PERGAMON

Chemosphere 45 (2001) 245–259

CHEMOSPHERE

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The occurrence of xenoestrogens in the Elbe river and the North Sea

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Accepted 10 November 2000

Abstract

The xenoestrogens Bisphenol A (BPA), *p*-alkylphenols and *p*-alkylphenol ethoxylates were determined in water samples of the North Sea, the Elbe river, and its tributaries Schwarze Elster, Mulde, Saale and the Weisse Elster. The sampling sites of the Elbe river reached from Schmilka at the German–Czech border to Cuxhaven at the estuary. Samples of the North Sea were taken in the German Bight. Additionally, freshly deposed sediments of the River Elbe and its tributaries were analyzed. Partitioning coefficients of these compounds for the distribution between suspended particulate matter (SPM) and the aqueous phase were calculated for samples of the River Elbe at sampling site Geesthacht.

The analytical procedure consisted of liquid–liquid extractions of the acidified water samples using dichloromethane. Sediments and SPM samples were extracted by Accelerated Solvent Extraction with *n*-hexane/acetone. Following a clean-up by HPLC, the analytes were derivatized with heptafluorobutyric acid anhydride and quantified using GC–MSD.

The concentration ranges of the compounds analyzed in water samples of the Elbe river were as follows (in ng l^{-1}): BPA 9–776, alkylphenols 10–221 and alkylphenol ethoxylates 18–302. In sediment samples the concentrations were (in μg kg^{-1} dry mass): BPA 66–343, alkylphenols 17–1378 and alkylphenol ethoxylates 30–1797. In samples of the North Sea the concentrations were generally about 1 order of magnitude lower. As shown by the concentration profiles following the River Elbe into the North Sea, the Elbe river must be considered as a major pollution source for the North Sea concerning the compounds analyzed. The SPM/water-partitioning coefficients calculated (mean values) amounted to: BPA 4.50, alkylphenols 5.52–5.58 and alkylphenol ethoxylates 5.60–6.38.

A comparison of the results with data from other surface waters showed that concentrations of these xenoestrogens in the River Elbe and its tributaries were relatively low. The evaluation of the data based on the lowest observable effect concentration (LOEC) for alkylphenols (endpoint: vitellogenin synthesis in male trout) indicated that the concentrations were well below the effectivity threshold. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Bisphenol A; Alkylphenols; Alkylphenol ethoxylates; North Sea; River Elbe; Sediments; Water samples; Partitioning coefficients

1. Introduction

In both the scientific and popular literature, disorders of the endocrine system resulting from the influence of natural or synthetic substances (xenoestrogens) have been discussed. A Danish study from 1995, showing

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PII: S0045-6535(00)00570-1

possible changes in both human and animal reproduction systems resulting from hormones and xenobiotics, formed the basis of this discussion (Danish Environmental Protection Agency, 1995). Epidemiological studies showed disorders in the development and the function of the human male reproduction system (Seibert, 1996) as well as disturbances in the sex-differentation of molluscs and fish populations. Investigations of rainbow trout (*Oncorhynchus mykiss*) exposed to effluents of sewage treatment plants in England have shown that there are substances present in the treated water which elicited vitellogenin synthesis in both male and female fish (Purdom et al., 1994). Vitellogenin is a protein produced in the liver of egg-laying animals like birds, reptiles, amphibians and fish which is normally not found in males or juvenile females. The conclusion of this study was that xenoestrogens were responsible for the increased vitellogenin levels and the prevalence of hermaphroditism in the fish population. Further studies examining environmental estrogens in sewage water using bioassays confirmed this assumption (Jobling et al., 1996; Harries et al., 1996; Harries et al., 1997).

International and national research activities are investigating the possible effects and implications of natural and synthetic substances exhibiting endocrine influences. Nevertheless, information is incomplete and fundamental research into active molecular mechanisms is necessary as well as monitoring the emission of estrogenic chemicals which are produced in large quantities and are released into the environment. A joint study of the ARGE ELBE and the Federal Maritime and Hydrographic Agency investigated the occurrence and distribution of selected xenoestrogens in the Elbe river, its tributaries Schwarze Elster, Mulde and Saale and in the Weisse Elster, a tributary of the Saale. Selection criteria for the compounds investigated were the relative estrogenic potential of these substances, as well as physical and chemical properties. The estrogenic potential can essentially be derived from in vivo and in vitro test results. For example, in the case of the steroid 17β-estradiol or 17α-ethinylestradiol, the estrogenic activity is estimated to be within the ng l^{-1} range for certain fish species (Purdom et al., 1994). In the case of xenoestrogens from municipal and industrial sources, the estrogenic potential is usually lower by one or two orders of magnitude for most compounds (Soto et al., 1995). Further criteria for the selection of target analytes were the annual production amount and the application spectrum of these chemicals. According to the aspects mentioned before, the following compounds were of interest.

1.1. Bisphenol A

2, 2′-Bis-(4-hydroxyphenyl)-propane (BPA) is a compound that is produced in large quantities worldwide. In 1995, BPA production in Germany amounted to 210,000 t and contributed approximately half of the West European annual requirement (Leisewitz and Schwarz, 1997). BPA is versatile in technical applications and is mainly used as an intermediate in the production of polycarbonate (133,000 t) and epoxy resin (56,000 t). Other applications include its use as a stabilizing agent in plastics, as an antioxidant in tyre production, as a basic chemical for the production of the common flame retardant Tetrabromobisphenol A, and as an additive in thermal papers or paper coatings. According to production reports, the release of BPA into the environment is estimated to be about 1 t/a via the air- and water-pathways during production and processing (Leisewitz and Schwarz, 1997). BPA might, therefore, microbially decompose relatively quickly in water, with a half-life of between 2.5 and 4 days (Staples et al., 1998; Dorn et al., 1987). A decomposition time of 28 days when using a modified OECD-test is referred to by the US EPA (cited in Staples et al., 1998).

1.2. Alkylphenols and alkylphenol ethoxylates

Among the alkylphenols 4-nonylphenol (NP) and 4-octylphenol (OP) are the most important substances due to the annual production amounts. Technical NP is a mixture of various isomers. In 1995, Germany had an alkylphenol consumption of 20,000 t, of which approximately 14,000 t were NP. The rest of 6000 t was made up of octyl-, butyl- and other alkylphenols. The major amount of NP (11,500 t) was used in the production of nonylphenol ethoxylates (NP*n*EO) with 1–40 ethoxy units (Leisewitz and Schwarz, 1997). For over 40 years NP*n*EO have been applied in many industrial sectors, for example as non-ionic surfactant in the pre-treatment of wool, as a wetting agent, as a softener, in leather and paper production, as a cleaner in the metal industry, in the production of latex paints, as an emulsifying agent in pesticides, during the formulation of pesticides, as a resource in the production of drills, flotation devices, and as emulsifying agent in paints. The biodegradation of NP*n*EO leads to a shortening of the polyethoxylate chain (hydrolytic cleavage of the ethoxy units). The resulting nonylphenol monoethoxylate (NP1EO) and diethoxylate (NP2EO) are more difficult to decompose by microorganisms than higher ethoxylated compounds.

Due to the possible estrogenic activity of these substances surface water samples and sediments were investigated. Results from analysis of 19 sampling sites along the River Elbe from the German–Czech border at Schmilka as far as Cuxhaven at the North Sea, from the Elbe tributaries Schwarze Elster, Mulde, Saale, and the Weisse Elster are presented. To investigate the influence of the River Elbe as an input source of these compounds for the North Sea on the one hand, and the fate and

concentration range of these compounds on the other hand, two sampling campaigns were performed in the German Bight of the North Sea. Partitioning coefficients were calculated for the distribution of these compounds between suspended particulate matter and aqueous phase. In conclusion, results from water samples of the Elbe river are compared with data from other surface waters and an attempt is made to interpret the concentrations measured in terms of possible estrogenic impacts on aquatic organisms.

