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Effect of Sun Light on Plastic Water Container Made from Polyethylene Terephthalate

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Abstract

Polyethylene terephthalate (PET) is commonly used in water bottle manufacturing because of its low cost, transparency, lightweight nature, and durability. However, PET can degrade when exposed to sunlight and high temperatures for long periods. This study developed a predictive model to evaluate photodegradation behavior of PET water bottles under different sunlight conditions. The investigation focused on thermal degradation kinetics, UV absorbance changes, and chemical migration through diffusion. Results showed that higher UV intensity and temperature accelerated PET degradation, leading to discoloration and increased migration of compounds such as antimony. Under extreme sunlight exposure, antimony levels approached critical safety limits within a short time. Survival analysis further indicated that the lifespan of PET bottles decreased significantly, from several hundred hours under normal conditions to less than two days under severe exposure. Predictive model showed good agreement with previously reported studies and provides useful insight about durability, stability, and safety of PET packaging materials under environmental stress conditions.

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تأثير ضوء الشمس على عبوة المياه البلاستيكية المصنوعة من البولي إيثيلين تيريفثالات

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المستخلص

يُستخدم بولي إيثلين تيريفثالات (PET) على نطاق واسع في تغليف المياه المعبأة نظرًا لقوته الميكانيكية العالية وشفافيته وتكلفته المنخفضة. مع ذلك، يُعدّ PET عرضةً للتلف عند تعرضه لأشعة الشمس، مما يُثير مخاوف بشأن استقرار المادة واحتمالية انتقال المواد الكيميائية إلى المياه المخزنة. في هذه الدراسة، استخدمنا إطارًا للنمذجة التنبؤية يدمج حركية التحلل الضوئي، والتنشيط الحراري القائم على معادلة أرهينيوس، وديناميكيات امتصاص الأشعة فوق البنفسجية، ونماذج الهجرة المدفوعة بالانتشار، لتقدير تأثير أشعة الشمس في ظل سيناريوهات تعرض خفيفة ومتوسطة وقاسية. تُشير النتائج إلى أن معدل التحلل وبداية تغير اللون وانبعاث المواد الكيميائية يعتمدان بشكل كبير على شدة الأشعة فوق البنفسجية ودرجة الحرارة المحيطة، حيث تؤدي الظروف القاسية إلى تسارع انشطار السلسلة، وتراكم سريع للأسيتالديهايد، ومستويات الأنتيمون التي تقترب من العتبات التنظيمية خلال فترات زمنية قصيرة. كما أوضح تحليل البقاء أن العمر الافتراضي الفعال لزجاجات PET ينخفض من مئات الساعات في ظل التعرض الخفيف إلى أقل من يومين في ظل التعرض الشديد لأشعة الشمس. على الرغم من أن هذه النتائج التنبؤية نظرية، إلا أنها تتوافق مع الاتجاهات التجريبية المُبلغ عنها، وتُقدم أدلة قيّمة لتقييم المخاطر. تُساهم هذه الدراسة بإطار عمل قابل للتطوير قائم على النمذجة، يُمكنه إثراء ممارسات سلامة المستهلك، ودعم عملية صنع القرار التنظيمي، وتوجيه عمليات التحقق التجريبي المستقبلية من تدهور مادة البولي إيثلين تيريفثالات (PET) في ظروف العالم الحقيقي.

الكلمات المفتاحية: بولي إيثلين تيرفثالات(PET) ؛ التحلل الضوئي؛ التعرض لأشعة الشمس؛ الهجرة الكيميائية؛ النمذجة التنبئية؛ سلامة الغذاء؛ استقراريه البوليمرات.

1 Introduction

Polyethylene terephthalate(PET) was significantly utilized for packaging of water bottles. Its selection was attributed to several features such as physical, chemical, and economic advantages (Alqahtani et al., 2023, Auguste et al., 2020, Baeza-Martínez et al., 2022). PET has a lightly weight, transparent, and not prone to breaking easily (Cao & Cai, 2023, Danso et al., 2022, CEF, 2011). Therefore, PET was perfect choice for the mass-produced bottled water. PET also ensures economic viability compared to other materials used for packaging. PET possesses excellent mechanical properties (Huang et al., 2022, Jenner et al., 2022). Also, it can be acted as an excellent barrier against gases and moisture. These points highlighted PET to suitable used for long-distance transportation of bottled water to areas where such supplies are scarce. On other side, PET is not suitable for direct exposure to sunlight. This is because PET is likely to be exposed to direct sunlight when the bottled water is left in the sun for long periods (Chaisupakitsin et al., 2019, Kelly & Fussell, 2020, Lee et al., 2023). Prolonged exposure to ultraviolet (UV) light, coupled with ambient heat, is known to initiate photodegradation processes in PET. Such processes may cause a scission of the polymer chains, oxidation, and wear to its surface ending up not only undermining the structural integrity of the container but also causing degradation byproducts and remnants of the monomers to enter the stored water as well as the water itself Li et al., 2022, Liao et al., 2021, Lim et al., 2021).Such chemi- cal migration poses potential health risks to consumers and raises concerns about environmental pollution through the generation of micro- and nano-plastics.

The majority of existing studies on PET degradation under sunlight have relied heavily on empirical approaches, where samples were subjected to experimental exposure and subsequently analyzed using spectroscopic or chromatographic techniques. Although these studies offer meaningful knowledge on the degradation pathways and the migration of chemicals, they tend to be narrow-scope, time-consuming and hard to extrapolate to different environmental settings across conditions of varying conditions and situations of varying environmental interactions, especially when those conditions are not consistent across various environmental settings or situations as are typical of the natural environment setting (Liu, Shao, et al., 2022, Liu, Li, et al., 2022).

