U.P.B. Sci. Bull., Series B, Vol. 87, Iss. 4, 2025 ISSN 1454-2331

PRELIMINARY STUDY OF THE BEHAVIOR OF PACKAGING IN CONTACT WITH VARIOUS AQUEOUS ENVIRONMENTS

Georgeta TEODORESCU (DIACONESCU)[1], Alexa-Maria CROITORU[2,3], Dobrita ALEXANDRA[4], Florentina Laura CHIRIAC[5], Claudia BUTEAN[6], Florina IONITĂ[1], Daniela Simina STEFAN[7]*

Plastic packaging is widely used for the marketing of beverages and food. For a long time, they were considered chemically inert, meaning they do not interact with the substances stored in them. This myth was dispelled with the technological evolution of analytical measurement methods when concentrations of micro and nanograms per liter of various toxic compounds began to be identified. Thus, it was revealed that components of the packaging migrate from the packaging into beverages and food. Thus, it was revealed that BPA, used as an additive in polymers, is found in water and food in concentrations of nanograms per liter. It was also identified that [8]BPA is an endocrine disruptor that seriously affects the health of consumers of products packaged in plastic. In the present study, we wanted to highlight the concentrations of BPA that migrate from polystyrene, PS, and polyethylene terephthalate, PET, plastic packaging into aqueous solutions at two exposure temperatures of 20 and 30 ºC, at a pH variation in the range of 1.5-9 and a contact time of maximum 50 days. We also studied the changes that appear in the IR spectra of the packaging following the contact of PS and PET packaging with aqueous media under the conditions mentioned above. It was found that all these parameters influence the release of BPA, the extremes of basic and acidic pH favor the release of BPA, both for PS and PET and generate structural changes, especially the PS polymer matrix.

---

[1] Doctoral School, Specialization of Environmental Engineering, Faculty of Chemical Engineering and Biotechnologies, National University of Science and Technology POLITEHNICA Bucharest, Romania, diaconescu_gina@yahoo.com

[2] Faculty of Chemical Engineering and Biotechnologies, Department of Science and Engineering of Oxide Materials and Nanomaterials, National University of Science and Technology POLITEHNICA of Bucharest, Romania; e-mail: alexa_maria.croitoru@upb.ro

[3] National Centre for Micro- and Nanomaterials, National University of Science and Technology POLITEHNICA, No 313, Spl. Independentei, 060042, Bucharest, Romania

[4] A.L.S. Life Sciences Romania, Ploiesti, Romania, e-mail: aalexandradorita@gmail.com

[5] National Institute for Research and Development for Industrial Ecology—INCD ECOIND, Bucharest, Romania; laura.badea88@yahoo.com

[6] Department of Chemistry and Biology North University Centre of Baia Mare, Technical University of Cluj Napoca, 430122 Baia Mare, Romania, e-mail: Claudia.BUTEAN@cb.utcluj.ro

[7]* Faculty of Chemical Engineering and Biotechnology, National University of Science and Technology POLITEHNICA Bucharest, Romania, *Corresponding author, e-mail: daniela.stefan@upb.ro

Keywords: packaging, polystyrene, polyethylene terephthalate, bisphenol A release, IR spectrum

1. Introduction

Global plastics production reached 390.7 million tonnes in 2021, according to Plastics Europe, with around 40% of this used in packaging. Plastic packaging contains various polymers to which numerous additives, colourants, solvents and other components are added [1]. Additives in plastic packaging play a critical role in protecting products, extending the shelf life of the packaging, and improving processing and aesthetics. They contribute to food safety, UV resistance, flexibility, and recyclability [2]. The studies showed it was revealed that components of the packaging migrate from the packaging into beverages and food [3]. Bisphenol A (BPA) is a chemical compound primarily used in the manufacture of polycarbonate and epoxy resins, which is used to impart durability, transparency, and heat resistance to plastics. It is commonly used in food packaging, reusable bottles, epoxy-coated metal cans, medical equipment, water bottles, baby bottles (formerly), bottle caps, and bottle tops [4].

Bisphenol A migrates from packaging under various conditions and can contaminate food, beverages, fruits and vegetables with which it comes into contact. The European Union first regulated its use through Directive (EEC) No. 90/128, which imposed a specific migration limit for BPA of 3 mg/kg. The Directive 2002/72/EC on plastic materials and articles intended to come into contact with foodstuffs reduced the limit to 0.6 mg/kg. In addition the Regulation (EU) No. 213/2018 on the use of BPA in materials for the inner lining of containers intended to come into contact with foodstuffs imposed the limit to 0.05 mg/kg [5, 6].

Bisphenol is a toxic compound that interferes with hormonal secretions, the secretion of sex hormones, causing disruption of reproductive function, which can lead to prostate cancer, breast cancer, metabolic problems manifested by obesity, diabetes, cardiovascular problems, the release of high concentrations in urine, etc. [7-10].

Studies in the literature have shown that BPA is rapidly absorbed in mammals (including humans), and it is converted into BPA glucuronide and BPA sulfate in the digestive tract and kidneys. Based on assessments by the European Food Safety Authority (EFSA), the maximum daily exposure limit for BPA from food is 4 μg per kg body weight per day (μg/kg body weight/day) [11].

Analyzes of various canned foods have shown that BPA concentrations can reach: in meat and meat products - in the range 20 - 400 μg/kg [12], in fish - between 1 - 550 μg/kg, in fruits - between 0.3 - 2, vegetable like sweet corn - in the range 0.01 - 145 μg/kg, and in peas - in the range 2 - 303 μg/kg, [5], in bottled drinking water - BPA concentrations are ranging from 8.5 - 90 ng/L, depending on the type of packaging [13].