2. Materials and methods

2.1. Compounds investigated

Substances analyzed were: 2,2′-Bis-(4-hydroxyphenyl)-propane (Bisphenol A), 4-tert-butylphenol, 4-tert-pentylphenol, 4-tert-octylphenol, technical 4-nonylphenol, 4-tert-octylphenol monoethoxylate, 4-tert-octylphenol diethoxylate, technical 4-nonylphenol monoethoxylate and 4-nonylphenol diethoxylate.

2.2. Sampling and sampling sites

2.2.1. Water samples

Surface water samples were taken from the Elbe river (10 sites), the mouth of the Schwarze Elster, Mulde and Saale in July 1998, and from the Weisse Elster (tributary of the Saale, six sites) in October 1998. Sampling was performed from the riverbank using a sampling device made of Teflon to which a 2-l glass bottle was attached. The sampling sites along the Elbe started below the Czech border at Schmilka and ended at the Elbe estuary at Cuxhaven (Fig. 1). Samples from the tidal part of the Elbe were taken during high tide (Bunthaus, stream km 609.8) and at the turning point of the tide (Grauerort, km 660.5). Sampling sites at the Weisse Elster were: (1) Nosswitz, (2) downstream Greiz, (3) Greiz, (4) Wünschendorf, (5) Bad Köstritz, and (6) Crossen.

Samples of the North Sea (and of the tidal part of the River Elbe) were taken during research cruise A 099 (RV Atair, Federal Maritime and Hydrographic Agency) in Mai 1998 and during research cruise G 325 (RV Gauss, Federal Maritime and Hydrographic Agency) in January 1999. Water samples were taken at a depth of 3 m

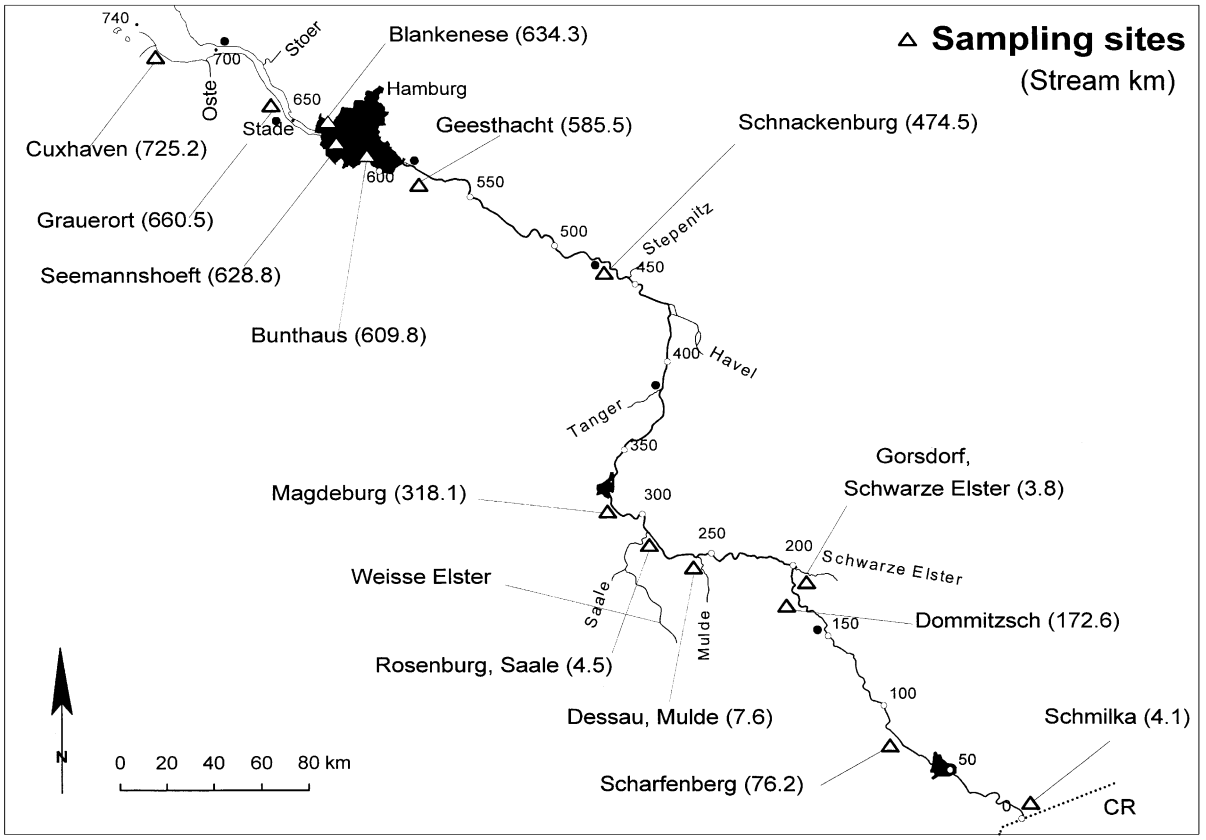

Fig. 1. Sampling sites of the Elbe river, the Schwarze Elster, Mulde, Saale and the Weisse Elster.

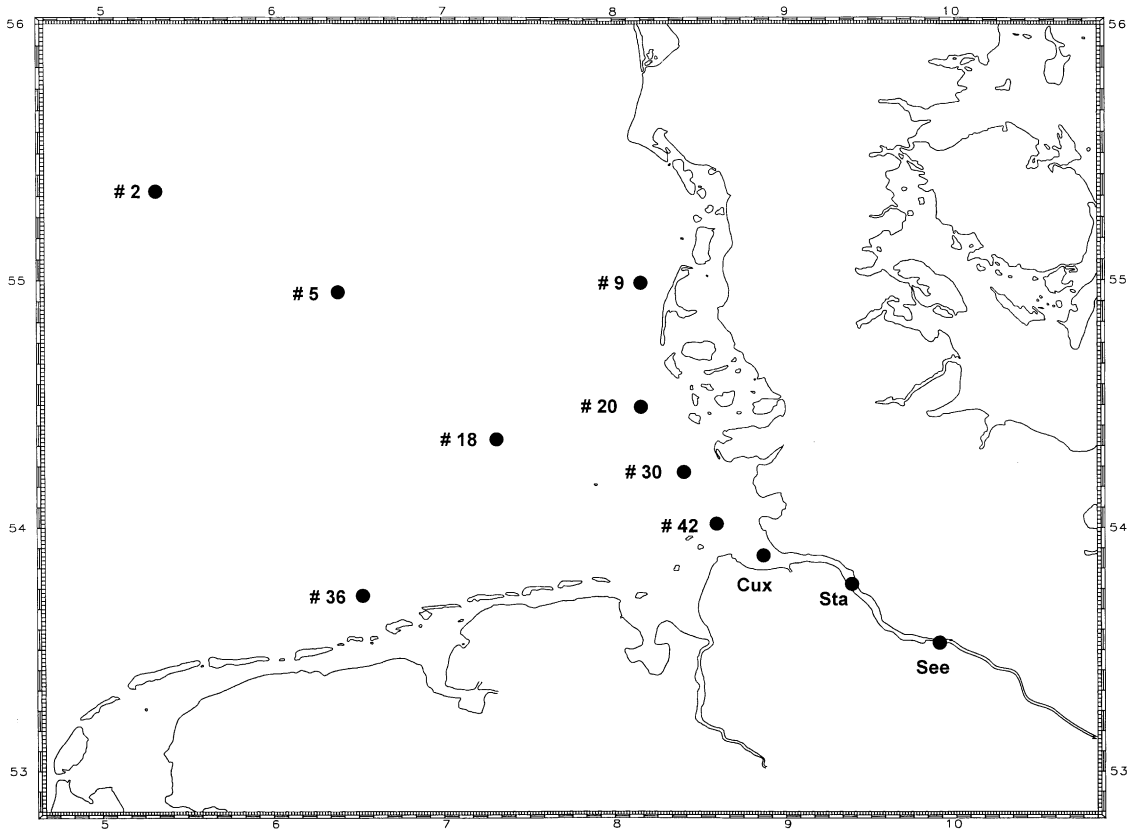

Fig. 2. Sampling sites of the North Sea (German Bight).

below surface with 10-l glass bottles. For a detailed description of the sampling procedure see Theobald et al. (1990). All sampling sites are shown in Fig. 2. The sampling points of the North Sea were selected in dependence of the prevailing hydrographic conditions. Sampling points #42, #30, #20, and #9 are dominated by the inflow of the River Elbe and to some extent by inputs of the river Weser. Sampling points #2, #5 and #18 are mainly influenced by the Atlantic inflow and usually show low concentrations of anthropogenic contaminants. Sampling point #36 is temporarily influenced by inputs of the River Ems.