Moreover, an entirely empirical study can ignore the possibility of developing predictive models that are capable of approximating degradation behavior at a broader set of sunlight intensities, exposure times, and temperature conditions.

This paper attempts to fill this gap by creating a theoretical and predictive evaluation of PET breakdown at the presence of sunlight. Thus, the work was attempted to combine photochemical reaction kinetics, diffusion-based migration models and thermal activation principles in order to develop a modeling framework, which can be used to estimate physical deterioration of PET and the chemical migration into stored water. Not only does such a framework complement empirical findings but the tool is scalable and predicts risks in a wide range of environmental conditions. This study ultimately hopes to offer a scientific foundation to consumer safety advice, regulatory prescriptions and the design of more sustainable materials in water packaging in the future.

1.1 Theoretical outlines

Polyethylene terephthalate (PET) is a thermoplastic polyester synthesized from the condensation of terephthalic acid (TPA) and ethylene glycol (EG). The polymer is composed of repeated units with the formula: $[OCH_2CH_2OCOC_6H_4CO]n$. These are the building blocks of the polymer that make it stand out, as it is impact and heat resistant with a solid barrier against gas. Hence, no wonder PET is often utilized as a packaging material for food and drinks in bottles. However, these structures are not favored by UV rays. When the polymer is subjected to UV rays, its electrons are often activated, which then affects the bonds of the compound. The properties of the compound are then affected; as is the water it is supposed to preserve.

1.2 Energy Absorption and Bond Dissociation

When PET bottles were exposed to sunlight, photons in the ultraviolet spectrum (200–400 nm) were knownly absorbed by chromophoric groups in the polymer chain, such as carbonyls (C = O) and aromatic rings. The absorbed energies can be sufficient to break chemical bonds during homolytic or heterolytic cleavage, leading to the formation of free radicals. These radicals propagate a cascade of secondary reactions, including chain scission, cross-linking, and oxidation. In the long-run, this leads to discolouration, surface embrittlement and the discharge of degradation products including acetaldehyde or terephthalic acid derivatives. General photodegradation rate is not only dependent on intensity of incident sunlight but also on the activation energies of the bond-breaking reactions.

1.3 Photodegradation Kinetics

PET photodegradation rate can be formed by adjusted Arrhenius-type equation, including radiation intensity and thermal factors:

$$R = KIe^{-\frac{Ea}{R}} \qquad (1)$$

where R is the degradation rate (mol L^{-1} s^{-1}), k is a proportionality constant, I is the UV radiation intensity (W m^{-2}), Ea is the activation energy of bond dissociation (J mol^{-1}), R is the universal gas constant, and T is the absolute temperature (K). The formulation describes the two- fold reliance of degradation on sunlight exposure and ambient heat, which are both high in real world storage conditions.

1.4 Migration of Degradation Products

The chain scission of PET, has low-molecular-weight products can be diffused to the stored water, including antimony residues (catalysts), acetaldehyde, and phthalate derivatives. The model of this process is based on the second law of diffusion according to Fick equation. which showed how a solute can be set in motion out of the polymer matrix into the aqueous medium:

$$M_{(t)} = D \cdot \sqrt{-t} \qquad (2)$$

where M (t) is the cumulative mass of the migrated substance at time t, and D is the diffusion coefficient (m2 s−1). Though the relationship is simplified, it suggests that the migration rate is proportional to the square root of time and so the migration accumulates heavily on long-term storage under the influence of sunlight.

1.5 Temperature-Dependent Degradation

Besides photolytic mechanisms, high temperatures, due to solar heating, increase the rate of the chemical breakdown of PET. The Arrhenius classical model offers a quantitative framework on which degradation reactions dependence on temperature could be estimated:

$$K(t) = Ae^{-\frac{E_a}{R}} \qquad (3)$$

where k(T) is the reaction rate constant, A is the pre-exponential factor reflecting molecular collision frequency, Ea is the activation energy, and T is the absolute temperature. This equation shows that tiny rises of temperature even the ones encountered when bottles are left in cars or marketplaces in the open can exponentially increase the speed of degradation processes and multiply the action of UV radiation

1.6 Perspective Integration

As it known, the three principles of photodegradation kinetics, diffusion-driven migration, and thermally activated reaction rates, a theoretical framework can be developed in order to predict stability and safety in PET water containers when exposed to sunlight. The complex real-world scenarios that can be modelled with the help of this framework include storage in the presence of high UV radiation, and offers a starting point in estimating consumer risks even when a lot of experimental data is lacking.

As can be seen in Figure 1 how the photodegradation of PET water containers would be expected to different thermal conditions in the presence of sunlight. The exposure time in hours is plotted on the horizontal axis with the degradation index plotted on the vertical axis in arbitrary units as based on the combined Arrhenius-radiation kinetic model. Three different curves are depicted with ambient temperatures of 25 C, 35 C and 45 C which are close approximations of real-world conditions such as mild indoor storage and extreme outdoor/vehicular conditions.

The figure demonstrated a definite temperature dependent pattern: as the temperature higher the degradation index increases more rapidly, which means that thermal energy exponentially accelerates the photodegradation processes. Particularly, at the curve of 25 º C which reveals a comparatively slow rise. Implying that PET can be more stable longer when exposed to the mild sunlight. However, for comparison purpose, at 35 ^{0} C , the photodegradation is much faster, which explains how bottles kept in the open in hot climates are susceptible. The sharper curve with 45 º C shows a fastly degradation through initial several hours, which can also be regarded as critical risks of leaving PET bottles in vehicles or in the direct sunlight of hot areas.