The release of toxic compounds such as BPA, benzyl butyl phthalate (BBP), di-n butyl phthalate (DBP), and di (2-ethylhexyl) phthalate (DEHP) was identified after contact of the packaging with water. It was identified that the concentrations of BPA, BBP, DBP and DEHP were of 5.7, 12.11, 82.8 and 64.0 μg/L respectively, the highest concentration being that of DBP, with a share of 23.7% of the Tolerable Daily Intake (TDI) [14]. Adriana C. Mârşolea and collaborators identified that the migration of BPA from polyethylene terephthalate, PET, packaging, is influenced by the environmental temperature and the contact time. The concentrations of BPA released ranged between 0.1 and 58 ng/L, depending on the working conditions. [15]. The content and release of BPA from polystyrene into food and aqueous media can reach very high concentrations depending on the country of origin of the raw material [16]. The release of BPA from PS is temperature dependent, directly proportionally with temperature, and ranging from 0.13 to 1,000 μg/kg for a temperature range of 40 to 100 ºC [17].

By contact with water, the packaging polymers suffer not only the release of additives from the composition, but also structural changes. These have been highlighted by changes in the IR spectrum of the plastic, for example oxidative degradation generates bands attributed to OH and C=O stretching vibrations [18, 19].

The study aimed to identify the behavior of polystyrene (PS) and polyethylene terephthalate (PET) packaging in contact with various aqueous media, at various pHs and temperatures over a period of 50 days of contact. In this regard, the release of bisphenol A (BPA) and the structural changes in the IR spectra were analyzed.

2. Materials and Methods

2.1 Identification of structural changes

To carry out the experiments, polystyrene (PS) and polyethylene terephthalate (PET) packaging with mass 0.15 g and 0.25 g respectively, was used, which were introduced into 50 ml of aqueous medium. The pH of aqueous solutions was in the range of 1.5 – 9, namely (1.5±0.1; 3±0.1; 5±0.1; 7±0.1 and 9±0.1). The pH of the solutions was maintained constant by using buffer solutions at different pHs. We worked at two temperatures of 20 °C and 30 °C. The packaging materials used from PS and PET were cut into various geometric shapes (circle, rectangle, rhombus, triangle, square, trapezoid), with relatively equal surfaces. Each geometric shape was assigned a sampling time, namely: the 6th, 10th, 21st, 36th, 44th and 50th day, respectively. Samples were taken from the system, washed with distilled water and dried. The IR spectra of the samples were analyzed and compared with the IR spectra of the control samples. The chemical properties of the scaffolds were examined under Fourier transform infrared spectroscopy (FT-IR) using a Nicolet iS50FT-IR (Nicolet, Massachusetts, USA) spectrometer equipped with a DTGS detector which provides information with a high sensitivity in the range of 4000 cm^{-1} and 100 cm^{-1} at a resolution of 4 cm^{-1}. The samples were shaken using an ES20 orbital shaker, 18 positions for the temperature of 20 °C and an ES20 orbital shaker, 18 positions for those at 30 °C at a frequency of 3500 rpm.

2.2 BFA release study

The study of BPA release from PS and PET packaging was carried out, at pHs of 1.5±0.1; 3±0.1; 5±0.1; 7±0.1 and 9±0.1 and at the two temperatures of 20 °C and 30 °C. Systems of 6 identical samples were made for each pH (48 ml distilled water and 2 ml buffer solution, with the same type and quantities of packaging, 0.15 g for PS and 0.25 g for PET, at the same temperature). We mention that the mass of a PS and PET package was 27 and 45 g, respectively, for a volume of 1 l of water.

The samples were contacted for different times (0, 6, 10, 21, 36, 44 and 50 days), and the BPA concentration was determined from them. Triplicates of the systems were used, the results presented being the arithmetic mean of the measured results. The BPA concentration was determined by the GC-MS method (Gas Chromatography and Mass Spectrometry). An Agilent 1260 series liquid chromatograph system (Agilent, Waldbronn, Germany), coupled with an Agilent 6410B triple–quadrupole mass spectrometer, MS, with an electrospray ionization source (ESI) was used.

The samples were shaken using an orbital shaker ES20, 16 positions for 20 °C, and an orbital shaker ES20, 18 positions for 30 °C, at a frequency of 3500 rpm. Buffer solutions were prepared from different ratios of 0.1 N hydrochloric acid - 0.1 N glycol for pH 1.5 and 3, and from different ratios of 1/15 M potassium dihydrogen phosphate, 1/15 M sodium monohydrogen phosphate, for pH 5 to 9. The substances used are analytical reagents produced by Fluka, Switzerland.

3. Results and Discussion

The analyses carried out highlighted the evolution of the IR spectra of PS and PET type packaging over a period of 50 days. The evolution of the BPA concentrations released from the packaging over the same period of time was also identified.

3.1. IR spectra of contacted with aqueous solutions at different pHs

3.1.1. IR spectra of PS

Figs. 1 and 2 present the characteristic IR spectra of polystyrene, PS, after 50 hours, at temperatures of 20 °C and 30 °C, respectively. From the analysis of the spectra, it can be observed that the signals at 1601 and 1492 cm^{-1} indicate the presence of the C=C stretching vibration of the benzene rings, the peaks at 906 cm^{-1}, and the peaks at 754 and 695 cm^{-1} being characteristic of the C-H bending vibration of the substituted benzene ring. The peaks at 2921 and 3025 cm^{-1} are assigned to aromatic and aliphatic C-H stretching, respectively. The peaks at 538 cm^{-1} are specific to substituted C-H bonds.

