

Project Notes:

Project Title:

Name: Palit, Jasmine

Note Well: There are NO SHORT-cuts to reading journal articles and taking notes from them. Comprehension is paramount. You will most likely need to read it several times, so set aside enough time in your schedule.

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Knowledge Gaps:

This list provides a brief overview of the major knowledge gaps for this project, how they were resolved and where to find the information.

Knowledge Gap	Resolved By	Information is located	Date resolved
HSPs	Muntasir	https://www.hansen-solubility.com/	8/31/25
How polymer dissolution and recovery works	Journal Article	Located in Project Notes	9/12/25
Using pandas the python library	Pandas Library	https://pandas.pydata.org/	9/15/25
What makes a green solvent	Journal Articles and Muntasir	Located in Project Notes	10/7/25

Literature Search Parameters:

These searches were performed between 8/15/2025 and 10/10/2025.

List of keywords and databases used during this project.

Database/search engine	Keywords	Summary of search
Google Scholar	"solvent dissolution"	I ended up using articles from this search listed below (#6)
Google Scholar	"types of polymer recycling"	I ended up finding a lit. Review as listed below.
Google Scholar	"multilayer films recycling"	I found good sources for my project proposal background.
Google Scholar	"green solvent plastic dissolution"	I found a really good article that I will read about modifying the STRAP process to use better solvents.

Tags:

Tag Name	

Article #1 Notes: Title

Article notes should be on separate sheets

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Source Title	
Source citation (APA Format)	
Original URL	
Source type	
Keywords	
#Tags	
Summary of key points + notes (include methodology)	
Research Question/Problem/ Need	
Important Figures	
VOCAB: (w/definition)	
Cited references to follow up on	
Follow up Questions	

Article #1 Notes: How Can AI Researchers Save Energy? By Going Backward.

Article notes should be on separate sheets

Source Title	How Can AI Researchers Save Energy? By Going Backward.
Source citation (APA Format)	von Hippel, M. (2025, May 30). <i>How Can AI Researchers Save Energy? By Going Backward</i> . Quanta Magazine. https://www.quantamagazine.org/how-can-ai-researchers-save-energy-by-going-backward-20250530/
Original URL	https://www.quantamagazine.org/how-can-ai-researchers-save-energy-by-going-backward-20250530/
Source type	Science News Article
Keywords	Reverse Computing, Transistors
#Tags	
Summary of key points + notes (include methodology)	<p>When a computer moves through a process, it deletes information. By doing this, it creates more entropy in the system, as the electrons are moving from known paths to unknown paths. This causes energy to be lost through heat, making the computer less efficient. Today, computer chips cannot get much smaller due to the physical limitations of the materials, but reverse computing is an alternative way to increase efficiency. By reverse computing, the computer goes through the computation backwards, leaving the electrons in a known state and reducing entropy. This idea was first explored by Laudner in 1961, as he realized that deleting data would generate heat. However, he soon gave up on his theoretical pursuit. Bennett proposed this idea again in 1973, but for it to be useful they had to construct chips with transistors that would not lose heat easily. In 1990, a group at MIT began constructing prototype chips with these new efficient transistors. Though these chips worked more slowly, they were able to save energy. Now, Hannah Earley and Frank are working together to create a commercial version of this reversible chip through Vaire Computing.</p>
Research Question/Problem/Need	How can scientists conserve energy in computer chips?
Important Figures	N/A
VOCAB: (w/definition)	<p>Transistor – semiconductor that can be used to amplify or modify electric signals/power</p> <p>Processor – part of computer that manipulates data</p>

Cited references to follow up on	https://ieeexplore.ieee.org/document/5392446 - Irreversibility and Heat Generation in the Computing Process https://dl.acm.org/doi/10.5555/163429.163468 - Practical implementation of charge recovering asymptotically zero power CMOS
Follow up Questions	How will these chips be implemented in computers? What kind of impact will they make on servers?

Article #2 Notes: There's a new acid in our rain — should we be worried? Scientists and regulators are divided over the threat posed by rising levels of a chemical called TFA.

Article notes should be on separate sheets

Source Title	There's a new acid in our rain — should we be worried? Scientists and regulators are divided over the threat posed by rising levels of a chemical called TFA.
Source citation (APA Format)	Lim, X. (2025, July 23). There's a new acid in our rain — should we be worried? Scientists and regulators are divided over the threat posed by rising levels of a chemical called TFA. <i>Nature</i> . https://www.nature.com/articles/d41586-025-02259-6
Original URL	https://www.nature.com/articles/d41586-025-02259-6
Source type	Science News Article
Keywords	TFA, PFASs, Forever Chemicals
#Tags	
Summary of key points + notes (include methodology)	Scientists and researchers have found an increase in trifluoroacetic acid (TFA) across the globe. While TFA is human-made, it can be found in the leaves of trees and ice cores, as well as rain. TFA contains carbon-fluorine bonds which are difficult to break down naturally. TFA is the smallest version or building block of larger chemicals called per- and poly-fluoroalkyl substances (PFASs). PFASs contain longer chains of carbon and fluorine or chlorine, and are extremely difficult to break down. This led scientists to categorize this group as forever chemicals, as they do not

naturally decompose. PFASs are known to be harmful and are banned in some countries. There are also initiatives to clean PFASs out of drinking water. However, while some organizations like the European Chemicals Agency (ECHA) have opened petitions for banning TFA, other organizations like the US Environmental Protection Agency do not consider it a toxic chemical. TFA can come from industrial plants, medications and inhalants, but it does not evaporate with water. The TFA found in rainwater is produced from different gases in the air; some of these precursor molecules can be found in insulation, inhalers, and even anesthetics. Scientists are also going back and forth over how TFA could be produced naturally. While a method for naturally forming TFA has not been discovered, some scientists believe that oceans could harbor this chemical, given that some marine life produced other types of fluorinated molecules. Though TFA is related to PFASs, it does not contain the same long carbon-fluorine chain and has been shown not to be toxic in many studies. Even though there is controversy over the toxicity of TFA, it is clear that the chemical is building up in rivers, plants, and animals to a degree much higher than previously recorded.

Research Question/Problem/ Need

Why is TFA in rainwater and is it toxic?

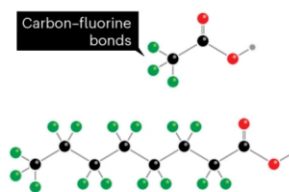
Important Figures

TFA: A CONTROVERSIAL MOLECULE

Levels of the human-made chemical trifluoroacetic acid (TFA) are rising in the environment. The molecule is a fluorinated analogue of vinegar (acetic acid), in which hydrogen atoms in the molecule's tail are replaced by fluorines.

● Carbon ● Fluorine ● Oxygen ● Hydrogen

TFA
By some definitions, TFA is the smallest of the per- and poly-fluoroalkyl substances or PFASs, also known as forever chemicals.



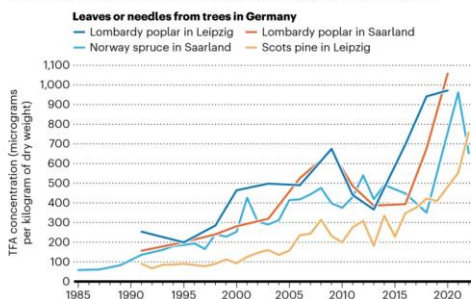
Perfluorooctanoic acid (PFOA)
The now-banned PFOA, a PFAS that is known to have harmful health effects, is shown for comparison. It has a much longer fluorinated tail than TFA.

©nature

This figure shows the controversy over whether TFA is toxic or not.

RISING LEVELS OF TFA

Trifluoroacetic acid (TFA) has been found in increased concentrations in various environments, including German forests (top) and Danish groundwater (bottom).

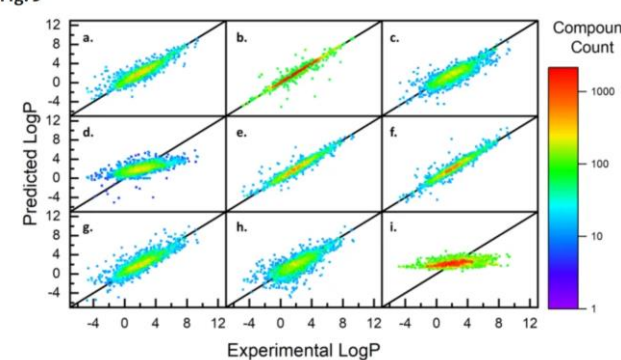


	This figure shows how TFA has been rising over time.
VOCAB: (w/definition)	PFASs - per- and poly-fluoroalkyl substances (forever chemicals) Hydrophilic – water – loving Hydrophobic – water -hating
Cited references to follow up on	https://pubs.rsc.org/en/content/articlelanding/2021/em/d1em00306b/unauth - Insufficient evidence for the existence of natural trifluoroacetic acid https://pubs.acs.org/doi/abs/10.1021/es0101532 - Trifluoroacetate in Ocean Waters
Follow up Questions	How can we prove if TFA is toxic? What other compounds are found in rainwater, and how do they affect the environment? Is there a way to break down ‘forever chemicals’?

Article #3 Notes: Dimensionally reduced machine learning model for predicting single component octanol–water partition coefficients.

Article notes should be on separate sheets

Source Title	Dimensionally reduced machine learning model for predicting single component octanol–water partition coefficients.
Source citation (APA Format)	K Kenney, D. H., Paffenroth, R. C., Timko, M. T., & Teixeira, A. R. (2023). Dimensionally reduced machine learning model for predicting single component octanol–water partition coefficients. <i>Journal of Cheminformatics</i> , 15(1). https://doi.org/10.1186/s13321-022-00660-1
Original URL	https://link.springer.com/article/10.1186/s13321-022-00660-1
Source type	Journal Article
Keywords	Molecular formula Feature engineering Model optimization LogP
#Tags	

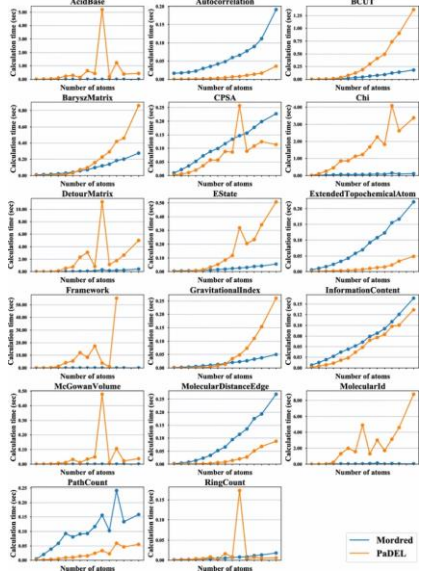
<p>Summary of key points + notes (include methodology)</p>	<p>LogP describes how a chemical dissolves in water as compared to a lipidlike substance. This property is important in biochemistry as the LogP values of certain drugs affect their ability to penetrate through lipid-like cell membranes. Thus, many models and predictors of a chemical's LogP value have been made. However, all of these models require structural information of the chemicals. In many cases, scientists will only know the chemical composition of the compound, and not the structure of it. As a result, the paper aims to create a model to predict LogP values based solely on molecular formula. The paper tested six different models: multivariate linear regression (MLR), ridge regression (RR), lasso regression (LR), random forest regression (RFR), gradient boosting regression (GBR), and k-nearest neighbor regression (KNNR). They found that RFR was the best performing, and KNNR came second. Both of these had issues with overfitting (when a model is good at only predicting training data and not data it has never seen) but still overall came out on top. This paper proved that a model using only molecular formula could accurately predict LogP values of different chemical compounds. However, it was noted that there were still some issues and inconsistencies as the model could not discern between isomers. All in all, they were successful in creating a model to help predict the behavior of chemicals with no information on their structure.</p>
<p>Research Question/Problem/ Need</p>	<p>Can a model be created to predict LogP properties of chemicals with only molecular formula as input?</p>
<p>Important Figures</p>	<p>Fig. 5</p>  <p>This figure shows how the model compares to the actual values for different types of models.</p>
<p>VOCAB: (w/definition)</p>	<p>LogP – a measure of how a compound dissolves in lipids vs in water Random forest regression – each “tree” is trained using different sample data, introducing diversity Isomers – compounds with the same molecular formula but different structures</p>

Cited references to follow up on	https://www.sciencedirect.com/science/article/abs/pii/S0169409X96004231 - Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings https://srđ.nist.gov/jpcrdreprint/1.555833.pdf - Octanol-Water Partition Coefficients of Simple Organic Compounds
Follow up Questions	What other properties can be predicted using a similar process? How can this be implemented to further scientific research?

Article #4 Notes: Mordred: a molecular descriptor calculator

Article notes should be on separate sheets

Source Title	Mordred: a molecular descriptor calculator
Source citation (APA Format)	Moriwaki, H., Tian, Y.-S., Kawashita, N., & Takagi, T. (2018). Mordred: A molecular descriptor calculator. <i>Journal of Cheminformatics</i> , 10(1). https://doi.org/10.1186/s13321-018-0258-y
Original URL	https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0258-y#Abs1
Source type	Journal Article
Keywords	Molecular descriptor QSPR Cheminformatics Calculation software Python
#Tags	
Summary of key points + notes (include methodology)	<p>Mordred is a molecular descriptor calculator which takes chemical information in and outputs properties of chemicals. It was designed to be superior to previous solutions, as it is faster, has a wider knowledge base, is open source, and easier to use. Mordred can calculate over 1800 2D and 3D descriptors, and is useful for studying the relationships between chemical structure and properties.</p> <p>Basic Methodology for Creating Testing Model:</p> <ol style="list-style-type: none"> 1. Split the dataset into training and test datasets to evaluate performance 2. From each compound in the datasets, calculate molecular descriptors 3. Use a model like regression or classification to check target values, for example: <ol style="list-style-type: none"> a. multiple regression analysis b. partial least squares regression c. support vector machine (SVM) d. random forest 4. Predict the target values of the compounds in the test dataset in order to evaluate the performance of the model

	<p>The algorithm in Mordred was further improved by using articulation points in the algorithm. This meant that the nodes were sectioned off by any nodes that would disconnect the web if removed, called articulation points. From there, it became much faster to search through the web of nodes.</p>
<p>Research Question/Problem/Need</p>	<p>Can a faster, more efficient, more knowledgeable, and more accessible molecular descriptor calculator be created?</p>
<p>Important Figures</p>	 <p>This figure shows how Mordred compares to a previous solution across multiple domains.</p>
<p>VOCAB: (w/definition)</p>	<p>NP-hard problem – a problem that is very difficult to solve efficiently CLI benchmark test – measures the performance of a command line interface PaDEL-Descriptor – previous software used to calculate molecular descriptors</p>
<p>Cited references to follow up on</p>	<p>https://books.google.com/books?hl=en&lr=&id=6Zp7Yrqzv8AC&oi=fnd&pg=PP2&ots=Jr-JI5JDh&sig=tGL2E1zKQhH4-Q-gEOfiTewHcng#v=onepage&q&f=false - Molecular descriptors from cheminformatics https://pubs.acs.org/doi/abs/10.1021/ci00053a005 - Atomic physicochemical parameters for three-dimensional-structure-directed quantitative structure-activity relationships. 2. Modeling dispersive and hydrophobic interactions</p>
<p>Follow up Questions</p>	<p>What other domains could use a calculator similar to this one (input structural information and output properties)? Can scientists use this calculator to predict side effects or properties of new chemicals after combining ones in the database? Can this calculator be reversed to identify chemicals based on their properties or recommend chemicals to a user based on properties they would like to have in their</p>

	chemicals?
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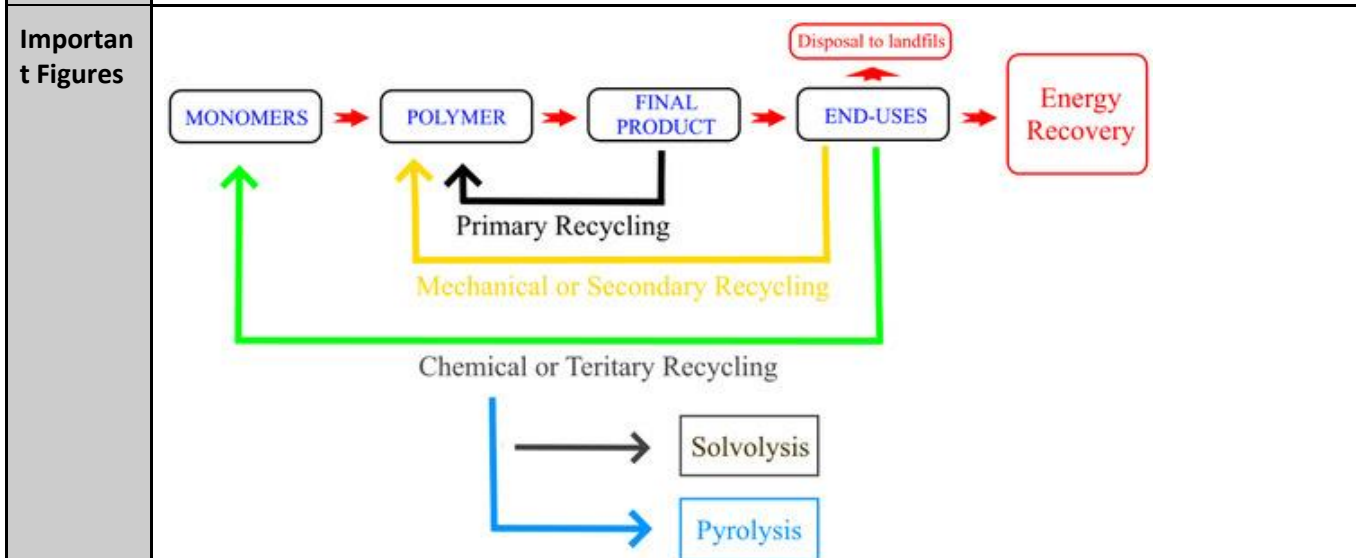
Article #5 Notes: A Journey from Processing to Recycling of Multilayer Waste Films: A Review of Main Challenges and Prospects