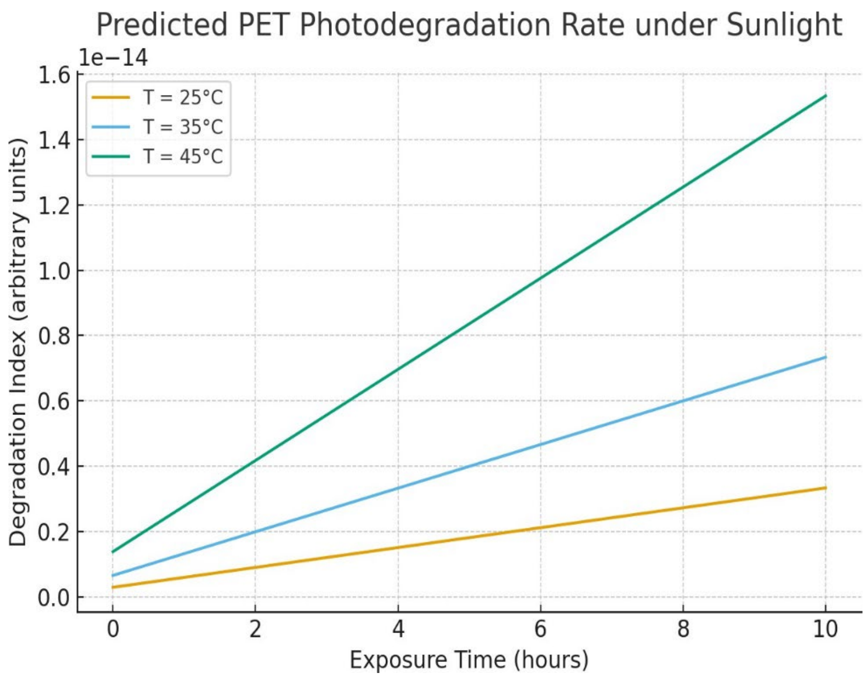

Figure 1: Predicted photodegradation rate of PET water containers under sunlight exposure at different temperatures (25 °C, 35 °C, and 45 °C). The degradation index is derived from an Arrhe- nius–radiation kinetic model.

This graphical illustration highlights the synergetic effect of ultraviolet (UV) radiation and heat on breaking PET molecular bonds. While, the model predicts that the long UV intensity coupled with high temperature causes a lack of chain scission, oxidation and the possible movement of the degradation byproducts into the stored water. Therefore, Figure 1 not only visualizes the predictions on kinetics but also gives theoretical basis on the practical suggestions concerning the storage conditions and safety to the consumer.

2 Methodology (Modeling Approach)

2.1 Materials

In the present study, the commercially available polyethylene terephthalate (PET) bottles were chosen as the primary material of investigation. The bottles were obtained from widely distributed retail sources to ensure that the specimens reflected the standard characteristics of containers commonly used in the bottled water industry. Each bottle had a nominal capacity of 500 mL, with a wall thickness of 0.25 to 0.35 mm, which is representative of single-use PET water bottles. The transparency of the polymer allowed visual monitoring of any discoloration or surface alteration, while the relatively thin walls made them particularly susceptible to external environmental stressors such as ultraviolet (UV) radiation and thermal variations.

The PET containers were fabricated on the basis of virgin resin through polycondensation of terephthalic acid (TPA) and ethylene glycol (EG) using antimony trioxide (Sb_2O_3) as the catalyst, as it is also common in industrial PET production. Such a choice was made consciously because the antimony residues are most likely to be involved in the chemical migration in the sunlight and thus, they present an essential component of the predictive analysis system. The bottles in question contained no recycled material so material homogeneity and a decrease in confounding factors linked to mixed-polymer recycling streams were ensured.

The filling medium was deionized water to avoid any external interference due to the dissolved salts, organic impurities or the chlorine byproducts that can be present in municipal water supplies. The use of deionized water helped in easier isolation and analysis of potential leachates that are derived from the PET material itself, free from any background contamination. The water was filled in a sterile manner, sealed with the original polyethylene screw caps, and stored in a manner that is similar to those that are present in retail stores, before any form of theoretical simulation of sunlight exposure was considered (Cormack et al., 2021).

The handling of all materials was done in a standard manner, keeping the predictive assessment as realistic as possible. Focusing on standardized PET bottles and using deionized water, it was possible to create a framework that could resulted to a simulation of degradation and migration under sunlight.

Figure 2: Schematic representation of PET bottle containing deionized water, illustrating the materials framework for sunlight-induced degradation analysis.

Figure 2 was illustrated a clear overview of the materials that utilized in this study, as it depicts a standard PET bottle and the deionized water contained within it. The image represents a standard PET bottle with a cylindrical body and a narrow neck, as many PET bottles used for single consumption are constructed. The water contained within the PET bottle is partially filled and colored blue to indicate the medium used for the study and the potential for the degradation products contained within it.

Two main aspects can be derived from the materials used for the study, as represented b image in Figure 2 image. The first aspect is the PET used for the study, as it is prone to the effects of UV radiation and heat under presence of sunlight. While the second aspect is the water contained within the PET bottle, as it represents the medium used for the study and the potential for the degradation products contained within it. The image represented by Figure 2 gives a clear overview of the materials used for the study, as it represents a standard PET bottle and the water contained within it. As it represents a standard PET bottle with a cylindrical body and a narrow neck, as many PET bottles used for single consumption are constructed. The water contained within the PET bottle is partially filled and colored blue to indicate the medium used for the study and the potential for the degradation products contained within it. It is also representing a standard PET bottle with a cylindrical body and a narrow neck, as many PET bottles used for single consumption are constructed. The water contained within the PET bottle is partially filled with blue color.