2.2.2. Sediment samples

Sediment samples of the Elbe river and its tributaries Mulde, Saale and Schwarze Elster were taken at Schmilka, Dommitzsch, Gorsdorf, Dessau, Rosenburg, Magdeburg, Bunthaus, Seemannshöft, Blankenese and Grauerort (Fig. 1). These samples were freshly deposed sediments, which were collected over a monthly period in sedimentation traps. Sampling was performed in June 1998. For an annual monitoring 12 sediment samples were taken at sampling site Schnackenburg covering the period from February 1998 to January 1999 (for details concerning the sampling devices see Stachel et al., 1995). After centrifugation and decanting the supernatant water sediment samples were air dried for three days in a clean bench prior to extraction.

2.2.3. Samples for the determination of partitioning coefficients

Samples were taken from the River Elbe at the weir Geesthacht (stream km 585.5) in September 1998. Four sampling campaigns were performed at one-week intervals. The SPM separation was carried out using a continuous flow centrifuge (Contifuge 17 RS, Heraeus) with a titanium rotor (Heraeus 8575) driven with 15,000 min^{-1}. The centrifuge was fed by a peristaltic pump (Watson-Marlow 503 U/RL) at a flow rate of 1 l min^{-1}, using Teflon tubes (ID 4 mm); those within the peristaltic pump were made of silicon. The centrifuge was run for 4–6 h resulting in SPM amounts between 4.8 and 7.2 g dm (at SPM contents of approx. 20 mg l^{-1}). After centrifugation, the SPM samples were collected using a metal spatula, transferred into glass bottles, and stored at −20°C until further work-up. During each centrifugation three 10-l samples of the centrifugate were collected in glass bottles. These centrifugate samples were

taken 1 h after the start, at the mid-point and 1 h before completion of the centrifugation. Sediment, SPM, and aqueous phase were extracted as described in the following section.

2.3. Analysis

2.3.1. Extraction of water samples

Water samples were acidified with concentrated sulfuric acid (10 ml for 2 l and 50 ml for 10-l samples). A triple extraction was done using dichloromethane (200 ml for 2 l and 500 ml for 10-l samples). Prior to the first extraction, 5–10 ml of an internal standard solution (containing D_{16}-Bisphenol A, 4-*n*-pentylphenol, 4-*n*-octylphenol, 4-*n*-nonylphenol monoethoxylate, D_3-2,4-dichlorophenol, $^{13}C_6$-pentachlorophenol) were added. After phase separation (0.5–1.5 h), the combined extracts were dried over sodium sulfate. The extracts were reduced to a volume of 0.5 ml under vacuum, taken up into *n*-hexane and concentrated to 100 μl by a gentle stream of nitrogen.

2.3.2. Extraction of sediment and SPM samples

Extractions were performed by accelerated solvent extraction (ASE) on a modified Suprex SFE 50 with a mixture of *n*-hexane/acetone (1:1; v/v) (Heemken et al., 1997). 200 mg of activated copper powder were added to 0.5–1 g of air-dried sediment samples in 10 ml extraction vessels. Extractions were carried out at a temperature of 100°C and 150 atm. The time for static extraction was 15 min after 5 min equilibration. Following the static extraction the extraction vessel was rinsed with 20 ml of solvent, and, as a final step, the vessel was purged with gaseous nitrogen. Prior to reduction to a volume of 100 μl the internal standard solution (50–100 μl) was added to the extracts.

2.3.3. Clean-up

In order to separate the non-polar substances from the analytes, water and sediment extracts were precleaned using HPLC. The HPLC unit consisted of a pump (L 6200, Merck/Hitachi, Darmstadt), an autosampler (HP Series 1050, Hewlett Packard), a fraction collector (L 5200, Merck/Hitachi, Darmstadt), a diode-array-detector (HP 1040 M Series II, Hewlett Packard) and a column oven (Techlab). A Nucleosil 100-5 (Machery/Nagel, Dülmen) was used as column; the temperature was kept at 20°C. The injection volume was 100 μl. The HPLC parameters were as follows: 2 min *n*-hexane/dichloromethane (95:5, v/v; 1 ml/min); in 6 min to 100% dichloromethane (1 ml/min); 4 min 100% dichloromethane (1 ml/min); 5 min 100% acetone (1.5 ml/min) to rinse the column, 10 min *n*-hexane/dichloromethane (95:5, v/v, 1.5 ml/min) to equilibrate the column. The fraction from 0 to 5 min was discarded, the fraction containing the analytes was taken from 5 to 18 min.

2.3.4. Derivatization using heptafluorobutyric acid anhydride (HFBA)

In order to facilitate the derivatization of the analytes the pre-cleaned extracts were reduced to 500 μl (*n*-hexane), 200 μl potassium carbonate solution (20 wt%) and 50 μl HFBA were added. These solutions were stirred for 15 min at 60°C in closed vials (sand bath). After reaction the hexane phase was collected with a pipette and the aqueous phase was extracted twice using 200 μl *n*-hexane. The combined extracts were reduced to 200–500 μl and quantification was carried out by GC–MSD.

In case of sediment extracts a second clean-up step after derivatization was necessary due to high amounts of co-extractable matrix compounds. For this purpose the extracts were fractionated by HPLC again as described in chapter "clean-up". The only difference was the initial solvent composition, which was made up by *n*-hexane/dichloromethane (60:40, v/v). In this case the fraction containing the analytes was taken from 0 to 7 min and reduced to 200–500 μl.

2.3.5. Quantification by GC–MSD

Quantification was performed by GC (Hewlett Packard 5890 Series II) coupled to a mass selective detector (MSD 5971 A). A 5% phenylmethyl-silicon capillary column with 0.2 mm ID, 0.33 μm film thickness and a length of 25 m (HP Ultra 2) was used, helium was used as carrier gas. The GC-temperature program was: 40°C for 1 min, heating rate 5°C/min to 320°C, 320°C for 8 min.

Parameters for the cold injection system KAS 3 (Gerstel GmbH, Mühlheim a.d. Ruhr, Germany) were as follows: 40°C for 10 s, heating rate 12°C/s to 330°C, 330°C for 10 min. Solvent venting time 10 s, splitless time 2 min, injection volume 5 μl.

The MSD was operated in the single ion monitoring mode (SIM) detecting the following masses: $m/z = 136$, 164, 361 (D_3-2,4-dichlorophenol); 321, 341, 421 (D_{16}-BPA); 242, 271, 468($^{13}C_6$-pentachlorophenol); 331, 346 (BP); 303, 360 (PP); 303, 331 (OP); 315, 331, 407 (BPA); 241, 375 (OP1EO); 241, 419 (OP2EO); 303, 317, 331, 345 (NP); 241, 375, 389, 403 (NP1EO); 107, 241, 419, 447 (NP2EO).

