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Screening Green Solvents for Multilayer Plastic Films Separation

Ugochukwu M. Ikegwu, Victor M. Zavala, and Reid C. Van Lehn*

University of Wisconsin-Madison, Department of Chemical and Biological Engineering, Madison, Wisconsin, USA.
* Corresponding Author: vanlehn@wisc.edu.

ABSTRACT

This paper introduces a computational framework for selecting green solvents to separate multilayer plastic films, particularly those challenging to recycle through mechanical means. The framework prioritizes the selective dissolution of polymers while considering solvent toxicity. Initial screening relies on temperature-solubility dependence, utilizing octanol-water partition coefficients (LogP) to identify non-toxic solvents (LogP ≤ 3). Additionally, guidelines from GlaxoSmithKline (GSK), Registration, Evaluation, Authorization, and Restriction of Chemical Regulation (REACH), and the US Environmental Protection Agency (EPA) are employed to screen for green solvents. Molecular-scale models predict temperature-dependent solubilities and LogP values for polymers and solvents. The framework is applied to identify green solvents for separating a multilayer plastic film composed of polyethylene (PE), ethylene vinyl alcohol (EVOH), and polyethylene terephthalate (PET). The case study demonstrates the framework's effectiveness in identifying environmentally friendly solvents and balancing trade-offs between solvent toxicity and solubility. Furthermore, the framework informs process design by screening for suitable green solvents in selective dissolution processes, potentially leading to the development of more sustainable dissolution processes and the identification of easily recyclable polymer blends in multilayer plastic films.

Keywords: Plastics Recycling, Green Solvents, Process Design, Life Cycle Analysis, Technoeconomic Analysis, Polymer, COSMO-RS.

INTRODUCTION

Multilayer plastic films have been pivotal in enhancing product safety, security, and handling [1]. These films, mostly comprised of polyethylene (PE), ethylene vinyl alcohol (EVOH), polyethylene terephthalate (PET), polyvinyl acetate (PVA) polymers, etc., serve diverse functions in prolonging the shelf life of food products [2]. Nevertheless, the intricate mix of these polymers complicates the recycling process, resulting in only 5% of multilayer plastic films being recycled in the United States; the rest are disposed of through incineration or in landfills. Various technologies have been utilized for recycling plastic waste, including thermochemical methods such as pyrolysis and thermal oxo-degradation, chemical processes, supercritical fluid application, and mechanical processes, but these processes are often not suitable for multilayer films.

As documented in previous studies, solvent-based separation technologies have exhibited significant potential in recovering virgin resins from multilayer plastic films [3]. An illustrative embodiment of this methodology is the solvent-targeted recovery and precipitation (STRAP™) process introduced by Walker et al. [4]. This approach systematically segregates the polymer constituents of multilayer plastic films by employing selective solvents, capitalizing on the temperature-dependent solubility of polymers in solvents, anti-solvents, or a combination of both, as expounded by Sánchez-Rivera et al. [5]. A critical step in achieving this separation lies in the solvent screening, which serves as the linchpin of the entire procedure. Therefore, prediction of temperature-dependent polymer solubility is a critical requirement. To address this need, molecular-scale models have been harnessed to expediently predict the temperature-dependent solubilities of various plastic components,

including but not limited to PE, EVOH, PET, and PP, across a spectrum of ~1000 solvents [6]. This was realized by modeling polymers as short oligomers, employing molecular dynamics simulations, and the COnductor-like Screening MOdel for Real Solvents (COSMO-RS), grounded in quantum chemistry principles for solubility determinations.

Furthermore, establishing a predictive framework for polymer solubility, as elucidated by the researchers mentioned above, underscores the influence of selective solvent availability in shaping the sequence of polymer resin recovery. This, in turn, informs the design of the overall process and its associated economic and environmental implications.

In addressing critical environmental challenges, deploying solutions like STRAP™ is essential. However, it is imperative to mitigate the emergence of new toxic waste streams proactively. In dissolution-based recycling methods, solvents typically remain unconsumed. Nonetheless, over repeated usage, minute quantities of these solvents tend to escape into the environment or are deliberately disposed of, potentially creating new waste streams. The ecological impact of such waste streams can be substantial when the solvents in question possess toxic attributes. Moreover, using toxic solvents may pose risks to the safety of operation personnel. Therefore, it is crucial to incorporate process safety and toxicity considerations in selecting solvents, influencing both process design and economic factors [7].