Article notes should be on separate sheets

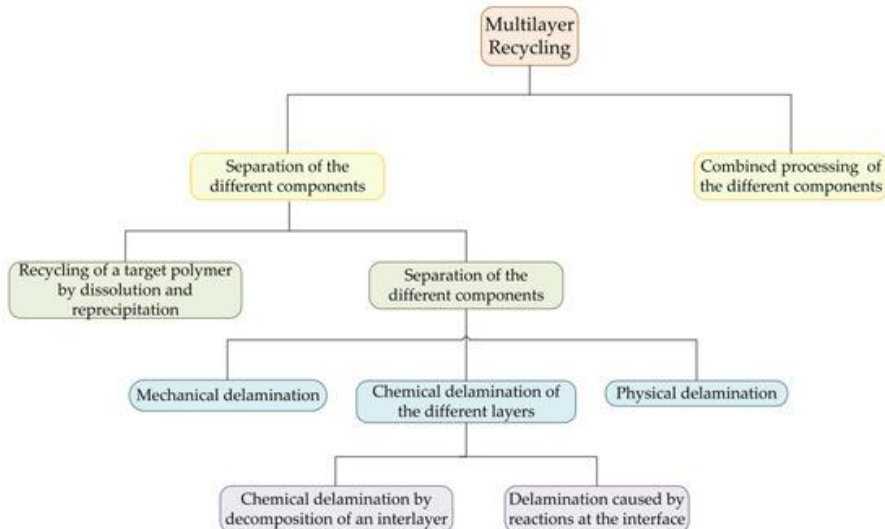
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Source Title	A Journey from Processing to Recycling of Multilayer Waste Films: A Review of Main Challenges and Prospects
Source citation (APA Format)	Cabrera, G., Li, J., Maazouz, A., & Lamnawar, K. (2022a). A journey from processing to recycling of Multilayer Waste Films: A review of main challenges and prospects. <i>Polymers</i> , 14(12), 2319. https://doi.org/10.3390/polym14122319
Original URL	https://www.mdpi.com/2073-4360/14/12/2319
Source type	Journal Article
Keywords	circular economy; recycling; eco-design; coextrusion; multilayers
#Tags	
Summary of key points + notes (include methodology)	Plastic use is spread across many different industries, but many can be confined to consumer packaging. Solid Plastic Waste (SPW) is generated as a result but takes a toll on the environment. The most common plastic waste from consumers is LPDE, HPDE, LLPDE, PET, and PP. The paper then describes different methods that countries use to sort and distinguish plastics. Usually, recycled plastic either gets recycled to its original form, turned back into its monomers, gets used for thermal energy/ chemical reactions, or used in another industry. Closed-loop recycling is when a polymer is returned to its original function, whereas open-loop is when the polymer becomes something else after recycling. For multilayer plastics, recycling often includes removing target polymers through specific solvents or dissolving the products that adhere multiple polymers together. The article then discusses different ways in which polymers are produced and different types of polymers.

Research Question /Problem / Need How is plastic recycled and what kinds of plastics are recycled?



This figure shows different routes for plastic recycling.



This figure shows the process of multilayer recycling.

VOCAB: (w/definition) Bioplastics – plastics that are contain organic matter
 Depolymerization- process of converting polymer to monomer
 fluid-catalytic cracking- a process using a powdered catalyst to break down heavy hydrocarbons into lighter ones
 Petrochemical- chemical derived from petroleum
 Chemolysis- dissolution by chemical

Cited reference https://www.sciencedirect.com/science/article/pii/S0956053X17305354?casa_token=zoxkKRb3rJY

<p>s to follow up on</p>	<p>AAAAA:Ctvi8mx9nVSaxcbdc3eO8LkzigoHHh-2gNkbO78oUwyK_dLjoqm6AnqawZ_6WVXfpM0Ry0BQJg - Mechanical and chemical recycling of solid plastic waste</p> <p>https://journals.sagepub.com/doi/full/10.1177/0734242X16678066?casa_token=PoO4GXmZrAIAA AAA%3AeqArpWvBqOPTfP31Xln3l0fBuH1EO46DACvQu4jszyp_wjfpLb1pzVC9ysq1F7NEal4sqV3VUV1Eng- - Characterization of plastic blends made from mixed plastics waste of different sources</p>
<p>Follow up Questions</p>	<p>How can post-industrial plastic waste be reduced? How can we better repurpose/dispose plastic? Does plastic recycling release toxic chemicals and greenhouse gases?</p>

Article #6 Notes: Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation

Article notes should be on separate sheets

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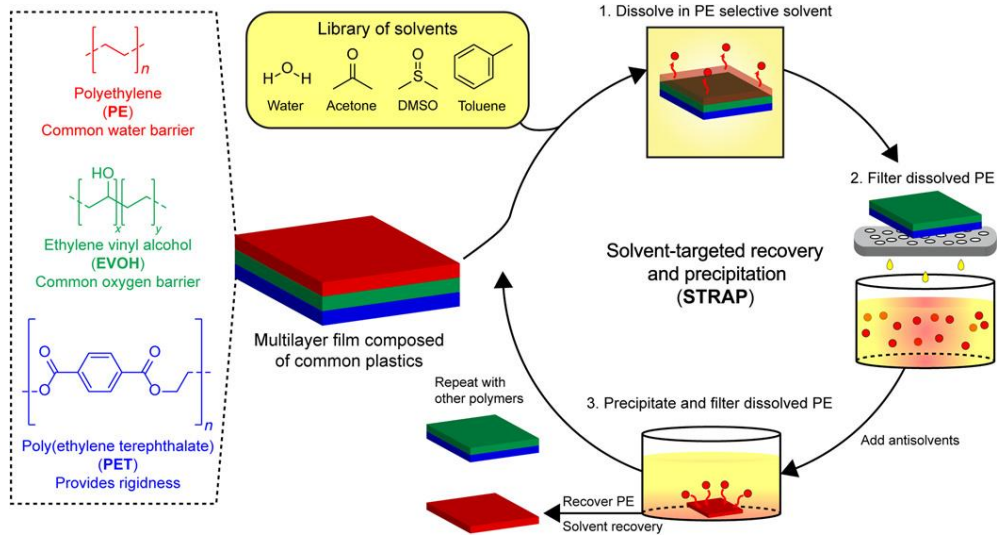
<p>Source Title</p>	<p>Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation</p>
<p>Source citation (APA Format)</p>	<p>Walker, T. W., Frelka, N., Shen, Z., Chew, A. K., Banick, J., Grey, S., Kim, M. S., Dumesic, J. A., Van Lehn, R. C., & Huber, G. W. (2020). Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation. <i>Science advances</i>, 6(47). https://doi.org/10.1126/sciadv.aba7599</p>
<p>Original URL</p>	<p>https://doi.org/10.1126/sciadv.aba7599</p>
<p>Source type</p>	<p>Journal Article</p>
<p>Keywords</p>	<p>Precipitation, STRAP, dissolution, multilayer polymer</p>
<p>#Tags</p>	
<p>Summary of key points + notes (include methodology)</p>	<p>The article looks to separately dissolve polyethylene (PE), ethylene vinyl alcohol (EVOH), and polyethylene terephthalate (PET). Past solutions to plastic recycling do not account for multilayer polymers or only work for very specific types.</p> <ul style="list-style-type: none"> - “Here, we prescribe a guided approach to rationally select solvents using calculations of Hansen solubility parameters (HSPs), molecular dynamics (MD) simulations, and a combined quantum chemical and statistical mechanical approach called the conductor-like screening model for realistic solvents (COSMO-RS)”

After selection, they compared the HSPs of the materials to the HSPs of the solvents. Similar values translate to good solubility. They then calculated the COSMO-RS which is based on statistical thermodynamics. After successfully separating the layers and recovering them, they tested them to make sure they were still in viable condition.

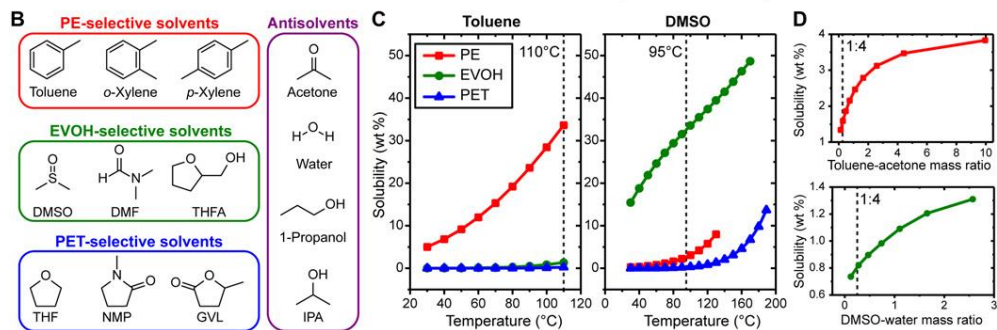
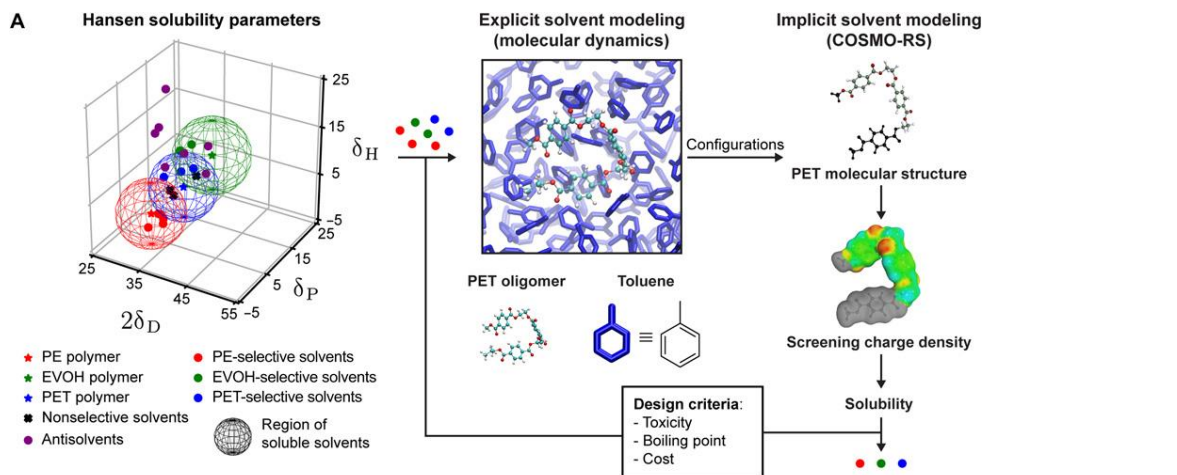
Research Question/Problem/Need

How can we separately dissolve and precipitate different layers of a multilayer plastic polymer?

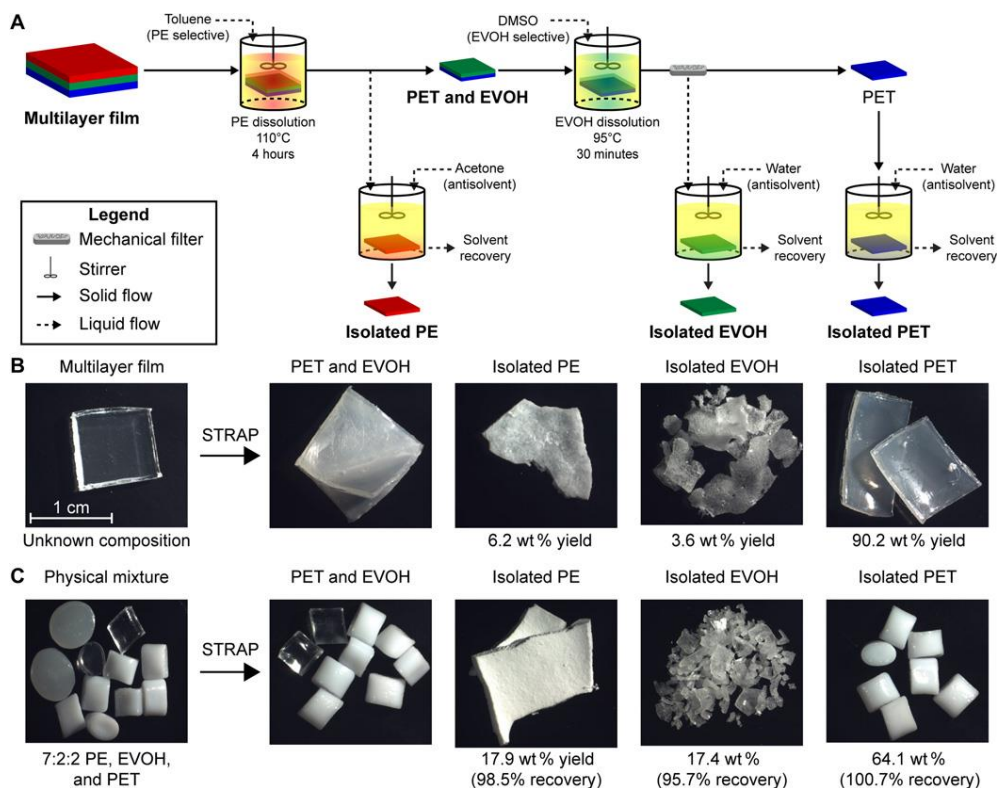
Important Figures



This figure shows the process explained by the article.



This figure explains some of their methodology and choices.



This figure shows actual photos of their abilities to recover substances.

VOCAB: (w/definition)	HSP – Hansen Solubility Parameters – describe dipole, polar, and h-bonds interactions vacuum filtration – separates solid from liquid (ATR)–FTIR spectra – specific absorbed wavelength which can identify compounds gel permeation chromatography – separates molecules by size multiangle laser light scattering- measures absolute molecular weight by scattering light
Cited references to follow up on	https://core.ac.uk/download/pdf/219382696.pdf - Chemical Recycling of Plastics by Dissolution https://pubs.acs.org/doi/full/10.1021/es5055786?casa_token=DQh6SeUMIVgAAAAA%3AIsfBIVmSlaYX4fGsF2PbW52QTnLNk81Da_woFi3R71zeqAGUYLfEDy8geNFhY-KuYR2gG3GbcmDvA2RG - Method for Efficient Recovery of High-Purity Polycarbonates from Electronic Waste
Follow up Questions	Wha other types of multilayer plastics need to be dissolved? Can environmentally friendly solvents be used instead? How can HSP be useful in matching solvents in other contexts?

