

Comparative Analytical Characterization and Chromatographic Profiling of Virgin and Recycled Polyethylene Terephthalate (PET)

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Abstract

Polyethylene terephthalate (PET) and its copolymeric variants represent a critical class of thermoplastic polymers widely deployed in packaging, industrial textiles, and consumer products due to their tensile strength, dimensional stability, and chemical resistance. PET materials are broadly categorized into virgin polyester (vPET), derived directly from petrochemical feedstocks, and recycled polyester (rPET), produced via the mechanical or chemical reprocessing of post-consumer polymer waste. While functional performance across both forms remains comparable, structural differences in chain morphology, thermal degradation history, and comonomer distribution persist. In this study, gas chromatographic (GC) profiling following depolymerization, extraction, and derivatization was evaluated as a qualitative and quantitative diagnostic methodology to differentiate vPET and rPET matrices based on residual monomeric markers. Method validation according to IS 16481-2016 demonstrated successful detection of isophthalic acid (IPA) across five commercial food-contact plastic substrates. Chromatographic comparison revealed distinct profile signatures, wherein rPET exhibited a secondary retention peak ($t_R=8.565$ min) attributable to residual monomeric IPA, whereas vPET displayed a singular internal standard peak ($t_R=6.386$ min). These findings demonstrate the viability of chromatographic profiling for verification, quality assurance, and traceability of recycled polymer fractions within commercial supply chains. The article aims to improve awareness of the origin and applications of polyester fibres and to highlight how recycling existing polyester waste can contribute to resource conservation and waste reduction.

Keywords

Polyethylene terephthalate (PET); Isophthalic acid (IPA); Gas chromatography; Textile fibres; Awareness; Sustainability.

Citation

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1.0 Introduction:

Polyethylene terephthalate (PET), commonly known as polyester is an aromatic semi-crystalline polyester widely synthesized via the polycondensation of terephthalic acid (TPA) or dimethyl terephthalate (DMT) with ethylene glycol (EG) (given in Fig. 1). Due to its high barrier efficiency against gases, structural rigidity, and optical clarity, PET constitutes a major fraction of post-consumer packaging materials and synthetic textile fibers. Virgin PET (vPET) is synthesized through direct petrochemical routes, producing

highly uniform macromolecular chains characterized by low polydispersity, high intrinsic viscosity, and minimal contamination. Conversely, recycled PET (rPET) is derived from post-consumer streams (e.g., mineral water bottles, packaging films, and discarded textiles) via mechanical sorting, shredding, thermal extrusion, or chemical depolymerization (1). Visual representation of Virgin PET and recycled PET is given in Fig. 2. While advanced processing can yield rPET with mechanical properties approaching those of vPET, repeated mechanical recycling inevitably induces chain scission, thermal-oxidative degradation, and hydrolytic cleavage.

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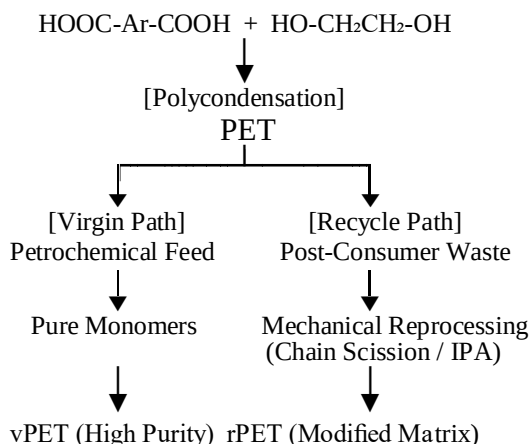


Fig. 1: Synthesis process of PET

Key characteristics of virgin polyester are;

- **Uniformity & purity:** Highly consistent molecular weight distribution with zero contamination or structural variation.
- **High tenacity:** Superior tensile strength, elasticity, and dimensional stability due to unbroken polymer chains.
- **Color clarity:** Pure white optical properties that easily absorb light, bright dyes without color contamination.
- **Environmental impact:** High carbon footprint, intensive energy consumption, and reliance on non-renewable fossil fuel resources.



Fig. 2: Virgin and recycled polyester fiber

Uses of virgin polyester includes activewear, home textiles like curtains, baby wipes, bedcovers, pillows etc. The schematic presentation is depicted in Fig. 3.



