



Investigation of carbonyl compounds in bottled waters from Poland

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Abstract

Poly(ethylene terephthalate) (PET) bottles are commonly used for storing mineral water. The migration of carbonyl compounds from PET bottles into mineral water was observed. **Carbonation of water, sunlight and high temperature enhance the process of migration. Formaldehyde, acetaldehyde and acetone were the most important carbonyls identified in series of bottled water samples.** The concentration of carbonyls can change depending on the time of storage as well as storage conditions. **It was identified particularly high concentration of acetaldehyde (more than $100 \mu\text{g l}^{-1}$) in samples of mineral water saturated with CO_2 gas.** © 2002 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The consumption of bottled water has been increasing in Poland for the last 12 years. Mineral water is used as a replacement for tap water, which is always chemically disinfected. The disinfection process generates a variety of disinfection by-products that have often in the public mind been associated with adverse health effects. According to Polish regulations, bottled water cannot be treated with chemical disinfectants. Therefore, ultra-filtration or UV disinfection is applied to make water microbiologically safe. Usually, manufacturers do not inform consumers about water treatment technology and about the organic compound content. However, the quality of bottled waters can often be questionable. Current regulations for bottled waters [1] require only the analysis of very few organic contaminants (DDT, phenol, anionic detergents and PAHs with benzo(a)pyrene). There are two sources of organic compounds in bottled waters: natural organic matter (NOM) in addition to organics migrating from the bottle material.

The chemical content of water can change during bottle storage. The use of poly(ethylene terephthalate) (PET) bottles for packaging mineral water has become more popular, owing to the desirability of its physical and chemical properties such as strength, transparency, light weight and toxicological safety [2].

Many authors [2–9] have studied the effect of thermooxidative and chemical degradation of PET material. Before being filled the bottle has to pass through a series of steps. During this treatment, hydrolysis or thermal degradation within the plastic bottle material can occur [10]. All polymers degrade under such external factors as sunlight and temperature [9], thus the storage of the bottles under uncontrolled conditions can also be a source of organic contaminants in water. The UV-degradation is due to the combined effects of photolysis and oxidative reactions.

The thermal stability of thermoplastic polyesters like PET is of great technological importance [11]. The thermal degradation takes place mainly during the polycondensation stage and is caused by high temperatures. The principal PET thermal degradation products are aldehydes, water, CO_2 and carboxyl end groups [8]. The degradation of PET proceeds through a free radical mechanism in the presence of air and thus phosphorous

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compounds are applied to inhibit the thermooxidative degradation of PET [2–4,11].

The products of PET degradation can migrate to water in bottles. As for all food packaging, the quality of plastic bottles must be in accordance with the principles of inertness of the packaging and the purity of the foodstuff in contact with it [12]. Page et al. [13] detected a variety of volatile organic contaminants in bottled waters. Benzene, toluene, cyclohexane, chloroform and dichloromethane were detected in a set of 182 samples of bottled waters. Buiarelli et al. [14] identified and determined erucamide and cyclic PET oligomers (from dimer to pentamer) in water stored in PET bottles. Erucamide is added to the plastic material as a plasticizer while PET oligomers are formed during the

polymerisation process. Water is a medium in which polar chemicals readily dissolve. Volatile carbonyls may change the organoleptic properties of water. The odour and taste threshold ranges for acetaldehyde is from 4 to 65 ppb [15]. In another paper, the odour threshold of acetaldehyde in water ranges from 20 to 40 ppb and is assumed to be influenced by carbonation of the water [16]. PET manufacturers declare that there is <1 ppm acetaldehyde in the material. Therefore, one 1.5 l bottle weighing approximately 40 g could be a source of 40 µg of acetaldehyde. Thus, the concentration of 27 µg l⁻¹ of acetaldehyde could be expected as a result of the compound migration from the bottle material. However, acetaldehyde has been found at much higher concentrations [15,16]. We have also determined higher