Numerous investigations have sought to elucidate the concept of "green" solvents within the framework of green chemistry principles. Saleh and Koller [8] characterize green solvents as those possessing low reactivity and flammability, exemplified by ionic liquids, per the 12th principle of green chemistry. Choi et al. [9] initially identified natural deep eutectic solvents (NADES) and deemed them environmentally friendly due to their derivation from plant sources.

Considering these different perspectives of green solvents, as discussed in the literature, Figure 1 depicts the ideal green solvent and its life cycle. This ideal green solvent, designed to harmonize sustainability and technical efficiency, should ideally originate from a renewable source, notably plant-derived solvents, and maintain cost-effectiveness as a fundamental criterion. Its utility in dissolution-based procedures should also be distinguished by enhanced solubility and reduced energy consumption, exemplifying its advantageous influence on process efficacy. It should also have benign health, safety, and environmental hazards throughout its life cycle. It should also be easily recyclable and biodegradable for disposal. Although it is necessary to find an ideal green solvent that satisfies all these criteria, it is difficult to achieve these metrics.

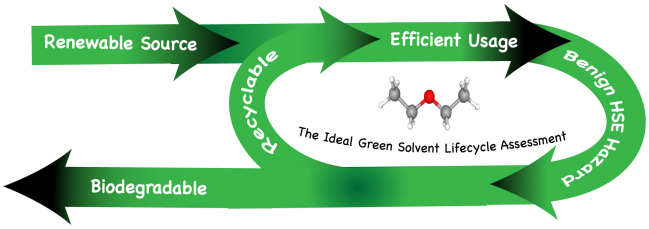

Figure 1. The Ideal green solvent.

The assessment of solvent greenness is subject to variations in ranking based on the chosen metrics. This was demonstrated by the different perspectives considered by the authors mentioned above to classify solvents as green. Nevertheless, Hessel et al. [10] assert that the principal objective of green solvents should be the mitigation of health, safety, and environmental risks. Therefore, it is vital to adopt a holistic approach in screening solvents for specific purposes, hence this study. To date, no existing study in the literature has formulated a comprehensive framework for the systematic evaluation and selection of environmentally friendly solvents designed explicitly for the separation of multilayer plastic films.

Therefore, in this study, we aim to develop a fast green solvent-screening framework for separating multilayer plastic films into virgin resins that considers solvent solubility and toxicity and how they impact process design and economics. Although this framework was developed in the context of multilayer plastic film separation, it can be extrapolated to any dissolution-based process. This work also elucidates the need to redesign multilayer plastic films, accounting for the ease of recycling food packaging materials. It also motivates the development of new green solvents to separate multilayer plastic films.

FRAMEWORK DEVELOPMENT

As previously detailed, this study introduces a multistep framework for the fast screening of green solvents in the context of efficiently separating multilayer plastic films into their respective virgin resins, as depicted in Figure 2. The framework starts by predicting solubilities in various solvents at a standard temperature of 120 °C to avoid the thermal degradation of the polymer while providing adequate temperature leeway to achieve optimal solubilities, as per Zhou et al. [6]. While steps (2) through (5) pertain specifically to selective dissolution-based procedures conducted at standard atmospheric pressure, other aspects of this framework are generalizable to solvent-based processes.

Solubility Prediction and Octanol-Water Partition Coefficient (LogP)

In this investigation, we employed the solubility prediction framework introduced by Zhou et al. [6] to predict the solubilities of target polymers in ~1000 solvents at