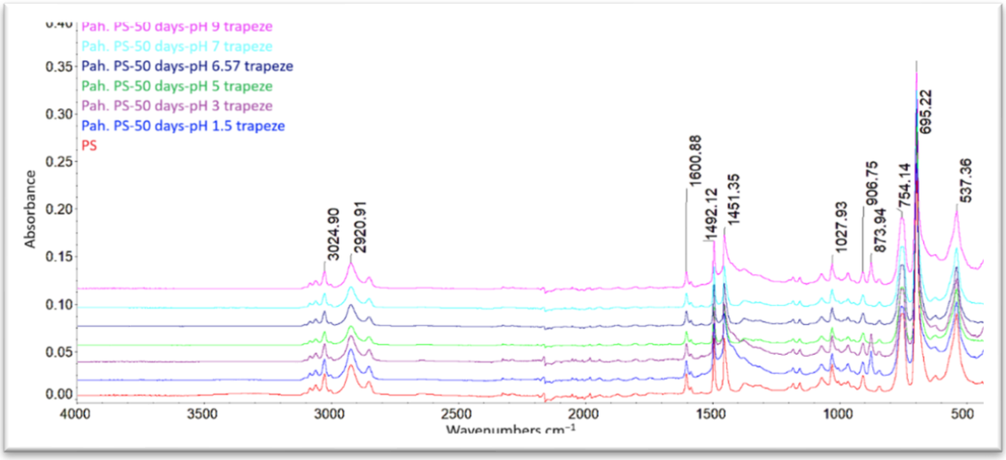


Fig. 1. IR spectra of PS at various pHs after 50 days of contact at T=20 °C

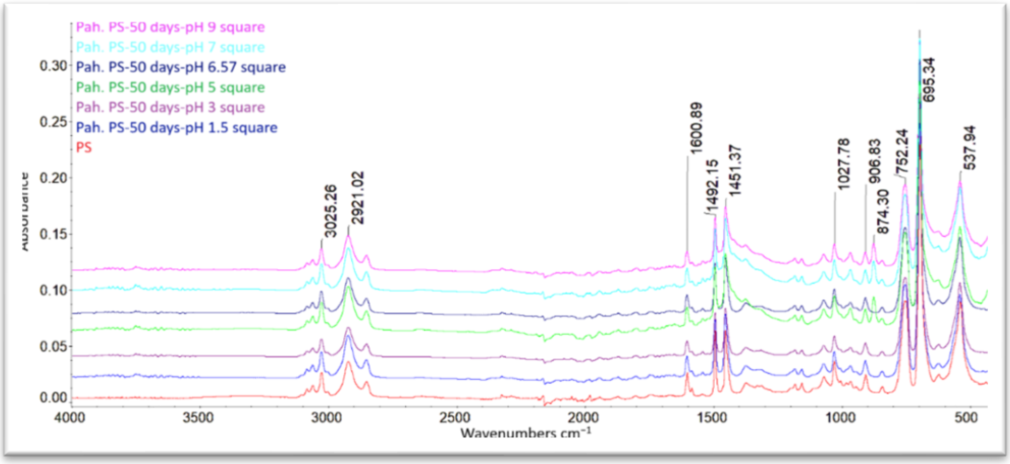


Fig. 2. IR spectra of PS at various pHs after 50 days of contact at T=30 °C

After treating PS samples with different aqueous solutions with different pH, significant changes can be observed. An increase in the relative intensity and a visible broadening of the bands: of around 1200 - 1650 cm^{-1} was found in PS samples at pH 1.5, 3 and 9. This proves that, important structural changes occur in the polymer matrix of polystyrene after 50 days, by rearrangements of atoms in the polymer chains, but also by the introduction of hydroxyl groups manifested by changes in the band at 1640 cm^{-1} [20, 21]. In order to better highlight when these changes in the structure occur, IR curves were plotted for 6 times intervals, namely: 6, 10, 21, 36, 44 and 50 days. Figs. 3 and 4 show the IR spectra for PS at pH=9, at different time intervals during the 50 days.

