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Research Article

The Impact of Temperature, Sunlight and Time on the Quality of Drinking Water Stored in Polyethylene Terephthalate Bottle in Yola Metropolis, Nigeria

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ABSTRACT

The present study examined how sunlight radiation, temperature and time in Yola climate can affect the physicochemical properties of drinking water in polyethylene terephthalate (PET) bottle in Yola Metropolis Nigeria. Conductivity, total dissolved solids (TDS), chemical oxygen demand (COD), pH, Cl^-, and NO_3^- were analyzed using standard methods for 42 days. Solvent extraction and GC-MS analysis were conducted periodically to monitor the appearance and identity of any migrant organic compounds. Sunlight exposure had the highest impact wherein conductivity, TDS, and COD trended upwards while pH decreased over time. However, Cl^- and NO_3^- stayed constant. The GC-MS results showed the highest concentration of organic compounds in the sunlight exposed samples showing the molecular ion peak of benzene. Conversely, the negative control samples, stored in a cool dry place, showed no signs of leachates.

Keywords: Bottled water quality, Polyethylene terephthalate, PET packaging, Physicochemical properties, Leachates

Résumé

La présente étude a examiné comment le rayonnement solaire, la température et le temps dans le climat de Yola peuvent affecter la contamination moléculaire organique de l'eau potable dans une bouteille de polyéthylène téréphtalate (PET). La conductivité, les solides dissous totaux (TDS), la demande chimique en oxygène (DCO), le pH, le Cl- et le NO3- ont été analysés pendant 42 jours. L'extraction par solvant et l'analyse GC-MS ont été effectuées périodiquement pour surveiller l'apparence et l'identité de tout composé organique migrateur. L'exposition au soleil a eu l'impact le plus élevé, la conductivité, le TDS et la DCO ayant tendance à augmenter tandis que le pH diminuait avec le temps. Cependant, Cl- et NO3- sont restés constants. Les résultats de la GC-MS ont montré la concentration la plus élevée de composés organiques dans les échantillons exposés à la lumière du soleil montrant le pic d'ions moléculaires du benzène. A l'inverse, les échantillons témoins négatifs, conservés dans un endroit frais et sec, ne présentaient aucun signe de lixiviat.

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1 INTRODUCTION

The earliest polyesters from aliphatic dibasic acids and diols could not be commercialized as they were susceptible to degradation by hydrolysis. In order to remedy this drawback, stiffer, and higher boiling point polyesters were made by substituting the aliphatic dibasic acid monomers with more rigid aromatic monomers (Scheirs & Long 2005). As a result, terephthalic acid (TPA) and aliphatic diols were used, in a condensation polymerization process, to synthesize a high melting point polyester known as polyethylene terephthalate (PET). PET is the highest produced polyester with an average annual global production of 25.9 million tons (Rogers & Long 2003). It is a semi-crystalline polymer with a glass transition temperature (T_g) of about 72°C. In its amorphous state, it is transparent while in the crystalline state, it appears translucent. Furthermore, it possesses dielectric properties (Sima *et al.* 2017; Reddish 1950), dimensional stability, and excellent gas barrier characteristics. PET is a thermoplastic material widely used in textiles (Chen *et al.* 2008) and packaging many food products such as carbonated beverages, edible oils, and bottled water. This widespread use of this plastic material is attributable to its strength, high resistance to chemical attack and weathering, and see-through features.

Over recent years, drinking bottled water has gained widespread popularity with over 200 million liters having been consumed globally in 2017 alone (Diduch *et al.* 2013). People's preference for bottled water over other water types such as tap water can be attributed to the characteristic chlorine smell and taste associated with tap water (Samadi *et al.* 2009), coupled with the prestige attached to drinking bottled water. The storage conditions of such packaging materials are of growing interest due to the potential leaching of organic and inorganic materials from PET bottles into the contained foods or drinks at elevated temperatures, exposure to UV radiation, and overextended storage time (Schmid *et al.* 2008). The leachates, also known as non-intentionally added substances (NIAS), are often the products of the degradation of the polymer itself by such agents as chemical attack, light, radiation, heat, mechanical stress, and others (Diduch *et al.* 2013). Generally, when a polymer synthesized via condensation polymerization is placed in a medium containing the small molecule that was given off during the polymerization process and at high temperature, the polymer degrades by hydrolysis. For example, PET and other polyesters in the presence of water at elevated temperatures under basic, acidic, and even neutral conditions begin to hydrolyze (Massey 2006).

