



Project Proposal

Project Title: Green Solvent Selection

Author: Palit, Jasmine

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Project Description:

Existing solutions for recycling multi-component plastic waste often use solvent dissolution and precipitation to separate plastic into the original polymer components for reuse. However, these solvents have historically been toxic and harmful to the environment and human health. The overall aim of this project is to create a method to devise what environmentally friendly solvents will be effective at dissolving certain polymers by incorporating machine learning on polymer thermodynamics and validating with physical testing.

Background:

Certain plastics contain multiple types of polymers—long chains of molecules—in order to benefit from a variety of properties; however, these polymers need to be separated to be reused. Currently, there are minimal processes that use polymer dissolution for plastic recycling, and these solutions often use solvents that are toxic. The goal of this project is to create a method to devise environmentally friendly solvents that will be effective at dissolving certain polymers.

Plastic Waste

Plastic has become an integral part of daily life, due to its wide variety of properties and applications. However, it was estimated in 2015 that 55% of manufactured plastic was discarded, leading to adverse environmental effects (Jiang et al., 2020). Plastics do not break down well in the environment, often requiring methods other than microorganisms to degrade plastic polymers in contrast to other organic compounds. In turn, this leads to pollution and the creation of nanoplastics which can have negative impacts on ecosystems and human health. Plastic waste—through creation and end of life processes—also accounts for around 2% of global CO₂ emissions, furthering environmental costs (Vollmer et al., 2020). Thus, plastic waste in landfills and aquatic environment needs to be reduced in order to protect the health of the planet.

Recycling

Recycling is often used to combat the plastic that has long been piling up in our environment. It was estimated in 2015 that only 20% of plastic waste was recycled (Jiang et al., 2020). Although a wide variety of recycling methods exist, and more are emerging as this problem gets more pressing (Vollmer et al., 2020), it is clear that progress needs to be made to ensure that more waste actually goes through these processes. Not only does non-recycled plastic pollute the environment but not reusing plastic means needing to produce more. Each year, an estimated 400 million tons of greenhouse gases are released into the atmosphere through the production

of new plastics (Shershneva, 2021). Thus, progress needs to be made in the field of recycling to better combat these issues.

Mixed Plastics

One issue with current recycling processes is that they do not always have the capacity to separate polymers. Separation is often necessary for the reproduction of reusable materials that have specific polymer components with different functional characteristics. A specific example of multi-polymer plastic is the multilayer film. Multilayer films are films made of stacked layers of polymers. Their layered structure allows a material to benefit from specific properties from each layer, such as high barriers to gases (Tartakowski, 2010). Over 100 million tons of multilayer thermoplastics are produced each year around the world (Walker, et al., 2020) making up around 17% of global plastic production but often results in a large amount of plastic waste. However, a large majority of these films do not get recycled due to necessary complexities in the recycling process for multilayer films (Adam et al., 2025). Researchers have been forced to look deeper into how to recycle these films; a promising method that could address some of the limitations of existing methods for multilayer plastic film recycling could be solvent dissolution and precipitation.

Dissolution and Recovery of Polymers

Dissolution for the separation of layered polymers is a process that has been implemented before in a multitude of ways. However, they must be separated into their original polymer components to be reused. Solvents have been proven as a successful method in separating the layers, as shown in the method called Solvent Targeted Recovery and Precipitation (STRAP). This process used thermodynamics to dissolve each layer of the film separately and then recover each polymer from its respective solvent (Walker et al., 2020). However, the STRAP process utilizes toxic solvents that could potentially impact the environment and human health.