Table 1
List of water samples tested in our investigations

| Symbol of sample | Sample description | Tables and figures with presented water sample |
|--|--|--|
| <i>Sample of special pure water</i> | | |
| P1 | Distilled water (from our laboratory) | Table 2 |
| P2 | Deionized water (from Cobrabid-Aqua apparatus) | |
| P3 | Deionized water (from Millipore) | |
| P4 | Sterile water (sample P3 was additionally sterilized at 134°C) | |
| P5 | Ringer solution, used in intravenous drips | |
| P6 | Tap water | |
| <i>Samples of mineral water stored in PET bottles (purchased on the retail market, from 14 different manufacturers, marked in paper as numbers 1–14)</i> | | |
| 1As, 1Al | A—non-carbonated mineral water stored in: | Table 3 |
| 2Al | | s—0.5 l PET bottle |
| 3As, 3Am, 3Al | m—0.75 l PET bottle | |
| 4As, 4Al | l—1.5 l PET bottle | |
| 6Al | | Table 4a |
| 7Al | | |
| 8Al | | |
| 9Al | | |
| 10Al | | |
| 11Al | | Fig. 3 |
| 12Al | | |
| 13Al | | |
| 1Bs | B—carbonated mineral water stored in: | Table 3 |
| 2Bl | | s—0.5 l PET bottle |
| 3Bs | m—0.75 l PET bottle | |
| 4Bs | l—1.5 l PET bottle | |
| 5Bs, 5Bl | | |
| 6Bl | | Table 4b |
| 7Bl | | |
| 8Bl | | |
| 9Bl | | |
| 10Bl | | |
| 11Bl | | Fig. 3 |
| 12Bl | | |
| 13Bl | | |
| 14Bl | | Fig. 5 |

concentrations of acetaldehyde. According to Wegelin et al. [17], water in PET bottles contains formaldehyde and negligible amounts of acetaldehyde after disinfection by sunlight. The aim of this paper is to show that other carbonyl compounds in bottled waters are also present, sometimes at astonishingly high concentrations. Recognition of the sources of the carbonyl compounds is the other purpose of the paper.

2. Experimental

2.1. Waters

Tap water from local distribution network was used (the ground water in Poznań (pop. 600 000) is aerated and filtered to remove iron and manganese and then is disinfected with chlorine dioxide). Ringer solution was purchased from a local pharmacy. All of the mineral waters were purchased from the local markets and they were investigated before the expiration dates. List of water samples tested in our investigations is presented in Table 1.

2.2. Chemicals and materials

The *O*-(2,3,4,5,6-pentafluorobenzyl)hydroxylamine (PFBOA) and analytical standards (aldehydes and ketones) were purchased from Aldrich—Chemie (Steinheim, Germany) and BDH (Pool, UK; AnalaR and GPR grades). PFBOA was prepared gravimetrically as an aqueous solution in organic free water while aldehyde and ketone solutions were prepared in methanol. Hexane (J.T. Baker, Germany) was used as a solvent for extraction.

2.3. Derivatization with PFBOA

Twenty milliliters of water samples were collected in glass vials with glass caps. One milliliter of 1 mg ml^{-1} aqueous PFBOA solution was added to the sample and kept at room temperature for 1 h, then 2 drops of concentrated sulphuric acid (H_2SO_4) were added to

complete the derivatization reaction. The oximes (Fig. 1) were extracted by shaking the solution with 1 ml of hexane for 1 min. The extract was then purified with 3 ml of 0.2 N sulphuric acid solution. The hexane layer was separated and transferred to vials containing approximately 50 mg of sodium sulphate to dry the extract. Fig. 1 illustrates the derivatization reaction.

2.4. Chromatographic analysis

The extracts were analysed by gas chromatography using GC 6000 and GC 8000 series (Fisons Instruments) equipped with a ^{63}Ni electron capture detector. Injections of $0.5 \mu\text{l}$ of the extract were introduced via “on column” injector onto chromatographic column. The DB-5 (J&W) fused silica capillary column ($30 \text{ m} \times 0.32 \text{ mm} \times 0.25 \mu\text{m}$ film) was applied for analysis while the Rtx-1301 (Restek) fused silica capillary column ($30 \text{ m} \times 0.32 \text{ mm} \times 0.5 \mu\text{m}$ film) was used as a confirmation column. Helium and nitrogen were used as a carrier gas and a detector make-up gas, respectively. The temperature program for GC was as follows: 80°C held for 4 min, increased to 240°C at 5°C min^{-1} , then increased to 270°C at $20^\circ\text{C min}^{-1}$, held at 270°C for 5 min. A CWS (Chromatography Station for Windows, Version 1,7 Eval, Build 270598, Czech Republic) system for collecting and processing the chromatographic data was used. Fig. 2 presents a typical chromatogram of PFBOA-oximes obtained by the method. With most carbonyl compounds, except for symmetrical ketones and formaldehyde, two geometrical isomers of the derivatives are formed. Calibration curves were made by plotting concentration versus area or, in the case of isomeric peaks, combined areas. Calibration curves were linear from the detection limit $0.1 \mu\text{g l}^{-1}$ to at least $150 \mu\text{g l}^{-1}$.

