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Master's Thesis Engineering Technology

Optimizing the functionalization of polypropylene using a photocatalytic UV reactor for enhanced compatibilization in various polymer blends

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INTRO

Polymer blends and composites are an increasingly important area within the plastics industry due to their wide range of potential applications. However, a key challenge is the **lack of interfacial compatibility** between different polymers, which often leads to phase separation and suboptimal material properties. One effective solution is the use of a **compatibilizer**, an additive that **reduces interfacial tension** between immiscible polymers, promoting better dispersion and enhanced material performance [1]. This research explores the functionalization and application of polypropylene grafted with maleic anhydride (**PP-g-MA**) using a **photocatalytic UV reactor** under mild conditions, to develop an efficient compatibilizer for polymer blends and composites that preserves the molecular weight of polypropylene.

Compatibilizer functionalization

For the functionalization process, **maleic anhydride** (MA) was **grafted** onto polypropylene (PP). PP was combined with N-hydroxyphthalimide (NHPI), iron oxide (Fe_2O_3) as a photocatalyst, MA, and a stabilizer, all dissolved in ortho-dichlorobenzene as the solvent. Upon exposure to **UV light** in the reactor (Figure 1), the iron oxide was photoactivated, generating electron-hole pairs. These promoted the conversion of **NHPI** into the phthalimide-N-oxyl (PINO) radical. The **PINO** radicals **abstracted hydrogen atoms** from the polymer backbone, creating polymer radicals. These reactive polymer radicals then reacted with maleic anhydride (MA), forming the compatibilizer depicted in Figure 2 [2].

Figure 1: Reactor

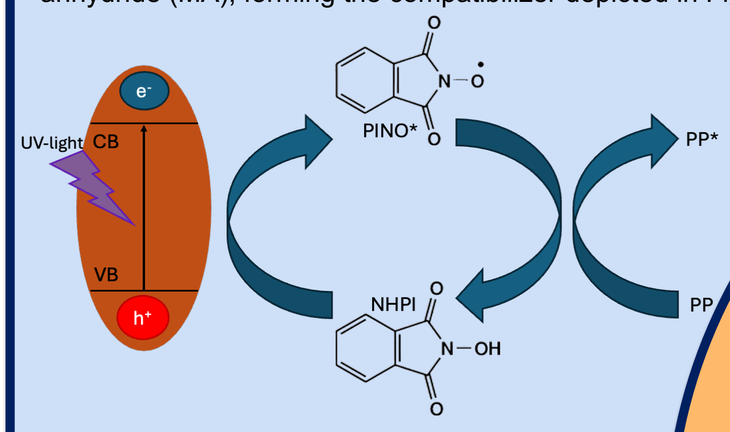
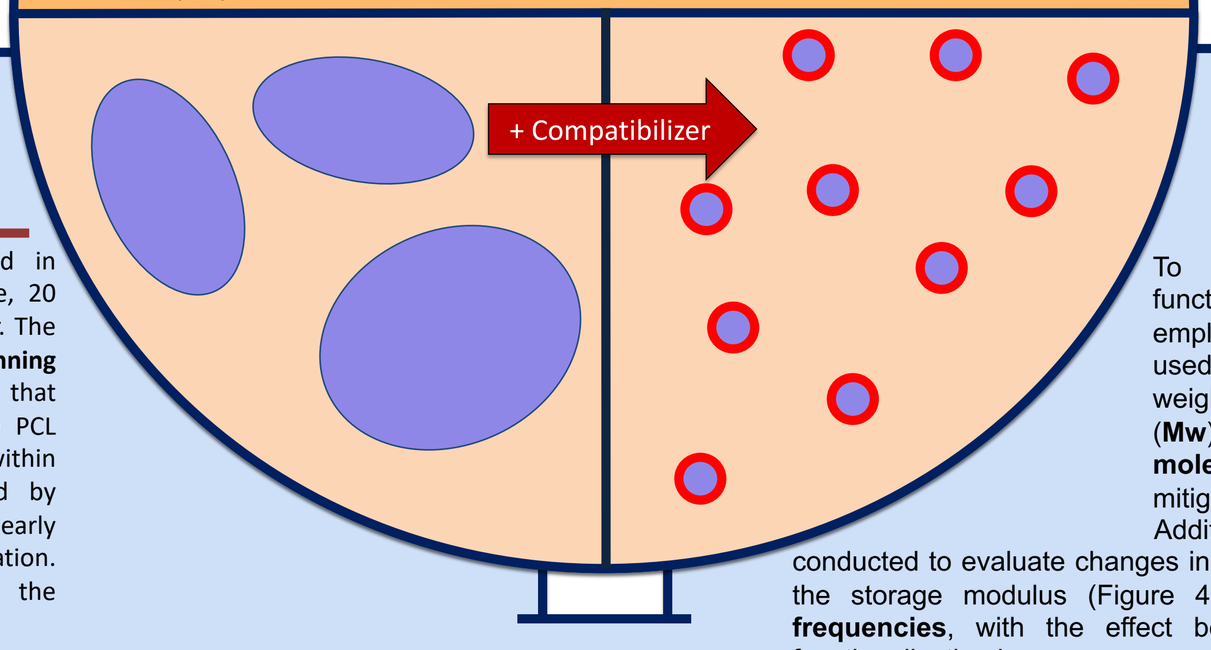


Figure 2: Reaction mechanism

CONCLUSION

It can be concluded that both an **extended reaction time** and a **higher concentration of maleic anhydride** result in a greater grafting degree on polypropylene. This improved functionalization enhances the effectiveness of the compatibilizer in polymer blends. Molecular weight also plays a role. A 1:20 BHT:NHPI ratio seems optimal to minimize the reduction in molecular weight. Blends containing compatibilizers with **higher grafting percentages** and **high molecular weight** demonstrate **better phase dispersion and interfacial adhesion**, which in turn lead to significantly improved mechanical properties of the final material.