Fig. 3: Schematic representation of uses of virgin polyester

At the same time, recycled polyester is manufactured by reprocessing the existing post-consumer PET waste (such as clear water bottles, packaging materials, or discarded textiles) into new usable fibers (1). The key characteristics of this are;

- **Performance parity:** Modern processing methods yield fibers that closely match virgin polyester in strength, durability, and texture.
- **Slight thermal/chain variations:** In mechanical rPET, slight thermal degradation can occur over repeated cycles, though chemical recycling restores virgin-equivalent purity.
- **Dyeing & dye Affinity:** Trace comonomers (such as isophthalic acid from original PET bottles) alter polymer crystallinity, which often improves dye uptake at lower temperatures.
- **Environmental Impact:**
 - Diverts plastic waste from landfills and ocean ecosystems.
 - Requires significantly less energy and generates fewer carbon emissions than virgin petro-chemical extraction.



Fig. 4: Schematic representation of uses of recycled polyester

The flowchart given in Fig. 5 outlines the step-by-step mechanical recycling process used to transform post-consumer PET bottle waste into high-quality recycled polyester fibers.

To optimize the crystallization kinetics, thermal stability, and stretch-blow molding behavior of bottle-grade PET, comonomers such as isophthalic acid (IPA; benzene-1,3-dicarboxylic acid, $\text{C}_6\text{H}_4\text{O}_4$, structure given in Fig. 6) are intentionally incorporated into the polymer backbone at fractions typically ranging between 1 to 5 wt%. The asymmetric meta-substitution of isophthalic acid disrupts chain regularity, lowering the rate of crystallization and increasing the amorphous fraction of the polymer matrix. This structural alteration enhances optical transparency in rigid packaging and alters dye susceptibility in textile fibers by increasing dye diffusion into amorphous domains.

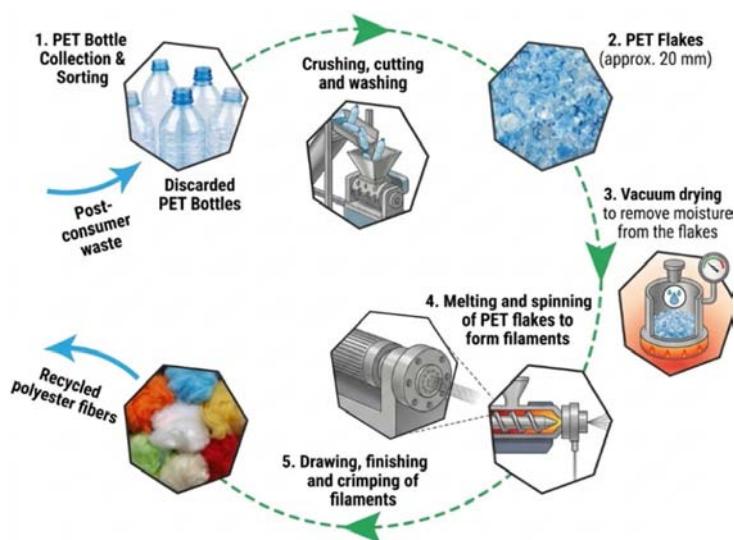


Fig. 5: Flow-chart showing the recycling process of PET bottles

During polycondensation, thermal processing, or subsequent service life, incomplete conversion or hydrolytic cleavage can yield unbound residual monomers and oligomers within the polymer matrix. Identifying and quantifying these unreacted or liberated small molecules is critical for quality control, material traceability, and evaluating mass migration into contacting media.

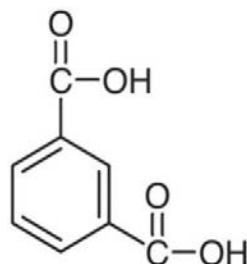


Fig. 6: Structure of isophthalic acid

Ideally, all monomers become chemically integrated into the polymer backbone during polymerization. However, trace levels of residual monomers may remain in the finished product due to incomplete conversion, manufacturing conditions, thermal degradation, or hydrolytic degradation during service. Monitoring residual aromatic acids in food-contact polymers is therefore important for product quality, manufacturing consistency, and migration studies (2, 3).

This study demonstrates a gas chromatographic screening methodology following chemical cleavage and derivatization to quantify residual IPA content in commercial food-contact packaging material and evaluate its utility as a diagnostic marker for differentiating vPET and rPET matrices. The method is intended for rapid screening and routine laboratory analysis. This analysis can create awareness among common public to minimize the use of recycled polyester as it contains IPA which is carcinogenic in

nature and continuous exposure if it to food, skin can cause cancer and other health related issues.