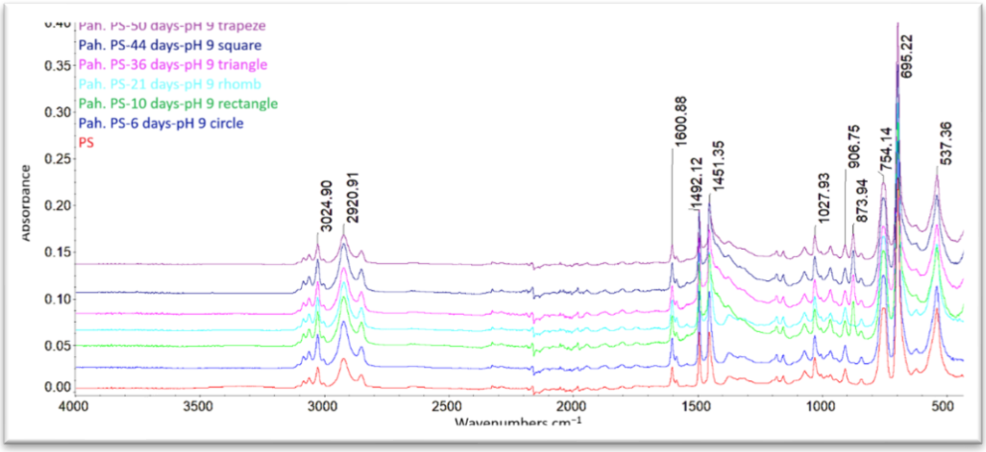
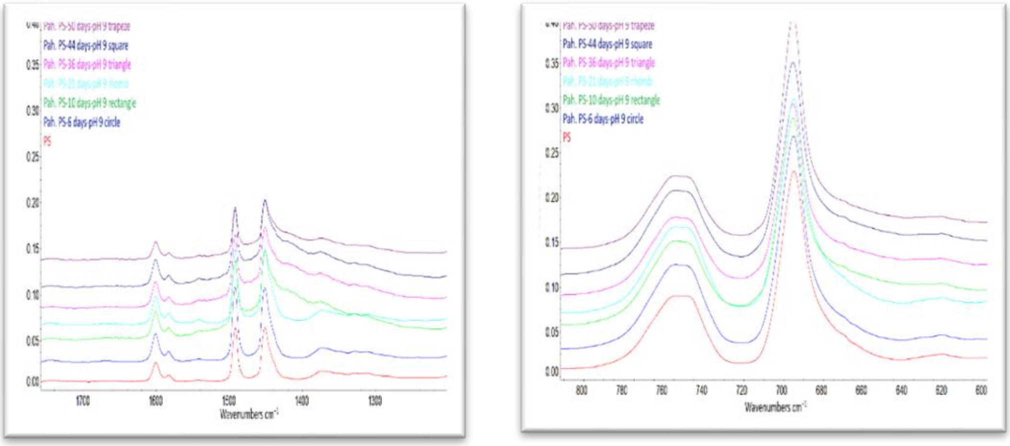


Fig. 3. IR spectra for PS at pH=9 at different time intervals during the 50 days at T=20 °C



.

Fig. 4. Details of IR spectra for PS at pH=9, at the Absorbance peaks at different time intervals over the 50 days at T=20 °C.

It can be seen that the above-mentioned changes appear in the IR spectra of PS at pH=9, after 10 days of contact. These changes become more pronounced as time passes. From the analysis of the details of the IR spectra in Fig. 3, for the 400 - 800 cm^{-1} range, it can be seen that, at the wavelengths of 754 cm^{-1} and 695 cm^{-1}

specific to the bending vibration of the C-H bond in the aromatic nuclei, an increase in amplitude occurs at 754 cm^{-1}, and a flattening at 695 cm^{-1}, which proves that substitutions occur at the level of the aromatic nucleus. The changes are much more evident after 21 days of contact. Another important change is at 538 cm^{-1}, when a rise in the vertical position and an amplification of the height occur. This change is determined by the substitutions that occur at the C-H groups. These changes prove that the polymer undergoes structural changes, with additions and substitutions.

3.1.2. IR spectra of PET

The FT-IR spectra of PET samples are shown in Figure 5. The characteristic bands of the C-O bond of the ester group are highlighted at 1237 cm^{-1} and 1090 cm^{-1}, respectively.