Three calibration standard solutions were used to generate response factors for each compound relative to internal standards. Analytes in the samples were identified by matching the retention time of each compound with the retention time in calibration standards and by the ratio of target and qualifier signal. For the quantification of NP and the NP*n*EO the ion traces with the smallest interferences were used. Concentrations were calculated, based on the recoveries of the internal standards.

Quantification limits were estimated as the 10-fold value of the noise close to target signals in standard

solutions and amounted to 0.5 pg μl^{-1} for BPA, BP, PP, OP, OPnEO and to 5 pg μl^{-1} for NP and NP*n*EO. Taking into account an enrichment factor of 10,000 the quantification limits for 2-l water samples were 0.05 ng l^{-1} for BPA, BP, PP, OP, OPnEO and 0.5 ng l^{-1} for NP and NP*n*EO (and about 5 times lower for 10-l samples). For 1 g sediment samples the quantification limits were 5 (NP, NP*n*EO) and 0.5 (all other) $\mu g\ kg^{-1}$ dm.

2.3.6. Chemicals

Sodium sulfate (p.A., Baker); sulfuric acid, potassium carbonate, 4-*n*-nonylphenol (p.A., Riedel de Haen AG, Seelze); 4-*n*-pentylphenol, 4-tert-octylphenol, Triton X 45 (p.A., Fluka, Buchs); heptafluorobutyric acid anhydride, 4-tert-pentylphenol (Derivatization Grade, p.A., Aldrich, Steinheim); Bisphenol A, 4-*n*-octylphenol, 4-*n*-nonylphenol monoethoxylate, D_3-2,4-dichlorophenol, $^{13}C_6$-pentachlorophenol (p.A., Promochem, Wesel); Marlophen NP 3 = tech. 4-nonylphenol (Hüls AG, Marl); D_{16}-Bisphenol A (p.A., Cambridge Isotope Laboratories, Andover); 4-tert-butylphenol (p.A., Chem Service, West Chester); acetone, *n*-hexane (Nanograde, Promochem, Wesel); dichloromethane (Lichrosolv, Merck, Darmstadt). All solvents were fractionally distilled before use. To avoid contamination of samples all glass devices used for sampling and sample preparation were consecutively rinsed with acetone and *n*-hexane and heated to 300°C for 12 h. Sodium sulfate was heated to 650°C for 12 h prior to use.

3. Results and discussion

3.1. Water samples

Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in water samples of the Elbe river and the tributaries Schwarze Elster, Mulde and Saale are shown in Table 1, concentrations of samples from the river Weisse Elster, a tributary of the Saale, are given in Table 2. Table 3 shows concentrations in water samples of the North Sea of two sampling campaigns from May 1998 and January 1999.

3.1.1. River Elbe and tributaries

In the Elbe river the concentration of BPA ranged from 17 ng l^{-1} (Cuxhaven) to 776 ng l^{-1} (Scharfenberg), the average being 47 ng l^{-1} (omitting Scharfenberg). At the German–Czech border at Schmilka the BPA concentration was 76 ng l^{-1}. The BPA probably originates from an industrial plant in Usti nad Labem, which manufactures epoxy resin using BPA. The wastewater is treated inadequately in the sewage plant, and flows into the Elbe via a small tributary, the Bilina, which is heavily polluted with organic and inorganic matter. An investigation of the effluent of this factory from October

Table 1
Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in water samples of the Elbe river and the tributaries Schwarze Elster, Mulde and Saale (in ng l^{-1})

	Elbe river, downstream											Tributaries		
Location	Cuxhaven	Grauerort	Blankenese	Seemannshoeft	Bunthaus	Schnackenburg	Magdeburg	Dommitzsch	Scharfenberg	Schmilka	Rosenburg (Saale)	Dessau (Mulde)	Gorsdorf (Schwarze Elster)
Stream (km)	725.2	660.5	634.3	628.8	609.8	474.5	318.1	172.6	76.2	4.1	4.5	7.6	3.8
BPA	17	57	19	22	27	58	57	87	776	76	125	37	8.9
BP	1.5	8.3	2.8	1.9	1.4	2.1	1.9	78	5.6	1.4	3.9	4.1	1.5
PP	0.7	0.3	0.2	0.3	0.4	0.6	0.5	0.1	0.4	0.2	0.5	0.4	0.2
OP	1.3	0.9	0.9	0.8	0.8	1.0	1.0	0.7	0.9	0.4	2.0	2.1	1.0
NP	13	12	12	9.5	7.3	9.5	12	9.1	52	14	32	13	1.0
OP1EO	1.3	1.0	0.9	1.0	1.0	1.3	1.5	0.8	6.3	1.1	1.8	1.7	0.9
OP2EO	1.1	0.8	0.8	0.6	0.9	1.0	1.1	0.61	6.8	1.4	1.5	1.3	0.8
NP1EO	15	10	12	12	18	26	35	27	205	47	83	41	13
NP2EO	3.8	4.2	4.6	3.6	7.9	9.1	11	9.8	84	21	25	9.8	4.3

Table 2
Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in water samples of the Weisse Elster (in ng l^{-1})

Sampling site	#1	#2	#3	#4	#5	#6
BPA	24	59	62	73	75	72
BP	1.6	2.3	2.0	5.3	1.0	1.5
PP	n.d.[a]	n.d.	n.d.	0.02	n.d.	n.d.
OP	3.6	3.0	2.5	6.0	1.5	2.4
NP	78	167	143	161	221	156
OP1EO	3.0	5.7	5.6	5.9	6.2	4.8
OP2EO	1.5	4.1	2.4	3.4	3.7	2.9
NP1EO	30	84	44	66	115	84
NP2EO	8.8	32	14	24	68	38

[a] n.d.: not detected.

Table 3
Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in water samples of the North Sea (in ng $l^{-1)}$

	See	Sta	Cux	#42	#30	#20	#09	#36	#18	#05	#02
May 1998											
BPA	25	249	7.0		n.d.[a]		n.d.	n.d.		n.d.	n.d.
BP	13	43	1.3		0.1		0.1	0.1		0.02	0.7
PP	<BG	0.3	0.3		n.d.		n.d.	n.d.		n.d.	n.d.
OP	12	1.6	1.4		0.7		0.1	0.4		0.02	0.1
NP	53	18	8.7		4.2		1.4	0.7		1.0	0.8
OP1EO	2.5	0.5	0.8		0.3		0.2	1.2		0.1	0.7
OP2EO	1.4	0.4	0.7		0.3		0.5	6.4		0.4	1.7
NP1EO	111	39	24		14		9.3	2.2		4.4	2.6
NP2EO	24	9.0	2.4		3.2		10	1.9		0.1	0.9
January 1999											
BPA	40	41	20	6.0	4.8	1.6	n.d.	n.d.	n.d.	n.d.	n.d.
BP	6.2	6.7	6.2	3.1	4.9	2.8	2.8	0.1	0.2	0.5	0.4
PP	7.6	7.7	1.9	3.8	7.7	3.8	3.8	1.1	0.9	n.d.	n.d.
OP	17	18	9.2	4.4	16	5.1	4.6	3.6	3.6	0.3	0.1
NP	69	84	58	34	63	32	32	21	21	0.5	0.3
OP1EO	12	11	5.7	6.7	11	5.8	5.8	1.3	1.6	0.4	0.3
OP2EO	21	20	15	11	19	9.8	9.8	6.9	7.0	0.1	0.1
NP1EO	47	46	57	18	29	3.8	15	8.5	5.3	1.6	0.7
NP2EO	9.3	11	12	4.6	2.7	0.8	0.5	1.0	1.8	0.2	0.6

[a] n.d.: not detected.