2. Experimental

2.1. Reagents and Materials

Chromatographic grade benzyl alcohol, titanium tetraisopropoxide ($\text{Ti}(\text{OCH}(\text{CH}_3)_2)_4$), and chloroform (CHCl_3) were obtained from commercial suppliers and used without further purification. Commercial post-consumer polymer samples representing direct food-contact packaging applications were acquired from local commercial suppliers:

- Sample-A: Fruit juice containers (PET)
- Sample-B: Mineral water packaging (PET)
- Sample-C: Disposable cutlery (Spoons)
- Sample-D: Rigid food storage containers
- Sample-E: Transparent thermoformed food packaging

2.2. Sample Preparation and Depolymerization

The polymer samples were rinsed with ultrapure water, dried under vacuum, and mechanically comminuted to a uniform particle size of approximately 3-5 mm. Quantitative samples weighing 0.20–1.00 g were transferred into sealed reaction vessels. Chemical cleavage and extraction of the bound and unreacted isophthalic acid fractions were conducted in accordance with the standard IS 16481-2016. To render the non-volatile dicarboxylic acid suitable for gas chromatographic separation, the extracted analytes were subjected to esterification/derivatization to yield volatile dialkyl esters prior to injection.

2.3. Instrumental Analysis

Qualitative and quantitative evaluations were conducted using a Gas Chromatograph equipped with a Flame Ionization Detector (GC-FID) / Total Ion Chromatogram (TIC) acquisition setup.

- Injection Volume: 1.0 μL
- Separation Profile: Isothermal / program-optimized to achieve baseline resolution of derivatized IPA from background matrix components.
- Quantification: Standard addition and peak area integration methods according to IS 16481-2016 parameters.

3. Results and Discussion

3.1. Quantitative Determination of IPA Content

The developed method produced well-resolved chromatographic peaks for the derivatized IPA with minimal interference from polymer additives or extraction solvents. Adequate chromatographic separation was achieved within a relatively short analytical run, allowing efficient routine

sample through put. Good linearity was observed over the investigated concentration range, demonstrating the suitability of the method for quantitative analysis. Repeat injections produced reproducible peak areas and retention times, indicating satisfactory instrumental precision and stable chromatographic performance. Sample preparation was a critical step in the analysis because direct chromatographic determination of the target acid is limited by its physicochemical properties. Therefore, hydrolysis followed by derivatization was employed to convert the analyte into a more suitable volatile derivative for GC analysis (4-6). The derivatization step improved chromatographic response and peak symmetry, thereby facilitating reliable detection and quantification. The determined IPA contents of the investigated packaging materials are presented in Table 1. IPA was detected in all five samples, with concentrations ranging from 1.78% to 2.10%. Sample-B and Sample-C showed the highest measured concentration (2.10%), followed by Sample-A and Sample-D (2.00%), while Sample-E showed the lowest concentration (1.78%). The mean IPA content across the five investigated samples was approximately 2.00%.

Table-1: IPA content of different packaging materials

Samples	IPA content (%)
Sample-A	2.0
Sample-B	2.1
Sample-C	2.1
Sample-D	2.0
Sample-E	1.78

The corresponding chromatogram is given in Fig. 6 (virgin polyester) & Fig. 7 (recycled polyester). The relatively narrow range of measured values in Table-1 indicates that IPA was present at comparable levels across the investigated packaging materials. The observed variation may be associated with differences in polymer formulation, manufacturing conditions, raw-material composition and processing history.