Article #7 Notes: Solvent-based plastic recycling technologies

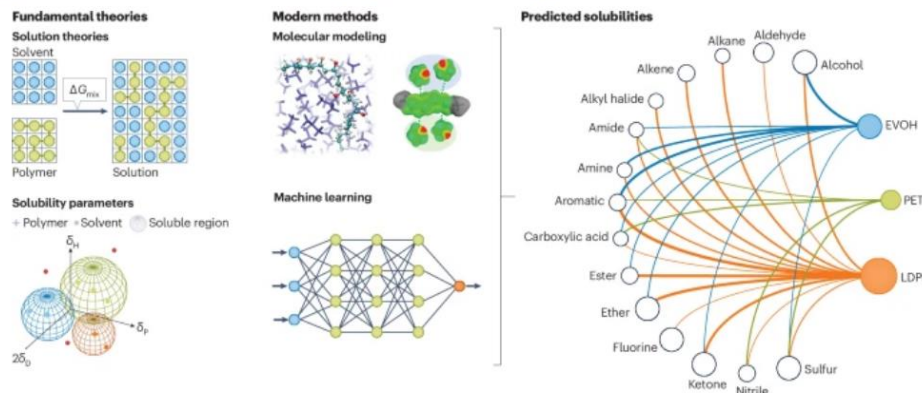
Article notes should be on separate sheets

Source Title	Solvent-based plastic recycling technologies
Source citation (APA Format)	Xu, Z., Sanchez-Rivera, K., Granger, C., Zhou, P., Munguia-Lopez, A. del C., Ikegwu, U. M., Avraamidou, S., Zavala, V. M., Van Lehn, R. C., Bar-Ziv, E., De Meester, S., & Huber, G. W. (2025). Solvent-based plastic recycling technologies. <i>Nature Chemical Engineering</i> , 2(3), 407-423. https://doi.org/10.1038/s44286-025-00247-1
Original URL	https://doi.org/10.1038/s44286-025-00247-1
Source type	Journal Article
Keywords	Recycling, Polymer Dissolution
#Tags	
Summary of key points + notes (include methodology)	<p>The method of using chemical recycling has multiple steps.</p> <ul style="list-style-type: none"> • Preprocessing: <ul style="list-style-type: none"> ○ Clean/sorting materials • Dissolution: <ul style="list-style-type: none"> ○ Dissolving the polymer in a specific solvent <ul style="list-style-type: none"> ▪ Need specific solvents and temperatures • Separation: <ul style="list-style-type: none"> ○ It is necessary to separate undissolved polymers from the solution <ul style="list-style-type: none"> ▪ Can use centrifuges • Cleaning: <ul style="list-style-type: none"> ○ After dissolution, some dyes and other contents can be present in the solution <ul style="list-style-type: none"> ▪ Absorption is often used to rectify this • Precipitation <ul style="list-style-type: none"> ○ After dissolution, the solution needs to be broken down into the polymer and the solvent. Options to do this are: <ul style="list-style-type: none"> ▪ adding antisolvent ▪ changing the temperature or pressure of the solvent ▪ evaporation of the solvent ○ These methods allow the separation of the solvent and solute ○ Decantation and filtration are often used for separation of precipitated solvent and the solvent • Solvent Recovery and Cleaning

	<ul style="list-style-type: none"> ○ Solvents can be reused, so they need to be purified and cleaned <ul style="list-style-type: none"> ▪ Distillation works for this • Testing of recovered polymers to confirm strength and usefulness <p>Many models have been developed to qualitatively predict solubility, but not quantitatively. Increasing density is possibly route to increasing solubility. Thermodynamic and kinetic factors such as viscosity also need to be taken into account, along with other factors like polymer crystallization, all of which affect solubility.</p> <p>Some commercial scaled implementations of this include CreaSolv, APK NewCycling, PolyStyvert, Purecycle, and STRAP.</p> <p>All of these processes use polymer targeted dissolution to dissolve and recover recycled polymers.</p> <p>After recovery, properties such as strength and flexibility need to be tested. Most studies found that there was not a large change in these properties, but further research needs to be done on separating dyes and other substances out of polymers.</p> <p>On the economic side, some processes can be profitable, but it depends on the specific process. For instance, using antisolvents costs more money than using just cooling.</p> <p>For environmental purposes, it is important to look at factors such as carbon emissions, toxicity, water used, energy used, etc.</p> <p>To put this on an industrial scale, organizations would need to understand the potential risks and hazards. They would also need to identify solvents that dissolve target polymers and no other ones. Finally, they would need to take into account the financial and environmental aspects of putting this at a large scale.</p> <p>For future steps, researchers need to look more into preprocessing, solvent selection, additives, solvent reuse, and post-recovery properties.</p>
Research Question/Problem/ Need	How can targeted dissolution of polymers lead to polymer recovery in recycling?

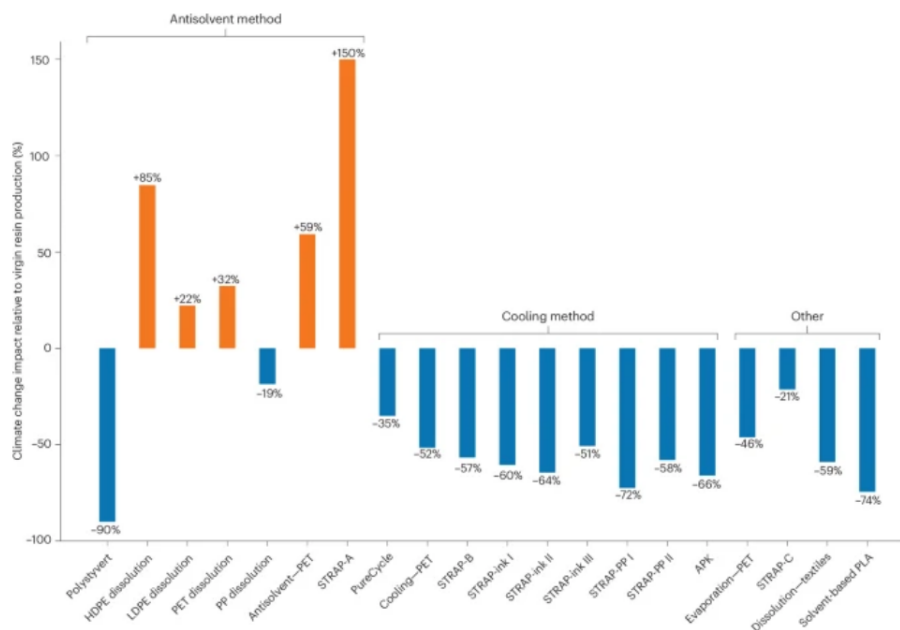
Important Figures

Fig. 2: Theories and models for polymer solubility prediction.



This figure shows how polymers and solvents interact.

Fig. 3: Comparison of climate change impact (kg CO₂e per kg resin) for reported dissolution recycling processes and their respective virgin resin counterparts.



Dissolution-based processes are compared with virgin resin production. The processes are differentiated by precipitation method: antisolvent, cooling or other. A positive percentage represents an increase in GHG emissions while a negative percentage represents a decrease in GHG emissions. All referenced values can also be found in Table 3.

This figure describes the climate change impact of recycling processes as compared to create the virgin polymer.

VOCAB: (w/definition)

Nucleation – beginning of conversion to new state
 non-combinatorial entropy – entropy not due to microstates, like vibration, etc.

	<p>Supercritical fluid - mix of properties of gases and liquids ambient pressure - pressure of surrounding environment Fourier transform infrared spectra – uses how molecules absorb light and vibrations to predict bonds</p>
Cited references to follow up on	<p>Karim, S. S. et al. Model analysis on effect of temperature on the solubility of recycling of polyethylene terephthalate (PET) plastic. <i>Chemosphere</i> 307, 136050 (2022).</p> <p>Walker, T. W. et al. Recycling of multilayer plastic packaging materials by solvent-targeted recovery and precipitation. <i>Sci. Adv.</i> 6, eaba7599 (2020).</p>
Follow up Questions	<p>How can dye be effectively separated from plastics? How does reducing plastic in landfills impact climate change? How does the toxicity of solvents impact the surrounding environment?</p>

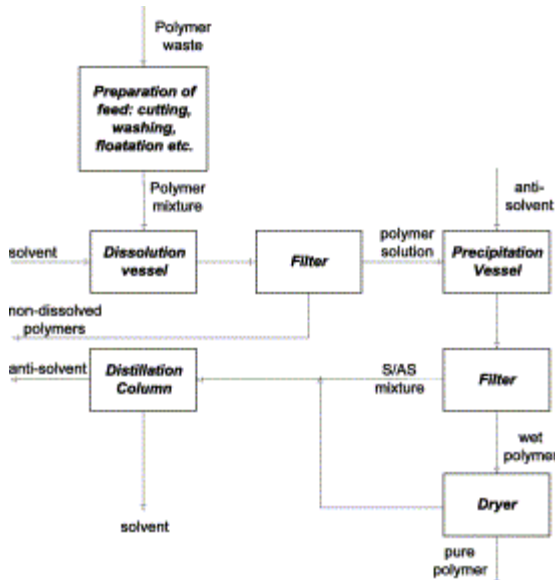
Article #8 Notes: The selective dissolution/precipitation technique for polymer recycling: a pilot unit application

Article notes should be on separate sheets

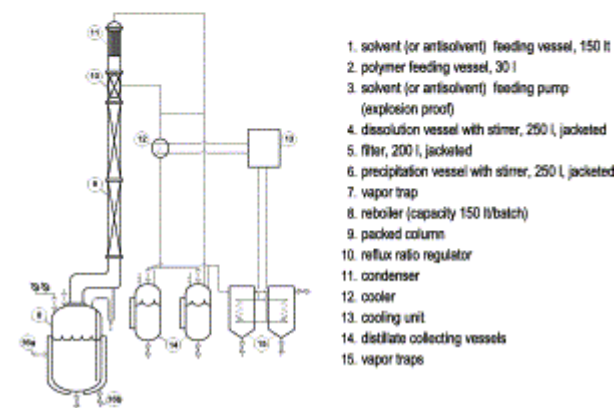
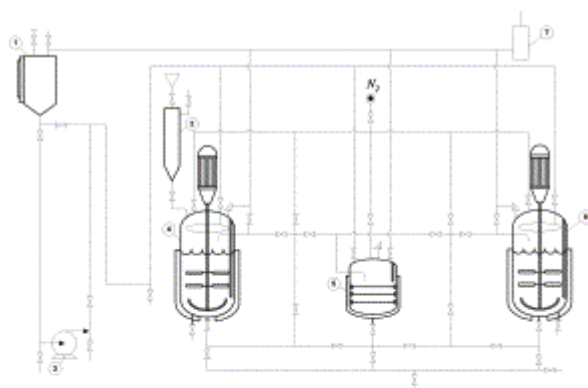
Source Title	The selective dissolution/precipitation technique for polymer recycling: a pilot unit application
Source citation (APA Format)	Pappa, G., Boukouvalas, C., Giannaris, C., Ntaras, N., Zografos, V., Magoulas, K., Lygeros, A., & Tassios, D. (2001). The selective dissolution/precipitation technique for polymer recycling: A pilot unit application. <i>Resources, Conservation and Recycling</i> , 34(1), 33–44. https://doi.org/10.1016/S0921-3449(01)00092-1
Original URL	https://doi.org/10.1016/S0921-3449(01)00092-1
Source type	Journal Article
Keywords	Selective dissolution/precipitation Polyolefins Plastic waste PolymersR ecycling
#Tags	

Summary of key points + notes (include methodology)	<p>Plastic waste makes up a decent amount of waste by volume, taking up space in landfills and hurting the environment. Very little is recycled, and combustion releases harmful chemicals into the air. This study looks at using solvent dissolution and precipitation to separate low and high density PE as well as PP. They can separate the low and high density first by floatation in a liquid.</p> <p>Methodology (Quoted):</p> <ul style="list-style-type: none"> • Cutting the waste into smaller pieces and, if necessary, washing with water. • Preliminary separation of the initial mixture to two or more mixtures by floatation in water or another liquid. • Addition of a solvent (S) that selectively dissolves only one of the polymers at certain conditions. • Filtration to remove the non-dissolved polymers. • Addition of an antisolvent (AS) to precipitate the dissolved polymer. • Filtration and drying of the precipitated polymer. • Separation of the S/AS mixture by distillation for reuse. • Application of the same procedure for each polymer of the mixture. <p>The unit can take up to 10kg of waste at a time and is insulated to reduce energy loss.</p> <p>They used melt flow index to assess how the properties of the polymers changed, and found at most an increase of 10%.</p> <p>Differential scanning calorimetry (DSC) showed only a small difference.</p> <p>For amounts higher than 30,000 t/year, the price of recycling is comparable to the price of the virgin material.</p>
Research Question /Problem / Need	<p>How can mixed plastics be broken down and recycled effectively?</p>

Important Figures

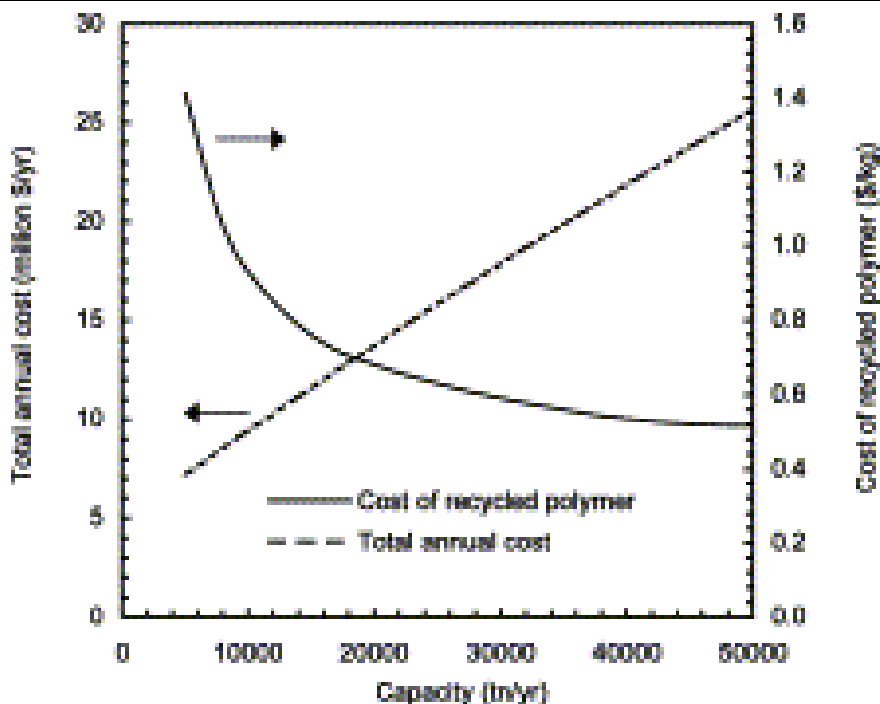


This figure describes the process used in the study.



1. solvent (or antisolvent) feeding vessel, 150 l
2. polymer feeding vessel, 30 l
3. solvent (or antisolvent) feeding pump (explosion proof)
4. dissolution vessel with stirrer, 250 l, jacketed
5. filter, 200 l, jacketed
6. precipitation vessel with stirrer, 250 l, jacketed
7. vapor trap
8. reboiler (capacity 150 l/batch)
9. packed column
10. reflux ratio regulator
11. condenser
12. cooler
13. cooling unit
14. distillate collecting vessels
15. vapor traps

This is a schematic of the physical unit they put together.



This figure looks at the cost of the recycled polymer vs total annual cost.