Toxic Solvents

One of the primary issues associated with using the process of dissolution is the toxicity of the solvents. Commonly, solvents can cause harm due to toxicity in a variety of different ways. They can accidentally or intentionally be released into the environment, risk the safety of those working with them, and potentially remain in the plastics treated with them which go on to be used in industries such as food packaging (Winterton, 2021). The STRAP process defined by Walker et al. (2020) as mentioned above utilized toluene to dissolve polyethylene (PE). However, this solvent is considered toxic and poses a serious health hazard (Ikegwu et al., 2025). Thus, there is a call for more environmentally friendly solvents to be used in recycling processes, especially with PE and PP. Thermodynamic capabilities used in these studies also highlight a pathway that can be used to find suitable solvents for specific polymers, such as the use of Hansen Solubility Parameters (HSPs) (Walker et al., 2020). A new method to identify and validate potential plastic solvents using HSPs and computational and lab-based methods is needed to mitigate the toxicity and improve the use in the recycling industry.

Experimental Design/Research Plan Goals:

IDV: Selected Solvents

DV: How well they dissolve the target polymer

Materials List:

Polymers: PE and PP

Solvents: Unknown until after solvent selection

Pump: Used for dosing specific amounts of solvent

3D Printer: Used to dose solvent as well as print parts for the solvent dosing mechanism.

Procedure:

Goal 1: Collect Solvent Data

Specific: This part of the process includes collecting data such as molecular weight, molecular formula, and SMILES strings. SMILES strings are a format of conveying chemicals which includes information about compounds present as well as bonds. The SMILES strings are then fed into the Mordred molecular calculator to retrieve around 1800 properties for each solvent. Mordred is an API that uses SMILES strings to find molecular properties such as the number of bonds or charge distributions.

Measurable: This goal will be measured by having the data for the solvents.

Achievable: This goal is achievable as I have experience working with Python.

Relevant: This goal is relevant to my project as I need it to train my model, which will then predict the best solvents.

Time-bound: This goal should be (and was) completed before the end of October.

Goal 2: Find most impactful variables

Specific: This goal is specific as I want to know which of the 1800 properties most affect the Hansen Solubility Parameters (HSPs).

Measurable: This goal can be measured by whether the most impactful properties are found.

Achievable: This goal is achievable as I have a background in machine learning as well as access to many resources.

Relevant: This goal is relevant as solvent predictions cannot be made without narrowing down properties.

Time-bound: This goal should be completed by the end of December

Goal 3: Train Model for Predictions

Specific: This goal includes creating a model that will predict HSPs based on SMILES strings.

Measurable: This goal is measurable by testing the accuracy of the model using validation and other metrics.

Achievable: This goal is achievable with the resources I have a background in machine learning.

Relevant: This goal is important to my project as I need to know what solvents will most likely work.

Time-bound: This goal should be completed by the end of January.

Goal 4: Test Predictions

Specific: I will test the chosen solvents on the polymers PP and PE. This experiment will be repeated many times over in well plates to ensure accurate data. I plan to use a modified 3D printer as a dosing mechanism. The printer head will have a pump that takes in specific amounts of solvents and deposits them into a well plate. This process ensures that trials can be repeated many times for accurate data.

Measurable: I will compare these results to the predicted ones to see if my model is accurate.

Achievable: I have access to space and equipment to complete this.

Relevant: This goal is important as it shows that my work is accurate at finding good solvents.

Time-bound: This goal should be completed by the end of March

Risk/Safety Concerns:

Solvents: Since this experiment focuses on green solvents, there is little risk associated with using them.

Data Analysis:

Data will be analyzed in many ways.

For the feature selection, this can be done using regression analysis.

For the model, features like percent accuracy and MSE can be applied.

For the overall project, data can be analyzed by comparing the solubility of the polymers in predicted solutions with whether they should have dissolved or not.

References:

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Timeline:

Goal 1: End of October

- Getting SMILES strings: end of Sep.
- Getting Mordred parameters: end of Oct.

Goal 2: End of November

- Getting basic regression analysis: end of Oct.
- Using Boruta: Thanksgiving break
- Finalizing parameters: end of Nov.

Goal 3: End of December

- Choose model: First week of Dec.
- Preliminary Training Data: December Fair
- Poster: December Fair
- Finalized model: End of December

Goal 4: End of January

- Acquire materials and begin testing: First week of Jan.
- Finish testing: End of Jan.
 - Overall Analysis and Comparisons: Feb. Fair
 - Poster and Written Materials: Feb. Fair