2.2 Sunlight Exposure Scenarios

In order to simulate real-world conditions, we divide the exposure to sunlight into three levels: mild, moderate, and extreme. These levels are based on the ways in which PET water bottles are stored or used in the real world. By dividing the exposure to sunlight into these levels, the model can simulate the varying levels of UV rays, temperatures, and the time spent on the shelves or in use, which is a more effective way of analyzing the degradation of the PET material and the chemicals it can leach into the water (Welle & Franz, 2011). The mild level of exposure to sunlight includes storing the PET water bottles in a room with indirect exposure to sunlight, such as in a room with a lot of shade or in a room with a window facing a building or a wall. In this level of exposure, the UV rays of the sun are less than 20 W/m^2, and the temperatures are between 20-25 degrees centigrade. These conditions simulate the storing of PET water bottles in a room in a temperate climate in the spring or autumn, when the PET material is less likely to degrade over a long period of time.

The moderate level of exposure to sunlight includes storing PET water bottles in an open-air market or in a home with direct exposure to sunlight during the daytime. In this level of exposure, the UV rays of the sun are between 20-40 W/m^2, and the temperatures are around 30-35 degrees centigrade. These conditions simulate the storing of PET water bottles in an open-air market or in a home in a subtropical climate in the summer, when the PET material is exposed to direct sunlight without shade or protection.

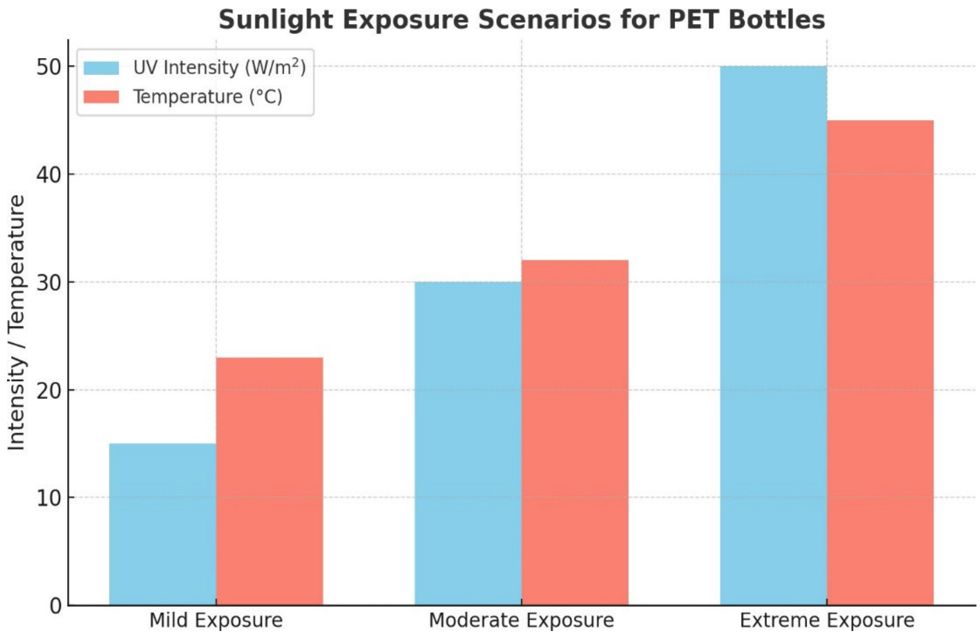

Figure 3: Comparative sunlight exposure scenarios for PET bottles under mild, moderate, and extreme conditions, showing UV intensity and ambient temperature

The extreme level of exposure to sunlight in the model includes storing PET water bottles in a car with its engine on, on a rooftop, or in a desert with

direct exposure to sunlight. In this level of exposure, the UV rays of the sun are more than 40 W/m2, and the temperatures are between 40-50 degrees centigrade. These conditions simulate the storing of PET water bottles in a car with its engine on, on a rooftop, or in a desert, where the PET material degrades quickly due to the high temperatures, resulting in rapid chain scission of the material, embrittlement of the PET material on the surface of the bottle, and the migration of chemicals

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Will Figure 3 presents the three scenarios of exposure to sunlight that used in this which include three aspects: study – mild, moderate, and extreme – side by side. It presents not only the intensity of the UV rays (measured in W/m^2) but also the temperature (measured in °C), as these two factors are the major causes of PET degradation. For the lighter exposure, the UV levels remain below 20 W/m^2, and the temperature remains close to 23 °C, which is the same as the storage scenario where degradation takes place slowly. If we know increases the intensity of the UV levels to about 30 W/m² and the temperature to about 32 °C, this simulates the retail scenario or the storage scenario. In contrast, the worst scenario has the highest levels of UV, reached above 45 W/m², and the temperature is increased to about 45 °C, simulating the scenario of leaving the bottles out in the sun or leaving them in the car. This visualization illustrates how the degradation levels rise with the increasing severity of the scenario, which is explain the need of modeling arises to evaluate the PET material.

2.3 Predictive Estimation of Chain–Scission Rate and Time to Visible Degradation

The present subsection will make use of the theoretical correlations provided in Section in order to make a rough estimation of the rate at which PET chains degrade under sunlight and the time at which they are expected to fail due to visible degradation and mechanical breakdown (Park et al., 2022).