VOCAB: (w/definition)	Feedstock recycling - recycling by breaking polymers into monomers Polyolefins- made of alkene monomers and make up things like pp and pe differential scanning calorimetry (DSC)- looks at how much heat a material can absorb Melt Flow Index – looks at how much melted polymer can moved through a controlled capillary in a certain amount of time
Cited references to follow up on	<p>https://www.sciencedirect.com/science/article/abs/pii/0361365887900622 - A model recovery process for scrap polystyrene foam by means of solvent systems</p> <p>https://onlinelibrary.wiley.com/doi/abs/10.1002/adv.1995.060140307?casa_token=dtHw137sR0kAAAAA%3A6KeLKDzfQp9118DroBqcpMlyULdTeNmC_CK1LbGzTRHD5GDEh0fv39x_b95s2mBy_Zizc7TP7HPNhMr</p> <p>The dissolution reprecipitation technique applied on high-density polyethylene. 1. Model recycling experiments</p>
Follow up Questions	<p>How can we predict what solvents we will need for different types of plastics?</p> <p>How will this process work with other types of contamination present?</p>

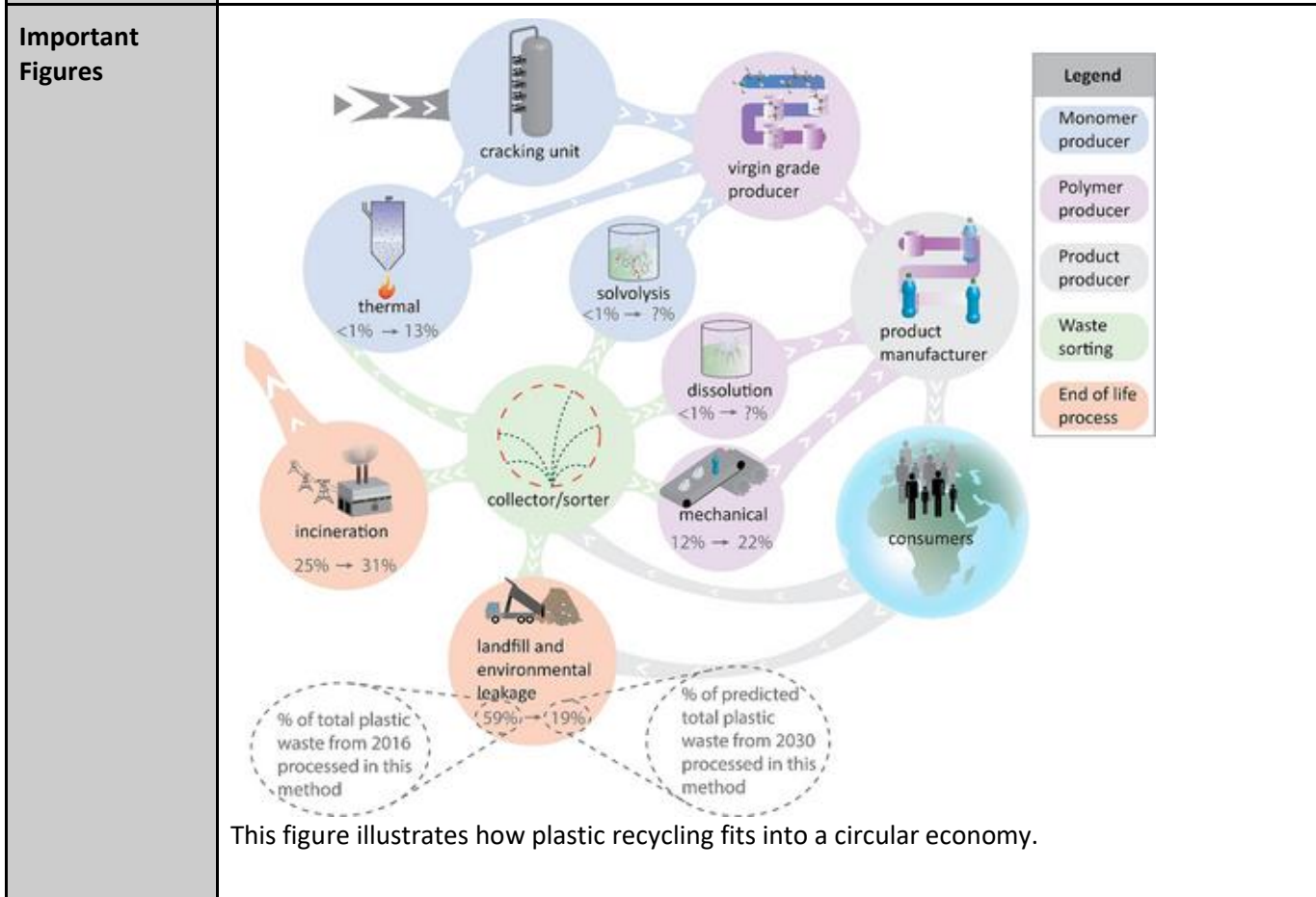
Article #9 Notes: Beyond Mechanical Recycling: Giving New Life to Plastic Waste

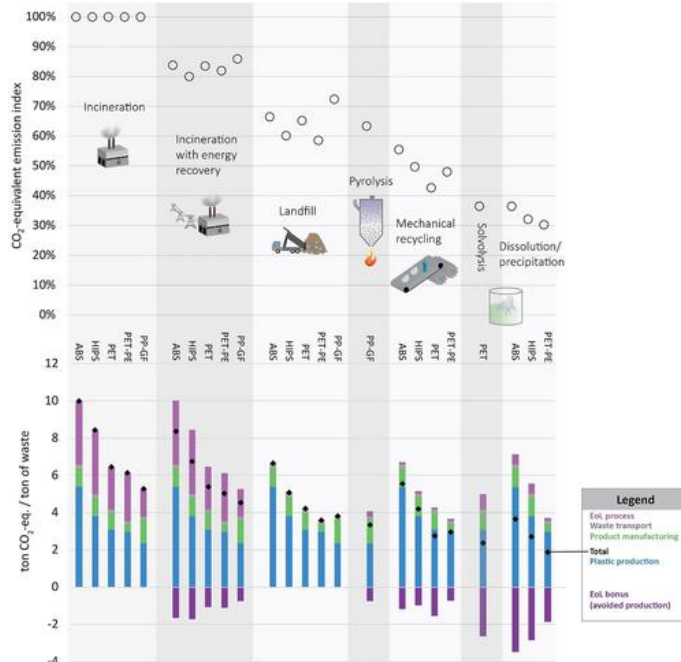
Article notes should be on separate sheets

Source Title	Beyond Mechanical Recycling: Giving New Life to Plastic Waste
Source citation (APA Format)	Vollmer, I., Jenks, M. J. F., Roelands, M. C. P., White, R. J., van Harmelen, T., de Wild, P., van der Laan, G. P., Meirer, F., Keurentjes, J. T. F., & Weckhuysen, B. M. (2020). Beyond mechanical recycling: Giving new life to plastic waste. <i>Angewandte Chemie – International Edition</i> , 59(36), 15402–15423. https://doi.org/10.1002/anie.201915651
Original URL	https://doi.org/10.1002/anie.201915651
Source type	Journal Article /Lit. Review
Keywords	catalysis chemical recycling circularity plastic waste solvolysis
#Tags	
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - Lots of plastic waste, but other materials are costly and have environmental downsides. - Governments and organizations are calling for solutions to plastic waste. - Solvolysis is used to break down PET into monomers or smaller parts which can then be remade into PET. - Dissolution/precipitation processes like CreaSolv dissolve certain polymers and then leave others to be dissolved in a different solution. - APK NewCycling also uses a similar process to separate multilayer films - This process can have issues with toxicity as well as removing chemicals like dyes or plasticizers. - Some companies take plastic waste and make more valuable compounds. - Pyrolysis has been applied to burn plastics for energy. - 5 main recycling types: <ul style="list-style-type: none"> o incineration with energy recovery o pyrolysis o mechanical recycling o solvolysis o dissolution/precipitation - D/P is lowest carbon emissions while incineration is highest - Landfilling is also low but is not a proponent of circular economy and releases toxins into the ground while taking up space - Some options include biology to break down plastics. - High pressure mechanics can be used to depolymerize plastics. - Some enzymes have been shown to effectively break down certain types of plastics. - Another solution is to design polyolefins for recycling by not adding additives that break them down during recycling. - Dissolution and precipitation work well, but it may be difficult to find solvents that work well and quickly. <ul style="list-style-type: none"> o Also concerns about leftover solvents in material

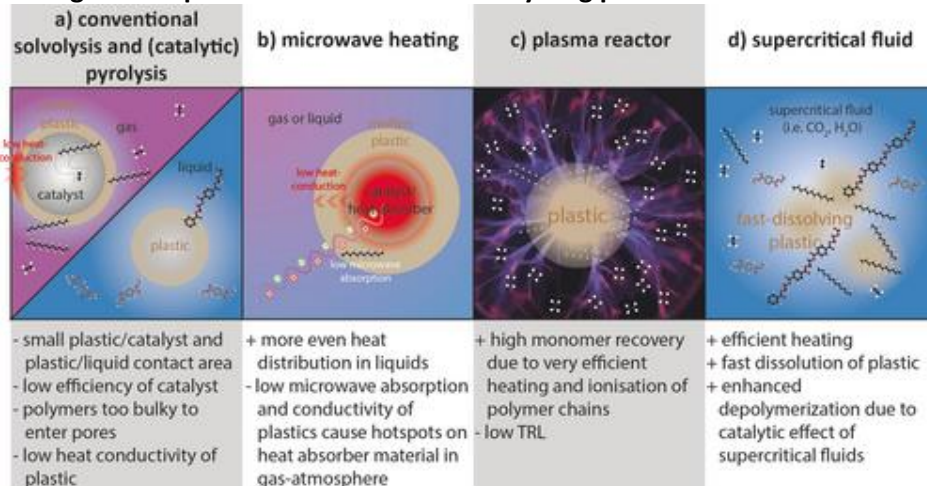
- Catalysts can be used to speed up pyrolysis, but some issues are viscosity as well as slowing down heat transfer.
- Pyrolysis is the most common method and has been implemented and changed in a variety of ways.

Research Question/Problem/ Need
 What are different ways to solve the issue of recycling plastic?

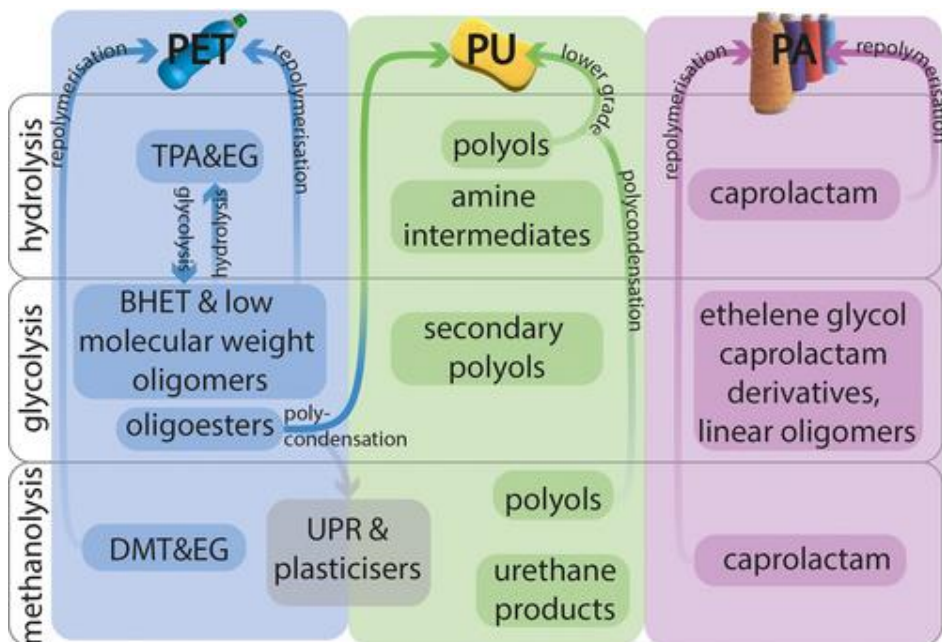




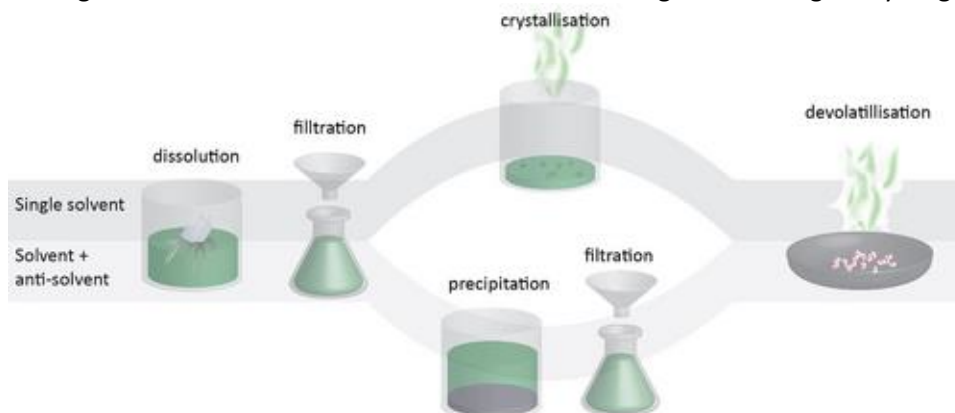
This figure compares different chemical recycling processes and carbon emissions.



This figure shows up and coming recycling methods.



This figure describes how certain methods can work together through recycling.



This figure describes a basic process for dissolution and precipitation.

**VOCAB:
(w/definition)**

Pyrolysis – using heat to decompose polymers
 Solvolysis – a chemical reacts with polymers to break bonds
 Hydrolysis – solvolysis using water
 Catalysis – using a catalyst to speed up the reaction
 Hydrocracking – uses hydrogen gas to break down polymers
 Coke – carbon- rich by product of many of these processes

**Cited
references to
follow up on**

https://www.sciencedirect.com/science/article/pii/S0956053X17305354?casa_token=CZUEC-UccdxoAAAAA:DWP62-nzDiftp6L0yvfhJvlsaV44uo4ZxPLdyquYU7fn6RKuZfQlqg-pwy6Fgg3DBQPKw - Mechanical and chemical recycling of solid plastic waste
<https://link.springer.com/article/10.1007/S10924-008-0106-7>-
 Pet Waste Management by Chemical Recycling: A Review

**Follow up
Questions**

How can these processes be combined to contribute towards a circular economy?
 Can the CO₂ released by incineration be captured and used to make new polymers?

Article #10 Notes: Mechanical and thermal properties of thermoplastic acetylated starch/poly(ethylene-co-vinyl alcohol) blends

Article notes should be on separate sheets

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Source Title	Mechanical and thermal properties of thermoplastic acetylated starch/poly(ethylene-co-vinyl alcohol) blends
Source citation (APA Format)	Jiang, W., Yu, J., & Li, Z. (2006). Mechanical and thermal properties of thermoplastic acetylated starch/poly(ethylene-co-vinyl alcohol) blends. <i>Carbohydrate Polymers</i> , 64(3), 354-361. https://doi.org/10.1016/j.carbpol.2006.01.005
Original URL	https://doi.org/10.1016/j.carbpol.2005.12.038
Source type	Journal Article
Keywords	Acetylated starch EVOH DMA DSC TGA
#Tags	
Summary of key points + notes (include methodology)	<ul style="list-style-type: none"> - Starch has a melting temp. Greater than its decomposition temp. Which leads to interesting properties - Acetylation can be used to make starch more water resistant - They chose EVOH to combine with the starch - They used techniques to test tensile strength, as well as DSC, DMA, and TGA - High amounts of EVOH can make the substance brittle - For DMA, the mixtures stay in order for testing of the properties, i.e. they stay in order a-e. - For the DSC they noticed that pure EVOH is much higher, which means that their process interrupts crystallization of EVOH. - For the TGA, they noticed most mass loss occurred between 280 and 350 degrees Celsius. - EVOH crystallization process is interrupted as it can help provide more thermal stability for the whole compound.
Research Question/Problem/ Need	How does creating compounds of different compositions of TPAS and EVOH affect its properties?