2.5. TOC measurement

TOC was analysed by a LABTOC system (Pollution and Process Monitoring Ltd., England) total organic carbon analyser by the sodium peroxydisulfate/orthophosphoric acid wet oxidation/UV radiation method.

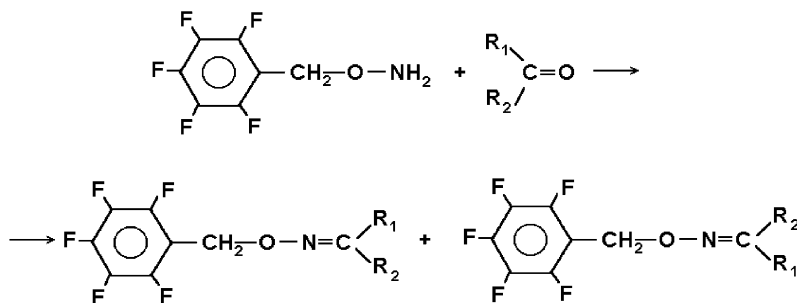


Fig. 1. Derivatization of carbonyl compounds with PFBOA.

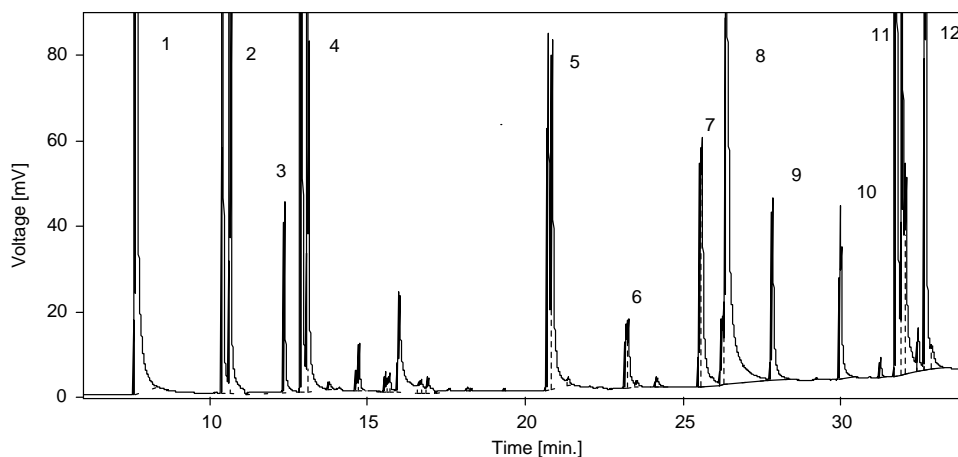


Fig. 2. Typical chromatogram of PFBOA-derivatives of carbonyl compounds. 1—formaldehyde, 2—acetaldehyde, 3—acetone, 4—propanal, 5—hexanal, 6—heptanal, 7—octanal, 8—benzaldehyde, 9—nonanal, 10—decanal, 11—glyoxal, 12—methylglyoxal.

3. Results and discussion

3.1. Evaluation of organic pure water

Aldehydes are present everywhere in the environment: in air as well as in water. Carbonyl compounds are identified even in organic free water for laboratory use [18]. This is confirmed also in our experiments. The determination of carbonyl compounds in the background is essential for a successful analysis of water samples. We have determined the aldehydes and ketones in various samples of purified water. These results are presented in Table 2.