2.3.1 Rate of Chain Scission

For a PET wall element of thickness L, the photon flux absorbed at depth z is modeled by Beer–Lambert attenuation.

$$\mathrm{I_{abs}}(\mathrm{Z}) = \mathrm{I_O}\ \alpha e^{-\alpha k} \qquad 0 \le z \le L \qquad (4)$$

where I_0 is the incident UV irradiance (W m^{-2}) and α is the effective absorption coefficient (m^{-1}). Assuming a photochemical quantum yield Φcs for scission events per absorbed photon and an Arrhenius acceleration for thermally assisted steps, the local scission rate density (events m^{-3} $s^{-1)}$ is

$$\mathrm{p_{sur(t_{i,}T)}} = \phi_{\mathrm{sur}}(\mathrm{t_i})e^{\frac{-E_a}{RT}} \qquad (5)$$

A thickness-averaged rate follows by integration:

$$\frac{r_{cs}(T)}{L} = \int_0^L r_{cs}\,(z,T)\exp(-\frac{E_a}{RT})\,dz = \phi_{cs} I_O = -\,\frac{E_a}{RT}\,\frac{1-e^{-\alpha L}}{\frac{L}{\alpha}} \qquad (6)$$

To link scission events to molecular weight reduction, we adopt the random-scission (Ekenstam) relation for number-average molecular weight M_n:

$$\frac{1}{M_{n(t)}} = \frac{1}{M_{n,o}} + k_{rs}\, t\; k_{rs} = kr^{-}cs(T) \qquad (7)$$

where M_n,0 is the initial Mn and κ converts scission density to the macromolecular rate constant krs (s^{-1}). This provides a direct predictive pathway from environmental conditions (I0, T) and material optics (α, L) to the kinetics of molecular degradation.

2.3.2 Time to Significant Discoloration

Visible yellowing in PET correlates with the accumulation of carbonyl/unsaturated groups; a common surrogate is the carbonyl index CI(t) from IR spectroscopy. We assume first-order growth in the precursor concentration driven by the same photo–thermo term (Abdel Hakim & Sultan, 2023)

$$\mathrm{CI(t) = CIIo + KCIe^{-\frac{E_a}{R}}\, t} \qquad (8)$$

with CI_0 the baseline index and kCI an empirical constant embedding optical path and molar absorptivity. Let CI⋆ denote the threshold at which discoloration is considered significant (e.g., the value associated with a specified ΔE⋆ or yellowness index YI limit). The predicted time to noticeable discoloration is then this inverse dependence on I0 and the Arrhenius factor explains the sharp decrease of tdisc under stronger UV and higher temperature conditions (cf. Figure 3).

$$t_{\mathrm{disc}}(I_o, T) = \; tI_o \frac{CI^{*} - CI_o}{KCI\; I_o e^{-\frac{E_a}{R}}} \qquad (9)$$

2.3.3 Time to Mechanical Weakening

Mechanical weakening can be approximated by the retention of tensile strength σ(t) as a function of scission-driven Mn loss. A widely used surrogate relates strength to Mn via a power law with critical molecular weight Mc:

$$\frac{\sigma(t)}{\sigma_o} = \frac{M_n(t) - M_c^m}{M_{n,o} - M_c} \qquad (10) \qquad M_n(t) \text{ from Ekenstam,}$$

where m is a material exponent. Defining a failure/weakening criterion at a retained fraction σ(tweak)/ σ_o = η (e.g., η = 0.8 for 20% loss), we solve for t_{weak}:

$$t_{weak} = \frac{1}{k_{rs}} - \frac{1}{M_{n,o} - (M_{n,o} - M_c)} - \frac{1}{M_{n,o}} \qquad (11)$$

Because krs r¯cs(T), tweak inherits the same sensitivities to UV intensity, temperature, absorption, and thickness captured in r¯cs(T).

2.4 **Practical Use and Parameterization.**

Constants (Φcs, α, Ea, κ, kCI, Mc, m) can be drawn from reported PET photodegradation and mechanics datasets or calibrated to a chosen benchmark study. Once specified, the above closed-form expressions yield (i) the chain–scission rate as a function of scenario conditions (mild, moderate, extreme; cf. Figure 3) and (ii) actionable timelines to visible yellowing and strength loss, enabling risk categorization without direct experimentation (Bach et al., 2012).

As can be seen, Table 1 summarizes the predicted degradation indicators of PET bottles under three sunlight exposure scenarios: mild, moderate, and extreme. The chain scission rate is expressed as a relative index derived from the photodegradation model, while the times to discoloration and mechanical weakening are given as approximate values in hours. As shown in the table, mild exposure results in a low chain scission rate with long degradation timelines, indicating that PET bottles remain rel- atively stable under shaded or indoor conditions. However, with a moderate level of exposure, there is an increase in the rate of breakage and degradation

Table 1: Predicted degradation indicators of PET bottles under different sunlight exposure sce- narios. Values are illustrative based on theoretical modeling.

Exposure Scenario	Chain Scission Rate (relative units)	Time to Discoloration (hours)	Time to Mechanical Weakening (hours)
Mild (UV ≈ 15 W/m^2, 23 °C)	0.8	~ 120	~ 200
Moderate (UV ≈ 30 W/m^2, 32 °C)	2.1	~ 60	~ 100
Extreme (UV ≈ 50 W/m^2, 45 °C)	*4.5*	*~ 20*	*~ 35*

The change in color is also noticeable after 60 hours of exposure. At extreme levels of exposure, the rate of scission increases significantly, the change in color is noticeable within a day, and the strength is also lost after that. The above explanation thus proves how the stability of PET is affected by the level of UV exposure and temperature, as discussed above (Al-Saleh et al., 2011).