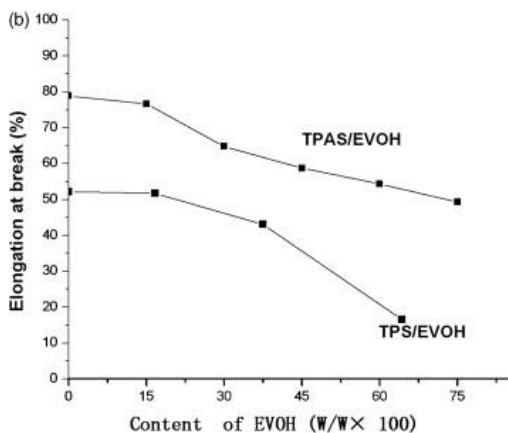
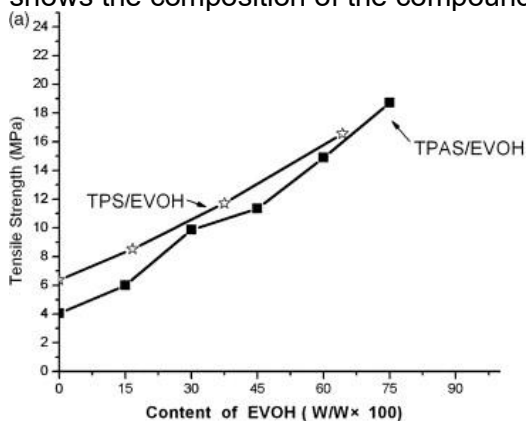
Important Figures

Table 1. Compositions of thermoplastic acetylated starch/EVOH blends (W/W_starch×100)

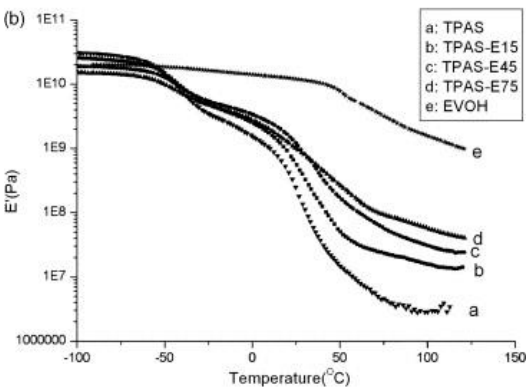
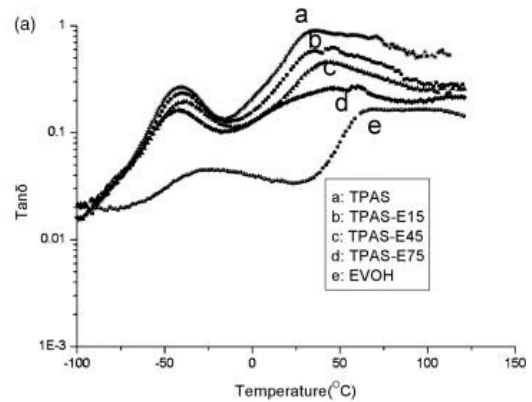
Component	TPAS	TPAS-E15	TPAS-E30	TPAS-E45	TPAS-E60	TPAS-E75
Acetylated starch	100	100	100	100	100	100
Glycerol	50	50	50	50	50	50
EVOH	0	15	30	45	60	75

This table

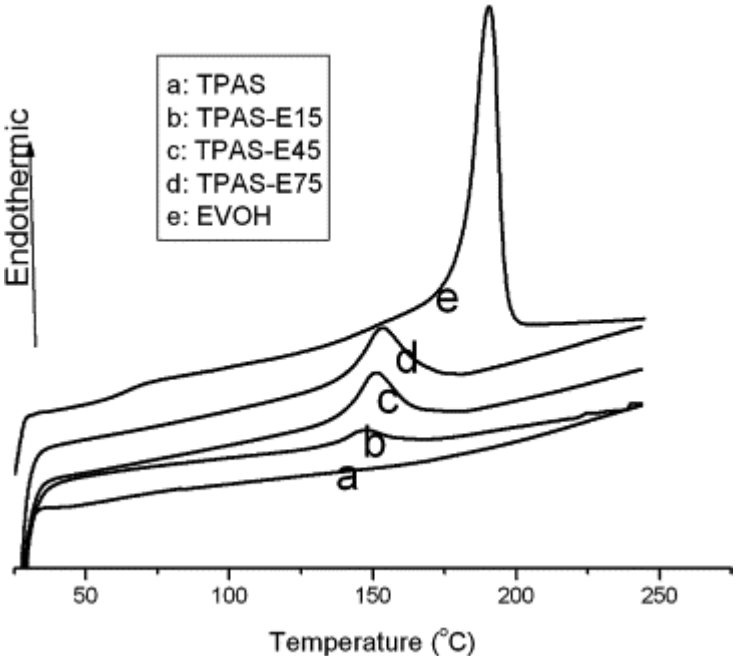
shows the composition of the compounds they created.



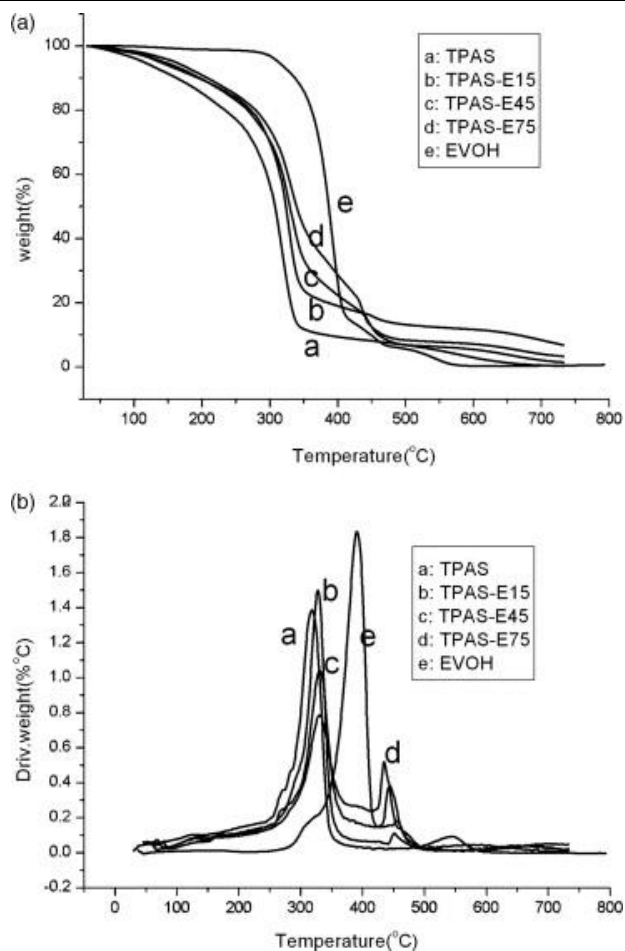
This figure shows EVOH content vs tensile strength and elongment at breaking.



This figure shows how the mixtures compare to properties of DMA.



This figure shows the results of the DSC scan.



This figure shows the results of TGA.

VOCAB:
(w/definition
)

Acetylation – adds acetyl group and makes substance more hydrophobic
 DMA - Dynamic Mechanical Analysis – looks at mechanical properties of compounds such as glass transition temperatures
 DSC - Differential Scanning Calorimetry – how much heat flow is needed to increase temperature
 TGA - Thermogravimetric Analysis – change in mass of a material during heating

**Cited
references to
follow up on**

Phase and glass transition behaviour of concentrated barley starch-glycerol-water mixtures, a model for thermoplastic starch -
<https://www.sciencedirect.com/science/article/abs/pii/S0144861797001331>

Effect of Acetylation on Some Properties of Rice Starch -
[https://onlinelibrary.wiley.com/doi/abs/10.1002/1521-379X\(200204\)54:3/4%3C148::AID-STAR148%3E3.0.CO;2-N?casa_token=VMzFULTMfD4AAAAA%3AOCrE2t4zLEBr0BPZfO0776EQ5KLPtWhJ_LWCxiYqWYobLSlp8UNzucOXb0fq3ryYps9FoOrKgPN](https://onlinelibrary.wiley.com/doi/abs/10.1002/1521-379X(200204)54:3/4%3C148::AID-STAR148%3E3.0.CO;2-N?casa_token=VMzFULTMfD4AAAAA%3AOCrE2t4zLEBr0BPZfO0776EQ5KLPtWhJ_LWCxiYqWYobLSlp8UNzucOXb0fq3ryYps9FoOrKgPN)

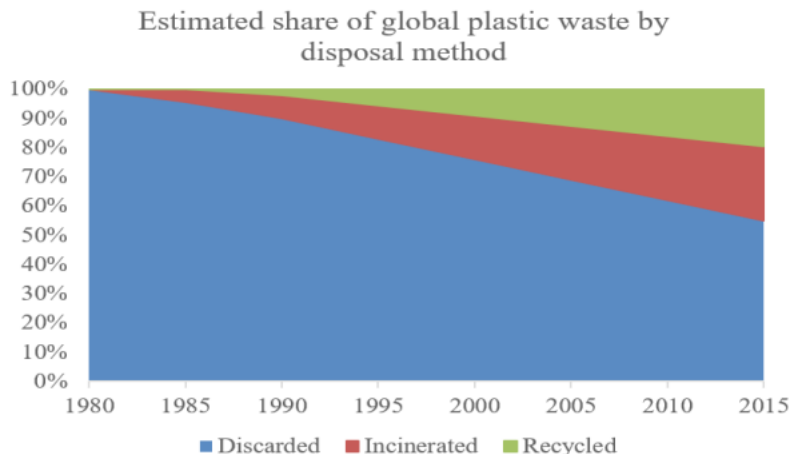
Follow up Questions	How can acetylation be used on other substances to make them more resistant to water like surgical gloves? What kinds of things can this TPAS_EVOH material be used for?
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Article #11 Notes: The Environmental Impact of Plastic Waste

Article notes should be on separate sheets

Source Title	The Environmental Impact of Plastic Waste
Source citation (APA Format)	Jiang, B., Yu, J., & Liu, Y. (2020). The environmental impact of plastic waste. <i>Journal of Environmental & Earth Sciences</i> , 2(2), 26–35. https://doi.org/10.30564/jees.v2i2.2340
Original URL	https://pdfs.semanticscholar.org/b00f/5500ab156bd3118358054d4e7030d757358e.pdf
Source type	Journal Article
Keywords	Multiple egression; Fuzzy hierarchy; Plastic waste; Environmental safety
#Tags	
Summary of key points + notes (include methodology)	Plastic is piling up and hurting the environment. They did a regression analysis to estimate the amount of plastic waste there would be overall. They also looked at how much plastic is recycled vs. incinerated vs. Discarded. They use an AHP to decide what factors were most important. They then tried using the DPSIR model too. They compared plastic waste data between Australia and China using these two models. They found that using their model Australia was more environmentally safe than China. They also noted that China's environmental safety level was lower than Australia's. They looked into why that was happening, including economic factors. They looked into what sectors produce the most plastic waste, and found that a lot of plastic waste comes from packaging. They used China to look at how plastic affected humans, businesses and the environment. They noted that countries that have more money and better education use more plastic but also do a better job of managing the waste. Finally, they made predictions about how plastic waste management will change in the future.
Research Question/Problem/Need	How is plastic waste distributed and affected by different variables?

Important Figures



This figure shows how plastic waste has been dealt with over time.

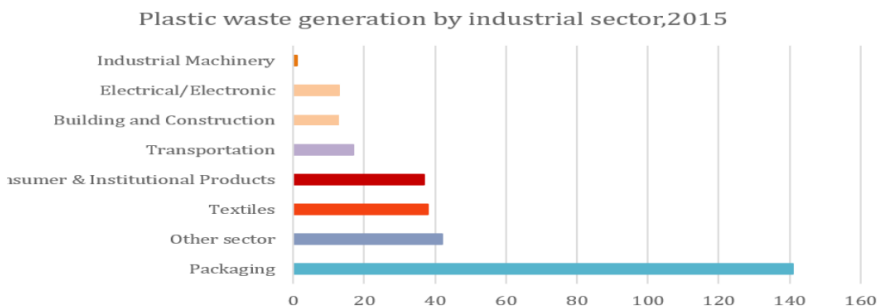


Figure 6. Plastic waste generation by industrial sector, 2015 [2]

This figure shows how plastic waste comes from different categories.

Comparing the indicators of Australia, China, India and Guinea, we get Figure 7:

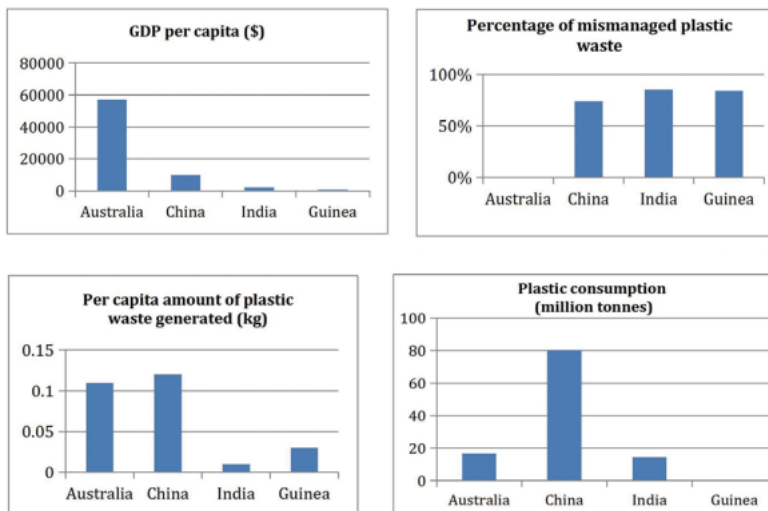


Figure 7. Comparison chart of indicators in Australia, China, India and Guinea

	This figure shows plastic waste as compared between different countries.
VOCAB: (w/definition)	Analytic Hierarchy Process – decision making method DPSIR Model – cause-effect for environmental problems Fuzzy Comprehensive Evaluation Method -
Cited references to follow up on	Mwanza B G, Mbohwa C, Telukdarie A. The Significance of Reverse Logistics to Plastic Solid Waste Recycling in Developing Economies[J].] Jambeck J, Hardesty B D, Brooks A L, et al. Challenges and emerging solutions to the land-based plastic waste issue in Africa[J]. <i>Marine Policy</i> , 2018, 96: 256-263
Follow up Questions	How can we alter these factors to reduce plastic waste? How do governments play a role in plastic waste?

Article #12 Notes: Plastic Waste: Global Impact and Ways to Reduce Environmental Harm

Article notes should be

Source Title	Plastic Waste: Global Impact and Ways to Reduce Environmental Harm
Source citation (APA Format)	Shershneva, E. G. (2021). Plastic waste: Global impact and ways to reduce environmental harm. <i>IOP Conference Series: Materials Science and Engineering</i> , 1079(6), 062047. https://doi.org/10.1088/1757-899x/1079/6/062047
Original URL	https://iopscience.iop.org/article/10.1088/1757-899X/1079/6/062047/pdf
Source type	Journal Article
Keywords	Plastic waste; climate change; biosphere
#Tags	
Summary of key points + notes (include methodology)	This study aimed to look at how effects of plastic waste can be minimized and identified how plastic affects the environment. They looked at what sectors were producing the most plastic over time. Main issues that they looked at: 1. Climate change and deterioration of hydro- and biosphere

2. Depletion of biotic resources and biodiversity
3. Acidification and photochemical oxidation of environment
4. Increase of oil and electricity power consumption
5. Toxicity to humans and growth of garbage

Plastic releases about 400 million tons of greenhouse gases, leading to rising temperatures. They also found that large amounts of marine life and other animals were impacted by plastic waste. Thus, they stated that policies needed to reduce the amount of plastic being consumed and improve recycling capabilities. They found that more developed countries use plastic. Finally, they looked at alternative uses for plastic waste like incineration for energy.

Research Question/Problem/ Need

How can we identify and minimize issues caused by plastic waste?

Important Figures

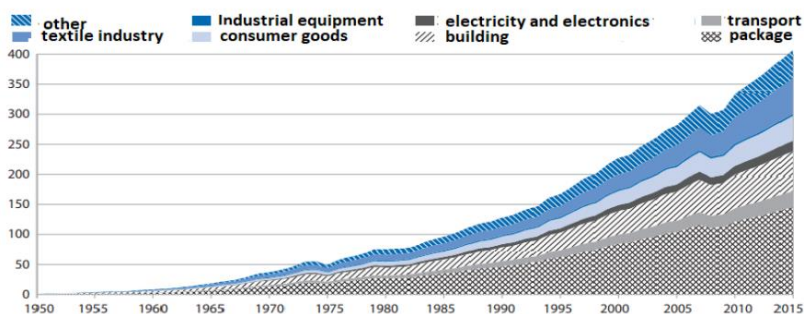


Figure 1. World production of plastic by economic sectors (millions of tons) [2].

This figure shows the distribution of plastic production.

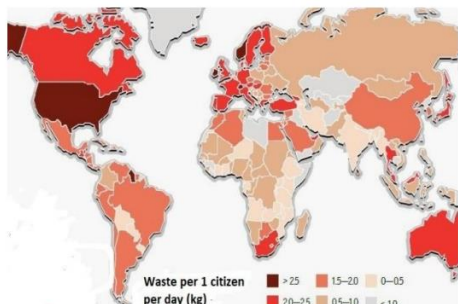


Figure 2. Distribution of waste in country, plastic takes up more than 10 % of waste volume [5].

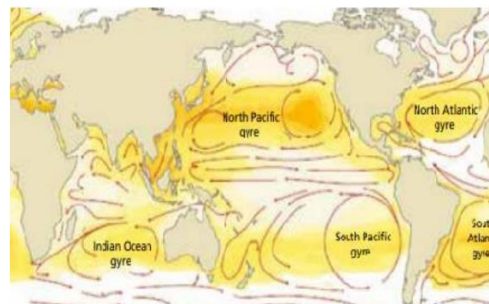


Figure 3. Distribution of plastic in oceanic and neritic waters, noticeably Great Pacific Garbage Patch [6].

These figures show the distribution of plastic waste by country and in the ocean.