In addition to the migration of substances that occur during storage, the migration of degradation materials sometimes also results from contaminants already existing in the water source or external contamination from the bottling plant. Thus, it is very important to note any possible interaction between the stored beverage and packaging material. Studies have shown that some contaminants include Antimony (Sb(III)) – the polymerization catalyst, acetaldehyde (Bashir *et al.* 2002; Mutsuga *et al.* 2006), Di (2-ethylhexyl) phthalate (DEHP) (Farhoodi et al. 2008), residual monomers/oligomers, additives (Abboudi & Odeh 2015), and some degradation by-products such as light gases (CO and CO_2), methane, ethane, benzene, TPA, ethylene, and biphenyl. The transfer of materials, albeit in trace amounts, needs to be closely checked to ensure it does not reach harmful levels. Studies have also shown that high levels of phthalates and its major metabolite, mono-(2-ethylhexyl) phthalate, are endocrine disruptors (Colón I *et al.* 2000) which lead to genetic disorders including decreased sperm count, testicular dysgenesis syndrome, lowered fertility in females, hormonal imbalance, damages to the uterus, and fetal defects (Montuori *et al.* 2008).

Given that the migration process of degradation products from the bottle into the contained beverage is a slow process, the compounds are usually monitored via a periodic analysis of selected water quality properties. Physicochemical properties include physical, solvation, and other properties that influence chemical reactivity. Some of these are total dissolved salts, pH, electrical conductivity, NO_3^-, Cl^-, F^-, NH_4^+, SO_4^{2-}, and chemical oxygen demand (COD). COD depicts the amount of oxygen required to oxidize present organic materials – a reflection of the concentration of organic matter that has migrated into the contained water (Geerdink *et al.* 2017; Li *et al.* 2018). In order to qualitatively identify the migrant organic compounds, the solvent extraction technique that separates a homogeneous mixture of two or more solutes (Ishizaka et al. 2019) can be employed alongside a GC-MS analysis.

The objective of our current study was to focus on the effects of sunlight, temperature, and time on stored PET bottled drinking water in Yola, Nigeria. The original aspects of this paper include (a) expanding this important water quality issue into Nigeria as not many studies have been conducted under harsh conditions, especially in Africa; (b) using the obtained data to further a better understanding of the quality of PET bottled water-related to human health with regards to organic contamination of drinking water. As in Yola northern Nigeria, the temperature is quite high; beverages are sometimes hawked under high sunlight intensity of 7.0 kWh/m^2 (25.2 MJ/m^2/day) (Sambo 2009), and beverage drink vendors sometimes display their products for buyers under the sun, the effects of these harsh storage conditions were assessed. The study also aimed at using its findings to draw conclusions on which common storage conditions most severely impact water quality, hence, underscoring the importance of proper storage practices.

2 MATERIALS AND METHODS

2.1 Samples and Materials

Six 750 ml PET-bottled water samples of a leading commercial brand were purchased in Yola, Nigeria. Three storage conditions were created: sunlight exposure (Group A), elevated temperature exposure (Group B), and a cool dry place as the negative control (Group C) – two samples for each condition. Group A was exposed between 10:00 am to 5:00 pm when the sunlight intensity was high. Similarly, Group B was stored in an incremental temperature of 35 to 65°C in order to mirror the natural outdoor temperature condition in Yola within the range of 38 to 42°C. All reagents used were analytical grade with high purity (>99%) and were purchased from Sigma Aldrich from New Jersey, USA. Our tests were done over 42 days (6 weeks) period with a 7 days interval starting from day zero of exposure.

2.2 Physicochemical Properties Analyses

2.2.1 Conductivity, TDS, pH, Cl^- and NO_3^-

Into three separate clean 100.0 mL beakers labeled A to C, 50.0 ml each of Group A, Group B, and Group C was poured respectively. Before testing the samples, the temperature of each sample was brought to 30°C, the average room temperature in the region, in order to achieve uniformity and remove temperature interferences. Following this, a computer, Vernier Computer Interface, and Logger Pro were used alongside various sensors for the physicochemical tests. The conductivity, TDS, pH, Cl^-, and NO_3^- probes were calibrated using standards. They include Vernier Chloride Ion-Selective Electrode (low standard (10 mg/L Cl^-) and high standard (1000 mg/L Cl^-), Vernier pH Sensor (pH 4 buffer solution and pH 9 buffer solution), Vernier Conductivity Meter (500 mg/L TDS standard solution and 50 mg/L TDS standard solution), Vernier Nitrate Ion-Selective Electrode (low standard (1 mg/L NO_3^-) and high standard (100 mg/L NO_3^-). Afterward, each property was analyzed by fully immersing each probe with the sample being gently swirled.