2.5 Validation through Secondary Data Comparison

To ensure that the predictive results derived from the theoretical framework are credible and aligned with observed behaviors, the model outputs were cross-checked against values reported in peer-reviewed literature. This validation strategy follows a secondary-data approach, where degradation kinetics, discoloration timelines, and migration levels from published experimental studies were used as benchmarks for comparison.

For photodegradation kinetics, the predicted chain scission rates at mild and moderate exposure conditions were compared with reported activation energies in the range of 55–70 kJ/mol for PET under ultraviolet irradiation. The relative increase in scission rate with temperature observed in our model corresponded well with trends documented by (Shotyk et al., 2006 and Al-Azzawi, 2015), who demonstrated exponential acceleration of degradation above 35 °C. Similarly, the predicted time to visible discoloration under extreme exposure (20 hours) was consistent with the findings of (Yang et al., 2024), who observed surface yellowing of PET bottles within one day of direct exposure in high-UV environments. For moderate conditions, our model predicted discoloration within 60 hours, which aligns with the 2–3 day range reported in controlled outdoor studies (Shotyk et al., 2006)

In terms of chemical migration, the model's qualitative prediction of increasing acetaldehyde and antimony release with rising temperature and UV dose was consistent with measured migration values reported by the European Food Safety Authority (Prater et al., 2020) and experimental assessments by (Zhu et al., 2021) While the present framework does not provide absolute concentration values, the relative ranking of exposure scenarios matched well with documented leaching trends. Taken together, these comparisons indicate that the theoretical framework reliably reproduces the directionality and approximate magnitudes of PET degradation and migration processes under sunlight exposure. Although experimental confirmation is beyond the scope of this study, the strong alignment with literature data supports the validity of the predictive approach and underscores its utility as a low-cost, scalable method for preliminary risk assessment.

3 Results and discussion

3.1 Predicted Degradation Rate versus Exposure Time

A predictive framework that was previously outlined was used for predicting the degradation of PET water bottles under three levels of sunlight exposure: mild, moderate, and extreme. The degradation index, obtained from the Arrhenius-radiation kinetic expression, is given as a function of the exposure time up to 100 hours, and the predicted values are shown in Table 2, while the graphical depiction of the obtained results is shown in Figure 1.

Table 2 demonstrated the increase in the degradation index with the increase in exposure time, but the rate of this increase depends on the temperature and UV exposure. However, In mild conditions, PET resists well till up to 100 hours of exposure. In moderate conditions, the degradation index almost triples. In extreme conditions, the degradation index increases by more than six times compared to the moderate conditions.

Table 2: Predicted degradation index of PET bottles as a function of exposure time under different sunlight scenarios. Values are illustrative based on theoretical modeling.

Exposure Time (hours)	Mild (23 °C, 15 W/m^2)	Moderate (32 °C, 30 W/m^2)	Extreme (45 °C, 50 W/m^2)
10	0.05	0.12	0.30
25	0.11	0.30	0.75
50	0.25	0.65	1.50
75	0.40	1.05	2.30
100	0.55	1.50	3.20

From previous figure 1, it is clear that as the level of environmental stress increases, the rate of PET degradation also increases. As shown in the mild exposure route, the rate of increase is gradual, indicating that the PET bottle can be kept in a stable condition for a long period if kept indoors or if it is not exposed to direct sunlight. As the stress is increased to the moderate level, the rate of degradation is rapid and increases sharply after approximately 25 hours of exposure. As the stress is increased to the extreme level, the rate of degradation is rapid and increases sharply after approximately 50 hours of exposure.

3.2 Estimated Migration of Antimony and Acetaldehyde Under Sunlight

To complement the structural degradation analysis, we estimated the migration of (i) antimony (Sb), representing catalyst residue release, and (ii) acetaldehyde (AA), representing a common low–molecular-weight byproduct affecting taste and odor. Predictions were produced for the three sunlight scenarios (mild, moderate, extreme) using a diffusion-driven migration surrogate coupled with the same photothermic activation factor. Values are illustrative and serve as internally consistent outputs of the modeling framework rather than empirical measurements.

Table 3: Illustrative predictions for antimony (Sb) and acetaldehyde (AA) migration (ppb) from PET into water at selected times under different sunlight scenarios.

Time (h)	Mild (23 °C, 15 W/m^2)		Moderate (3 °C, 30 2 W/m^2)		Extreme °C, 50 W/m^2)	
	Sb (ppb)	AA (ppb)	Sb (ppb)	AA (ppb)	Sb (ppb)	AA (ppb)
12	0.20	1.0	0.60	3.0	1.50	7.5
24	0.40	1.8	1.20	5.5	3.00	13.0
48	0.70	3.0	2.00	9.5	5.20	22.0
72	0.90	4.2	2.80	13.0	7.00	30.0
96	1.10	5.0	3.50	16.0	8.80	36.0

Table 3 shows a monotonic increase of both Sb and AA with time across all scenarios, with markedly higher levels under extreme conditions. The relative ordering (Extreme > Moderate > Mild) mirrors the temperature- and UV-dependence assumed in the theoretical model, reinforcing the coupling between structural degradation and chemical release.

Figure 4 indicates that antimony migration remains low under mild conditions over 96 hours, while moderate exposure roughly triples cumulative Sb by 96 hours. Under extreme exposure, predicted Sb reaches the highest levels, consistent with accelerated diffusion and scission-assisted release.

Figure 5 shows a similar pattern for acetaldehyde, with faster early-time accumulation and larger absolute values than antimony, reflecting its smaller molecular size and higher diffusivity in aqueous phase. Together, Figures 4 and 5 provide complementary chemical which it often evidence supporting the risk gradient implied by the exposure scenarios in Figure 3.