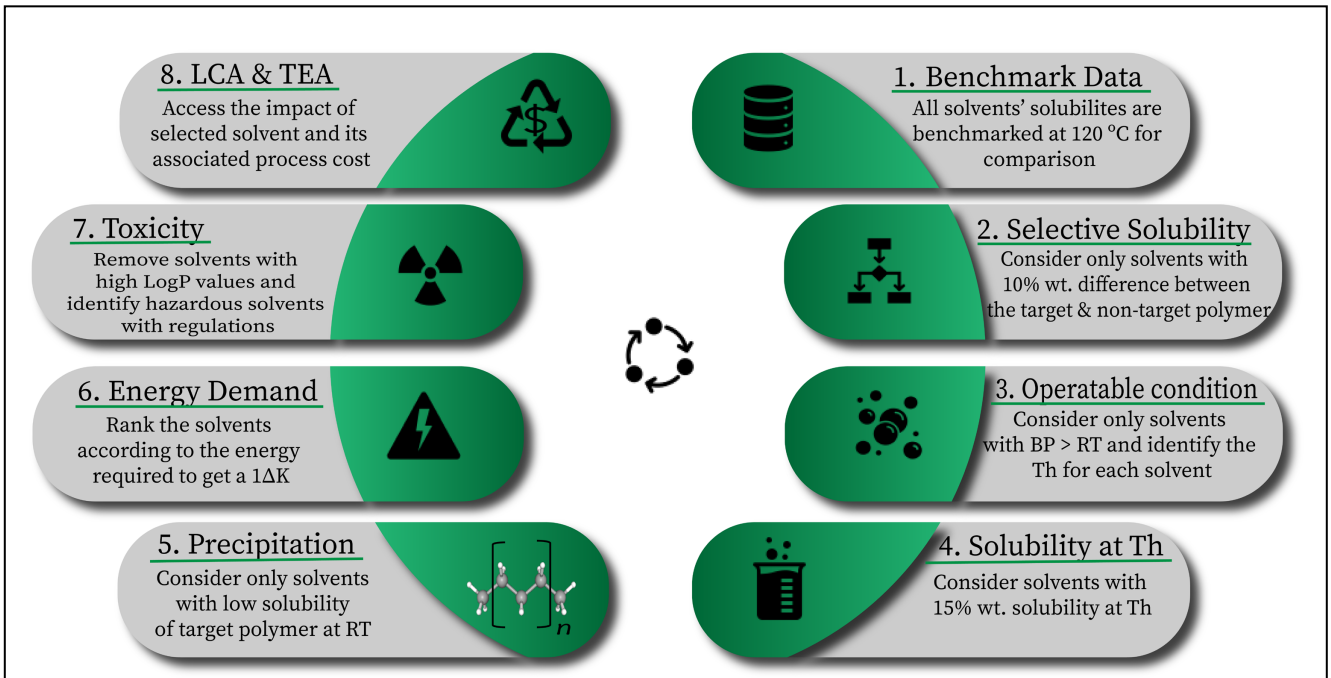

Figure 2. Green solvent selection framework for separating multilayer plastic films.

120 °C. The target polymers were first modeled as short oligomers in reference solvents using molecular dynamics simulations to obtain different conformational structures. These conformations in the form of trajectories are then optimized and served as inputs into COnductor-like Screening MOdel for Real-Solvents (COSMO-RS) to predict the temperature-dependent solubilities at infinite dilution as described in detail by the authors mentioned above.

The octanol-water partition coefficient (LogP) gives information about a solvent's tendency for bioaccumulation. It is often described as the ratio of concentrations of a chemical in a mixture of octanol (hydrophobic or nonpolar phase) and water (hydrophilic or polar phase) in equilibrium. This study employed the COSMO-RS method to predict the LogP values of all solvents.

Solvents with LogP > 0 are considered lipophilic and hence have the possibility of bioaccumulation, while solvents with LogP < 0 are considered hydrophilic. Although solvents with LogP > 0 are generally not regarded as green solvents due to their possibility of bioaccumulating in mammals and aquatic life, this study considered solvents with LogP ≤ 3 as an initial screening process. This choice was to assess the trade-offs among the different selected solvents.

Fast green solvent screening

Having benchmarked the solubilities of all target polymers in all solvents and computed the required molecular properties described in the preceding sub-section, python-based data analytical techniques were employed to screen for green solvents quickly. To ensure selective solubility, the solubility difference between the target polymer and other polymers in the multilayer plastic films must be greater than 10 wt.%.