We have found a relatively high background level of aldehydes in laboratory reagent waters (samples P1–P4) as well as in drinking water (sample P6). Formaldehyde is always present in water at single $\mu\text{g l}^{-1}$ concentrations. The common presence of acetone in water samples is also worth emphasising. Surprising results were obtained for the Ringer solution (sample P5). The total amount of carbonyl compounds in the sample was much higher than that in tap water. Ringer solution is usually distributed in the polyethylene (modified by polypropylene) containers. The final product undergoes a sterilisation process at a high temperature and can be stored for 3 years. Our sample was 1-year old. Thus, the organic containers are likely to be the source of formaldehyde, acetaldehyde and acetone.

3.2. Carbonyl compounds in bottled waters

We have analysed a selection of bottled waters commercially available in Poland and we have detected a very broad range of carbonyl compounds' concentrations. Some reports have been written on the presence of aldehydes in bottled waters but a very broad range of

Table 2

Aldehydes and ketones identified in pure water samples

| Compounds ($\mu\text{g l}^{-1}$) | Samples of pure water | | | | | |
|------------------------------------|-----------------------|-----|-----|-----|------|------|
| | P1 | P2 | P3 | P4 | P5 | P6 |
| Formaldehyde | 3.3 | 1.9 | 7.3 | 7.1 | 20.2 | 4.5 |
| Acetaldehyde | 1.4 | 0.1 | | | 20.1 | 4.5 |
| Propanal | 0.4 | 0.4 | 0.1 | | 2.8 | 1.0 |
| Hexanal | | | | 5.5 | 5.2 | 0.8 |
| Benzaldehyde | | | 1.3 | 0.4 | 15.1 | |
| Nonanal | 0.7 | | 0.8 | | 1.7 | 2.0 |
| Decanal | | | | | 1.4 | 0.5 |
| Glyoxal | | | | | | 0.4 |
| Methylglyoxal | 1.6 | | | | 1.0 | 1.0 |
| Total aldehydes | 7.4 | 2.4 | 9.5 | 13 | 67.5 | 14.7 |
| Acetone | 1.5 | 5.4 | 4.6 | 4.4 | 67.0 | 2.4 |

The samples P1–P6 are described in Table 1.

concentrations has also been reported. Acetaldehyde migration from PET material is most often identified as the source of the aldehyde, however the aldehydes are also detected in water packed in glass bottles. The most surprising result of the research is a common presence of acetone in bottled water. Acetone has been detected also within a broad range ($5.1\text{--}125 \mu\text{g l}^{-1}$) of concentrations in all samples of examined waters. That has not been reported so far. The formaldehyde concentration sometimes exceeds $50 \mu\text{g l}^{-1}$ that is allowed in tap waters by Polish regulations. Acetaldehyde frequently exceeds $20\text{--}40 \mu\text{g l}^{-1}$ that is considered to be the threshold of odour and taste. The presence of nonanal and (very common) methylglyoxal has also been detected in many of the waters. The results of the analysis are shown in Table 3. The analysed samples had very different origins and they were manufactured at undetermined times. Thus, we

Table 3
Carbonyl compounds identified in various bottled water samples

| Sample | Formaldehyde ($\mu\text{g l}^{-1}$) | Acetaldehyde ($\mu\text{g l}^{-1}$) | Acetone ($\mu\text{g l}^{-1}$) | Nonanal ($\mu\text{g l}^{-1}$) | Glyoxal ($\mu\text{g l}^{-1}$) | Methylglyoxal ($\mu\text{g l}^{-1}$) | TOC ($\mu\text{g l}^{-1}$) |
|--------|---------------------------------------|---------------------------------------|----------------------------------|----------------------------------|----------------------------------|--|------------------------------|
| 1As | 31.6 | 0.9 | 19.1 | 0.9 | | 0.9 | 2.95 |
| 1Al | 2.2 | 2 | 5.1 | 1.9 | | | 1.72 |
| 1Bs | 25.6 | 5.3 | 16.8 | 1.4 | | 0.8 | 3.76 |
| 2Al | 9.2 | 0.9 | 85.4 | | | 0.9 | 1.35 |
| 2Bl | 57.7 | 96.9 | 92.4 | 0.95 | | 2.6 | 2.12 |
| 3As | 4.6 | 2.4 | 101.3 | 2.1 | | 2.1 | 2.54 |
| 3Am | 5.1 | 2.8 | 105.7 | 2.3 | | 3.0 | 2.51 |
| 3Al | 7 | 2 | 107.6 | 1.2 | | 1.1 | 2.3 |
| 3Bs | 37.7 | 317.8 | 82 | 1 | | 2.4 | 4.51 |
| 4As | 37.7 | 96.5 | 97.9 | 11.3 | | 15.8 | 3.47 |
| 4Al | 64.6 | 133.8 | 95.7 | 7.7 | 5.9 | 3.8 | 3.02 |
| 4Bs | 96.1 | 148.8 | 93.3 | | | 4.6 | 3.08 |
| 5Bs | 39.5 | 4.7 | 125.6 | 7.9 | 0.9 | 2.8 | 3.92 |
| 5Bl | 35.1 | 170.9 | 93.9 | | | 1.4 | 1.11 |