1998 showed a BPA concentration of 118 μg l^{-1} which confirms the assumption that the BPA originated from this Czech factory. Investigations of a water sample taken from the Bilina in September 1998 by Gandraß (1999) showed a BPA concentration of 1.3 μg l^{-1}. The sampling site at Scharfenberg lying downstream of Dresden showed with 776 ng l^{-1} the highest BPA concentration. This can probably be attributed to the effluent from the municipal sewage plant in Dresden–Kadiz or from a factory further upstream. At Dommitzsch the BPA concentration was 87 ng l^{-1} and decreased at Magdeburg to a level of 57 ng l^{-1}. On the 160 km down the river as far as Schnackenburg the concentration remained nearly constant (58 ng l^{-1}). However, as a result of dilution and taking into account the relatively short half-life of 2.5–4 days, a reduction in concentration would be expected. One possible explanation for the unchanging BPA concentration is an additional input from the tributary Havel at river-km 428. In samples of the tidal-influenced part of the River Elbe at Bunthaus, Seemannshöft and Blankenese, the BPA concentration decreased to a level of 19–27 ng l^{-1}. At the Elbe estuary at Cuxhaven the BPA concentration was 17 ng l^{-1}. An obvious concentration increase from approximately 20 to 57 ng l^{-1} was determined at the sampling site Grauerort, which is downstream from Stade. This increase could be explained by an augmentation from a BPA producing factory in Stade. Other authors found a concentration level of 33 ng l^{-1} BPA from a water sample taken in September 1998 at Bützfleth, a few kilometers upstream from Stade (Gandraß, 1999). In the tributaries Schwarze Elster, Mulde, and Saale the BPA concentrations were 9, 37, and 125 ng l^{-1}, respectively.

Among the alkylphenols investigated, NP had the highest concentrations in the Elbe river and its three tributaries. NP is a mixture of isomers with different side chain branchings. As shown in Fig. 3, 16 isomers from a commercial NP mixture were separated by GC–MSD (as HFBA-derivates). For quantification, the concentrations of these isomeres were added up. The concentration of NP in the Elbe river was between 7.9 (Bunthaus) and 52 ng l^{-1} (Scharfenberg). The average concentration was 11 ng l^{-1} (omitting Scharfenberg). Considering the tributaries, the highest NP concentration was found in the Saale (32 ng l^{-1}) whereas the Schwarze Elster and Mulde exhibited similar concentrations of 10 and 13 ng l^{-1}, respectively. Among the other alkylphenols PP had the lowest concentrations (<1 ng l^{-1}). The OP concentrations were somewhat higher and remained relatively constant along the Elbe (average 0.9 ng l^{-1}). The highest OP concentrations were found in the Mulde (2.1 ng l^{-1}) and Saale (2.0 ng l^{-1}). The BP concentrations, however, were higher in both the Elbe river and its tributaries, the average value being approximately 3 ng l^{-1} (omitting Dommitzsch). The

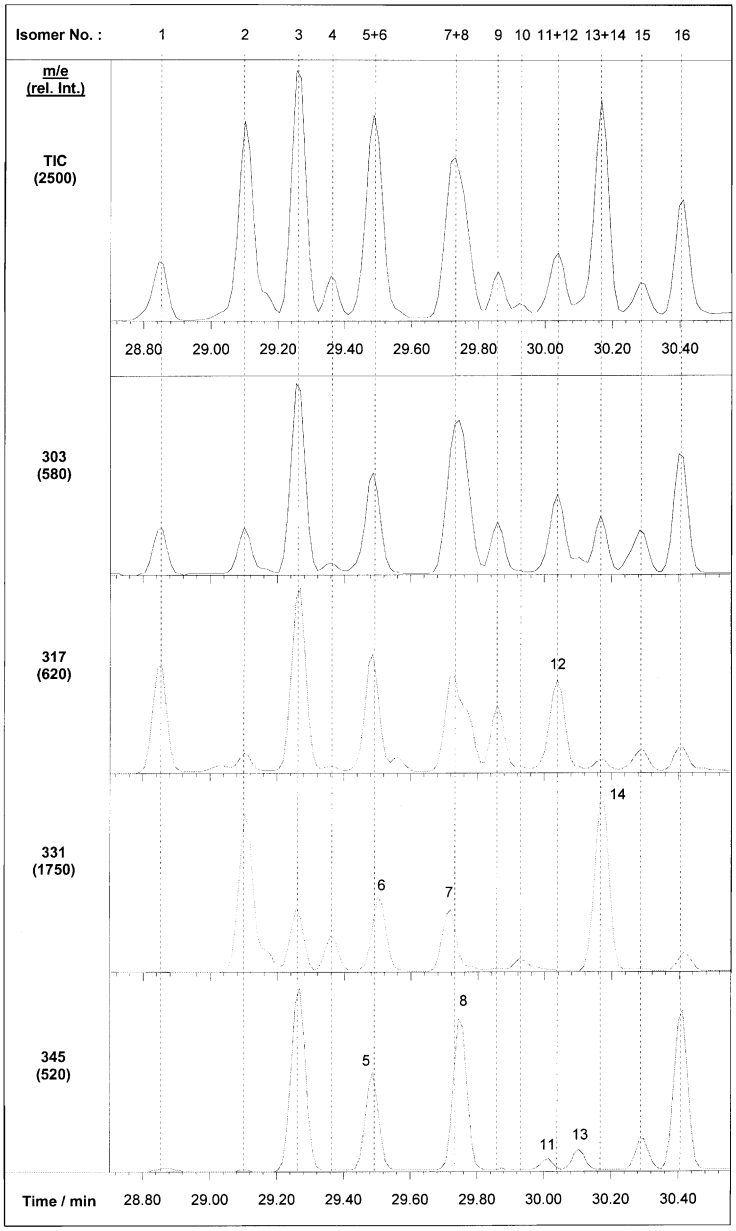

Fig. 3. Total ion chromatogram (TIC) and ion traces of NP (HFBA-derivates).

maximum concentration of 78 ng l^{-1} was found at Dommitzsch, followed by 8 ng l^{-1} at Grauerort.

Among the alkylphenols the concentrations of OP1EO in the Elbe were between 0.8 (Dommitzsch) and 6.3 ng l^{-1} (Scharfenberg); OP2EO concentrations ranged from 0.6 (Seemannshöft) to 6.8 ng l^{-1} (Scharfenberg). The average concentration of OP1EO and OP2EO was approximately 1 ng l^{-1} (omitting Scharfenberg). Similar concentrations were recorded at the three tributaries. Similar to NP the NPnEO consists of isomers with different branched alkyl-sidechains. In case of NP1EO 23 isomers and for NP2EO 22 isomeres were resolved in GC–MSD. Concentrations of NP1EO and NP2EO are given as the sum of these individual isomers. The concentrations of NP1EO and NP2EO in the water samples investigated were distinctly higher than concentrations of the OPnEO. The NP1EO concentration in the Elbe ranged from 10 (Grauerort) to 205 ng l^{-1} (Scharfenberg), the average value being 23 ng l^{-1} (omitting Scharfenberg). The concentration at Schmilka was 46 ng l^{-1}, twice as high as the average value. The tributaries exhibited concentrations of 12 (Schwarze Elster), 38 (Mulde) and 81 ng l^{-1} (Saale). The NP2EO concentrations in the rivers were found to be lower than the NP1EO concentrations (Table 1), the average being 8.3 ng l^{-1} (omitting Scharfenberg), the maximum being 84 ng l^{-1} (Scharfenberg). The concentration at Schmilka was 21 ng l^{-1}, considerably higher than the average concentration. NP2EO concentrations in the tributaries were between 4.3 (Schwarze Elster) and 25 ng l^{-1} (Saale); the Mulde had a concentration of 9.8 ng l^{-1}. The tidal-influenced part of the Elbe, at Seemannshöft, Blankenese, Grauerort and Cuxhaven, exhibited NP2EO concentrations of approximately 4 ng l^{-1}.