VOCAB: (w/definition)

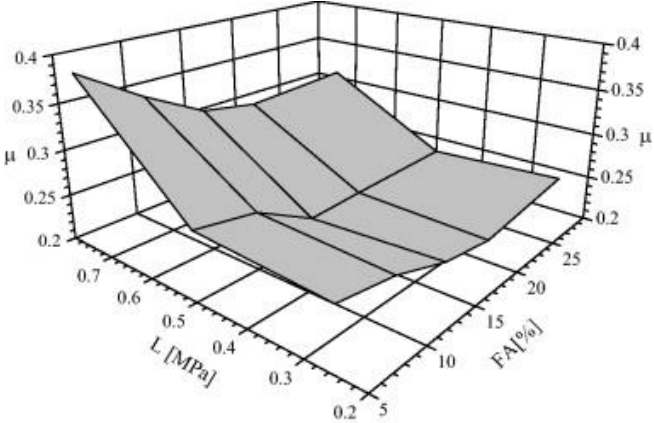
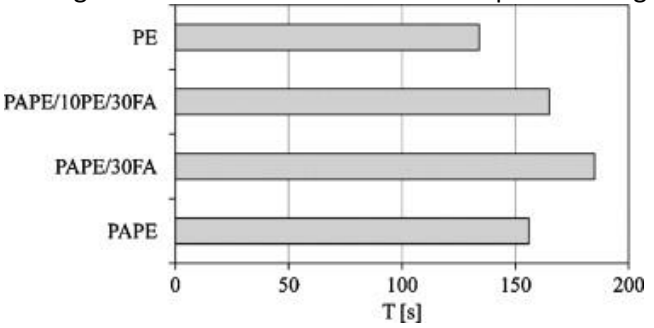
- photochemical oxidation – light catalyzed reaction of chemicals in the air
- Acidification – substances becoming more acidic
- Biopolymers – natural polymers made by living organisms
- Microfibrils – tiny chains of polymers

	elastic modulus – measure of stiffness
Cited references to follow up on	Hayelom D B 2014 Recycling of plastic waste into fuels (review) Int. J. of Science, Technology and Society vol 2 (6) pp 190–5 Welden N A and Lusher A 2017 Impacts of changing ocean circulation on the distribution of marine microplastic Integrated Environmental Assessment and Management doi:10.1002/ieam.1911
Follow up Questions	How can we make sure countries follow waste regulations? Why do less developed countries have less plastic? How can we mitigate the greenhouse gases produced through incineration?

Article #13 Notes: Recycling of packaging multilayer films: New materials for technical products

Article notes should be on separate sheets

Source Title	Recycling of packaging multilayer films: New materials for technical products
Source citation (APA Format)	Tartakowski, Z. (2010). Recycling of packaging multilayer films: New Materials for Technical Products. <i>Resources, Conservation and Recycling</i> , 55(2), 167–170. https://doi.org/10.1016/j.resconrec.2010.09.004
Original URL	https://www.sciencedirect.com/science/article/pii/S0921344910002053
Source type	Journal Article
Keywords	Recycling; Packaging ; multilayer films; PAPE; Inorganic fillers
#Tags	
Summary of key points + notes (include methodology)	A lot of plastic tends to come from the packaging sector. These packaging films are usually multilayer films made of different layers of polymers. This is because different polymers provide different properties that are useful for packaging, like gas and liquid barriers. However, they can cause environmental harm. The researchers looked at how recycled materials from multilayer films can be applied to other areas. Composite polymers are created when multilayer films are recycled without separation. They can be used in applications like bearings. They can also be

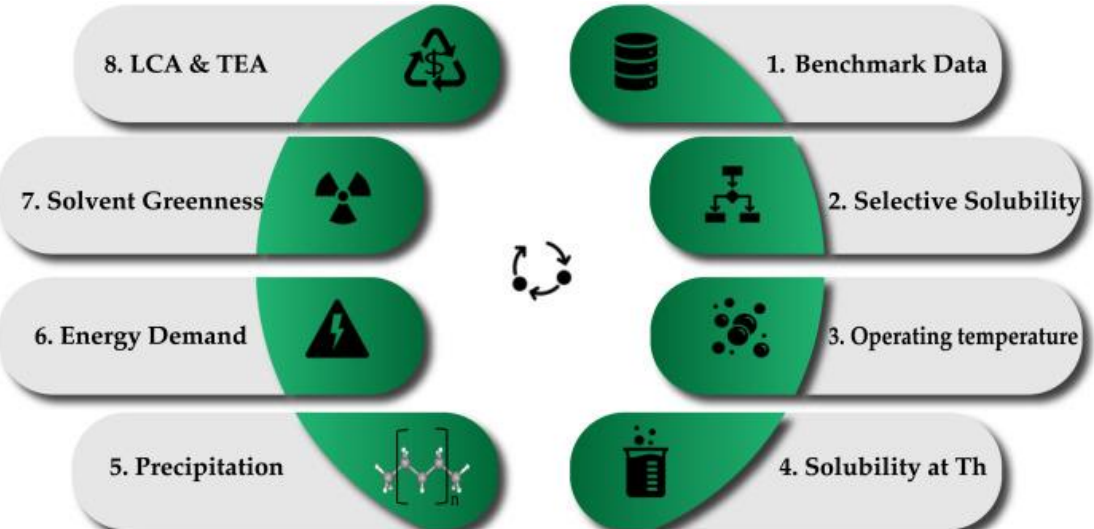
<p>gy)</p>	<p>made into other mechanical parts. They also looked at the electrical conductivity and resistance of the recovered composite materials. This showed that certain ratios of compounds could be implemented in places where insulators or resistors were needed. Overall, they found multiple ways for composite recycled material from recycled multilayer films to be reused in parts and tested the physical properties so that it was clear what applications they would be best suited for.</p>
<p>Research Question/Problem/Need</p>	<p>How can the recycled composite mixture from multilayer films be applied in different contexts?</p>
<p>Important Figures</p>	 <p>This figure shows how friction of the composite changes.</p>  <p>This figure shows the electrical resistance of different composite materials.</p>
<p>VOCAB: (w/definition)</p>	<p>Fly ashes - byproduct of coal burning Dielectric strength - maximum voltage before a substance conducts or breaks down tribological properties - how objects slide or roll PAPE modified - substance that can be added to modify properties of a polymer Agglomerate – cluster of small particles</p>
<p>Cited references to follow up on</p>	<p>https://onlinelibrary.wiley.com/doi/abs/10.1002/masy.19920570111?casa_token=RaKbMQLcShIAAAAA%3ArgPF29EaOad8HAQ53pIFkbquEexqvejRDmqE1Uv2QScM-dkHO0Z5XHtRAqxe7UtGbY56H60nHB46Vw - Identification and segregation of materials in mixed waste</p>

	https://www.sciencedirect.com/science/article/pii/S0142941806000079?casa_token=RmjHYFckOggAAAAA:8rTwzFph5HRKx17g4NU3zORb87huN39o-pNY59v4a9wv0l_Qh8o59QN398trXX9qUxenVrc - Resistance of high-content polypropylene/wood composites to low-current arc discharges
Follow up Questions	<p>Can recovered plastics be used in batteries?</p> <p>How would recovered plastics work in 3D printing?</p> <p>How can we alter properties of composite polymers?</p>

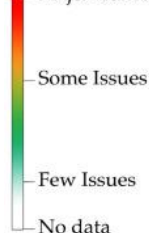
Article #14 Notes: Screening green solvents for multilayer plastic film recycling processes

Article notes should be on separate sheets

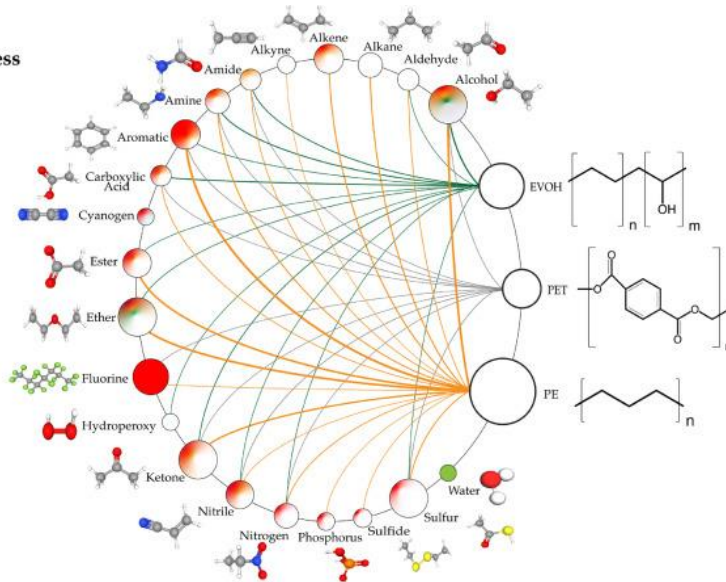
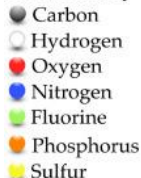
Source Title	Screening green solvents for multilayer plastic film recycling processes
Source citation (APA Format)	Ikegwu, U., del Carmen Munguía-López, A., Van Lehn, R. C., & Zavala, V. M. (2025). <i>Screening Green Solvents for Multilayer Plastic Film Recycling Processes</i> . https://doi.org/10.26434/chemrxiv-2025-zrmnp
Original URL	https://www.sciencedirect.com/science/article/pii/S0098135425001334?casa_token=8N5eFD58hscAAAAA:KMI-pCehadNV90k9tCRyy48qhDRY4tLhIQoit5nj6680-NOTBDIlwR2zqcX2uEcYuktDoKSRZg
Source type	Journal Article
Keywords	Green solvent; dissolution; precipitation; multilayer films
#Tags	
Summary of key points + notes (include methodology)	Multilayer films are common in the packaging industry since they can benefit from properties of multiple different polymers at once. For instance, different polymers may provide barriers to liquids or gases. However, only around 5% of these films are currently recycled. Past solutions include pyrolysis and mechanical recycling, which do not always account for the multiple types of polymers present. Processes like STRAP have been successful at separating these types of substances. Some of these use COSMO-RS to determine which solvents to use. However, solvents used in these were often toxic and not safe for the environment or humans. They decided 'greenness' would be based on whether they are derived from a renewable source, their usage

	<p>efficiency, health, safety, environmental hazards, recyclability, and biodegradability. They developed a holistic framework to decide what solvents should be used. First, they predicted polymer solubilities in over 1000 solvents at 120 degrees Celsius to prevent thermal degradation. Then, they made sure there was enough difference between the solubility of the target polymer and that of the other polymers of the mixture. This would ensure that only one polymer dissolved out of the mixture at a time. Following this, the researchers made sure the solvent boiling points were at least room temperature and then set them to one degree less than their boiling point. Then, they looked at solvents that had at least 15% wt solubility. Finally, they chose solvents with low solubility at room temperature so that precipitation could be done by cooling. They looked at the heat energy used to understand how much energy each solvent would require to heat. They also looked at logP values to determine if a solvent was bioaccumulative; a higher logP meant it would be more bioaccumulative. They compared their findings to databases of toxic solvents in order to better understand how the solvents would impact the environment. They then conducted technoeconomic analysis to see whether or not their process was economically viable. Finally, they used a life cycle assessment to look at the long term picture of their work. They conducted a case study using the STRAP process but replacing the solvents used by STRAP with their own.</p>
Research Question/ Problem/ Need	<p>How can green solvents be used to separate multilayer films?</p>
Important Figures	 <p>This figure shows their considerations in deciding what solvents to use.</p>

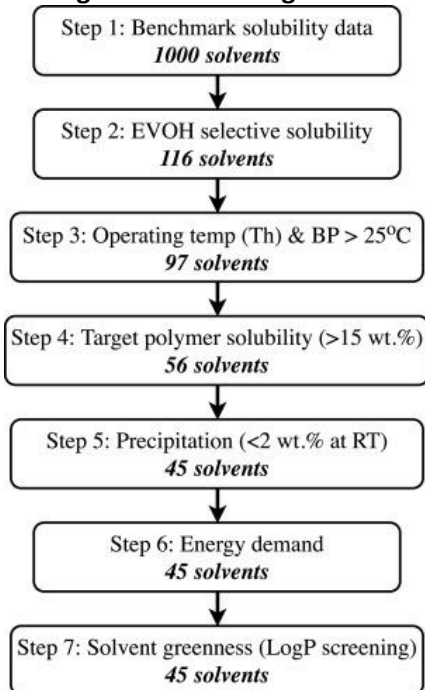
Solvent Greenness
Major issues



Structure Key



This figure shows how green solvents are that can dissolve the polymers mentioned in STRAP.



This figure shows how their methodology narrowed down which solvents to use.

<p>VOCAB: (w/definition)</p>	<p>Biomass - organic waste from organisms ex. wood LCA – assess environmental impacts over entire life cycle from start to finish TEA – looks at economic viability based on what currently exists Freshwater ecotoxicity – how a substance affects freshwater systems aprotic dipolar solvent – highly polar but does not h-bond</p>
<p>Cited references to</p>	<p>Quantifying the environmental benefits of a solvent-based separation process for multilayer plastic films -</p>

follow up on	https://pubs.rsc.org/en/content/articlehtml/2023/gc/d2gc04262b?casa_token=rCtsQNAfulwAAAAA:lrDL0k5pkIjodw2Itc0rMmjNct8FDOQkHba8tRIF00KhguqR_d34xVXn0yEvowC1NWZDDq-Wipl5tsc Integrating model-based design of experiments and computer-aided solvent design - https://www.sciencedirect.com/science/article/pii/S0098135423002156
Follow up Questions	How can other methods of recycling be made more environmentally friendly? What effects do polymers themselves have on toxic outputs of recycling plants? How can this process be applied to other scenarios other than just packaging?

Article #15 Notes: Pigment removal from reverse-printed laminated flexible films by solvent-targeted recovery and precipitation (TBR)

Article notes should be on separate sheets

Source Title	Pigment removal from reverse-printed laminated flexible films by solvent-targeted recovery and precipitation
Source citation (APA Format)	Yan, T., Granger, C., Sánchez-Rivera, K. L., Zhou, P., Grey, S., Nelson, K., Long, F., Bar-Ziv, E., Van Lehn, R. C., Avraamidou, S., & Huber, G. W. (2025). Pigment removal from reverse-printed laminated flexible films by solvent-targeted recovery and precipitation. <i>Science Advances</i> , 11(11). https://doi.org/10.1126/sciadv.adt5841
Original URL	https://www.science.org/doi/10.1126/sciadv.adt5841
Source type	Journal Article
Keywords	STRAP; ink; polymers
#Tags	
Summary of key points + notes (include methodology)	Plastic has been piling up and causing environmental issues. When recycling films, layers generally need to be separated and purified. However, dyes in films end up tainting the color or accumulating in black flecks. Color is important for consumers as well as pricing; clear films tend to be sold for

more money. Pigments are small dots of color whereas dyes are meant to be dissolved. Pigments need to be bound to plastic. Sometimes, pigments are printed on an inner layer of the plastic, making them harder to get rid of during recycling. During STRAP, some pigments get filtered out if they are not solubility in the solvents. Since the coloration never increased during STRAP, they decided the coloring was likely not due to polymer degradation. Red 57:1, Blue 15:4, Green 7, Yellow 110, and Violet 19 are common pigments used in films. The researchers looked at the inks in groups as there is a large variety of them. PE tends to have a bright yellow color after STRAP, so the violet is not the cause of that. Most common inks are not soluble in dodecane. For Orange 13 and Yellow 12, at 20C they were not soluble but after heating to 120C and then cooling back down to 20C, they were still present in a bright yellow color. This is because during heating, the pigments decompose from diarylides to monoazos, which means they are a different chemical species than at the start. They noticed the absorbance depended on both initial concentration and temperature, which does not follow standard equilibrium principles. During STRAP, lots of colorant gets deposited on the PE, which is why it becomes so yellow. One way to reduce this is to reduced the amount of solvent left in the substance, as the solvent deposits more ink. This is because when they dry the polymer, only the solvent evaporates. Adding absorbants like carbon can decrease color by absorbing pigment.

Research Question/Problem/ Need

Why do certain polymers become colored after the STRAP process?

