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Innovation in Active Packaging: Biodegradable PBAT/Molybdenum Oxide Systems with Nanoparticles for Microplastic Reduction

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Abstract

This study proposes the development of nanocomposite films based on poly (butylene adipate-co-terephthalate) (PBAT) incorporated with different concentrations of molybdenum trioxide (MoO_3) for use in biodegradable packaging. The films were produced by extrusion followed by calendering and characterized using Fourier-transform infrared spectroscopy (FTIR), time-domain nuclear magnetic resonance (TD-NMR), water activity (aW) analysis, and contact angle measurements. FTIR results indicated physical interactions between the polymer matrix and the nanoparticles, particularly in the carbonyl group region. TD-NMR analysis revealed restricted molecular mobility of the PBAT chains in samples with lower MoO_3 content, suggesting good nanoparticle dispersion. Water activity decreased with increasing MoO_3 concentration, indicating improved barrier properties. Contact angle measurements showed that the formulation with 0.1% MoO_3 exhibited greater hydrophilicity, due to the generation of more heterogeneous materials, which is in agreement with the TD-NMR measurements. The results suggest that controlled incorporation of MoO_3 can enhance the structural and functional properties of PBAT, reinforcing its potential as a material for active and sustainable packaging.

Keywords

PBAT, MoO_3, Nanocomposites, Biodegradability, Active Packaging, Moisture Barrier

1. Introduction

The growing concern over the environmental impact caused by plastic waste has driven the search for innovative alternatives in the packaging sector [1]. The accumulation of materials derived from non-degradable synthetic polymers poses a serious environmental issue, encouraging research into biodegradable materials that can replace conventional packaging. In this context, nanotechnology represents an important technological frontier for improving biodegradable polymers, enabling the development of high-performance applications such as active packaging [2].

Among biodegradable polymers, poly (butylene adipate-co-terephthalate) (PBAT), a fully biodegradable aliphatic-aromatic polyester, has gained attention due to its flexibility and ability to decompose under appropriate environmental conditions [3]. Although it exhibits low resistance to water vapor transmission, PBAT offers a remarkable oxygen barrier, superior to that of low-density polyethylene (LDPE). These characteristics make PBAT a viable and accessible alternative to conventional petrochemical-based polymers [4]. PBAT combines good biodegradability—attributed to the aliphatic units in its molecular chain—with excellent mechanical properties derived from its aromatic components [5].

Nanotechnology has shown great promise for enhancing the properties of polymers and expanding PBAT applications. Shankar and Rhim [6] developed three different types of zinc oxide nanoparticles (ZnONPs) and incorporated them into PBAT nanocomposite films. The resulting films showed improvements in optical and mechanical properties and demonstrated strong antimicrobial activity. In addition, PBAT-based films containing silver nanoparticles (AgNPs) were synthesized [7] showing enhanced mechanical strength and water vapor barrier, making them promising for UV-barrier and antimicrobial packaging.

Molybdenum trioxide (MoO_3) is an inorganic material with antioxidant, antimicrobial, and gas barrier properties [8], making it a promising additive for polymer matrices [9]. Moreover, the structural reinforcement provided by these nanoparticles can reduce polymer fragmentation during degradation, minimizing microplastic formation [10].

Recent studies have highlighted the potential benefits of incorporating MoO_3 into biodegradable polymer matrices, with applications in photocatalysis, antimicrobial activity, and environmental remediation. Fakhri and Afshar Nejad [11] reported the antimicrobial, antioxidant, and cytotoxic properties of MoO_3 nanoparticles, as well as their effectiveness in ketamine degradation under varying light conditions. Regarding PBAT, da Rocha *et al.* [12] found that the incorporation of MoO_3 increased the opacity of the materials, which may protect packaged goods and enhance photooxidative degradation.

Therefore, this study aims to propose a nanocomposite formulation using PBAT as the polymer matrix and MoO_3 as the nanoparticle, and to analyze material properties relevant to the technical and environmental performance of active food packaging and the potential to reduce microplastic generation in the environment. The new packaging should be compostable.

2. Methodology

2.1. Materials

The polymer matrix used in this study was poly(butylene adipate-co-terephthalate) (PBAT), supplied by BASF S.E. under the commercial name Ecoflex® F Blend C1200. This polymer has a density between 1.25 and 1.27 g/cm^3 at 23˚C, a melt flow index ranging from 2.5 to 4.5 g/10 min, and a melting point between 110 and 120˚C. PBAT was used in the form of white pellets with an average diameter of approximately 5 mm. Molybdenum trioxide (MoO_3, 99.5%) was purchased from Sigma-Aldrich®.