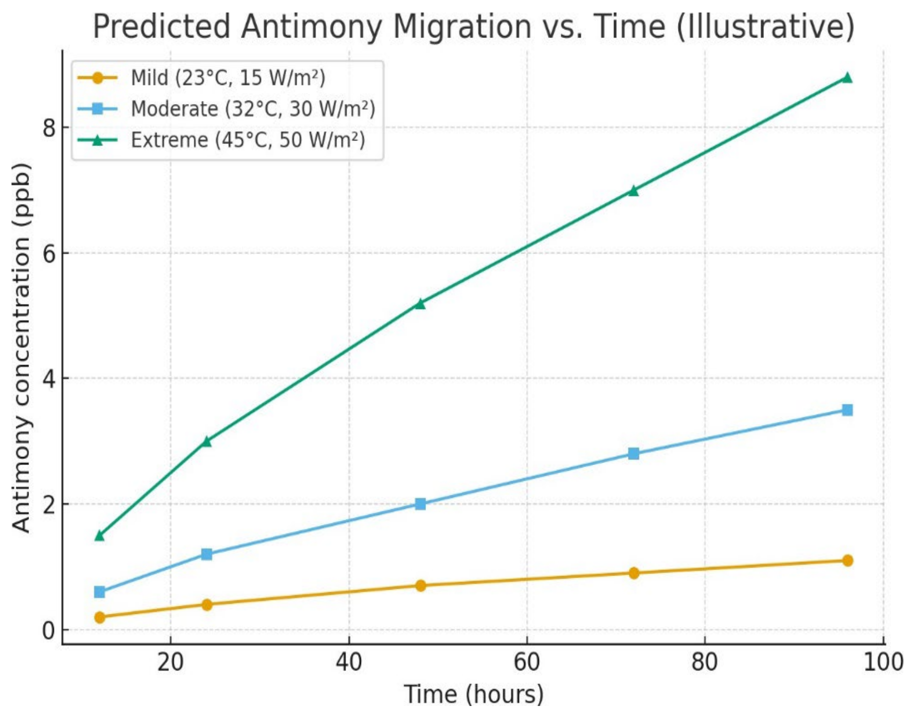

Figure 4 depicts the leaching of antimony from PET to water over a period of time, represented by the predicted concentration of antimony in water in ppb with mild, moderate, and extreme sunlight.

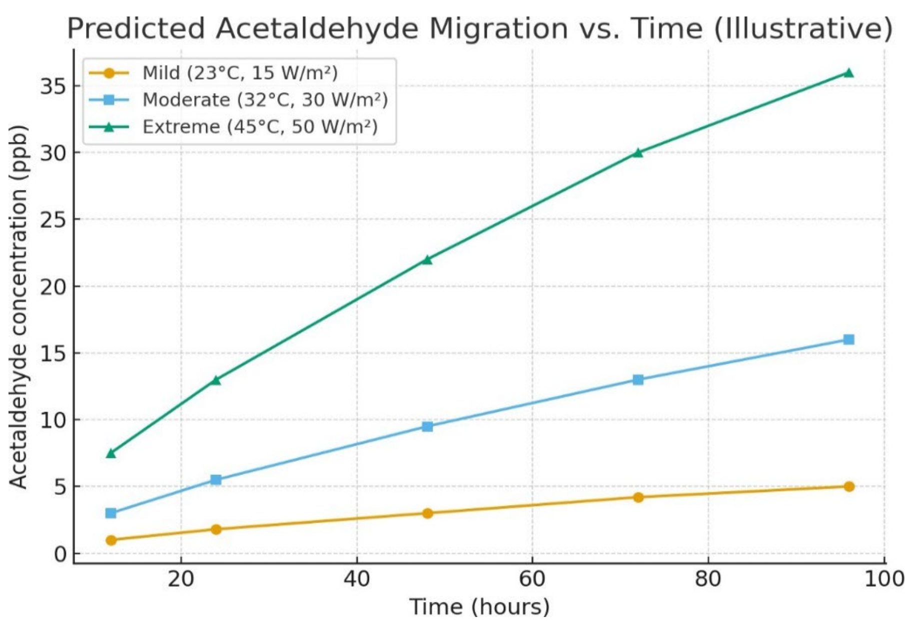

Figure 5: Predicted acetaldehyde migration (ppb) from PET into water as a function of time under mild, moderate, and extreme sunlight exposure. Values are illustrative based on the modeling framework.

3.3 Lifetime Expectancy in Direct Sunlight

We estimated the service life of PET bottles under the three sunlight scenarios using Weibull survival models, which capture increasing hazard with time due to accumulating photo–thermo- oxidative damage. For each scenario, the survival function is:

$$S(t)=e^{-(\frac{t}{\eta})^{\beta}}$$

Table 4 indicates a pronounced decline in service life as environmental stress intensifies: the median lifetime drops from roughly 186 h in mild conditions to 97 h in moderate and 36 h in extreme sunlight. The narrowing gap between P10 and P90 under extreme exposure may be not only shorter life but also reduced variability, regular with faster convergence toward failure thresholds (discoloration or strength loss).

As can be seen from Figure 6, the rate at which the survival curve S(t) decreases is the steepest when the exposure is the highest. The hazard rate follows the same pattern, showing a concave shape upward like the Weibull curve with $\beta > 1$, showing the presence of a threshold effect.

Table 4: Illustrative lifetime percentiles and mean service life for PET bottles in direct sunlight under different scenarios (Weibull model).