3.1.2. Weisse Elster

The results of the previous chapter showed relatively high concentrations of compounds analyzed in the Saale river (see Table 1). Because of this, a further study was carried out to find the input source of the Saale. The Weisse Elster is a small river which flows into the Saale. There is a chemical factory at this river, which produces antioxidants and stabilizing agents for plastics. Some villages and small towns are also found on its shores, and the effluents of sewage plants flow into the Weisse Elster. This river was investigated in October 1998 (six sampling sites). As seen in Table 2 at sampling point 1 the concentrations of nearly all compounds were considerably lower than at the other sampling points. Concentrations were of about 24 ng l^{-1} for BPA, 78 ng l^{-1} for NP, 26 ng l^{-1} for NP1EO and 9 ng l^{-1} for NP2EO. The concentrations of the other compounds were below 5 ng l^{-1}. Between sampling points 1 and 2 is the above-mentioned chemical factory. Downstream from this factory, at sampling point 2, the concentrations raised by a factor of about 3 (BPA), 2 (NP, NP1EO), and 4 (NP2EO). Further downstream between sampling points 2–6 the concentrations remained at the same order of magnitude. Summarized, these data show that the Weisse Elster is a source of contamination for the Saale river.

3.1.3. North Sea

The sampling campaigns of the North Sea showed for nearly all compounds decreasing concentration profiles following the River Elbe into the German Bight (see Table 3). BPA was detected only in the tidal part of the River Elbe and the outer estuary. The concentration of BPA at these sampling points was in the range of 7 and 249 ng l^{-1} in May 1998 and between 1.6 and 41 ng l^{-1} in January 1999. The highest concentration was measured at Stade near the effluent of a BPA producing factory (a parallel sample taken at Stade was filtrated prior to extraction and showed a BPA concentration of 178 ng l^{-1} for the aqueous phase). At all other sampling locations of the North Sea the concentration of BPA was below the detection limit. This effect may be attributed to dilution of the inflowing Elbe water and/or to the short half-life of BPA (about three days).

The alkylphenols showed concentrations ranging from below 1 to 84 ng l^{-1}, the highest concentrations being measured for NP. The alkylphenol ethoxylates had concentrations between 0.1 and 111 ng l^{-1}. Generally, the concentrations of alkylphenols and – ethoxylates were higher in samples of January 1999. A probable reason for this can be a reduced microbial degradation of these compounds during the winter months. Among the sampling sites of the North Sea, which are not influenced by the River Elbe, station #36 showed comparable high concentrations of the compounds analyzed. Depending on the current, this can be caused by inputs of the River Ems.

Summarizing, it can be seen that the River Elbe is one major input source of the compounds investigated for the North Sea. Other sources like spills caused by tank washings offshore with non-ionic tensides were not ascertained.

3.2. Sediment samples

From the *n*-octanol/water-partitioning coefficients ($\log K_{OW}$ values) of alkylphenols and – ethoxylates (between 4.12 and 4.48) it can be expected that these compounds adsorb onto suspended particulate matter to a considerable extent. To complete the data concerning the occurrence of xenoestrogens in the different environmental compartments, freshly deposed sediments of the River Elbe and its tributaries were analyzed. The concentrations of compounds analyzed in sediment samples are given in Table 4. Data of an annual screening of the River Elbe at sampling site Schnackenburg are shown in Table 5.

Table 4
Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in sediment samples of the Elbe river, the tributaries Schwarze Elster, Mulde and Saale (in μg kg^{-1} dm)

Location	Elbe river, downstream								Tributatries		
	Grauerort	Blankenese	Seemannshöft	Bunthaus	Schnackenburg	Magdeburg	Dommitzsch	Schmilka	Rosenburg (Saale)	Dessau (Mulde)	Gorsdorf (Schwarze Elster)
Stream (km)	660.5	634.3	628.8	609.8	474.5	318.1	172.6	4.1	4.5	7.6	3.8
BPA	96	66	68	187	230	194	278	343	121	76	132
BP	30	24	24	64	75	23	24	37	77	31	93
PP	36	31	26	66	77	17	19	29	83	33	n.d.
OP	40	35	32	66	77	21	24	39	86	41	38
NP	483	404	367	852	997	448	387	485	1378	507	705
OP1EO	94	102	113	78	91	31	30	51	91	51	93
OP2EO	126	140	139	100	110	52	45	86	113	79	110
NP1EO	760	754	886	712	967	464	323	568	809	553	624
NP2EO	972	1003	1144	1434	1611	774	546	980	1593	1009	1121

Table 5
Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in sediment samples of the Elbe river at sampling site Schnackenburg (in μg kg^{-1} dm)

	February 97	March 98	April 98	May 98	June 98	July 98	August 98	September 98	October 98	November 98	December 98
BPA	191	192	156	244	230	251	155	242	127	131	260
BP	44	26	19	73	75	81	31	67	37	82	82
PP	44	24	19	75	77	79	21	67	37	89	96
OP	37	33	24	78	77	79	23	67	45	103	116
NP	857	544	484	989	997	1029	454	884	790	704	736
OP1EO	81	44	35	93	91	92	36	81	88	79	62
OP2EO	95	66	66	119	110	107	57	98	125	119	79
NP1EO	586	600	666	981	967	1000	568	777	843	1027	795
NP2EO	1091	838	1259	1573	1611	1503	1068	1330	1426	1797	1381

The concentrations of BPA in sediment samples ranged from 66 to 343 μg kg^{-1} dm. The highest concentration was found at sampling site Schmilka, while the lowest concentrations were found in the Mulde and the tidal influenced part of the River Elbe (Seemannshöft, Blankenese and Grauerort). As in the case of water samples, there was slight increase in the tidal influenced part of the Elbe from about 70 μg kg^{-1} dm at Blankenese and Seemannshöft to 96 μg kg^{-1} dm at Grauerort, which can be attributed to the emission of a BPA producing factory. The annual monitoring at sampling site Schnackenburg showed BPA concentrations ranging from 127 to 322 μg kg^{-1} dm (Table 5), the maximum being in January 1999.

Among the alkylphenols NP had the highest concentration in sediment samples of the Elbe river, ranging from 367 to 997 μg kg^{-1} dm. The highest concentration of 1378 μg kg^{-1} dm was ascertained in the sample of the Saale, while the concentrations in the Mulde and the Schwarze Elster were 507 and 705 μg kg^{-1} dm. The concentrations of BP, PP, and OP were about 1 order of magnitude lower, they ranged from 17 to 93 μg kg^{-1} dm. During the annual monitoring at sampling site Schnackenburg the concentration of NP was between 454 and 1029 μg kg^{-1} dm. The concentrations of BP, PP, and OP ranged from 19 to 116 μg kg^{-1} dm during the sampling period.

The OP*n*EO in sediments of the River Elbe and tributaries showed concentrations lying between 30 and 140 μg kg^{-1} dm. The concentrations of NP*n*EO were in the range of 323 and 967 μg kg^{-1} dm for NPE1O and between 774 and 1611 μg kg^{-1} dm for NP2EO. The annual screening at sampling site Schnackenburg showed OP*n*EO concentrations ranging from 35 to 119 μg kg^{-1} dm. The NP*n*EO concentrations were between 568 and 1797 μg kg^{-1} dm. In all sediment samples investigated the alkylphenol diethoxylates had higher concentrations than the alkylphenol monoethoxylates The concentrations of the corresponding alkylphenols were usually lower or similar to the concentration of the monoethoxylates.

Summarizing, these results show, that alkylphenols and – ethoxylates have a strong tendency to enrich in the particulate phase. Even BPA with a reported half-life of 2.5–4 days (in water samples) was detected in all sediment samples investigated. Considering that these sediments were sampled for the duration of one month, it can be assumed that the decomposition process of BPA in the particulate phase takes much longer.