2.2.2 Chemical Oxygen Demand (COD)

The COD analysis was done to determine the amount of oxygen required to oxidize the organic materials in the samples. Four COD vials with lids were obtained. Into each vial, 2.5 mL of distilled water (serving as a blank), Group A, B, and C was added. After that, standard potassium dichromate (1.5 mL, 0.25N) and sulfuric acid (3.5 mL, conc.) were added to each vial and capped tightly; then placed in a COD digester (150°C, 2 hours). After the digestion reaction, ferrous ammonium sulfate (0.1N) was titrated against each of the vial contents. Two drops of ferroin indicator were used under gentle constant stirring, and at the endpoint, the color changed from bluish-green to reddish-brown. The titer values were documented. The COD of the samples were calculated in mg/L as according to equation (1) where A = the volume of ferrous ammonium sulfate for blank, B = the volume of ferrous ammonium sulfate for sample, N = Normality of ferrous ammonium sulfate:

$$\mathbf{COD(mg/L)}=\frac{(A - B) \times N \times 8 \times 1000}{\text{volume of sample taken (mL)}} \qquad (1)$$

2.3 Solvent Extraction

The liquid-liquid extraction technique was employed as the GC-MS system available only analyzes organic compounds. In the solvent extraction method for water organic matter analysis, organic materials present in the aqueous water sample layer are able to transfer into the organic solvent layer based on the solubility differences between the two immiscible layers (Reyes & Crisosto 2016). We used hexane as an organic solvent. Into three separatory funnels, 50.0 mL of each sample was poured. A 50.0 mL of hexane was divided into five portions (10.0 mL each). The first 10.0 mL was added to the funnel and stoppered, followed by a 15 seconds vigorous shake with venting to reduce gas build-up. The separatory funnels were then placed in their holders and allowed to separate into two distinct layers. Afterward, the valve was opened to remove the aqueous layer below the organic layer on top. The separated aqueous layer from the step above was placed back into the funnel and the separation procedures were repeated for the remaining four hexane sets (10.0 ml each).

2.4 GC-MS Analysis

GC-MS analysis was done to identify the organic materials that may have migrated from the PET bottle into the contained water. The hexane extracts (1 µL) of each sample was injected via the inlet of an Agilent GC-MS system (Agilent 7890A GC, 5975C MS) equipped with a capillary column (DB-35MS 30m × 0.25mm × 0.25µm). The instrument parameters included: the inlet temperature of 50°C with an increase in temperature by 10°C per minute to 200°C and a hold time of 1 minute. Injection mode was splitless, carrier gas flow was high purity helium, and a total run time of 34 minutes. The identity, structure, and molecular weight of the unknown samples were obtained from interpreting the mass spectra from the National Institute Standard and Technology database (NIST 2014 and NIST 2011).

3 RESULTS AND DISCUSSION

First, the potential migration of organic materials from polyethylene terephthalate bottles into water under elevated temperature, sunlight radiation, and incubation time was monitored. The tests were categorized into the physicochemical analyses including conductivity, total dissolved solids, pH, chlorides, nitrates, and COD, as well as GC-MS analysis supported by organic solvent extraction.

3.1 Physicochemical Properties Results

3.1.1 pH Results

The pH values measured on day zero before any exposure for all sample groups showed an average pH value of 8.03 (s = 0.03, n=3); a slightly alkaline pH although not reported on the product label by the manufacturer. Over the course of the exposure, the pH values for all samples averaged 7.56 (s = 0.44, n=21) (Fig. 1a). The sunlight exposed samples exhibited the largest decline in pH, whereas the pH of the negative control group fluctuated the least. This can be attributed to the migration of slightly acidic materials such as terephthalic acid monomer into the water with extended exposure to sunlight (Bach et al. 2012). Our pH values ranged from 8.07 to 6.60 and are comparable with the World Health Organization (WHO) and the International Bottled Water Association (IBWA) standards for quality of water which stand at 6.5 to 9.5 and 6.5 to 8.5, respectively.

3.1.2 Conductivity and Total Dissolved Solids

Conductivity (Fig. 1b) and total dissolved solids (Fig. 1c) increased over the study period. For the samples at elevated temperature, we observed a rapid change in conductivity and TDS values from 60 to 65°C (day 35 – 42), as the conductivity increased by 17% from 37.7 to 44.0 ìS/cm; whereas the control group stored in a cool dry place remained constant for the same period. The conductivity values for all samples ranged from 27.1 to 45.0 ìS/cm, while TDS was from 12.9 to 25 mg/L within the IBWA limit of 500 mg/L.