The samples are described in Table 1.

Table 4
Concentration of TOC and carbonyl compounds

| Sample no. | TOC ($\mu\text{g l}^{-1}$) | Formaldehyde ($\mu\text{g l}^{-1}$) | Acetaldehyde ($\mu\text{g l}^{-1}$) | Acetone ($\mu\text{g l}^{-1}$) | Total carbonyl compounds ($\mu\text{g l}^{-1}$) |
|--|------------------------------|---------------------------------------|---------------------------------------|----------------------------------|---|
| <i>(a) In non-carbonated bottled water</i> | | | | | |
| 6Al | 4.33 | 0.8 | 0.9 | 11.4 | 13.1 |
| 7Al | 2.80 | 27.7 | 2.6 | 42.1 | 72.4 |
| 8Al | 1.93 | 38.8 | 2.0 | 43.1 | 83.9 |
| 9Al | 1.33 | 3.5 | 0.6 | 81 | 85.1 |
| 10Al | 0.26 | 18.4 | 39.1 | 6.6 | 64.1 |
| <i>(b) In carbonated bottled water</i> | | | | | |
| 6Bl | 5.87 | 1.7 | 2.2 | 8.8 | 12.7 |
| 7Bl | 3.86 | 66.7 | 130.4 | 29.8 | 226.9 |
| 8Bl | 1.70 | 9.5 | 107.2 | 32.7 | 149.4 |
| 9Bl | 3.48 | 25.6 | 105.6 | 84.0 | 215.2 |
| 10Bl | 0.81 | 10.4 | 48.6 | 8.9 | 67.9 |

For sample description see Table 1.

have started to investigate the influence of the various parameters on the carbonyl content.

3.3. Correlation between TOC and concentration of carbonyl compounds

We have not observed the correlation between TOC and carbonyl compound concentration in different types of water packed in PET bottles.

The two types of samples (carbonated and non-carbonated water) were collected from various manufacturers and then TOC and carbonyl compounds were determined.

Table 4a and b leads us to the conclusion that there is no correlation between TOC and the level of aldehyde

concentration in bottled mineral water. The results indicate that the carbonyl compounds are more likely to originate from PET bottles than from the natural organic matter present in water. Nijssen et al. [16] reported on the presence of acetaldehyde in carbonated water, however carbonyl compounds are also present in significant amounts in non-carbonated water. A comparison of randomly chosen brands of bottled water show significantly higher concentrations of acetaldehyde in carbonated water. Relatively high concentrations of acetone were found in all examined types of water. Acetone is also usually present in tap water, but at significantly lower concentrations (usually at a single $\mu\text{g l}^{-1}$). The presence of acetone in bottled water has not been reported on as yet in a paper. According to our