Functionalization Confirmation

To evaluate the **success of the functionalization**, both Fourier transform infrared (**FTIR**) spectroscopy and **acid-base titration** were employed. FTIR analysis was used to detect carbonyl peaks around **1750 cm^{-1}**, characteristic of the **carbonyl groups** in maleic anhydride. To obtain a more accurate quantitative assessment, acid-base titration was performed to determine the grafting percentage. As shown in Table 1, **longer reaction times** and **higher MA content** both led to increased incorporation of MA.

Table 1: Grafting percentage for various reaction settings

Reaction time (h)	Added MA (mg)	Grafting (wt%)
1	720	1.71
2	720	1.26
4	720	3.54
20	720	4.45
20	500	2.55
20	1000	6.40

Application in Polymer Blends

Finally, a series of compatibilizers were evaluated in **polymer blends** composed of 75 wt% polypropylene, 20 wt% polycaprolactone (PCL), and 5 wt% compatibilizer. The blend morphology was initially examined using **Scanning Electron Microscopy** (Figure 5-6). The results indicate that when a **more grafted compatibilizer** was used, the PCL phase became more dispersed and **better integrated** within the PP matrix. This effect was further enhanced by **increasing the compatibilizer content**, resulting in a nearly homogeneous morphology with minimal phase separation. Lastly, bending tests were performed to measure the mechanical performance of the blends

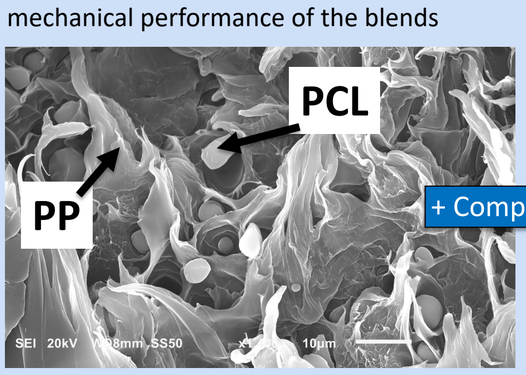


Figure 5: PP/PCL blend without compatibilizer

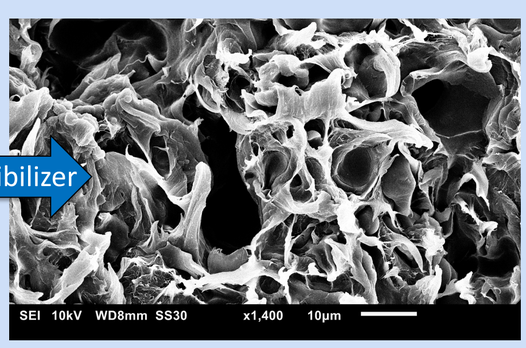


Figure 6: PP/PCL blend with 10 wt% compatibilizer

Effect on Material Properties

To assess changes in the material after functionalization, several analytical techniques were employed. Gel permeation chromatography (**GPC**) was used to observe **changes** in number average molecular weight (**Mn**) and weight average molecular weight (**Mw**). The results (Figure 3) indicate a **decrease in molecular weight** after functionalization, which can be mitigated by increasing the amount of stabilizer.

Additionally, **rheological measurements** were conducted to evaluate changes in **flow behavior**. These measurements reveal that the storage modulus (Figure 4) shows a distinct **upturn at lower angular frequencies**, with the effect becoming more pronounced as the degree of functionalization increases.

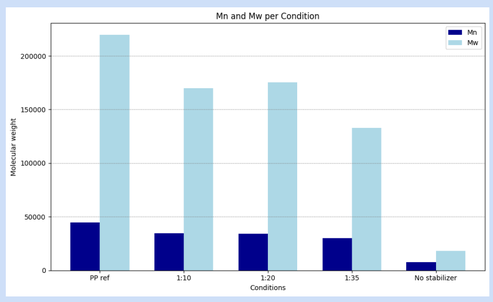


Figure 3: Mw and Mn of different stabilizer amounts compared to standard PP

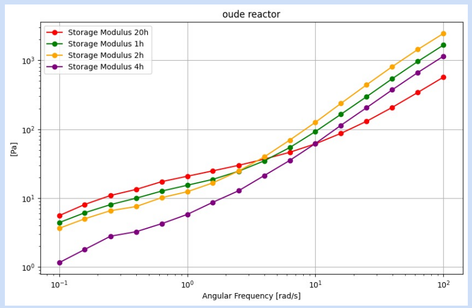


Figure 4: Storage modulus vs. reaction time for various compatibilizers

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[1] L. A. Utracki, "Compatibilization of polymer blends," 2002, *Canadian Society for Chemical Engineering*. doi: 10.1002/cjce.5450800601.
[2] C. Zhang, Z. Huang, J. Lu, N. Luo, and F. Wang, "Generation and Confinement of Long-Lived N-Oxyl Radical and Its Photocatalysis," J Am Chem Soc, vol. 140, no. 6, pp. 2032–2035, Feb. 2018, doi: 10.1021/JACS.7B12928/SUPPL_FILE/JA7B12928_SI_002.PDF.