles analysed by UPLC-MS and HPLC