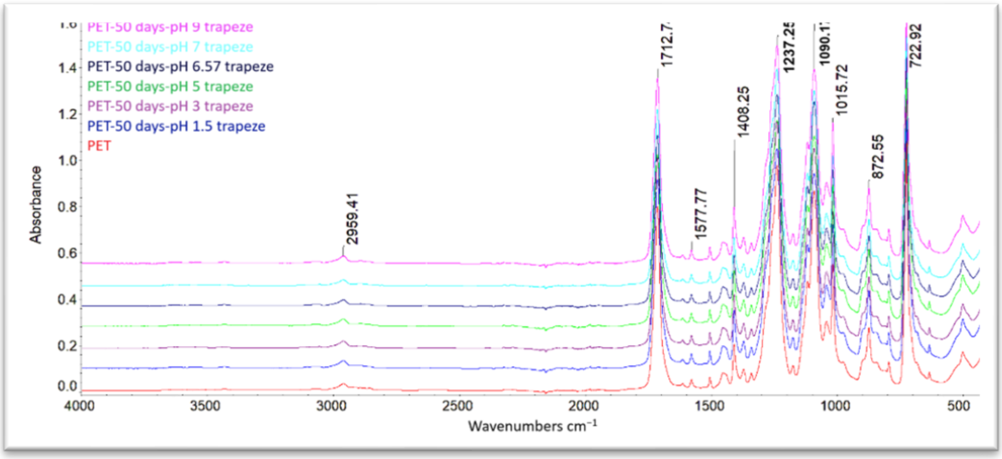


Fig. 5. IR spectra of PET at various pHs after 50 days of contact at T=20 °C

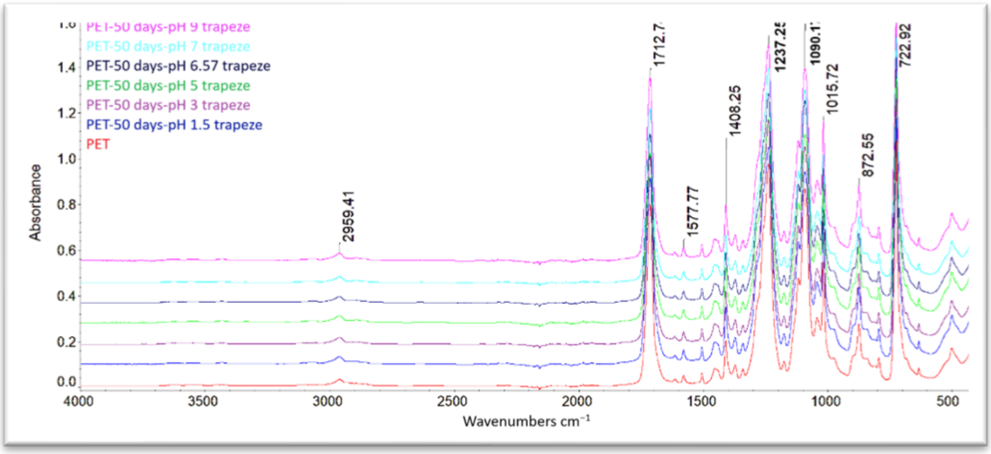


Fig. 6. IR spectra of PET at various pHs after 50 days of contact at T=30 °C

Also, in the fingerprint region (between 500 and 1500 cm^{-1}), a series of absorption bands are highlighted, such as the C-H band of the aromatic ring at 722 cm^{-1}, the CH_2 rocking at 872 cm^{-1} and the O-CH_2 stretching vibration at 1041 cm^{-1}. The strong peak at 1712 cm^{-1} is attributed to the stretching of the C=O bond of the ester group. The stretching vibration of the aromatic ring occurs at 3431 cm^{-1}, and the peak at 2958 cm^{-1} is attributed to the average C-H stretching bond [22].

After contacting the PET samples with aqueous solutions of different pH, no significant differences can be observed between the FT-IR spectra of the samples. However, a slight increase in the intensity of the peaks can be observed, which occurs with the increase in pH value. This proves that after 50 days no significant structural changes occur in the polymer matrix.

3.1.3. Study of BPA released in liquid samples

Fig. 7 shows the variations in BPA concentrations in the aqueous solution after 50 days of contact for the two types of materials, PS and PET, at the working pHs and temperatures mentioned above.

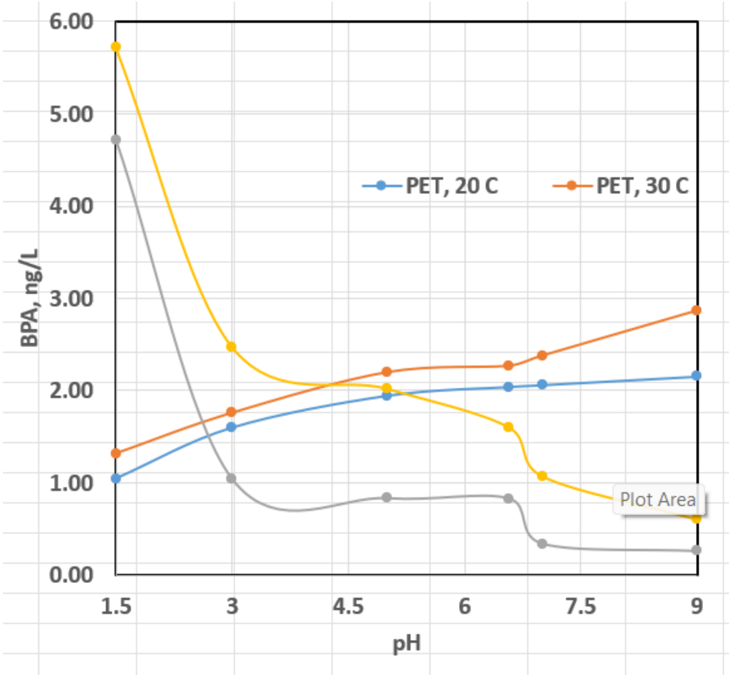


Fig. 9. Variation of BPA concentration released from PET and PS plastic packaging as a function of pH at 20 °C and 30 °C, after 50 days.

At a temperature of 20 °C, it can be observed that, in an acidic medium pH=1.5, PS releases the maximum amount of BPA the solution concentration being 4.72 ng/L, after which its concentration drops suddenly, so that, at a pH=3, it reaches 1.04 ng/L and then, up to a pH lower than 7, it is relatively constant, having the value 0.83 ng/L. At a pH higher than 7, the BPA concentration drops suddenly in the liquid medium, tending to zero. At a temperature of 30 °C, it can be observed that, in an acidic medium at a pH=1.5, PS releases the maximum amount of BPA, the solution concentration being 5.72 ng/L, after which its concentration drops suddenly, so that, at a pH=3, it reaches 2.47 ng/L, and shows a constant decrease in the BPA concentration, its value at a pH higher than 8 being 0.60 ng/L. PET has a completely different behavior from PS. At 20 °C, the maximum amount of BPA is released at a basic pH, this is 2.15 ng/L. At an acidic pH of 1.5, it is 1.04 ng/L, and slowly increases to values of 1.60 ng/L for pH=3, and around 2 ng/L for pHs higher than 3 and lower than 8. At 30 °C, the maximum amount of BPA is released at a basic pH, this is 2.87 ng/L. At an acidic pH of 1.5, it is 1.32 ng/L, and slowly increases to values of 1.76 ng/L for pH=3, and around 2.20 - 2.40 ng/L for pHs higher than 3 and lower than 8. The amounts of BPA released from PS and PET packaging are in large quantities, and pH is a very important factor in the economics of the process.

Figures 10 and 11 show the variations in BPA concentrations over time, for each type of material, PS and PET respectively, at each pH, at a temperature of 20 °C. From Figure 10, it can be seen that the release of BPA from PS at pH=1.5, very acidic, is slow in the first 20 days, after which the release is very rapid, the concentration increasing from 0.43 ng/L to 4.72 ng/L in the next 30 days. This demonstrates what was expected, that a stationary acidic environment in a polystyrene container causes a very high release of BPA.