2.2. Preparation of Nanocomposites

The nanocomposite films were prepared by incorporating MoO_3 nanoparticles into PBAT at different concentrations (0.1%, 0.3%, and 0.5% w/w). These concentrations of MoO_3 were selected based on preliminary tests and previous literature reports [12] indicating that low concentrations of metal oxides can provide significant functional effects—such as antimicrobial activity—without compromising the polymer matrix. These specific concentrations allowed the authors to investigate the threshold at which functional improvements occur while maintaining desirable mechanical and optical properties, as well as ensuring homogenous dispersion of the nanoparticles.

Initially, PBAT was ground in a knife mill and mixed with the nanoparticles in a V-mixer for 30 minutes to ensure proper homogenization of the solid phase. The mixtures were then processed by extrusion in a single-screw mini-extruder (model 1626, Ax Plásticos), equipped with a calendering system for direct film production. The extrusion process was carried out at 60 rpm, with the following temperature profile in the heating zones: 115˚C (zone 1), 112˚C (zone 2), and 103˚C (zone 3). The speed of the calendering rolls was adjusted to 48 rpm.

2.3. Film Characterization

2.3.1. Fourier Transform Infrared Spectroscopy (FTIR)

The films were characterized by chemical interactions and structural modifications using FTIR spectroscopy, employing a Nicolet iS5 spectrometer (Thermo Scientific) coupled with an attenuated total reflectance (ATR) accessory. The spectra were recorded directly on the films in the 4000 - 500 cm^{-1} range, with a resolution of 4 cm^{-1} and 60 consecutive scans per sample.

2.3.2. Time-Domain Nuclear Magnetic Resonance (TD-NMR)

Longitudinal relaxation (T_1) analyses were performed using low-field NMR on an MQ spectrometer (Oxford Instruments), with a hydrogen nucleus observation frequency of 23 MHz. The inversion-recovery pulse sequence was used to determine the T_1 distribution, allowing insight into the molecular dynamics of the samples. For the analysis of structural rigidity and matrix homogeneity, the Magic Sandwich Echo (MSE) sequence was also employed, focusing on transverse relaxation times (T_2*).

2.3.3. Water Activity (aW) Measurement

The water activity of the films was determined using an AquaLab 4TE (METER Group LatAm Ltda) device, operating with a dew point system at 20˚C. All water activity (aW) tests were performed under controlled and consistent storage conditions. Samples were stored in a temperature—and humidity-controlled environment to avoid fluctuations that could influence aW measurements. This ensured the reliability and reproducibility of the results throughout the analysis.

The films were analyzed without prior preparation. The obtained aW values were compared to the recommended limits for inhibiting microbial growth, considering 0.90 aW as the upper limit for pathogenic bacteria and 0.60 aW as the safe maximum for most microorganisms [13].

2.3.4. Contact Angle Measurement

The surface wettability of the films was assessed by measuring the static contact angle with distilled water using an OCA 15EC (Dataphysics Instruments) system. Three droplets were applied to different regions of each sample, and the average values were used for analysis. The results were classified according to the literature: angles below 90˚ indicate hydrophilic surfaces, while values above 90˚ indicate the formation of more hydrophobic surfaces [14].

3. Results and Discussion

3.1. Fourier Transform Infrared Spectroscopy (FTIR)

The structural characterization of the samples was performed using Fourier Transform Infrared Spectroscopy (FTIR), as illustrated in **Figure 1**. The spectrum of pure PBAT displayed the characteristic bands of the polymer's copolyester structure. Among them, the intense band at approximately 1715 cm^{-1}, attributed to the C=O stretching vibration of the ester groups, stands out. In the 2950 - 2850 cm^{-1} region, bands corresponding to the stretching of the methylene groups ($–CH_{2}–$) can be observed, while the band between 1260 - 1240 cm^{-1} is related to the C–O stretching vibrations of the ester groups. The band around 730 cm^{-1} can be attributed to the out-of-plane bending of the aromatic rings, confirming the presence of the terephthalic segment in the PBAT structure.

With the incorporation of MoO_3 small changes in the intensity and relative position of some bands were observed, particularly in the 1715 cm^{-1} region [15]. At concentrations of 0.1% and 0.3%, this band showed a slight shift and reduced intensity, which may indicate multiple interactions between the carbonyl groups of the matrix and the surface of the metal oxide. The attenuation of this band in the sample with 0.5% MoO_3 strengthens this hypothesis, suggesting that the presence of the nanofiller may limit the mobility of the polymer chains through physical interactions with the polymer. Furthermore, no additional bands specifically attributed to MoO_3 were observed, which is in agreement with the literature, as this metal oxide does not form direct covalent bonds with the polymer matrix [16].

