Enzymatic deinking of LDPE films: Mechanistic insights into surfactant-enhanced catalyzed hydrolysis

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Keywords: Enzymatic deinking, Polyurethane adhesive degradation, Nonionic surfactant-assisted catalysis
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For printed plastic films, the quality of recycled materials is often affected by residual ink and layers related to adhesives. From an industrial perspective, de-inking is not only a cleaning step but also a potential way to improve the availability and value retention of recycled plastics in the recycling material system. Although current de-inking technologies mainly rely on washing, surfactants, solvents or chemical reagents, there are still relatively few studies on selective biocatalytic methods for this type of material. In this research, we combined structure-guided enzyme priority selection, experimental verification, and surfactant-assisted treatment to study the de-inking process of printed single-layer plastic films assisted by enzymes. This study focused on the adhesive structure related to polyurethane as the target layer for selective weakening, aiming to support a more gentle and selective de-inking concept in future plastic film recycling.

In order to establish a reasonable enzyme selection process, the enzymes related to PU were first organized and incorporated into a screening process, which combined sequence comparison, structure alignment, catalytic pocket analysis, and molecular docking. It was not merely based on the docking score, but rather by generating effective conformational analysis to evaluate whether the substrate could adopt a catalytically significant conformation within the active site. This process can prioritize the most promising PU-related scaffolds and support the conversion of reported candidate enzymes into commercially available enzymes for experimental verification.

Based on this structure-oriented workflow, we selected two commercial enzymes - CRL and HiC for further testing. Subsequently, these enzymes were combined with six representative non-ionic surfactants at three concentration levels to treat the printed LDPE films of the PU adhesive for de-inking. The initial screening identified the enzyme-surfactant combination that exhibited the most favorable de-inking effect, and then the selected system was further optimized through response surface design.

The results of both the computational screening and the experimental tests indicate that HiC is more suitable than CRL. In the experimental screening, compared with the use of enzymes alone, surfactants alone, or buffer controls, the combination of HiC and TX114 provided the strongest de-inking effect. Time-dependent film observations further demonstrated that the ink removal effect produced by the HiC–TX114 combination system was significantly better than that of either HiC or TX114 alone, indicating a clear synergistic effect between catalytic action and interface assistance. Response surface optimization indicates that the deinking system is mainly controlled by temperature, followed by the HiC concentration, while the influence of the TX114 concentration is smaller but still significant. Importantly, the significant interaction between HiC and TX114 confirms that TX114 does not act independently but enhances the performance of the enzymatic system.

Overall, this study proposes a framework that combines computation and experimentation to perform de-inking of single-layer plastic films through enzyme-assisted methods. The research results indicate that the prioritization of enzymes based on their structure can support the actual selection of enzymes, and the assistance of non-ionic surfactants, when properly matched with the enzyme system, can significantly enhance the de-inking effect. Particularly, the combination of HiC–TX114 highlights the importance of integrating catalytic activity with interface regulation. Therefore, this work not only provides a screening strategy but also offers a mechanistic basis for developing more selective, milder, and more environmentally friendly de-inking methods for printed plastic films.