3.1.3 Chlorides and Nitrates

For the samples tested in this study, the chloride and nitrate values measured before exposure were negligible at 0.1 mg/L apiece. Upon exposure and the interval physicochemical tests performed after every 7 days, the recorded values of Cl^- and NO_3^- remained fairly constant throughout as shown in Fig. 1d. Chloride ions for all samples stayed at 0.1 mg/L while nitrate ions fluctuated between 0.1 mg/L and 0.2 mg/L, all below the international permissible limit of 250 mg/L for Cl^- and 44 to 50 mg/L for NO_3^-. These trace values are expected given that chlorides and nitrates are neither used in making PET bottles, thus, not expected to migrate out; nor are they used by the manufacturer for water treatment.

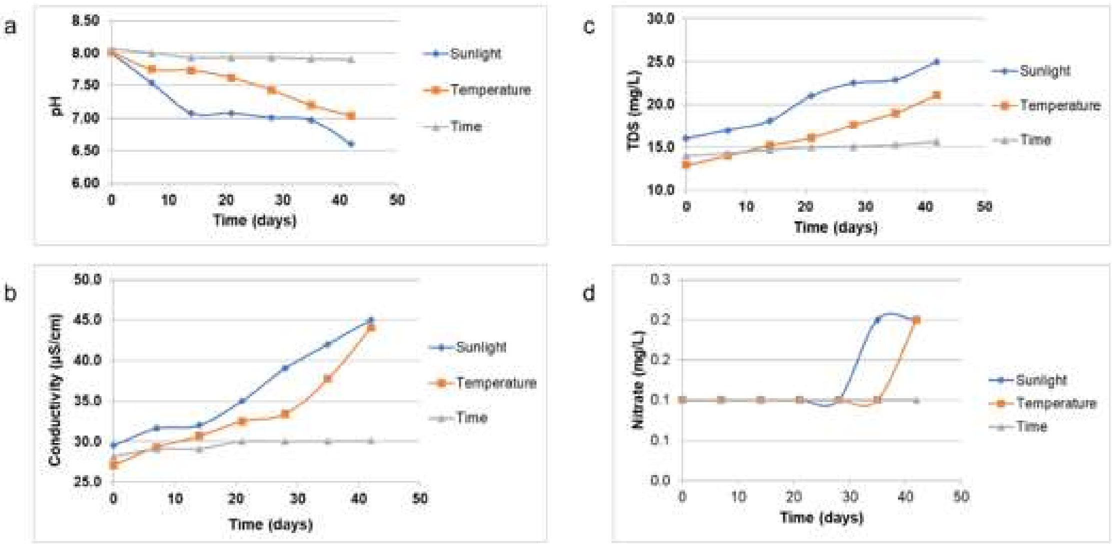

Fig. 1 Variation in the measured physicochemical properties of the three sample groups stored under sunlight, elevated temperature, and optimum conditions from 0 to 42 days of exposure. a – trends in pH values; **b** – variation of conductivity (ìS/cm); **c** – changes in total dissolved solids (mg/L); and **d** – trends in nitrate ions (mg/L)

3.1.4 Chemical Oxygen Demand

The recorded chemical oxygen demand values represent the amount of dissolved organic materials in the water samples stored under the different experimental conditions. Fig. 2 shows the variations in COD values for the samples in Groups A, B, and C during the 42 days exposure period. The most significant increase in COD value was observed for the sunlight exposed samples which more than doubled by the end of the exposure of the period from 3.01 to 8.03 mg/L. Muhammad et al. (Muhamad *et al.* 2011) who studied the effects of temperature and sunlight exposure on PET bottled water in a similar hot and sunny clime to northern Nigeria, Kurdistan in Iraq (Asia) with temperatures as high as 45 °C during summers (Rasul *et al.* 2015), reported a similar upward trend in COD values; albeit at a significantly lower rate of increase. They reported a 2.5% rise in the COD values of the sunlight exposed sample from 6.634 to 6.797 mg/L after 30 days of exposure; while that of high temperature exposed samples increased by 5.2% from 6.739 to 7.091 mg/L. In comparison to our results, however, we observed a doubling in our COD value for the sunlight exposed samples for the same period of time from 3.01 to 6.78 mg/L. The discrepancy in the rate of our COD value growth could be attributable to a combination of factors including the difference in sunlight intensities, differences in polymer packaging material, and elusive method errors. Nonetheless, the measured COD values for all samples did not exceed the international standard permissible limit of 225 mg/L and they ranged from 25.6 to 80.30 mg/L.