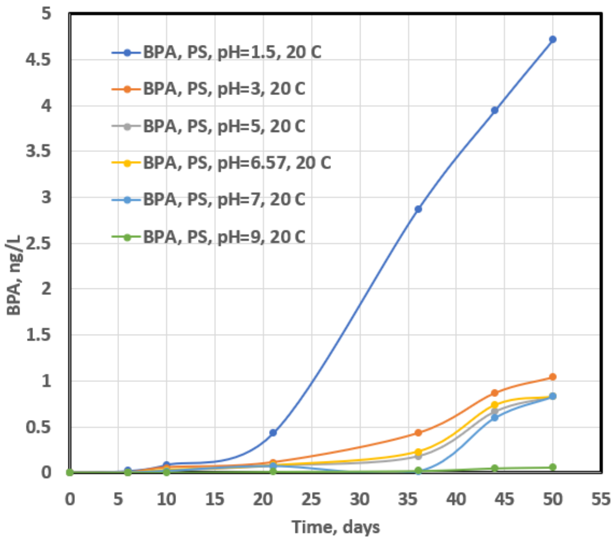


Fig.10. Variation of BPA concentration released from PS, over time, at different pHs, at T=20 °C.

At less acidic pHs, from pH=3 to basic pH, the release is much reduced, reaching 0.11 ng/L after 21 days at pH=3, 0.43 ng/L after 36 days, and only 1.04 ng/L after 50 days. The concentrations of BPA released gradually decrease with increasing pH, so that, at pH 6.57 specific to distilled water, the release in the first 21 days is only 0.08 ng/L, reaching 0.83 ng/L after 50 days.

At a pH of 9, the amount released tends to zero in the first 21 days, increasing to a maximum of 0.26 ng/L after 50 days.

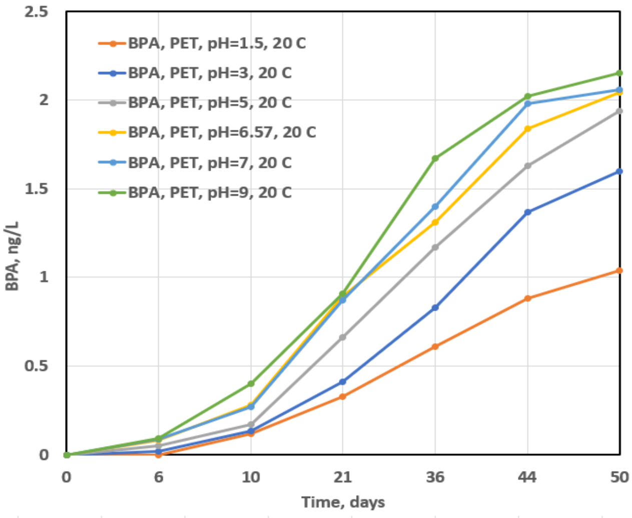


Fig. 11. Variation of BPA concentration released from PET, over time, at different pHs, at T=20 °C.

From the analysis of Figure 11, it can be seen that the release of BPA from PET is very slow in the first 21 days of contact, and increasing with increasing pH. After 21 days, it increases more and more with pH increasing, reaching a level where, at neutral pH, it doubles or even triples within 30 days. So BPA is released from PET over the entire pH range in significant quantities, this quantity increasing over time proportionally to pH.

Figures 12 and 13 show the variations in BPA concentrations released from PS and PET packaging, respectively, over a 50-day contact period at 30 ºC. It can be seen that for both packaging, BPA release increases with increasing contact time and temperature. Increasing pH has a negative effect on BPA release from PS and a positive effect on BPA release from PET. After 50 days of contact of PS packaging with aqueous solutions with different pHs, BPA release is maximum at pH = 1.5 and reaches 5.72 ng/L at 30 ºC, 1 ng/L more than at 20 ºC. At higher pHs, the release of BPA does not exceed 1 ng/L as seen in Figure 12.

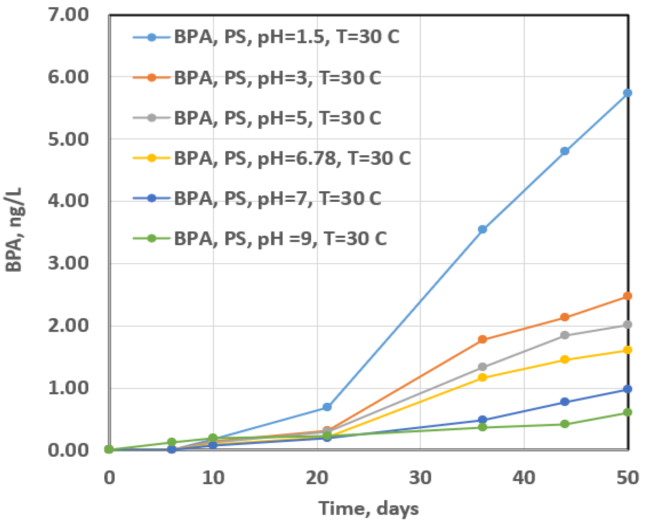


Fig. 12. Variation of BPA concentration released from PS, over time, at different pHs, at T=30 °C