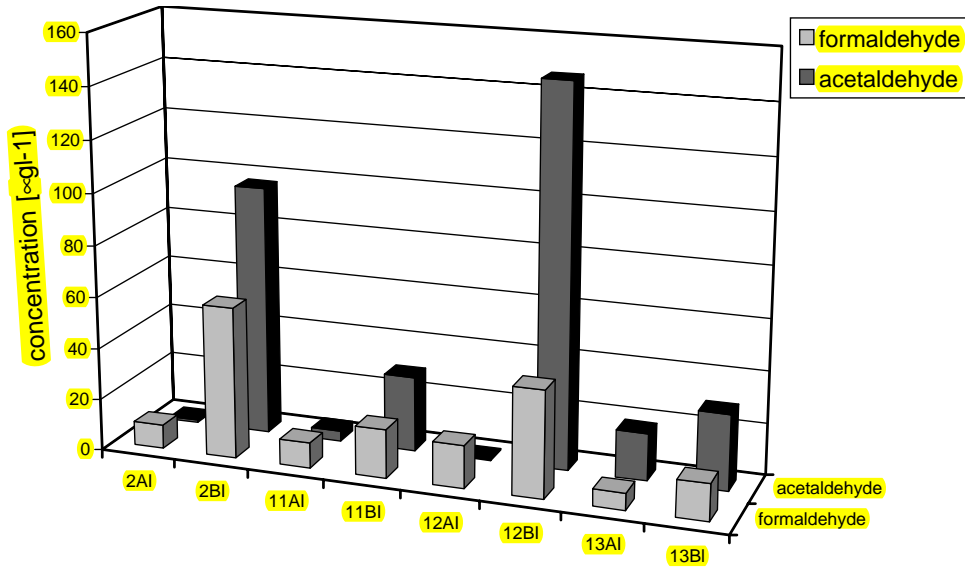


Fig. 3. Influence of carbonation on aldehyde concentration in different kinds of bottled water (for sample description see Table 1).

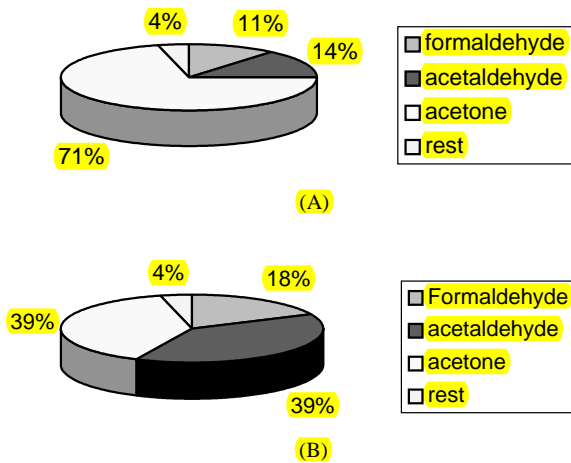


Fig. 4. Average distribution of carbonyl compounds in: A—non-carbonated and B—carbonated mineral water (for sample description see Fig. 3 and Table 1).

results, presented in this paper, acetone seems to be as abundant organic impurity as aldehydes.

3.4. Influence of carbonation process on aldehyde concentration in bottled water

We have noted a significant difference between the amounts of formaldehyde and acetaldehyde in carbonated and non-carbonated water of the same brand. Four brands of bottled water manufactured by four manufacturers have been tested. Fig. 3 illustrates the differences between noncarbonated and carbonated

waters. The carbonation of water significantly increases the amount of acetaldehyde in water. This was previously found by Nijssen et al. [16] who reported acetaldehyde concentrations of up to $100 \mu\text{g}\cdot\text{l}^{-1}$.

The carbonation changes also the distribution of carbonyl compounds in bottled water and that is shown in Fig. 4. On average acetaldehyde comprises 14 percent and it can comprise up to 39 percent of the total carbonyl compound content in non-carbonated water. The presence of CO_2 or lower pH of carbonated water is responsible for the increase in carbonyl compounds concentration in bottled water. High concentrations of acetaldehyde in spring or mineral water can be an important factor in determining the quality of the water as the odour and taste threshold of acetaldehyde is estimated as $20\text{--}40 \mu\text{g}\cdot\text{l}^{-1}$ [16].

3.5. Influence of storage condition on amounts of carbonyls

The influence of the storage conditions on the content of the carbonyl compounds was examined. A reference sample was taken from a freshly filled PET bottle (sample 14BI). The second sample was obtained from a bottle that had been kept for 4 days in the dark at 4°C , while the third sample was from bottle that had been exposed to $\sim 30^\circ\text{C}$ and sunlight for 4 days. The results are presented in Fig. 5.