Furthermore, the solvents having boiling points lower than room temperature (RT) were removed. This rule only applies to processes that wish to operate at standard atmospheric pressure. Similarly, the elevated temperature (Th) was set to a degree less than the solvent's boiling point to maintain this operating condition. Solvents with at least 10 – 15 wt.% at Th are then selected. This solubility range has been identified to be reasonable for multilayer plastic film separation [7]. To recover the dissolved layer after hot filtration, the solvent must exhibit low solubility of the target polymer at room temperature for easy precipitation [5]. To assess the first environmental impact of the selected solvents, the minimum energy required by each solvent was determined using Equation 1, and these solvents were ranked accordingly.

$$Q = m\, C_p\, \Delta T \tag{1}$$

$m(g)$ denotes the mass of solvent, $C_p(J/gK)$ denotes the heat capacities of the solvents at the operating temperatures, and ΔT is the temperature difference between room temperature and the elevated temperature. Furthermore, solvents with LogP greater than three were removed since these would have a high bioaccumulation tendency. Further solvent screening was subsequently done using data from publicly available industrial solvent selection guidelines. Finally, an LCA and TEA analysis will be done within a process such as STRAP™ to assess the environmental impact and the associated process cost

attached to each selected solvent.

Solvent toxicity database and regulatory framework

Using a toxic solvent in any solvent-based process runs beyond contributing to the inefficiency of the process. It constitutes the most significant environmental burden to processes resulting from its energy demand and end-of-life fate. This observation has led to different societies and companies developing quantitative toxicity metrics for common solvents as a guide for solvent selection. These guides mostly contain the environmental implications of each solvent's usage. Some of these include guides developed by GlaxoSmithKline (GSK) [11], the ACS Green Chemistry Institute Pharmaceutical Roundtable (ACS GCI-PR) [12], and AstraZeneca (AZ) [13].

The GSK guideline categorized 111 solvents with over ten primary functional groups under six headings. These categories include wastes, environmental impact, health, flammability, reactivity, and life cycle. Scores between 1 and 10 were given to each solvent, with 1 indicating the solvents with the most concern and 10 indicating the solvents with the least concern. Two extra categories were included to classify solvents based on legislation and restriction bans placed by the Environmental Health Services (EHS). Conversely, AZ and ACS GCI-PR guidelines categorized 46 and 63 solvents, with a score of 10 indicating the solvent with the most concern and 1 with the least concern. Although these guidelines contain different metric categories, they all seek to rate solvents based on the Health, Safety, and Environment (HSE) metrics.

This study employed only the GSK solvent guideline because it contains the most solvents, covers the HSE metrics, and includes the legislation and regulatory ban information about some solvents. Although the GSK guide can be used with other guides, the difference in the meaning of the rank assigned to each solvent makes it more difficult. Moreover, using these guides is not the sole toxicity check in this framework, as these guidelines do not contain information about most of the solvents in our database. Hence, other solvent regulatory standards are considered.

The Registration, Evaluation, Authorization, and Restriction of Chemical Regulation (REACH) initiative, a European Union regulation, focuses on limiting the adverse effects of chemicals on human health and the entire ecosystem [14]. This initiative guides the use of solvents both for large-scale processes and our day-to-day lives. This initiative also places restrictions on both common and uncommon chemicals. For example, as of the period of conducting this study, benzene and toluene were enlisted on the list of restricted substances under the REACH [15]. Similarly, the US Environmental Protection Agency (EPA) aims at securing human lives and the environment from toxic chemicals. The Toxic Substances Control Act (TSCA), established in 1976, provides the EPA with the authority to demand full disclosure of any process relating to chemical substances and mixtures [16].

Furthermore, as of the period this study was conducted, common chemicals like toluene, formamide, and fluorine were included in the list of chemicals covered by the Toxic Release Inventory (TRI) [17]. Processes that use chemicals in this list are generally required to disclose their operations due to their toxicity. Other chemical regulatory frameworks include the Chemical Hazards and Toxic Substances (OCHA) framework, which strives towards similar goals, but rather than enforcing restrictions on chemicals, this framework implements operational standards and handling of chemicals to ensure safe working conditions for personnel.

This study will use the REACH and EPA TSCA solvent list of concern to access the selected solvents from the automated screening process.

Process Economics and Environmental Impact Assessment

Techno-economic analysis (TEA)

A techno-economic analysis is done to assess the process cost associated with using a choice solvent within the context of the selected process. This will determine the minimum selling price of the recovered polymer. As illustrated in Figure 1, the ideal solvent must exhibit high efficiency. This translates into a balance across different metrics mentioned in previous sections and process costs. The TEA is done on BioSTEAM, an open-source python-based steady-state process simulator that has been benched marked against existing proprietary software like Aspen Plus [18]. The choice of solvent for multilayer plastic film separation can also inform the dissolution sequence. Hence, the TEA of all possible sequences will be evaluated to consider all scenarios and assess the trade-offs. Although this TEA does not include the process cost associated with the process safety equipment needed for each choice solvent, this can be introduced to this framework in future studies.