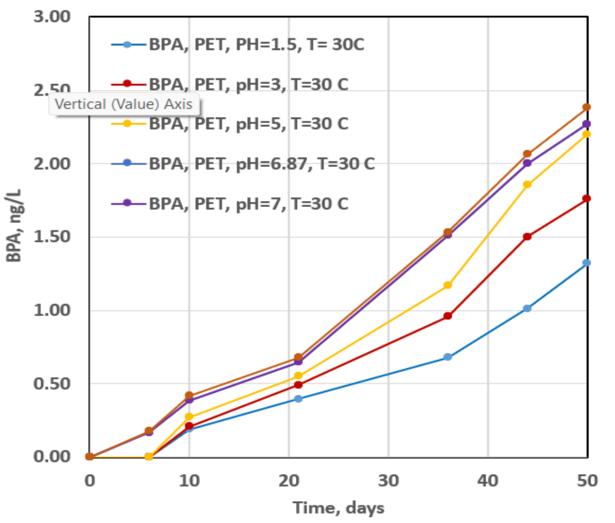


Fig. 13. Variation of BPA concentration released from PET, over time, at different pHs, at T=30 °C

A significant release is identified after 21 days when the BPA concentration increases from 0.8 ng/L to 5.72 ng/L at 50 days, this type of behavior was also identified at 20 ºC. The release of BPA from PET packaging increases constantly over time, reaching values of 2.87 ng/L at a pH of 9. The BPA concentration values after 50 days of contact, at 30 ºC for the studied pH range of 1.5 - 9, are between 1.32 and 2.87 ng/L, higher than at 20 ºC with values ranging between 0.6 and 2.2 ng/L as shown in the comparative analysis of Figures 11 and 13.

4. Conclusions

The analyses showed that it was found that polymers have been recently declared to be chemically inert, release additives used as plasticizers into the environment, but also undergo structural changes.

Following the analyses carried out, it was found that, in contact with water at different pHs, polystyrene, PS, releases both BPA-type compounds used as additives to increase its plasticity. The maximum concentration is obtained at pH=1.5 when 4.72 ng/L and 5.72 ng/L of BPA appear in the liquid medium after 50 days of contact, at temperatures of 20°C and 30°C, respectively. The release for both temperatures is slow in the first 21 days, after which it is very rapid, the concentration increasing 4.5 times in the following/ next 30 days. The release of BPA decreases with increasing pH. PS also undergoes structural changes; these are best seen at basic pH. The changes are very clearly evident after 10 days of contact, for both working temperatures, these being supported both at the level of the aromatic nucleus, and at the level of the aliphatic chains, where various substitutions take place, and/ as well as introductions of oxydryl and hydroxyl groups into the matrix.

Polyethylene terephthalate (PET) has a different behavior compared to PS, the release of BPA increases proportionally with pH. Thus they increased from the value of 1.04 ng/L at pH=1.5 of 2.1 5 ng/L at pH=9, respectively from the values of 1.32 ng/L at pH=1.5 of 2.87 ng/L at pH=9, at 30°C after 50 days of contact. At a temperature of 20°C, the release of BPA from PET is slow in the first 21 days, reaching values between 0.33 and 0.91 ng/L, and then, the release reaches values 3-4 times higher. For 30 °C, the behavior is similar, with values increasing from the range 0.42 -1.03 ng/L to 1.3 – 2.87 ng/L.

From the analysis of the IR spectra, it can be seen that the PET does not suffer major changes in the polymer matrix during the 50 days in which the experiment was carried out at both working temperatures. The stability of the polymer matrix of polyethylene terephthalate (PET) is much higher than the stability of polystyrene (PS).

REFERENCE

[1] Plastics Europe – Plastics – the Facts 2022, World plastics production evolution, Plastics - the Facts 2022 • Plastics Europe, accesat aprilie 2025.

[2] Xusen Chemicals, Classification and Role of Plastic Additives, August 17th, 2019, Https://Ro.Xusenchemicals.Com/Info/Classification-And-Role-Of-Plastic-Additives-41755487.Html

[3] Petronela-Andreea Vereş, Claudia Maria Simonescu, Oana Ciocîrlan, Carmen Deleanu, Effect of the Packaging Type on the Quality Parameters of Sea Buckthorn Syrup, U.P.B. Sci. Bull., Series B, Vol. 85, Iss. 3, 2023.

[4] Y. Xiang *et al.*, Microplastics and environmental pollutants: Key interaction and toxicology in aquatic and soil environments, *J Hazard Mater*, vol. 422, Jan. 2022, doi: 10.1016/j.jhazmat.2021.126843.

[5] Proiect 22N/2019 „The pakaging, instrument – system for information and protection, essential for management of foodsafety", PN 19 02 03 02, Faza 4/2020 Evaluarea conținutului de bisfenol A din alimente și ambalaje de uz alimentar, 2019-2022, responsabil Gabriel Mustățea, Evaluarea conținutului de bisfenol A din alimente și ambalaje de uz alimentar

[6] Bofill J., 'Microplastics and micropollutants in water Contaminants of emerging concern, European Investment Bank, Project - EIB sector paper - ENR/Water Management February 2023 (www.eib.org/projects), 2023, Microplastics and Micropollutants in Water,

[7] Herath, C.B., Jin, W., Watanabe, G., Arai, K., Suzuki, A.K., Taya, K. (2004). Adverse effects of environmental toxicants, octylphenol and bisphenol A on male reproductive functions in pubertal rats. Endocrine vol. 25(2):163-172.