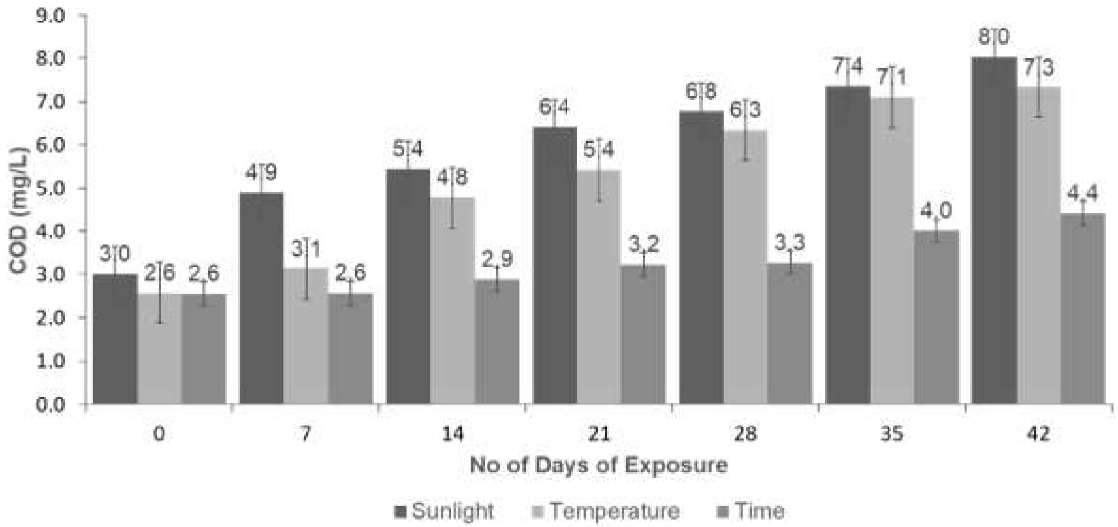

Fig. 2 Variation in chemical oxygen demand (mg/L) values for the three sample groups stored under sunlight, raised temperature, and optimal conditions from 0 to 42 days of exposure.

3.2 Effects of Migration/ Polymer Degradation Agents

3.2.1 Effect of Sunlight Radiation

Table 1 shows the results of the physicochemical properties of the Group A samples exposed to sunlight radiation and analyzed every 7 days for 6 weeks. Although UV light comprises only 5% of sunlight, UV light has been found to be the main agent of degradation for plastics stored outdoors under a process termed photodegradation caused by UV-rays in a wavelength range of 300 -330 nm (Liu et al. 2009; Curtzwiler et al. 2017). Our experiments show that conductivity, total dissolved solids, and chemical oxygen demand increased steadily over time. Comparing the pre-exposure values to the final values, it can be seen that conductivity, TDS, and COD increased by 52.5%, 56.3%, and 64.2% to 45.0 ìS/cm, 25.0 mg/L, and 8.03 mg/L, respectively. On the other hand, the pH of the water, which was initially slightly alkaline at 8.00, became slightly acidic at a pH of 6.60 by the end of the exposure period. Whereas the chloride and nitrate values remained mostly constant. Similarly, Muhamad et al. (Muhamad et al. 2011) reported an increase in conductivity, TDS, and COD from 342 to 360 ìS/cm, 171 to 180 mg/L, and 6.63 to 6.79 mg/L, respectively after exposing 17 brands of PET bottled water in the Kurdistan region of Iraq. Although there are no published studies on the effects of harsh storage conditions in other developing countries in Africa, we expect to see similar results for other countries with high sunlight intensities such as Djibouti, Burkina Faso, Mali, Senegal, Mauritius.

The reduction in pH may be due to oxidative and hydrolytic chemical degradation of PET polymer via chain scissions and cross-linking which yield acidic products that further catalyze the degradation process (Shultz & Leahy 1961; Sang et al. 2020). The scission reactions usually commence at the ester linkage – the weakest bond – which leads to the formation of radicals that terminate to produce small molecules like carbon monoxide, carbon dioxide, in addition to polymer chains that have end groups such as hydroxyl, carboxyl, ketones, and aldehyde groups (Abboudi & Odeh 2015). The organic compounds that are formed then dissolve in the water contents of the PET bottle.

Table 1 Effect of sunlight on the physicochemical properties of the stored water samples (Sample Group A)

No of days of Exposure	Conductivity (µS/cm)	TDS (mg/L)	pH	COD (mg/L)	Cl^- (mg/L)	NO_3^- (mg/L
0	29.50	16.00	8.00	3.01	0.10	0.10
7	31.60	17.00	7.54	4.89	0.10	0.10
14	32.00	18.10	7.08	5.44	0.10	0.10
21	35.00	21.00	7.08	6.41	0.10	0.10
28	39.00	22.50	7.01	6.78	0.10	0.10
35	42.00	22.90	6.97	7.36	0.10	0.20
42	45.00	25.00	6.60	8.03	0.10	0.20

3.2.2 Effect of Temperature

Elevated temperatures can lead to parts or whole of the polymer to melt, hence, inducing thermochemical reactions (Saha & Ghoshal 2005; Das & Tiwari 2019). Thermal decomposition of polyesters usually initiates by a random scission of an in-chain ester bond which gives rise to carboxyl and vinyl ester end groups. Then, via transesterification, the vinyl ester is converted to vinyl alcohol which is converted with acetaldehyde as the major by-product (Özlem 2008). Acetaldehyde formation can be explained using the McLafferty rearrangement mechanism which involves a six-membered transition state occurring through a hydrogen shift in the methylene group located at a â-position to the carbonyl group (McIntyre 2004).