3.3. SPM/water-partitioning coefficients

As shown in the previous chapters, all compounds investigated were detectable in both the aqueous and the particulate phases. For this reason partitioning coefficients of BPA, alkylphenols, and -ethoxylates were determined in order to estimate the partitioning between the aqueous phase and suspended particulate matter. In the case of lipophilic compounds, the adsorption process is mainly affected by the content of total organic carbon (TOC) of the particulate phase. The partitioning coefficients (K_{OC}) calculated according to Eq. (1), were therefore related to the TOC of the SPM samples.

$$K_{OC} = C_S/C_W, \tag{1}$$

where C_S is the concentration of a compound in SPM (ng/kg TOC), and C_W is the concentration of a compound in the aqueous phase (ng/l).

The concentrations of compounds analyzed in the aqueous and particulate phases and the resulting partitioning coefficients in logarithm form ($\log K_{OC}$) are given in Table 6. All extractions of the aqueous phase were performed in triplicate to prove whether the concentrations were constant during each sampling campaign (taking about 6 h). The variability of concentrations, expressed by the relative standard deviation (RSD, see Table 6, values in brackets), was in the range of the analytical variation. It can be assumed, that the water samples taken showed no significant differences in the concentration levels of analytes during each of the four sampling campaigns.

The $\log K_{OC}$ values determined for BPA were in the range of 4.22–4.64, the mean value being 4.50 with an RSD of 4.3%. The $\log K_{OC}$ values of alkylphenols were about 1 order of magnitude higher. There was a slight increase of $\log K_{OC}$ values dependent on the degree of alkylation from BP to NP. The mean values were 5.58 for BP, 5.52 for OP and 5.86 for NP (for PP $\log K_{OC}$ values were not determinable because the concentration in SPM samples was below the detection limit). The RSD of the four determinations were 2.3 (BP), 0.8 (OP) and 4.7% (NP). Among the alkylphenol ethoxylates NP2EO had the highest $\log K_{OC}$ value with a mean value of 6.38 followed by OP2EO with 6.24. The RSD of the four experiments were below 2.5% in case of the ethoxylates.

A comparison of $\log K_{OC}$ values of the compounds analyzed with other environmentally relevant compound groups is given in Fig. 4. The results shown were calculated on the basis of water samples of the River Elbe also taken at sampling site Geesthacht (Heemken et al., 2000). It can be seen that the $\log K_{OC}$ values of alkylphenols and ethoxylates are located in the lower range of the strongly hydrophobic compound groups of PAH, PCB, and DDT and metabolites. According to the relatively high water solubility, BPA had the lowest $\log K_{OC}$ value. From the data presented it can be derived that alkylphenols and -ethoxylates are suitable parameters for sediment or SPM monitoring programs, while BPA preferably should be analyzed in water samples.

Table 6
Concentrations of BPA, alkylphenols and alkylphenol ethoxylates in the aqueous phase and suspended particulate matter of samples of the Elbe river at sampling site Geesthacht and resulting partitioning coefficients as log K_{OC}-values[a]

	Aqueous phase (ng/l)				SPM (mg/kg TOC)				log K_{OC}-values					
	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Exp. 1	Exp. 2	Exp. 3	Exp. 4	Mean	RSD (%)
BPA	12 (3.7)	19 (5.7)	20 (7.6)	20 (6.9)	n.d.[b]	0.31	0.86	0.90	n.v.[c]	4.22	4.63	4.64	4.50	4.3
BP	1.2 (12.8)	1.0 (14.6)	1.0 (18.3)	0.6 (9.8)	n.d.	0.26	0.38	0.34	n.v.	5.42	5.59	5.73	5.58	2.3
PP	0.03 (18.9)	0.01 (22.7)	0.04 (9.4)	0.02 (19.7)	n.d.	n.d.	n.d.	n.d.	n.v.	n.v.	n.v.	n.v.	n.v.	n.v.
OP	1.7 (15.3)	0.8 (8.5)	1.2 (10.1)	0.8 (3.5)	n.d.	0.22	0.42	0.28	n.v.	5.46	5.53	5.57	5.52	0.8
NP	7.5 (8.5)	4.5 (13.5)	5.5 (9.2)	3.3 (9.2)	2.07	2.76	5.73	4.97	5.44	5.79	6.02	6.18	5.86	4.7
OP1EO	0.4 (8.7)	0.7 (4.3)	0.6 (17.5)	0.4 (8.9)	n.d.	0.46	0.68	0.65	n.v.	5.83	6.05	6.19	6.02	2.5
OP2EO	0.4 (12.9)	0.5 (20.5)	0.5 (15.2)	0.3 (14.3)	n.d.	0.55	0.96	0.77	n.v.	6.02	6.31	6.39	6.24	2.5
NP1EO	13 (21.3)	8.9 (18.5)	16 (13.0)	9.5 (12.7)	n.d.	2.47	6.75	4.94	n.v.	5.44	5.64	5.72	5.60	2.0
NP2EO	4.4 (11.6)	2.4 (16.9)	4.9 (14.9)	3.3 (12.2)	n.d.	5.21	11.6	8.56	n.v.	6.34	6.38	6.42	6.38	0.5

[a] Values in brackets: RSD of triplicate determinations.
[b] n.d.: not detected.
[c] n.v.: no value, because the concentrations in one of the compartment was below detection limit.

3.4. Comparison with other surface waters

Environmental monitoring data concerning BPA are cited in Staples et al. (1998). In the Rhine river the concentration of BPA was below the detection limit of <10 ng l^{-1} (1989, seven sampling sites) and 119 ng l^{-1} (one sample). In various (industrially affected) Japanese surface waters, studies carried out between 1974 and 1978 showed BPA concentrations ranging from 60 ng l^{-1} to 110 ng l^{-1}. A sample taken at Tokyo had a BPA concentration of 1900 ng l^{-1}. Matsumoto et al. (1977) found concentrations of between 10 and 90 ng l^{-1} along the Tama river in Japan. Thus, concentrations of BPA in the Elbe river and its tributaries Schwarze Elster, Mulde and Saale are comparable with those of other surface waters. The estrogenic effect of BPA was shown in in vitro tests with cultured trout liver cells (endpoint: vitellogenin synthesis) by the transcription of recombined yeast cells (Celius et al., 1999) and the estrogen-dependent profileration of human breast cancer cells (Soto et al., 1995) as well as in in vivo studies (Christiansen et al., 2000). An indication for the estrogenic activity of this compound can be estimated by comparing it to 17β-estradiol. Therefore, relative estrogenic potency for BPA essayed in vitro is found to lie between 10^{-3} and 10^{-4} (Gaido et al., 1997).