[8] Shelley Ehrlich, Paige L. Williams, Stacey A. Missmer, Jodi A. Flaws, Katharine F. Berry, Antonia M. Calafat, Xiaoyun Ye, John C. Petrozza, Diane Wright, and Russ Hauser, Urinary Bisphenol A Concentrations and Implantation Failure among Women Undergoing in Vitro Fertilization, Environmentak Health Perspective, 120 (7) (2012), pp. 978 - 983, 10.1289/ehp.1104307

[9] Nadeem Ghani Khan, Jacinta Correia, Divya Adiga, Padmalatha Satwadi Rai, Herman Sunil Dsouza, Sanjiban Chakrabarty, Shama Prasada Kabekkodu, A comprehensive review on the carcinogenic potential of bisphenol A: clues and evidence, Environmental Science and Pollution Research (ESPR), 28, (2021), pp. 19643–19663, https://doi.org/10.1007/s11356-021-13071-w.

[10]Bin Wang, Wei Zhou, Wenting Zhu, Lin Chen, Weiye Wang, Ying Tian, Lisong Shen, Jun Zh ang, Associations of female exposure to bisphenol A with fecundability: evidence from a preconception cohort study, Environmental International, 117 (2018), pp. 139-145, 10.1016/j.envint.2018.05.003

[11] Md Abu bakar Siddiquem Sabine M. Harrison, Frank J. Monahan, Enda Cummins, Nigel P. Brunton, Bisphenol A and Metabolites in Meat and Meat Products: Occurrence, Toxicity, and Recent Development in Analytical Methods, *Foods* 2021, *10*(4),714; https://doi.org/10.3390/foods10040714

[12] Bemrah, N.; Jean, J.; Rivière, G.; Sanaa, M.; Leconte, S.; Bachelot, M.; Deceuninck, Y.; Le Bizec, B.; Dauchy, X.; Roudot, A.-C.; et al. Assessment of dietary exposure to bisphenol A in the French population with a special focus on risk characterisation for pregnant French women. Food Chemistry Toxicology 2014, 72, 90–97, https://doi.org/10.1016/j.fct.2014.07.005

[13] Ashwini Kumar, Daljit Singh, Rajan Bhandari, Ashok Kumar Malik, Sukhjeet Kaur, Baljinder Singh, Bisphenol A in canned soft drinks, plastic-bottled water, and household water tank from Punjab, India Journal of Hazardous Materials Advances, 9, 2023, 100205, https://doi.org/10.1016/j.hazadv.2022.100205

[14] Tatiana Sainara Maia Fernandes, Edmilson de Sousa Almeida, Juliene Tomé Oliveira, Jhonyson Arruda Carvalho Guedes, Guilherme Julião Zocolo, Francisco Wagner de Sousa and Ronaldo Ferreira do Nascimento, Potential risk of BPA and phthalates in commercial water bottles: a minireview Rouse da Silva Costa, Journal of Water and Health, 19.3 , 2021, doi: 10.2166/wh.2021.202

[15] Adriana C Mârşolea, Florentina L Chiriac, Cristina Orbeci, Liliana Bobirică, Constantin Bobirică, Migration and leaching behaviour of Bisphenol A from polyethylene terephthalate water bottles under different storage conditions, *International Journal of Food Science and Technology*, 58, 10, 2023, Pages 5609–5615, https://doi.org/10.1111/ijfs.16583

[16] Nan Zhao, Jianqiang Zhu, Meirong Zhao, Hangbiao Jin, Twenty bisphenol analogues in take-out polystyrene-made food containers: concentration levels, simulated migration, and risk evaluation, Environmental Science and Pollution Research (2023) 30:10516–10526, https://doi.org/10.1007/s11356-022-22890-4

[17] Tooraj Massahi, Abdullah Khalid Omer, Amir Kiani, Borhan Mansouri, Hamed Soleimani, Nazir Fattahi, Masoud Moradi, & Kiomars Sharafi, A simulation study on the temperature-dependent release of endocrine-disrupting chemicals from polypropylene and polystyrene containers, Scientific Reports, (2025) 15:19318, https://doi.org/10.1038/s41598-025-05036-7

[18] JASCO Global, Spectroscopy Group, Identification of Degraded Plastics Cross-checking IR Spectra using Machine Learning Classification and Library Search, 2025, Identification of Degraded Plastics Cross-checking IR Spectra using Machine Learning Classification and Library Search | JASCO Global

[19] Octavio Villegas-Camacho, Roberto Alejo-Eleuterio, Iván Francisco-Valencia, Everardo Granda-Gutiérrez, Sonia Martínez-Gallegos, Javier Illescas, FTIR-Plastics: A Fourier Transform Infrared Spectroscopy dataset for the six most prevalent industrial plastic polymers, Data in Brief, 55 (2024) 110612, https://doi.org/10.1016/j.dib.2024.110612

[20] Sorina Gabriela Șerban, Laura Maria Strugariu, Simion Jitian, The influence of solvents on the appearance of the absorption bands of the polystyrene films deposited from solutions on metal mirrors, Optica Applicata, Vol. LIII, No. 1, 2023 DOI: 10.37190/oa230101

[21] Vanessa Moll, Krzysztof B. Be, Justyna Grabska and Christian W. Huck, Investigation of Water Interaction with Polymer Matrices by Near-Infrared (NIR) Spectroscopy, *Molecules* 2022, *27*(18), 5882; https://doi.org/10.3390/molecules27185882.

[22] Brian C. Smith, Infrared Spectroscopy of Polymers, VIII: Polyesters and the Rule of Three, Spectroscopy, 2022, 37, 10, 25–28, https://doi.org/10.56530/spectroscopy.ta9383e3