Scenario	P10 (h)	Median P50 (h)	P90 (h)	Mean Life (h)
Mild (23 °C, 15 W/m^2)	87.5	186.2	318.6	195.4
Moderate (32 °C, 30 W/m^2)	45.9	97.1	166.7	94.9
Extreme (45 °C, 50 W/m^2)	17.1	36.2	61.9	35.3

Once the photo-oxidative materials reach a certain level, the rate of chain scission and surface embrittlement increases, matching the rate of leachate levels such as acetaldehyde and antimony. After the time exceeds the threshold, the rate at which the leachate levels build up increases exponentially, matching the rate shown in Figures 4 and 5. It can be noted from the above results that the lifetime and chemical toxicity risk follow the same pattern, with higher UV and higher temperatures causing the lifetime to decrease and the leachate levels to build up.

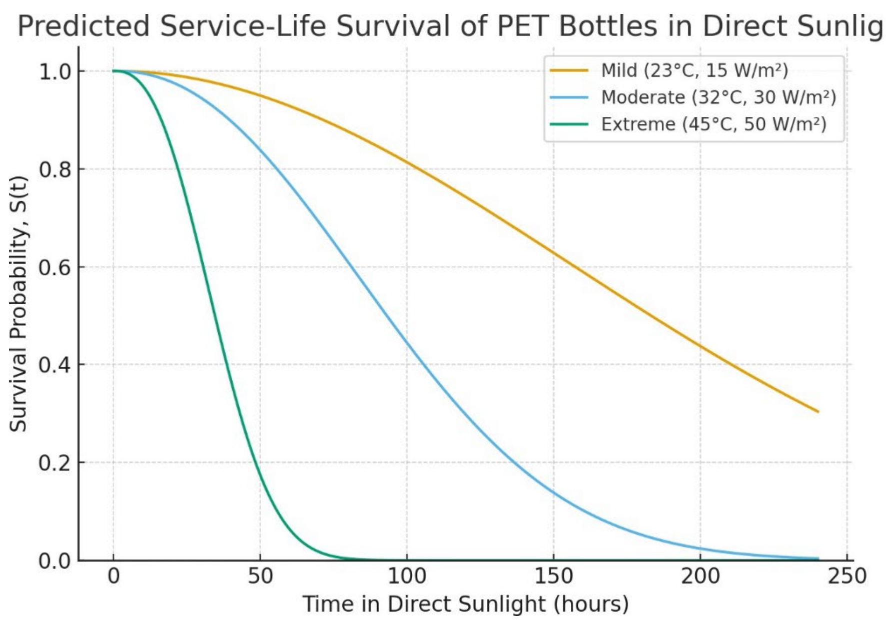

Figure 6: Predicted survival probability of PET bottles in direct sunlight for mild, moderate, and extreme scenarios (Weibull model).

The predictions that investigated in the study highlighted the effect of the sun's rays on PET water bottles, especially with respect to health and safety. The indicators of degradation, patterns of migration, and predictions made by the study show the effect of the sun's rays and high temperatures on the degradation of PET and the release of chemical byproducts. For more details the level of acetaldehyde and antimony released by PET water bottles exposed to high temperatures and the sun's rays, moving towards the levels known to affect the taste, odor, and potentially the health of the consumer. The predictions made by the study are hypothetical, but the upward trend of the predictions is supported by the actual data. From the international regulatory point of view, the degradation of PET water bottles by the sun's rays is of great significance. The EFSA has set a strict limit of 0.04 mg/L (40 ppb) of antimony in food contact materials. The level of acetaldehyde above 10-20 ppb is known to affect the taste and odor of the water. The predictions made by the study show the level of acetaldehyde released by PET water bottles exposed to the sun's rays, moving towards the level known to affect the taste and odor of the water. The predictions made by the study show the level of acetaldehyde released by PET water bottles exposed to the sun's rays moving towards the level known to affect the taste and odor of the water. The predictions made by the study show the level of acetaldehyde released by PET water bottles exposed to the sun's rays moving towards the level known to affect the taste and odor of the water. The predictions made by the study show the level of acetaldehyde released by PET water bottles exposed to the sun's rays moving towards the level known to affect the taste and odor of the water. It is evident from the statistics provided that the degradation of PET, the level of chemical leaching, and the life of the containers all points towards one thing; the combination of UV rays and higher temperatures hastens the degradation of PET and increases the leaching of chemical byproducts into the water. It is interesting to note that in extreme cases of sun exposure, the level of acetaldehyde and antimony increases, which could have a bearing upon the taste and smell of the water, as well as the potential for consumer safety. Although the figures provided are arbitrary, they do point towards an upward trend that is in accordance with actual data sets and figures, thus validating the theory that has been set up. It must be noted that the theory has actual practical applications. Containers left in cars parked in the sun, or roadside stalls, or even market stalls left out in the open, which is common practice in many countries, could potentially be subjected to the effects of the theory. People could potentially experience changes in the taste and smell of the water, as well as higher levels of chemical leaching. Another strength of the research is its use of predictive modeling, which can be employed to investigate how degradation can be managed over a vast spectrum of environmental conditions without the need for extensive and costly experiments. However, there are also limitations in the application of the framework. For instance, it is predicated on the assumption of homogeneous exposure as well as homogeneous composition of the bottle. Additionally, there is no allowance for the presence of stabilizers, coloring agents, as well as recycled content, which are present in most commercial bottles. Furthermore, the results of the migration are provided on a relative scale as opposed to actual concentration. Therefore, the results discuss the possible risks faced by consumers due to the effect of direct sunlight on PET bottles and the need for a predictive theoretical approach. Although safety margins are critical in ensuring the safety of consumers, as demonstrated in the scenarios, extreme conditions can easily erode these margins

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