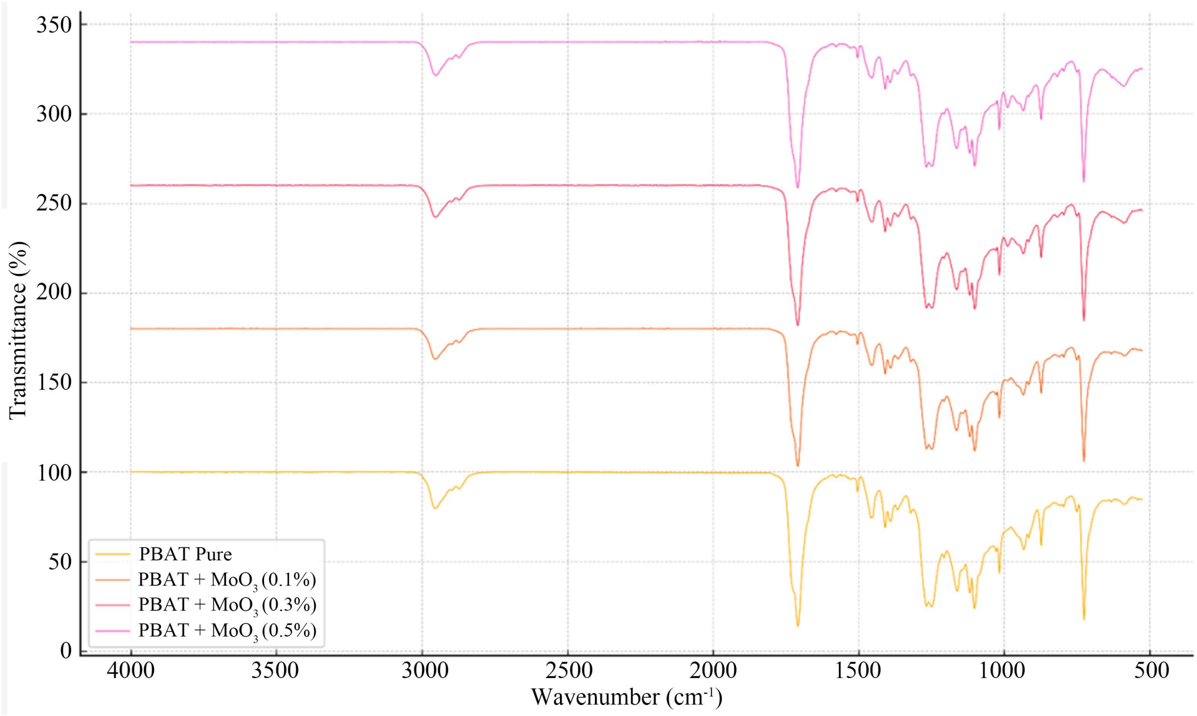

Figure 1. A series of FTIR spectra of PBAT/MoO_3 at different proportions.

3.2. Time Domain Nuclear Magnetic Resonance (TD-NMR)

The TD-NMR technique was employed to investigate the molecular mobility of the polymer chains and the interaction between the PBAT matrix and molybdenum trioxide (MoO_3). The longitudinal relaxation times (T_1) obtained for the different samples are presented in **Table 1**. The pure PBAT film exhibited two distinct T_1 populations, with average times of approximately 4 ms (water aborbed) and 62 ms (main domain) and a small third one related, probably to a small portion of an extreme rigid phase induced by the metal oxide; indicating the presence of regions with different degrees of mobility, ranging from more mobile domains to highly crystalline regions [12].

Table 1. Values of relaxation time data from the materials formed.

Sample			T_1 H (ms)	
			Main domain	
PBAT	4		**62**	1888
PBAT Mo_2O_3 (0.1%)	2.5	9.5	**61**	1156
PBAT Mo_2O_3 (0.3%)	7		**60**	
PBAT Mo_2O_3 (0.5%)	4		**55**	1680

With the incorporation of 0.1% MoO_3, a shift in the T_1 distributions towards shorter times was observed compared to pure PBAT (2.5 ms, 9.5 ms, with the main domain relaxation centered in 61 ms, and small domain located at 1156 ms). This behavior suggests a restriction in the molecular mobility of the polymer chains, possibly due to physicochemical interactions between the matrix and the oxide, such as hydrogen bonding or dipole-dipole interactions. For the intermediate concentration (0.3%), the peaks were concentrated around 7 ms, 60 ms, and 1680 ms, indicating a reorganization of the chains and a relatively efficient dispersion of the nanofiller. The presence of a peak at 60 ms, very close to the value observed in pure PBAT, may indicate the preservation of a fraction of the original matrix organization, while the small domain located at 1680 ms time suggests the formation of a very rigid region, induced by the nanoparticle oxide.

In the sample with the highest concentration (0.5%), the relaxation times returned to values close to those of the pure matrix (4 ms, 55 ms, and 1680 ms), which may be associated with formation of multiple intermolecular interactions between nanoparticle oxide and the matrix. This behavior may be linked to the saturation effect of the filler, where increasing the nanofiller content may not result in greater dynamic restrictions and may even compromise the uniformity of the dispersion [17].