Life Cycle Assessment (LCA)

The impact of using each chosen solvent within the multilayer plastic film separation process on the environment and climate (kg CO_2 eq.) will be measured using an LCA methodology. For simplicity, the functional unit considered in the LCA is the production of 1 kg of multilayer plastic film. Thus, we compare the impact of producing 1 kg of ML film using some choice solvents. BioSTEAM will also be used to perform this assessment. The case study will describe more details of the method employed. This framework does not include accessing the full Life Cycle

Assessment (LCA) of each solvent outside the context of the dissolution process. However, it can be incorporated as an additional step, demonstrating the adaptability of this framework.

RESULTS AND DISCUSSION

As described earlier, STRAP™, a solvent-based process, has been identified as a state-of-the-art technology for separating complex waste plastics containing multiple polymers as components. Moreover, three different variations of this technology have been developed [5]. STRAP™-A is anti-solvent dependent, whereby solvents and antisolvents dissolve and precipitate the polymer layers. STRAP™-B relies on the solubility dependence on temperature whereby after dissolution occurs at an elevated temperature, the polymer solution is cooled to precipitate the polymer. STRAP™-C employs both anti-solvent and temperature to achieve a similar purpose.

Munguía-López et al. [19] quantified the environmental impact of all three variants using the LCA tool to evaluate the carbon footprint, energy use, water use, and toxicity. It was observed that STRAP™-B (temperature dependent) when applied to a multilayer plastic film manufactured by Amcor, had the best metrics among the three variants. This STRAP™-B variant was also compared to the environmental impact of producing virgin films and outperformed fossil-based virgin films on all metrics. Hence, as this work also focuses on driving a sustainable process, STRAP™-B is adopted as a case study to elucidate the strength of this framework. The STRAP™-B process schematic can be seen in the study mentioned above.

This study delineates two distinct scenarios originating from a systematic, bottom-up approach. The first scenario focuses on selecting a green solvent to separate a two-component system comprising EVOH-PET plastic film. Subsequently, the second scenario pertains to selecting a green solvent for separating a three-component system, specifically involving PE-EVOH-PET plastic film. However, in this paper, only the former scenario will be presented. As depicted in Figure 2, the framework's initial phase involves assessing solubility data for all polymers and solvents at a temperature of 120 °C.

Two-component system (EVOH-PET)

Selective dissolution and precipitation

In alignment with the separation sequence outlined by Sánchez-Rivera et al. [5], our objective is to identify green solvents suitable for the selective dissolution of EVOH (ethylene vinyl alcohol) from a composition of EVOH-PET (polyethylene terephthalate) polymer blend. To ensure the targeted dissolution of EVOH, solvents exhibiting a minimum of 10 %wt. difference in solubility between EVOH and PET at 120 °C were retained. This initial screening resulted in the identification of 116 potential solvents.

Subsequently, we narrowed our selection to solvents amenable to operation at atmospheric pressure, i.e., those possessing boiling points above room temperature. This criterion led to the exclusion of 19 solvents, resulting in a remaining pool of 97 solvents. We then determined each solvent's elevated temperatures (Th) and selected only those exhibiting a minimum of 15 %wt. solubility at Th to ensure the solubility of EVOH. This refinement further reduced the solvent list to 56 candidates. To facilitate subsequent precipitation processes, we further refined our selection by retaining only those solvents with less than 2% weight solubility of EVOH at room temperature (RT). Consequently, the number of viable solvents was reduced to 45.

Energy Demand Evaluation

The minimal energy requirements for each of the 45 solvents were calculated using Equation 1. A representation of some solvents' respective minimum energy requirements is presented in Figure 3. The x-axis of Figure 3 denotes solvents, with each letter signifying a specific solvent and its EVOH solubility at Th in brackets. Although higher energy requirement equals higher carbon emissions, solvents were not screened solely based on energy demand. However, they were considered when quantifying the trade-offs amongst all the green metrics.