The concentration of carbonyl compounds in the reference sample (14BI) was very low, similar to that found in the background (see Table 2). However, the amount of carbonyls increases in water stored for only 4 days in PET bottles. As one can see in Fig. 5 sunlight

and higher temperature enhance the formation or migration of carbonyl compounds from PET bottles. Wegelin et al. [17], observed a similar correlation for formaldehyde only but not for the other aldehydes. However, they examined the migration (or formation) of formaldehyde over much longer period of time. The highest concentration of formaldehyde was observed after about 6 months of sunlight exposure. Contrary to Wegelin et al. [17] our results indicate that acetaldehyde and acetone are equally important carbonyl compounds migrating to bottled water.

3.6. Long-term storage and carbonated water quality in PET bottles

Carbonated, bottled water was collected from the same manufacturer (sample 14Bl, see Table 1) for a period of 9 months and stored in 1.5l PET bottles at room temperature. The water samples were collected between June 2000 and February 2001. All the tested water samples were analysed at the same time in May 2001. The change of the aldehyde content in water vs. manufacturing date is presented in Table 5 and in Fig. 6. The following conclusions can be drawn from the results: acetaldehyde is a dominant carbonyl compound in carbonated water, the content of aldehydes gradually

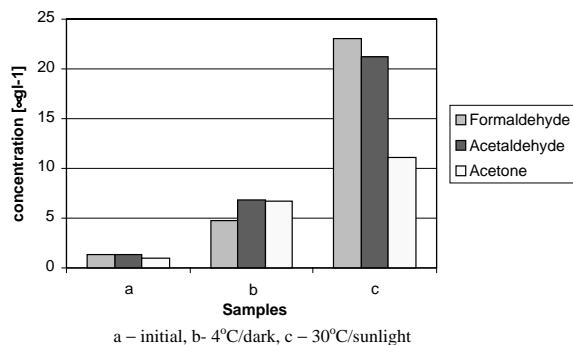


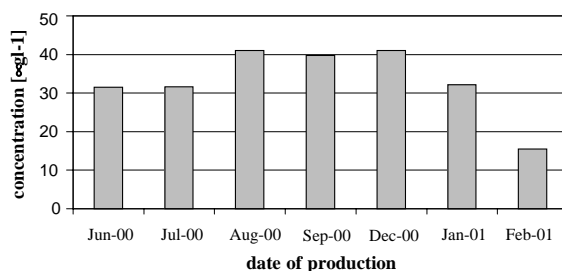
Fig. 5. Influence of storage conditions on the amount of carbonyl compounds in PET bottles (sample 14Bl).

increases over the period of 8–9 months and then begins to decrease. It is well known that the ageing process of carbonated water is due to the gradual loss of dissolved CO₂ as the bottles are not sufficiently tight for the gas.

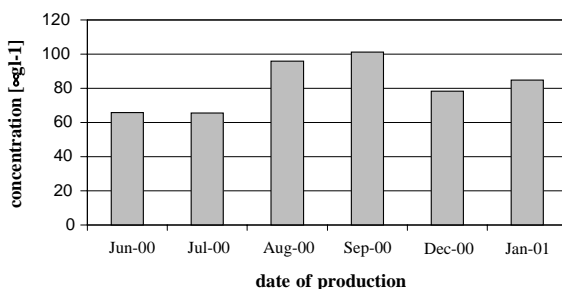
Nijssen et al. [16] suggest that the stability of acetaldehyde in carbonated water may be caused by the absence of oxygen. As a decrease of concentration is also observed for formaldehyde it can be assumed that the carbonyls diffuse through the bottle wall similarly to CO₂.

3.7. Extraction of carbonyl compounds from PET bottles

We have also tried to evaluate the influence of artificial ageing conditions on carbonyl compounds formation. One-half of a freshly blown and unused



(A) Formaldehyde concentration.



(B) Acetaldehyde concentration.

Fig. 6. (A, B) Aldehyde contents in water samples of various age (sample 14Bl).

Table 5
Aldehyde's contents in carbonated, bottled water produced at different time

| Aldehydes (µg l ⁻¹) | Date of production | | | | | | |
|---------------------------------|--------------------|--------|--------|--------|--------|--------|--------------|
| | Jun-00 | Jul-00 | Aug-00 | Sep-00 | Dec-00 | Jan-01 | Feb-01 |
| Formaldehyde | 31.5 | 31.6 | 41.0 | 39.7 | 41 | 32.2 | 15.5 |
| Acetaldehyde | 65.8 | 65.6 | 96.0 | 101.3 | 78.3 | 84.8 | ^a |
| Total aldehydes | 97.3 | 97.2 | 137.0 | 141.0 | 119.3 | 117.0 | |
| TOC (mg l ⁻¹) | 1.57 | 1.44 | 1.25 | 1.29 | 1.13 | 1.03 | 1.06 |

^aNot analysed.