During the 42 days of the study, several tests were conducted to monitor the changes in the physicochemical properties of the PET bottle water contents. A similar trend for conductivity, TDS, chlorides, nitrates, and COD was observed for the elevated temperature exposed samples as was seen in the sunlight exposed group presented in Table 2. Conductivity and TDS increased by

62.4% and 62.8% to 44.0 ìS/cm and 21.1 mg/L, respectively. The pH also trended downwards from 8.01 to 7.04, maintaining neutrality.

Table 2 Effect of temperature on the physicochemical properties of the stored water sample (Sample Group B)

Temperature (°C)	Conductivity (µS/cm)	TDS (mg/L)	pH	COD (mg/L)	Cl^- (mg/L)	NO_3^- (mg/L)
35.0	27.10	12.90	8.01	2.58	0.10	0.10
40.0	29.30	14.00	7.75	3.13	0.10	0.10
45.0	30.70	15.20	7.73	4.78	0.10	0.10
50.0	32.50	16.10	7.62	5.42	0.10	0.10
55.0	33.40	17.60	7.43	6.34	0.10	0.10
60.0	37.70	19.00	7.20	7.10	0.10	0.10
65.0	44.00	21.10	7.04	7.33	0.10	0.20

3.2.3 Effect of Time

Unlike the pronounced changes in the values of the measured physicochemical properties of the water stored under sunlight and raised temperature conditions over the 42 days period of the study, the control sample group stored under 25°C to 30°C in a cool dry place did not exhibit dramatic changes in the values of the measured properties (Table 3). Conductivity and TDS marginally increased by 10.0% and 12.1% from 28.1 to 30.9 ìS/cm and 14.0 to 15.7 mg/L, respectively. Likewise, COD values rose from 25.6 mg/L to 44.2 mg/L between days 7 and 42 of storage. The final COD value of the sunlight exposed sample (80.3 mg/L) and high temperature exposed sample (73.3 mg/L) are almost double that of the control group (44.2 mg/L). Nawrocki et al. (Nawrocki et al. 2002) reported that time is also a dominant factor influencing the leaching of substances. Irrespective of optimum storage conditions, prolonged storage durations can induce migration from the inner surface of the bottle in direct contact with the water.

Table 3 Effect of time on sample stored in appropriate conditions as control (Sample Group C). The storage temperature between 25°C – 30°C as obtainable within the region.

No of days of Exposure	Conductivity (µS/cm)	TDS (mg/L)	pH	COD (mg/L)	Cl^- (mg/L)	NO_3^- (mg/L)
0	28.10	14.00	8.07	2.56	0.10	0.10
7	29.01	14.30	8.00	2.57	0.10	0.10
14	29.05	14.70	7.93	2.88	0.10	0.10
21	30.03	15.00	7.93	3.23	0.10	0.10
28	30.03	15.10	7.93	3.27	0.10	0.10
35	30.07	15.30	7.91	4.01	0.10	0.10
42	30.09	15.70	7.90	4.42	0.10	0.10

3.3 Comparison with International Standards

Furthermore, the results of the physiochemical properties tests were compared with those of internationally recognized standards (Table 4). Our lowest and highest values for each property from all storage conditions were weighed against the WHO and IBWA guidelines for bottled water quality safe for human drinking. The values gotten, nevertheless, were within the WHO and IBWA international guidelines.

Table 4 Comparison between physicochemical properties measured in this work and WHO and IBWA regulations and standards for water intended for human consumption.