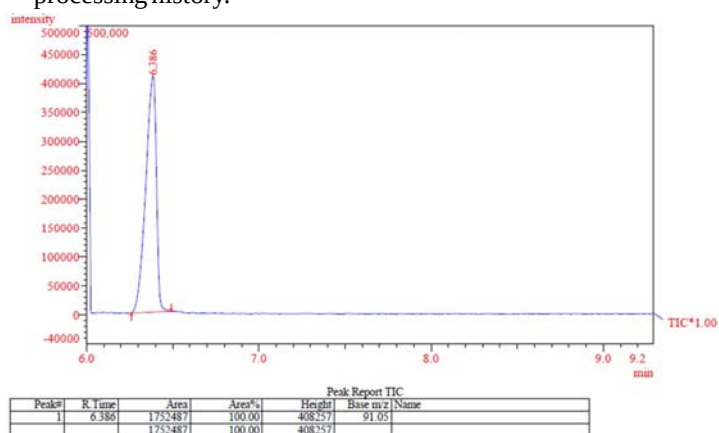


Fig. 6: Chromatogram of virgin polymer

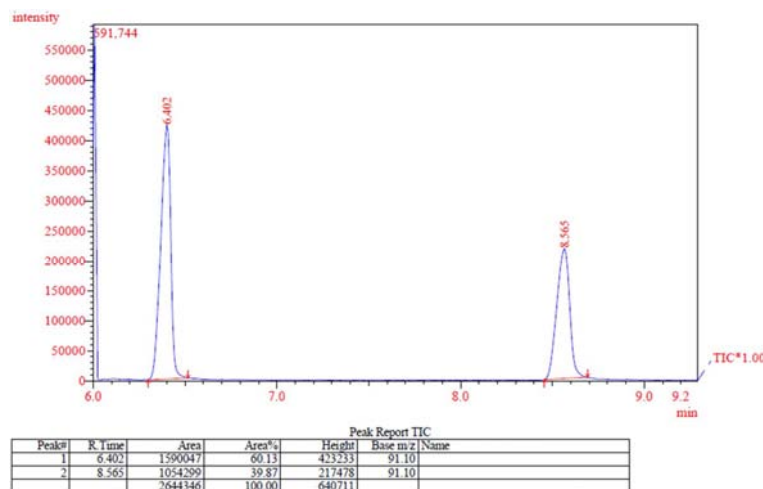


Fig. 7: Chromatogram of recycled polymer

3.2. Chromatographic Differentiation of vPET and rPET

Comparative chromatographic analysis demonstrated distinct structural and chemical differences between virgin and reprocessed polymer matrices.

- **Virgin Polyester Profile:** As shown in the representative chromatogram, vPET displays a single, sharp analytical response at retention time (Rt)=6.386 min corresponding to the added standard reagent, with complete absence of secondary volatile degradation products or unreacted monomeric peaks in the extended retention region.
- **Recycled Polyester Profile:** In contrast, the chromatogram for the reprocessed material shows the primary standard peak at retention time (Rt)= 6.402 min alongside a distinct secondary peak at Rt=8.565 min (Area %=39.87%). This secondary peak corresponds to liberated residual IPA. The appearance of this characteristic secondary peak (Rt≈8.56 min) serves as an analytical indicator of reprocessed PET content. During mechanical recycling, repeated thermal cycles and moisture-induced hydrolysis promote chain cleavage, releasing esterified IPA co-monomer units into free or low-molecular-weight oligomeric forms that are readily extracted and identified during derivatization.

3.3. Toxicological and Regulatory Considerations

It is critical to distinguish between total internal residual content (wt%) and specific chemical migration limits (SML) into contacting media. Regulatory frameworks (e.g., EU Commission Regulation No 10/2011) mandate that compliance for food-contact plastics be determined by mass transfer into liquid simulants rather than total constituent concentrations within the polymer matrix (7, 8). While internal concentrations of IPA average 2.00 wt%, actual health hazards depend on migration rates under intended conditions of use. Consequently, quantitative identification of IPA serves primarily as a quality and structural marker rather than direct evidence of toxicological non-compliance.

4. Conclusions

Gas chromatographic characterization following depolymerization and derivatization provides a reliable analytical method for evaluating co-monomer concentrations and processing history in polyethylene terephthalate (PET) materials. The quantitative analysis established a baseline average isophthalic acid (IPA) content of 2.00 wt% across common commercial food-contact packaging. Furthermore, comparative chromatographic profiling demonstrated clear differentiation between virgin and recycled matrices based on the presence of a characteristic residual IPA peak at retention time (R_t)=8.565 min in reprocessed samples. This analytical protocol

provides a useful approach for material verification, quality control, and supply chain audit within circular polymer manufacturing.

Conflict of Interest

The authors declare no competing financial or personal interests.

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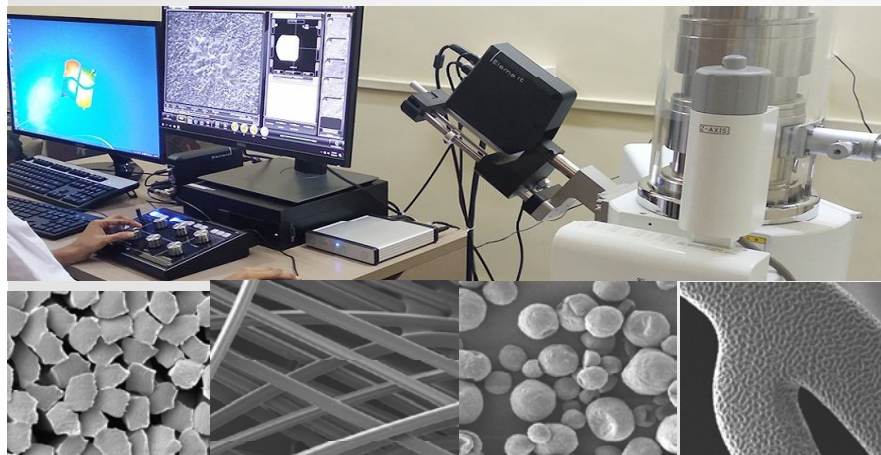
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In BTRA, advanced new JEOL JSM IT 200 LV SEM machine (Japan) have magnification capabilities ranges from 10X to 3,00,000X and resolution of about 10 nm. The surface view and cross-sectional view of the sample can be easily seen. In addition, the elemental composition and mapping of any solid material can be carried out by EDAX (U.S.A.) energy dispersive X-ray spectroscopy (EDS).

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