Toxicity Evaluation

Partition coefficients were next computed to remove solvents with a LogP greater than 3, indicating a propensity for bioaccumulation. Nevertheless, the solvent count remained at 45, and we performed additional screening steps 6 through 8. Furthermore, we aimed to identify solvents with less environmental concerns and regulations. For example, dimethyl formamide (DMF), ethylene glycol monomethyl ether, N,N-dimethyl acetamide, N-methyl formamide, and N-methyl-2-pyrrolidone all have restrictions placed on their usage by the United States Environment, Health, and Safety (EHS) [11]. However, as earlier mentioned, the GSK solvent guideline does not contain all ~1000 solvents studied in this work. Hence, other solvent guides/restriction lists are queried to screen the selected solvents further.

As shown in Figure 3, dimethyl sulfoxide (DMSO) fulfills the selective solubility criteria of this separation process. This observation agrees with the solvent screening process done by Walker et al. [4], showing that DMSO fulfills the selective solubility criteria without necessarily considering its HSE concerns. However, this study's framework considers solvent toxicity. Furthermore, as

Table 1: Selected candidate solvents for EVOH dissolution and its associated hazards

S/N	Solvent Name	Hazard	Flash Point (°C)	Operating Temp (°C)	Melting Temp (°C)	Solubility (% wt.)	LogP (-)	Energy (J/g)	Note
1	4-Ethyl Phenol	Corro-sive	104	120	46.0	18.2	2.3	760.5	Used as a flavor in pharmaceuticals.
2	Dimethyl Sulfoxide (DMSO)	Irritant	95	120	18.5	35.3	-1.5	770.3	Used as a pharma-ceutical.
3	Epsilon-Caprolac-tam	Irritant	110	120	70.0	18.3	-0.2	851.1	Used as monomer for plastics and paints.