Property	Unit	Results Recorded	WHO (2008)	IBWA (2009)
pH	N/A	6.60 – 8.07	6.50 – 9.50	6.50 – 8.50
COD	mg/L	25.60 – 80.30	-	225.00
TDS	mg/L	12.90 – 25.00	1,000.00	500.00
Cl^-	mg/L	0.10	5.00^f	0.10
NO_3^-	mg/L	0.10 – 0.20	50.00	10.00

^{f} = provisional guideline value

3.4 GC-MS Results

GC-MS analysis of the bottled water contents was performed to identify different unknown organic substances that have possibly migrated from the bottle into the contained water. This was following the solvent extraction technique using hexane to extract non-polar organic molecules from its homogeneous mixture with polar water molecules. An initial GC-MS analysis of the three sample groups was carried out on day zero prior to storage in order to compare them with the results to be obtained after storing in different conditions. Fig. 3a shows the total ion chromatogram of the initial run with only one major peak at about 1.7 – 2.2 mins retention time (RT) and as was expected. While Fig. 3b shows the mass spectrum at RT of 2.15 min, corresponding to the mass spectrum of hexane (Fig. 3c) used as the solvent.

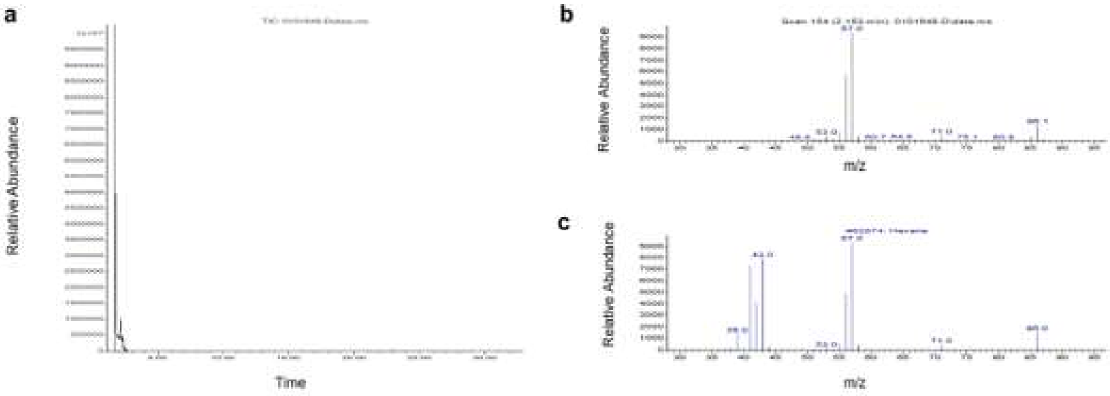

Fig. 3 GC-MS analysis of the solvent extracts of the three sample groups prior to storage. a - Total ion chromatogram of the solvent extract; **b** - m/z analysis of an unknown molecule at RT 2.153 mins showing m/z = 57 (base peak) and m/z = 86.1 (M^+); **c** - NIST database search showing hexane with m/z = 57 (base peak) and m/z = 86 (M^+)

After four weeks of exposure, another GC-MS analysis was performed on the three sample groups. Figure 4 shows the total ion chromatogram (Fig. 4a) and mass spectra (Fig. 4b) of the sunlight exposed samples monitoring organic compounds that may have migrated from the PET bottle into the contained water as a result of ultraviolet radiation. In addition to the hexane solvent peak, three additional peaks were observed at 9.339 mins, 22.373 mins, and at 22.864 mins. The unknown compound at RT of 9.353 mins (Fig. 4b) with base peak is 68.9m/z and the molecular ion (M^+) peak of 78.8m/z was inferred to be benzene with a molecular weight of 78.11gmol^{-1}. Benzene is a by-product of the ester bond-cleavage in polyethylene terephthalate which can be induced by UV radiation (Wang et al. 2019), thus, making benzene a plausible organic contaminant when PET packages are exposed to harsh sunlight conditions. In the same vein, additional peaks to the hexane peak were observed for the elevated temperature exposed samples at an RT of 26 mins (Fig. 5a). Finally, the control sample group was analyzed to depict the effect of time as a degradation factor in polyesters. The results (Fig. 5b) showed only the hexane solvent peak at RT 2.147 mins without other peaks. However, this was surprising as we had expected to see additional peaks to account for the organic materials which led to the increase in the chemical oxygen demand of the control group.