Evaluating the T_2* relaxation parameter from the MSE FID experiment, the results from each fraction are related in **Table 2**.

Table 2. Percentages of each fraction and their respective transverse relaxation times.

Sample	F_r (%)	T_{2^*r} (μs)	F_{sr} (%)	T_{2^*sr} (μs)	F_m (%)	T_{2^*m} (μs)
PBAT	41	20	33	141	26	420
PBAT Mo_2O_3 0.1	34	22	28	119	38	286
PBAT Mo_2O_3 0.3	35	22	34	122	31	317
PBAT Mo_2O_3 0.5	35	22	32	123	33	325

Standard deviation of fractions = ±2%. Standard deviation of times = ±3 μs.

These measurements confirm the results found by T_1H spin-lattice relaxation time, where three domains were found. The Fraction rigid comes from the rigid domain; fraction semi-rigid is related to the main domain and the mobile fraction is associated with water absorbed.

3.3. Determination of Water Activity (aW)

The water activity (aW) of the pure PBAT films and the nanocomposites with different concentrations of molybdenum trioxide (MoO_3) were evaluated to estimate the microbiological potential and the stability of the materials for food packaging applications. The obtained values were: 0.43 for pure PBAT, 0.37 for the formulation with 0.1% MoO_3, 0.38 for 0.3%, and 0.35 for 0.5%. It is observed that all films presented values below the 0.60 limit, considered safe for most pathogenic microorganisms, as established by Abbas Saleh *et al.* [13] and confirmed by recent studies [18]. This characteristic is important for biodegradable packaging, as it contributes to extending the shelf life of food and reducing microbial proliferation.

The incorporation of MoO_3 nanoparticles led to a significant reduction in aW compared to pure PBAT, with the composite containing 0.5% nanofiller showing the lowest value. This behavior can be attributed to the greater interaction between the nanoparticles and the polymer matrix, which hinders the diffusion and retention of water molecules in the system.

3.4. Contact Angle Measurement

The contact angle analysis of the PBAT samples and their nanocomposites with different concentrations of molybdenum trioxide (MoO_3) showed significant changes in the surface wettability of the films, as presented in **Table 3**.

Table 3. Average contact angle values for PBAT films with different MoO_3 contents.

Sample	Contact Angle (˚)
Pure PBAT	88
PBAT + MoO_3 (0.1%)	75
PBAT + MoO_3 (0.3%)	89
PBAT + MoO_3 (0.5%)	86

The analysis of the contact angles showed variations in the wettability of PBAT films with the addition of MoO_3. Pure PBAT exhibited a contact angle of 88˚, indicating a moderately hydrophobic surface. The incorporation of 0.1% MoO_3 reduced the angle to 75˚, suggesting an increase in hydrophilicity. However, higher concentrations of MoO_3 resulted in contact angles of 89˚ (0.3%) and 86˚ (0.5%), indicating a partial reversal of the initial trend. These results align with previous studies. Rocha *et al.* [12] observed that the addition of MoO_3 to PBAT increased the hydrophilicity of the films, as evidenced by the reduction in contact angles. However, higher concentrations may lead to nanoparticle agglomeration, compromising surface uniformity and, consequently, wettability.

The variation in wettability can be attributed to changes in the surface energy promoted by the MoO_3 nanoparticles. At optimal concentrations, they increase the surface polarity, favoring interaction with water. However, at higher concentrations, the formation of agglomerates may create surface irregularities, reducing wettability.

4. Conclusions

The results obtained in this study demonstrated the potential of PBAT nanocomposites containing molybdenum trioxide (MoO_3) for application in biodegradable packaging with enhanced functional performance. The incorporation of nanoparticles directly influenced the structural, dynamic, and surface properties of the films, as shown by the characterization techniques employed.

FTIR analysis indicated possible physical interactions between the polymer matrix and MoO_3, especially in the carbonyl stretching range, suggesting a restriction in chain mobility. This effect was corroborated by the NMR-TD results, which showed significant changes in the longitudinal relaxation times (T_1), particularly in the sample with 0.1% MoO_3, indicating an effective interaction between the additive and the polymer matrix.

The water activity of the films decreased with increasing MoO_3 concentration, indicating a greater barrier to moisture diffusion—an essential parameter for extending the microbiological stability of packaged food. Finally, the contact angle tests revealed that the 0.1% MoO_3 concentration promoted greater surface hydrophilicity, while higher concentrations resulted in a slight return to the initial hydrophobic character, possibly due to nanoparticle agglomeration.

The data suggest that the controlled addition of MoO_3 to PBAT can optimize critical properties for applications in active and sustainable packaging. The formulation with 0.1% nanofiller stood out as the most balanced in terms of structural modification and wettability, pointing to its promising use in systems with a lower environmental impact and potential for microplastic generation mitigation.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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