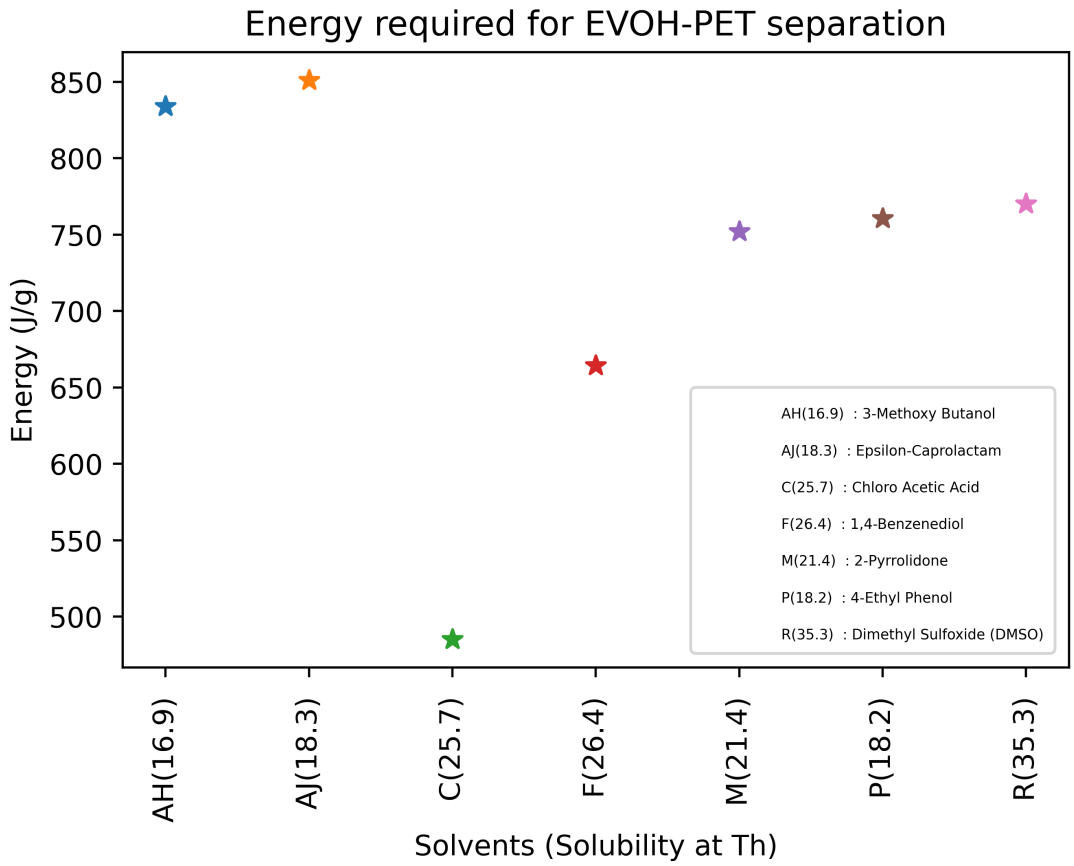

Figure 3. The minimum energy required by selected solvents for EVOH selective dissolution.

human health safety is paramount in any process, solvents that pose human health hazards are strongly discouraged from being considered to avoid trace amounts from contacting food. For example, diethanolamine, Ethylene Glycol Monomethyl Ether, and Hexamethylphosphoramide all pose serious health hazards.

Having considered the various hazards associated with each of the 45 solvents based on the data contained in the GSK solvent guidelines, the PubChem public database, the European Chemical Agency (ECHA), and the Environmental Protection Agency (EPA), three candidate solvents with the least known hazards have been identified as contained in Table 1.

CONCLUSION AND FUTURE WORK

This study presented a fast green solvent selection framework for multilayer plastic film separations. This work uses STRAP™-B, a variant of STRAP™, to elucidate the need to employ this holistic framework to guide green solvent selection. This will eliminate the risk of producing new toxic waste streams associated with solvent-based approaches.

The framework was developed by benchmarking

the solubilities of all target polymers in ~1000 solvents. This was done by adopting a similar solubility prediction workflow developed by previous researchers. This framework comprises two key components: selective dissolution and solvent greenness. This selective dissolution was achieved by ensuring a 10 %wt. difference between the target polymers and the non-target polymer(s). Subsequently, for a solvent to be selected, the solubility of the target polymer must be at least 15 %wt. at elevated temperatures, and its boiling point must be higher than room temperature to ensure its operability at standard atmospheric pressure.

The solvent greenness screening involved quantifying the energy requirement of each solvent and predicting the octanol-water partition coefficients (LogP) to eliminate solvents with LogP > 3. Selected candidate solvents were further subjected to the GSK solvent screening guide and regulatory frameworks such as the REACH and the EPA. The framework's final stage encompassed evaluating each candidate solvent's cost and environmental impact in a dissolution-based process. Furthermore, this framework was applied to a case study involving separating a 3-component multilayer plastic film (PE, EVOH, and PET) employing a two-step dissolution process. Additionally, the framework's robustness was demonstrated by its application in informing the process design of dissolution-based processes.

The case study employed a separation sequence of PE-EVOH-PET. Initial consideration focused on selectively dissolving EVOH from an EVOH/PET polymer blend, followed by PE selective dissolution from a PE/EVOH/PET polymer blend. In the first separation (EVOH), only 45 out of ~1000 solvents could dissolve EVOH selectively. Three solvents with the least hazards were identified through a solvent greenness screening process. While DMSO (770 J/g) demonstrated a lower energy requirement than epsilon-caprolactam (851 J/g), both solvents exhibited promising features, including negative LogP values. Additionally, epsilon-caprolactam is a precursor in plastic production.

We have demonstrated the efficacy of the initial seven steps within this framework for identifying environmentally friendly solvents in separating multilayer plastic films. In our immediate future work, we intend to apply this framework to the selective dissolution of PE from a PE/EVOH/PET polymer blend. Additionally, to demonstrate how this framework informs process design, we will apply this framework to select feasible separation sequences based on the availability of green solvents using a similar multilayer plastic film blend.

Furthermore, we intend to evaluate each solvent's Techno-Economic Analysis (TEA) and Life Cycle Assessment (LCA) in the context of the STRAP™ process. This assessment aims to establish the framework as a green solvent selection tool and a valuable resource for informing process design considerations.

While selective dissolution and LogP screenings offer rapid and automated assessments, solvent selection based on specified guidelines and regulatory frameworks is manual and time-consuming. This underscores the necessity to quantify solvent toxicity numerically, considering the diverse regulations imposed on each solvent. Our future research aims to achieve this, expediting the green solvent selection process.

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