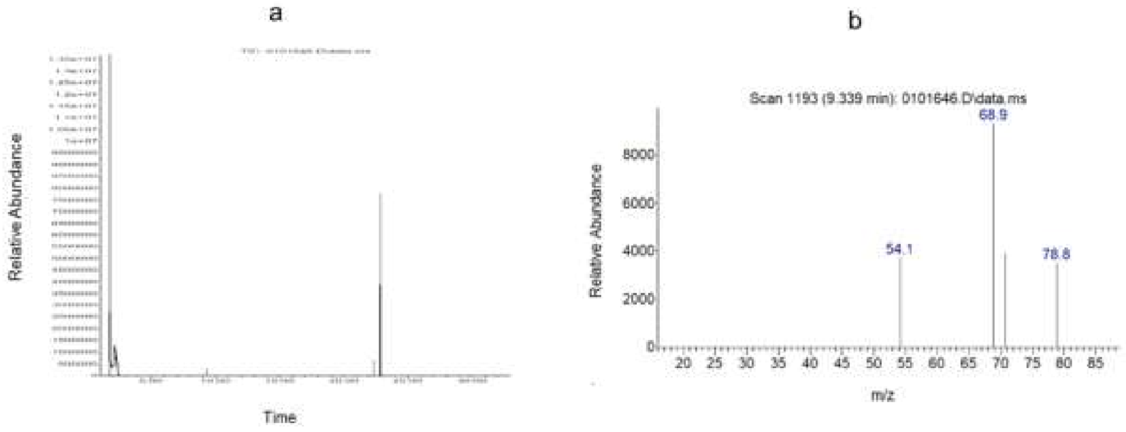

Fig. 4 GC-MS analysis of the solvent extracts of the sunlight exposed sample group after 4 weeks of exposure. a - Total ion chromatogram of the solvent extract showing additional peaks to the hexane solvent peak at 9.339 mins, 22.373 mins, and at 22.864 mins; **b** - m/z analysis of an unknown molecule at RT 9.339 mins showing m/z = 68.9 (base peak) and m/z = 78.8 (M^+) inferred to correspond to benzene (M^+ = 78.1)

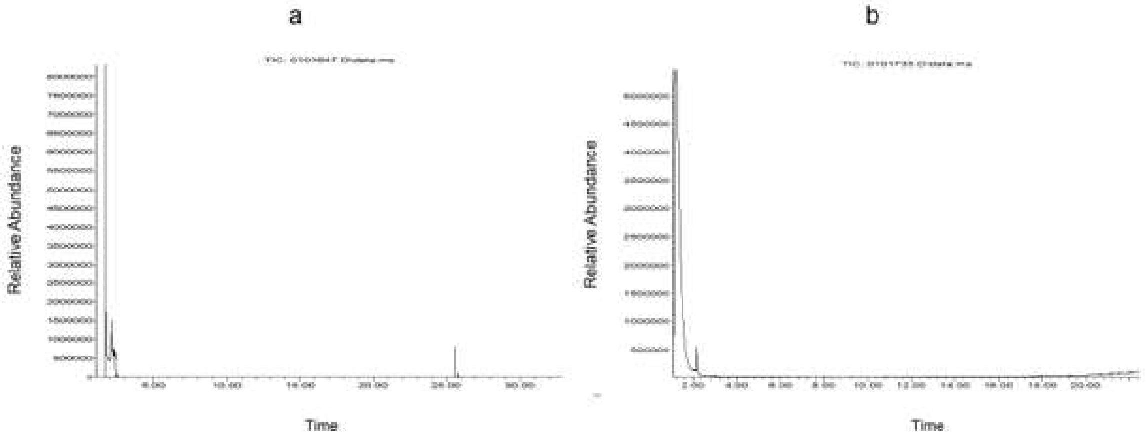

Fig. 5 GC-MS analysis of the solvent extracts of the higher temperature exposed and optimally stored sample group after 4 weeks of exposure. a - Total ion chromatogram of the solvent extract of the elevated temperature exposed sample showing additional peaks to the hexane solvent peak at 26 mins; **b** - Total ion chromatogram of the solvent extract of the optimally stored sample showing only the hexane solvent peak at 2.1 mins

4 CONCLUSIONS

The effects of environmental factors including sunlight radiation, temperature, and time on the water in PET has been determined. The periodic TDS, conductivity, COD, pH, Cl^-, NO_3^- and GC-MS analysis over a 42 days period revealed the migration activities in the samples. The results concluded that exposure to higher temperatures and sunlight radiation had marked impacts on the migration of organic materials from the bottle into the water in the PET bottle. Also, although studies have reported that increasing storage time can potentially lead to the migration of contaminants into the contained food, this finding supports that time only becomes a migration agent after an extended period of time. In spite of the changes to the physicochemical properties brought about by the harsh storage conditions, these properties for this particular commercial used in this study were still within the regulations and standards for water intended for human consumptions as directed by a combination of European Economic Community (EEC), World Health Organization (WHO), US Environmental Protection Agency (EPA), International Bottled Water Association (IBWA), and the US Food and Drug Administration (FDA). However, consumption of such waters containing these leachates, on a very long-term basis, can lead to potential disease initiation, especially genetic disorders. As supported by these results, it is strongly recommended that all polymer packaged beverages be stored in a cool dry place not more than 30 °C to reduce any potential contaminations.

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DECLARATION OF INTEREST STATEMENT

Conflict of interest: The authors declare that they have no conflict of interest to disclose.

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