Important Figures

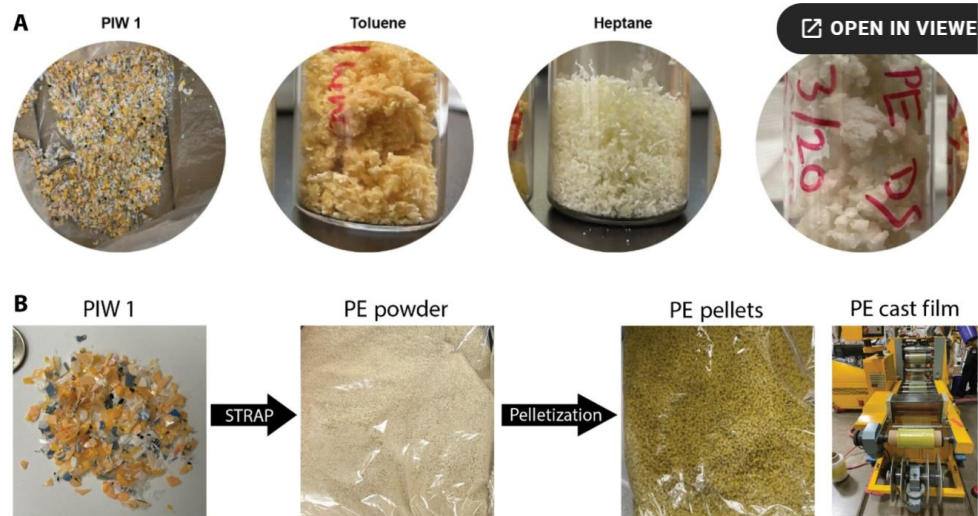
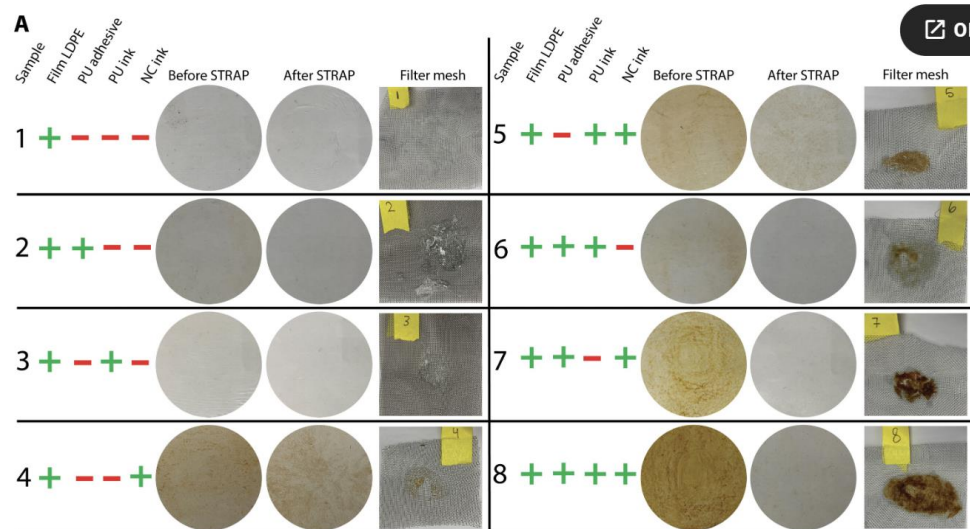
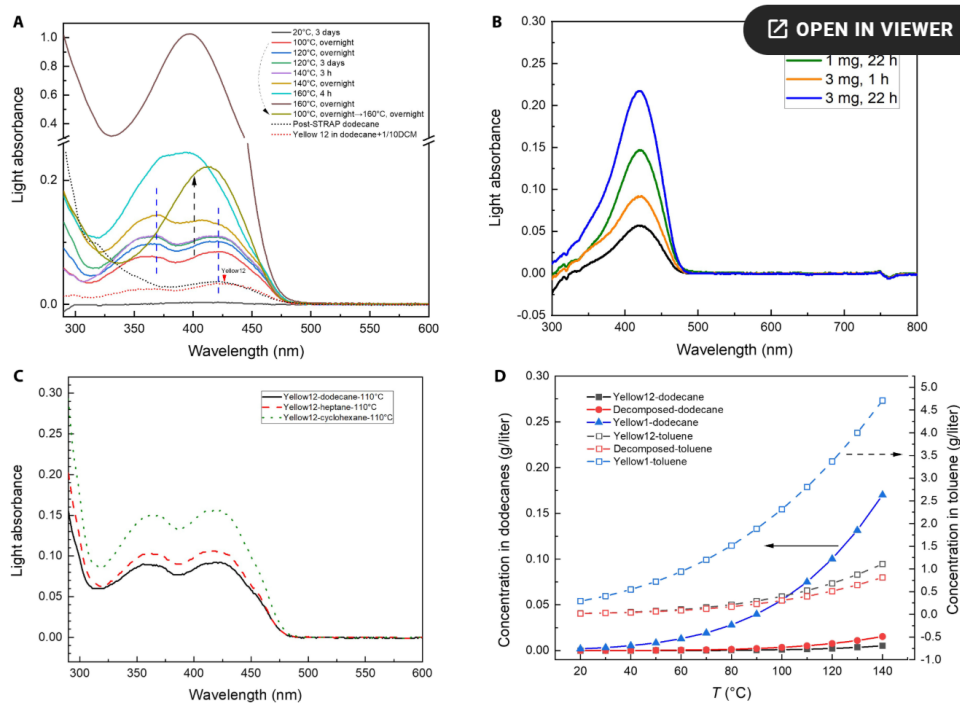


Fig. 2. Recovered PE from a reverse-printed laminated multilayer film via STRAP. This figure shows a past method of removing colorant from films.



This figure shows the color of films before and after STRAP.



This figure shows that the inks are a different chemical species before and after heating.

VOCAB: (w/definition)

Diarylides – type of compound with two rings
 Monoazo – type of compound with azo bond
 Dodecane - $C_{12}H_{26}$ - hydrocarbon
 Spectrophotometer – looks at light absorbance

Cited references to follow up on

Circularity in polymers: addressing performance and sustainability challenges using dynamic covalent chemistries - <https://pubs.rsc.org/en/content/articlehtml/2023/sc/d3sc00551h>

	The discoloration of polyethylene obtained from chemical separation of laminates: Investigating additives and other potential causes - https://lup.lub.lu.se/student-papers/search/publication/9055885
Follow up Questions	Can all ink be removed by using activated carbon? Can inks be designed to not be soluble in organic solvents? Can the inks be recovered and reused?

Article #16 Notes: Identification and segregation of materials in mixed waste

Article notes should be on separate sheets

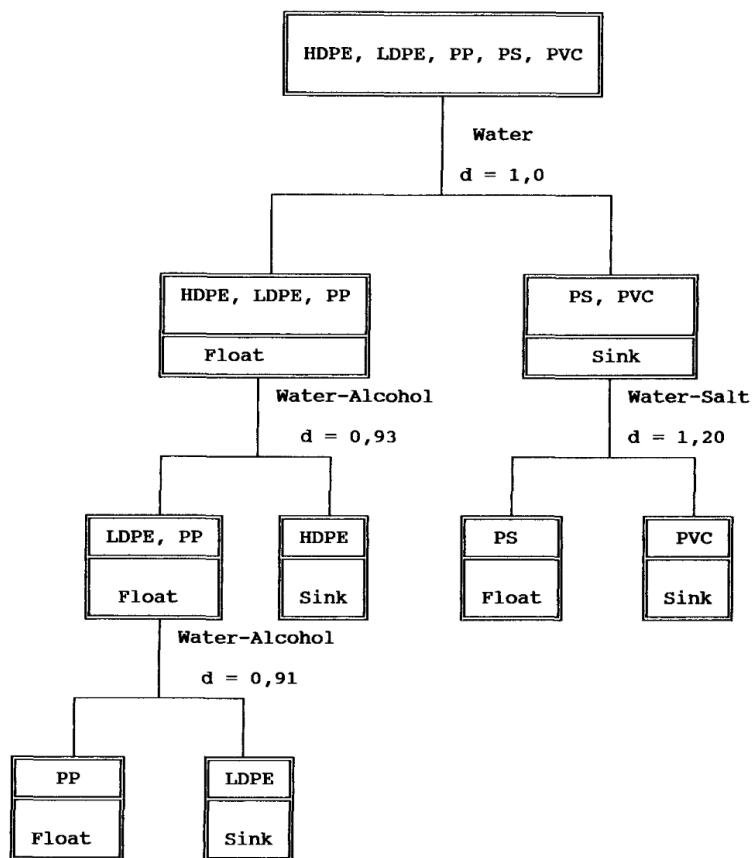
Source Title	Identification and segregation of materials in mixed waste
Source citation (APA Format)	Soler, T. O. (1992). Identification and segregation of materials in mixed waste. <i>Makromolekulare Chemie. Macromolecular Symposia</i> , 57(1), 123–131. https://doi.org/10.1002/masy.19920570111
Original URL	https://onlinelibrary.wiley.com/doi/epdf/10.1002/masy.19920570111?saml_referrer
Source type	Journal Article
Keywords	Triboelectric separation; plastic; solvents; chemical markers
#Tags	
Summary of key points + notes (include methodology)	Plastics are produced globally and tend to pile up at the end of their lives. They do not degrade well in the environment, leading to ecological problems. Other methods like incineration release harmful gases into the atmosphere. Thus, to recycle plastics, they must first be separated into different types. In general, plastics can be separated by physical properties, using solvents, or by looking at chemical markers for identification. Triboelectric separation has proven to be very effective at separating polymers. This process occurs by charging the polymers with friction and then projecting them in an electrostatic field. Physical separation has also been effective. One way to separate polymers physically is by float-sink separation, which uses varying densities of polymers to separate them. Another option is using solvents to dissolve out specific polymers and precipitate them out of the solution. One issue with these methods is that they usually require prior knowledge of what polymers are present within the mixture. This is not always the case, especially when it comes to mixed waste at recycling plants. A solution to this is to chemically mark the different types of polymers with small amounts of another chemical substance,

which would lead to easier identification. These chemical markers must not impact safety of the polymers or color. They should also be non-toxic.

Research Question/Problem/Need

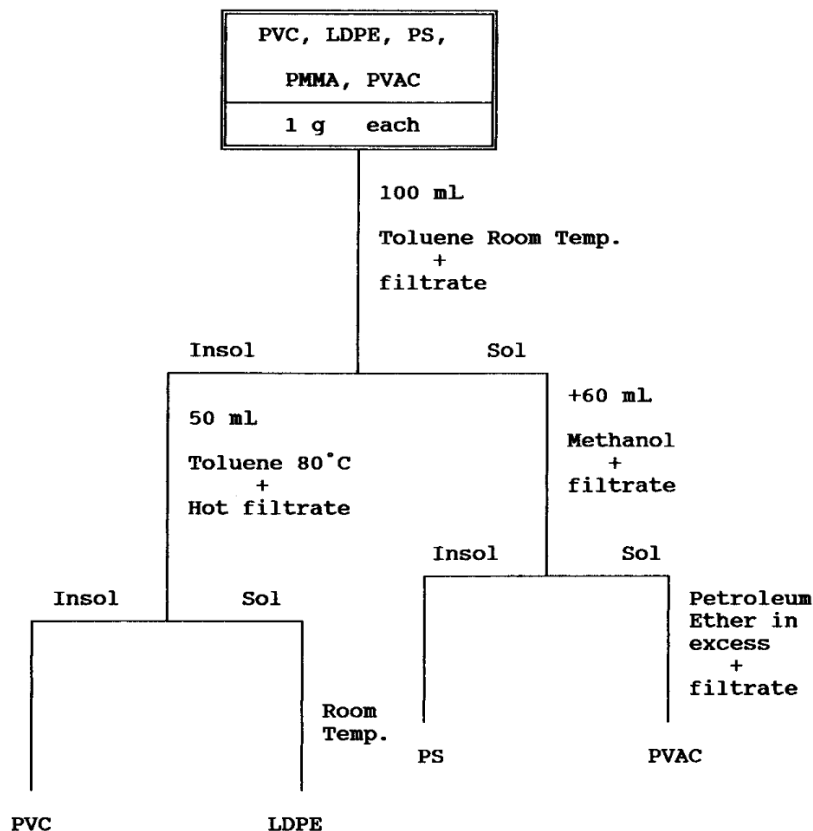
How can polymers be separated for better recycling?

Important Figures



This figure shows how polymers can be separated based on physical properties.

FIGURE 2



This figure shows separation based on dissolution.

VOCAB: (w/definition)

triboelectrical separation – separation based on electrostatic charging
 Hydrocyclone – uses centrifugal force to separate particles
 surfactant agents – reduce surface tensions/ tension between phases
 spectroscopic methods – how matter interacts with electromagnetic radiation

Cited references to follow up on

Drain, K. F., Murphy, W. R, Otterburn, M. S.. A solvent Techiquefor the Recycling of Polypropylene - Degradation on Recy-cling. Conservation and Recycling, 1983, 6, (3), pp.123-137
 Sperber, S.J., Rosen, S.L..Recycling of Thermoplastic Waste:Phase Equilibrium in Polystyrene-PVC-Polyolefin Solvent.Polymer Eng. and Science 1976, April, Vol. 16, NQ 4, pp. 246-251.

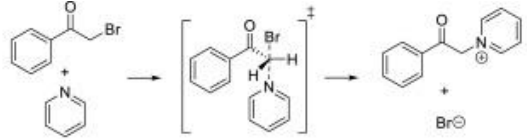
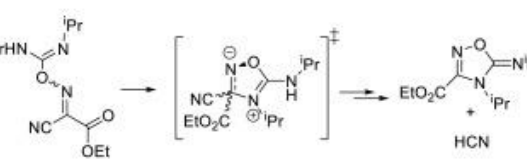
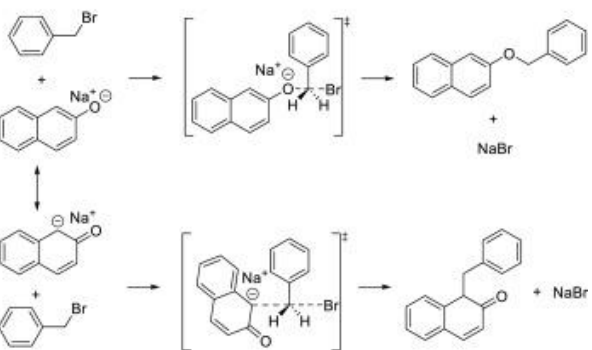
Follow up Questions

How can triboelectric separation be used to separate materials other than plastic?
 How could chemical markers be applied to current waste technologies?
 What can be done to mitigate the adverse impacts of solvents on the environment?

Article #17 Notes: Integrating model-based design of experiments and computer-aided solvent design

Article notes should be on separate sheets

Source Title	Integrating model-based design of experiments and computer-aided solvent design
Source citation (APA Format)	Gui, L., Yu, Y., Oliyide, T. O., Siougkrou, E., Armstrong, A., Galindo, A., Sayyed, F. B., Kolis, S. P., & Adjiman, C. S. (2023). Integrating model-based design of experiments and computer-aided Solvent Design. <i>Computers & Chemical Engineering</i> , 177, 108345. https://doi.org/10.1016/j.compchemeng.2023.108345
Original URL	https://www.sciencedirect.com/science/article/pii/S0098135423002156
Source type	Journal Article
Keywords	Model-based design of experiments; Computer-aided molecular design; Solvent design; Solvatochromic equation
#Tags	
Summary of key points + notes (include methodology)	<p>Reaction kinetics can affect the properties of the product. For this reason, understanding reaction kinetics is essential for fields like polymer creation and the food industry. Factors like pH, temperature, catalysts, and the solvent used all affect kinetics. For this study, they focused on how solvents impact reaction kinetics. However, conducting experiments in a lab setting has economic and environmental costs. So, the researchers looked into creating a computer simulation to solve this issue. Past computer programs include CAMD, which has looked at solvent selection for applications like crystallization. These programs look at specific features of a molecule to be optimized. Most molecular models use some form of multivariate linear regression. Specific examples are based on molecular properties, such as those generated by COSMO. Some other ways to predict properties of compounds include artificial neural networks; however, these often require large amounts of training data to be accurate which is not always available. Some studies focused more on actual reaction kinetics than molecular properties. For instance, one group looked at experimental reaction rate constants and used them to predict other reactions. Another model, also looking at rates, correctly predicted which solvent would be the best even though the actual calculations varied from reality. The researchers decided to build on these experiments with their own model. They focused their efforts onto three case studies: one about the Menschutkin equation, one regarding peptide synthesis, and the final one about the Williamson ether synthesis. They used a quantum mechanical model to calculate rate constants for the reactions and create a regression. Their goal was to be able to select the best solvents from a certain list using rate constants. Their model is a regression which has a similar design to a</p>

	neural network with weights and biases. They incorporated and related many different types of chemical properties and eventually ended up with a linear regression. They found that in general their model predicted the top 10 best solvents correctly.
Research Question/ Problem/ Need	How can rate constants be used in a computer model to decide which solvents work best for which reactions?
Important Figures	<p>a) </p> <p>b) </p> <p>c) </p> <p>This figure shows the three case studies and the chemical reactions for each one.</p> <div style="display: flex; flex-wrap: wrap; justify-content: space-around;"> <div style="border: 1px solid black; border-radius: 10px; padding: 5px; width: 45%; text-align: center;"> 1. Expand the solvent list in Formulation 1 with solvents* that have missing solvatochromic parameters </div> <div style="border: 1px solid black; border-radius: 10px; padding: 5px; width: 45%; text-align: center;"> 4. Solve Formulation 2 for optimal initial solvent set </div> <div style="border: 1px solid black; border-radius: 10px; padding: 5px; width: 45%; text-align: center;"> 2. Estimate the missing parameters using GC methods </div> <div style="border: 1px solid black; border-radius: 10px; padding: 5px; width: 45%; text-align: center;"> 3. Expand the candidate matrix in Formulation 1 with the new solvents to form Formulation 2 </div> </div> <p>This figure shows a workflow of their computing process.</p>