NP concentrations from rivers in southern Germany, analyzed in 1995, were found to lie between 6 and 340 ng l^{-1} at 14 different sampling sites (Zellner and Kalbfus, 1997). Extensive sampling of the Main river in 1990 showed NP concentrations of between 7 ng l^{-1} and 3300 ng l^{-1} (47 samples; 90 percentile value = 80 ng l^{-1}) (cited in Gülden et al. (1997)). In 1991, the NP concentrations were between 9 and 1300 ng l^{-1} (54 samples; 90 percentile value = 80 ng l^{-1}). NP concentrations of between 38 ng l^{-1} and 50 ng l^{-1} were analyzed in the Main river were analyzed by Trapp et al. (1992). A study published in 1994 reported data from samples of the Glatt river in Switzerland which showed NP concentrations of between <300 (detection limit) and 45,000 ng l^{-1} (Ahel et al., 1994a). In a further study of six rivers (29 samples) in Great Britain, NP concentrations of between 20 and 180,000 ng l^{-1} were reported (Blackburn and Waldock, 1995). In a Canadian study of surface waters, NP concentrations of between <10 (detection limit) and 920 ng l^{-1} and OP concentrations of between 5 and 84 ng l^{-1} were determined (Bennie et al., 1997). In comparison to these data from the literature, the NP concentrations of between 7 and 52 ng l^{-1} (average 11 ng l^{-1}) found in the Elbe river were relatively low. Likewise, concentrations in the tributaries were also low (the maximum concentration of 32 ng l^{-1} was found at the mouth of the Saale). Adequate in vivo dose-response data for an assessment are available for OP and NP (Gülden et al., 1997). Experiments concerning the concentration-dependent induction of vitellogenin synthesis in male fish

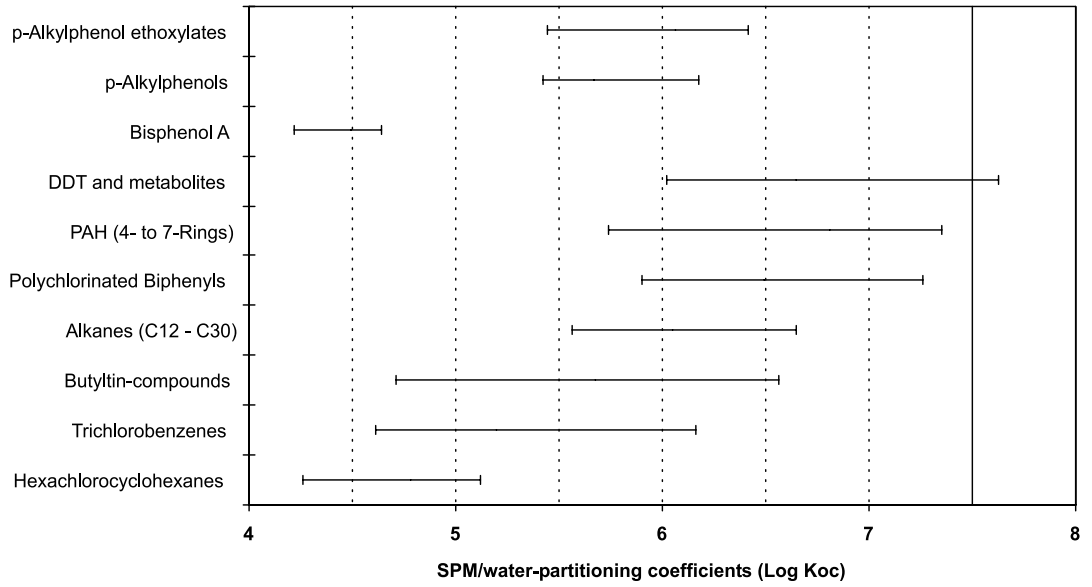

Fig. 4. Comparison of SPM/water-partitioning coefficients of different compound groups in samples of the River Elbe.

exist for OP and NP. LOEC-values were determined using the results of these experiments; 5000 ng l^{-1} for OP and 20,000 ng l^{-1} for NP. On the basis of these LOEC-values, one may infer that the alkylphenol concentrations in water samples of the Elbe river and the three tributaries are at least three orders of magnitude lower.

NP1EO concentrations of between <3000 (detection limit) and 69,000 ng l^{-1}, and NP2EO concentrations between <300 (detection limit) and 30,000 ng l^{-1} were found in river samples (Glatt) from Switzerland (1983–1986) (Ahel et al., 1994b). Concentrations of between 1100 and 4100 ng l^{-1} for NP1EO, and between 1300 and 5800 ng l^{-1} for NP2EO (Stephanou, 1985) were determined in Lake Geneva. According to the previously cited study of 35 surface waters in Canada (Bennie et al., 1997), the concentration range lay between 20 and 7800 ng l^{-1} for NP1EO and between 20 and 10,000 ng l^{-1} in the case of NP2EO. The presence of NP*n*EO is probably related to effluents from paper and pulp mills in the area. The NP1EO and NP2EO concentrations found in the Elbe amounted to <100 ng l^{-1}. At Scharfenberg where the maximum concentrations were found, the sum of both ethoxylate mixtures amounted to approximately 290 ng l^{-1}. These values show that the alkylphenol ethoxylate concentrations measured in the Elbe were considerably lower than in the cited surface waters. Considering an LOEC-value of 30,000 ng l^{-1} NP2EO (endpoint: vitellogenin synthesis in male trout) (Jobling et al., 1996), the total max. AP ethoxylate concentrations measured were two orders of magnitude lower than the LOEC-value.

4. Conclusions

In water samples of the North Sea, the Elbe river and the tributaries Schwarze Elster, Mulde and Saale, and the Weisse Elster the concentrations of BPA, alkylphenol- and alkylphenol ethoxylate (mono- and diethoxylate) ranged between <1 and <1000 ng l^{-1}.

The maximum concentrations for most of the compounds were found at the sampling site Scharfenberg (76.2 km). It is conceivable that the effluent from a sewage plant downstream of Dresden or of a factory leads to the high concentrations. Raised concentrations were also determined at the German–Czech border at Schmilka (4.2 km). Of the three tributaries investigated, the Saale exhibited the highest concentrations, followed by the Mulde and the Schwarze Elster. As one pollution source for the xenoestrogens found in the Saale the tributary Weisse Elster was recognized. Concentrations of compounds analyzed in samples of the North Sea were about 1 order magnitude lower than in samples of the River Elbe. The concentration of BPA was below the detection limit.

The LOEC values reported are 20,000 ng l^{-1} for NP and 30,000 ng l^{-1} for NP2EO (endpoint: induction of vitellogenin synthesis in male trout). The concentrations of these compounds in water samples of the North Sea, the Elbe river, its tributaries and the Weisse Elster were all well below these LOEC values. Assuming that BPA, alkylphenols and alkylphenol ethoxylates exhibit the same estrogenic activity, and adding up the analyzed concentrations, the average total concentration in the Elbe is approx. 50 ng l^{-1} which is about three orders of magnitude below the LOEC.

Investigations of freshly deposed sediments showed, that alkylphenols and – ethoxylates tend to enrich in the particulate matter. The concentration range of alkylphenols reached from 17 to 1378 μg kg^{-1} dm, levels of alkylphenols ethoxylates ranged from 30 to 1611 μg kg^{-1} dm. These findings were confirmed by the determination of SPM/water-partitioning coefficients which amounted to 5.52–5.58 for alkylphenols and 5.60–6.38 for alkylphenol ethoxylates. The adsorption rates of these compound groups are hence comparable to hydrophobic compound groups like n-alkanes. The SPM/water-partitioning coefficient of BPA was 4.50. In spite of this relatively low value and the short half-life of three days, BPA was detected in all sediment samples investigated. The concentration range was 66–343 μg kg^{-1} dm.

Acknowledgements

We would like to thank Mrs. U. Ehrhorn and Mr. M. Bergemann for the graphics.

Appendix A. List of abbreviations

BPA	Bisphenol A = 2,2′-Bis-(4-hydroxyphenyl)-propane
dm	dry mass
HFBA	Heptafluorobutyric acid anhydride
LOEC	Lowest Observable Effect Concentration
NP*n*EO	Nonylphenol ethoxylates (*n* = number of ethoxy units)
NP1EC	Nonylphenoxy acetic acid
NP2EC	Nonylphenoxy ethoxy acetic acid
BP	4-tert-Butylphenol
NP	4-Nonylphenol (technical)
NP1EO	4-Nonylphenol monoethoxylate (technical)
NP2EO	4-Nonylphenol diethoxylate (technical)
OP	4-tert-octylphenol
OP1EO	4-tert-octylphenol monoethoxylate
OP2EO	4-tert-octylphenol diethoxylate
PP	4-tert-pentylphenol
SPM	Suspended particulate matter
TOC	Total organic carbon

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