Table 6
Carbonyls determined in the fresh bottle extract

| Carbonyl compounds ($\mu\text{g l}^{-1}$) | Deionized water | Ageing at room temperature | | Ageing at 60°C | |
|---|-----------------|----------------------------|------|----------------|-------|
| | | 2.5 h | 15 h | 2.5 h | 15 h |
| | | Formaldehyde | 9.4 | 18.7 | 27.2 |
| Acetaldehyde | 2.2 | 6.4 | 26.3 | 57.2 | 135.9 |
| Acetone | 2.2 | 13.6 | 20.7 | 50.7 | 97.1 |
| Total amount | 13.8 | 38.7 | 74.2 | 145.9 | 310.5 |

Table 7
Carbonyls determined in one-month old bottle extract

| Carbonyl compounds ($\mu\text{g l}^{-1}$) | Deionized water | Ageing at room temperature | | Ageing at 60°C | |
|---|-----------------|----------------------------|------|----------------|-------|
| | | 2.5 h | 15 h | 2.5 h | 15 h |
| | | Formaldehyde | 9.4 | 21.1 | 26.4 |
| Acetaldehyde | 2.2 | 3.0 | 8.7 | 24.0 | 60.2 |
| Acetone | 2.2 | 43.8 | 44.7 | 59.8 | 68.8 |
| Total amount | 13.8 | 67.9 | 79.8 | 126.2 | 212.7 |

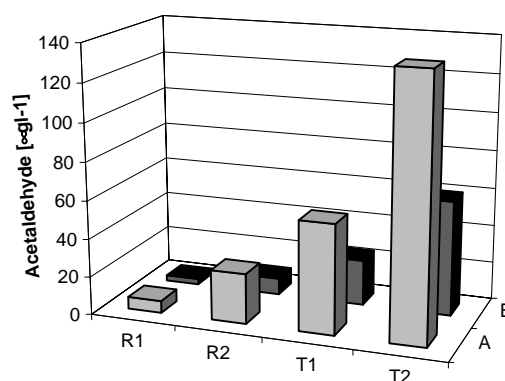
PET bottle was cut into pieces (approx. 20 mm × 20 mm) and in order to allow for the maximum interaction between water and the bottle surface, it was placed into Erlenmeyer flasks with 200 ml of deionized water. The same procedure was applied for empty bottles that had been stored for 1 month. Ageing process was performed (using magnetic stirrer) at room temperature and at 60°C for 2.5 and 15 h. The results of the formaldehyde, acetaldehyde and acetone determination in extracts are presented in Tables 6 and 7.

The experiment confirms that the carbonyls migrate (or are formed) from the PET bottle. Formaldehyde, acetaldehyde and acetone were found in all extracts. The concentrations of acetaldehyde in the fresh bottle extract are evidently higher than those from the 1-month old bottle (Fig. 7).

It might be speculated that the faster degradation of PET at higher temperature is responsible for the higher concentration of aldehydes found in the extract at 60°C.

4. Conclusions

- Formaldehyde, acetaldehyde and acetone are found also in organic free water.
- Formaldehyde, acetaldehyde and acetone are the most important carbonyls identified in bottled water.
- There is no correlation between TOC concentration and carbonyl concentration in bottled water.
- Migration or formation of aldehydes from PET bottle into the water is observed.



R1 – ageing at 20°C for 2,5 h, R2 - ageing at 20°C for 15 h, T1 - ageing at 60°C for 2,5 h, T2 - ageing at 60°C for 15h, A – fresh bottle, B- one-month-old bottle

Fig. 7. Acetaldehyde determined after ageing of PET bottles.

- Carbonation of water, sunlight and high temperature enhance the process of migration or aldehydes formation from PET bottles into water.
- The concentrations of carbonyls in water stored in PET bottles are not stable, they change over the time of storage as well as storage conditions.

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