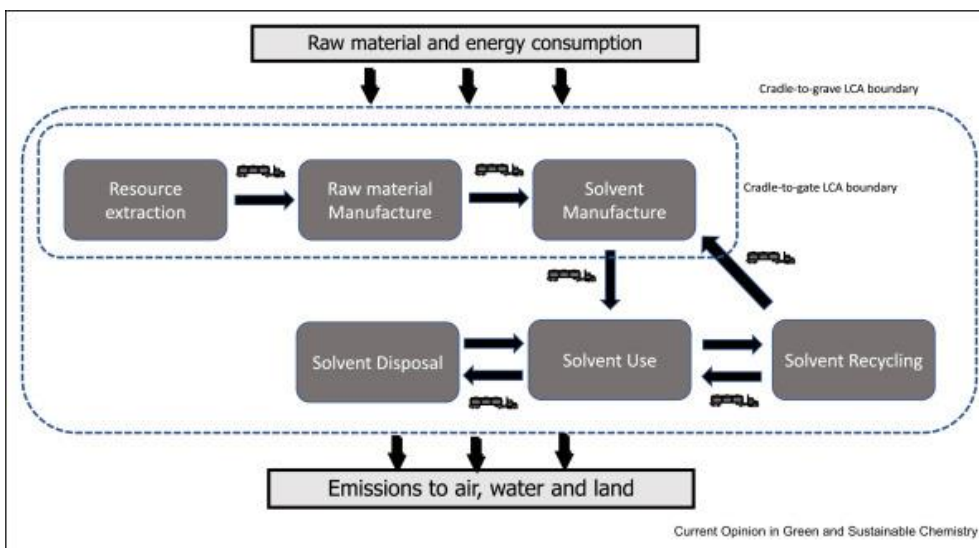
	<p>This shows a full workflow of how they were able to develop their model.</p>
VOCAB: (w/definition)	<p>Solvatochromic equation – how a molecules spectrum shifts w/ polarity Menschutkin reaction – a specific equation that is useful for studying solvent interactions with rate density functional theory – looks at distribution Abraham’s hydrogen bond basicity – how good of a proton acceptor something is σ profiles - surface charge density distribution in COSMO RS Bayesian optimisation – a way to train on large amounts of data/ make predictions A-optimality criterion - minimize average variance D-optimality criterion – maximize determinant of information matrix</p>
Cited references to follow up on	<p>Discrete and mixed-variable experimental design with surrogate-based approach - https://www.sciencedirect.com/org/science/article/pii/S2635098X24001967</p> <p>Optimal design of solvent blends for environmental impact minimization - https://aiche.onlinelibrary.wiley.com/doi/abs/10.1002/aic.690450415?casa_token=lrBOL5ICY9gA_AAAA:4v1TNqv3Cg0fCFh5XtZdMdNzwOkXIac31IPw6bVLup88LWrsEFJsrQva-_RqDfyVfkKxZQYQy30Qq3H5w</p>
Follow up Questions	<p>How can data about solvent toxicity be incorporated into this model? How easy is it to separate the products from the solvent? What applications does this model have outside of chemistry (ex. Engines)?</p>

Article #18 Notes: Life cycle considerations of solvents

Article notes should be on separate sheets

Source Title	Life cycle considerations of solvents
Source citation (APA Format)	Jimenez-Gonzalez, C. (2019). Life cycle considerations of Solvents. <i>Current Opinion in Green and Sustainable Chemistry</i> , 18, 66–71. https://doi.org/10.1016/j.cogsc.2019.02.004
Original URL	https://www.sciencedirect.com/science/article/pii/S2452223618301147?casa_token=B4ThLKXmiQEAAAAA:qXNKtrYsavxYlujwrRFoknHdbETIVgcDyAEYOkP2ci6CQxTYCPkFbpWj1pc2kL8_ONn4uVd3ROY
Source type	Journal Article / Lit. Review
Keywords	Life Cycle Assessment ; green solvents; environment
#Tags	
Summary of key points + notes (include methodology)	Solvents are used a variety of ways and industries. However, there are concerns about their possible adverse effects, including health and environmental hazards. Thus, it is important to look at the impacts of solvents throughout their entire lifecycle. Some substance are used in the formation of other products but not add to the purpose of that product. These substances should be eliminated if possible as they can cause negative impacts. To truly understand the impact of solvents, it is necessary to look at a solvents full lifecycle. This includes looking at emissions, energy, and toxicity starting at the creation of the solvent and following it through its uses and finally its disposal. Sometimes, solvents can release toxic chemicals through evaporation during use. At the end of a solvent's life, there are many aspects that need to be taken into consideration. For instance, a solvent can be recycled or released into the environment. One important factor to take note of is the cost of recycling relative to the cost of producing more virgin solvent. As for incineration, it will produce energy but often also carbon emissions. If a solvent can be recycled, however, it stops the need to produce more solvent. All of these different approaches to the end of life treatment of a solvent result in vastly different impacts on the environment and health. Thus, it is important to be clear and intentional about the LCA is measuring.
Research Question / Problem / Need	How can the life cycle of solvents be assessed?

Important Figures



This figure shows the entirety of the life cycle assessment.

Propanol	Propanal	Ethylene	Petroleum extraction/refinery		
			Water		
			Sodium Hydroxide	Sodium chloride	Salt rock
					Water
		Hydrogen	Natural gas		
			Oxygen	Air	
		Carbon monoxide	Natural gas		
			Steam	Water	
			Carbon Dioxide	Air	
				Natural gas	
	Water				
Hydrogen	Natural gas				
	Oxygen	Air			

Current Opinion in Green and Sustainable Chemistry

This figure shows the many processes involved in refining a specific solvent.

VOCAB: (w/definition)

Ancillary – things that support something else
 release potential – likelihood of something being released into the environment
 fugitive emissions - unintended leakage from equipment
 ionic liquids - salts as liquids

Cited references to follow up on	<p>https://pubs.acs.org/doi/full/10.1021/es048114o?casa_token=UwNFVx8wIwIAAAA%3AtXAut_JEmgPyMM-jot5s_bQk4bZg0tEJ7qOycLL474eQR1RA9_JjAp6SVsp6RI3q7SRuxb6NZHR0PXYm4g -- Life-Cycle Inventory of Waste Solvent Distillation: Statistical Analysis of Empirical Data</p> <p>https://pubs.rsc.org/en/content/articlehtml/2014/gc/c4gc01149j?casa_token=bxFCruSS-0IAAAA:zlt464whfGHF1nzilTHrzlWaSStycakwd47422K78WkTrShN49O6pDmK2T94VdfCB6bKatZoAzBEX2pQ - A survey of solvent selection guides</p>
Follow up Questions	<p>How can companies use this process in selection for their production?</p> <p>How can solvents be recycled into other industries?</p> <p>Can biodegradable solvents be created?</p>

Article #19 Notes: Ensemble machine learning to accelerate industrial decarbonization: Prediction of Hansen solubility parameters for streamlined chemical solvent selection

Article notes should be on separate sheets

Source Title	Ensemble machine learning to accelerate industrial decarbonization: Prediction of Hansen solubility parameters for streamlined chemical solvent selection
Source citation (APA Format)	Al-Sakkari, E. G., Ragab, A., Amer, M., Ajao, O., Benali, M., Boffito, D. C., Dagdougui, H., & Amazouz, M. (2025). Ensemble machine learning to accelerate industrial decarbonization: Prediction of Hansen solubility parameters for streamlined chemical solvent selection. <i>Digital Chemical Engineering</i> , 14, 100207. https://doi.org/10.1016/j.dche.2024.100207
Original URL	https://www.sciencedirect.com/science/article/pii/S2772508124000693#bib0094
Source type	Journal Article
Keywords	Machine learning; Biclustering algorithm; Decision fusion; Chemical analytics; Lignins; Smiles; Hansen solubility parameters

#Tags	
Summary of key points + notes (include methodology)	<p>AI driven chemistry methods are becoming more prevalent. Using AI to help understand lignin properties can prove beneficial to the use and understanding of them. Given the lack of data, ensemble based machine learning is attractive for prediction. Also, many datasets can over or underrepresent certain groups, impacting results. Many single focus ML models have lacked accuracy and precision that can be helped through a multifaceted approach. HSPs are useful to describe both polar and non polar solvents, allowing a wide range of applications. The traditional methods take too long and are not applicable for large amounts of data. SMILES strings were utilized to better represent chemicals for a machine learning model.</p> <p>Main Issues with past models (as stated by text):</p> <p>“</p> <ul style="list-style-type: none"> • Existing machine learning techniques exhibit suboptimal prediction accuracies. • Current feature selection methods are often inefficient, relying on manual selection as observed in some literature. • There is a prevalent issue of black-box modeling, leading to a lack of interpretability and explanation. • There is an imperative for a precise tool to predict Hansen solubility parameters for various materials, including solvents, which is crucial for optimizing industrial processes such as lignin valorization, carbon capture, and polymer manufacturing. <p>“</p> <p>Goals:</p> <ol style="list-style-type: none"> 1. Investigate the use of bi-clustering as a data finding method to perform features selection and use non-linear clustering techniques to optimize the parameters of bi-clustering graphically. 2. Create a decision method to improve the prediction accuracy based on using different machine learning models, with different benefits. 3. Validate the model that should predict Hansen solubility parameters using SMILES codes as inputs. This will help in the accurate definition of the Hansen sphere to select the best solvents to dissolve a certain material. 4. Interpret the black-box models by incorporating XAI techniques to extract knowledge and actionable insights that help the users, e.g., material and process designers accelerate the solvent selection and design optimization procedures afterwards. <p>To process the data, they removed outliers and began using clustering and biclustering methods. They utilize this method to help improve accuracy and visualization. They use UMAP, t-SNE, and k-means algorithm to visualize data. They also used PCA to transform their data. They use decision fusion to understand their modeling. They then had to decide what training and validation split to use. They looked at a variety of models such as CNNs, LSTMs, and SVR. In</p>

	<p>total, they utilized 8 models in their ensemble learning. They looked at data distribution and correlation. They later found that a bigger data size helped accuracy.</p> <p>Overall, they found their model and methods accurately predicted the HSPs.</p>
<p>Research Question/Problem/ Need</p>	<p>How can Hansen solubility parameters be predicted?</p>
<p>Important Figures</p>	<p>This figure demonstrates the project's methodology and flow.</p>



Different data forms & sources

Data cleaning
Omitting outliers, missing & invalid observations

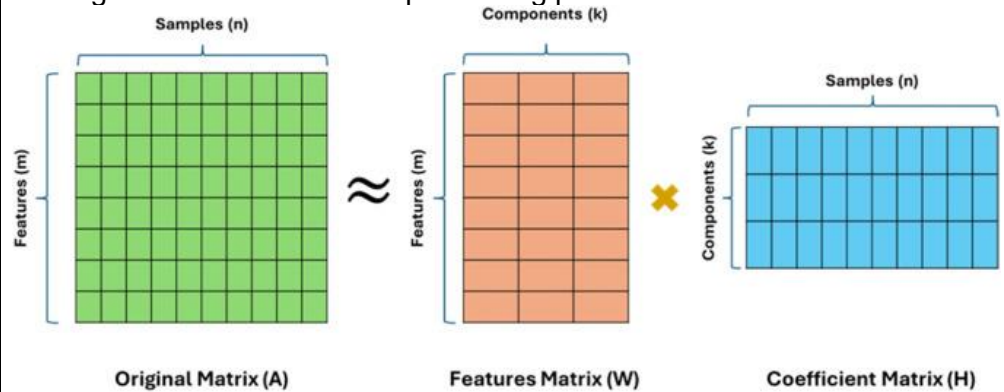
Features extraction
Extraction of different representative features & descriptors

Initial clustering
Definition of the optimum number of clusters & components required for bi-clustering

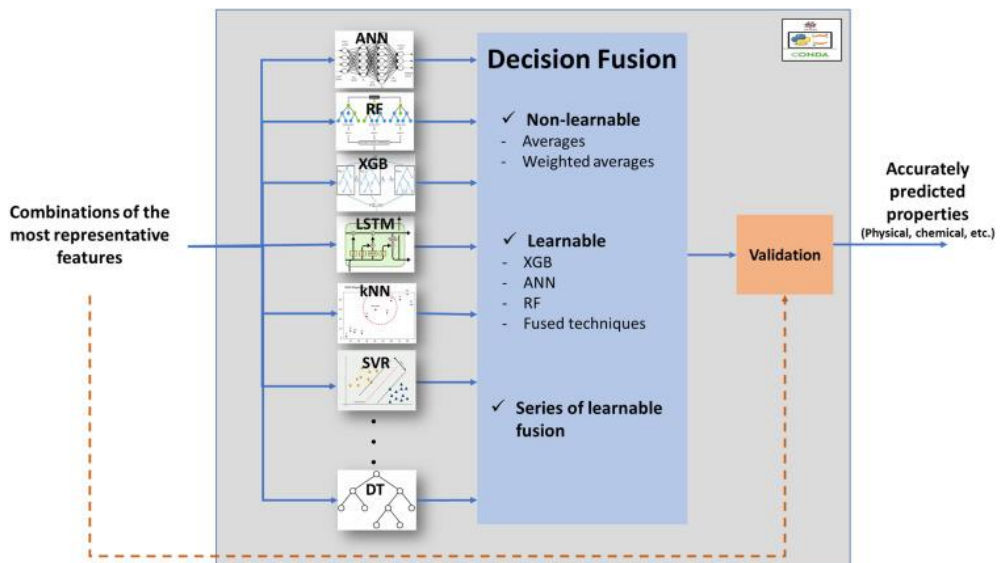
Bi-clustering (Features selection)
Definition of the most significant features & descriptors

The most significant features

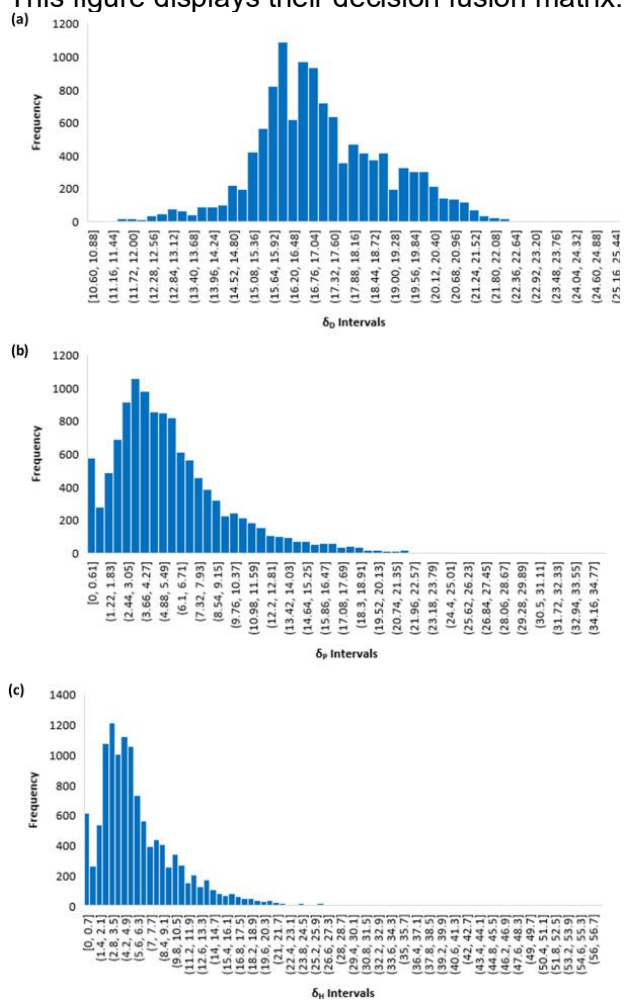
This figure describes the data processing process.



This figure shows how biclustering works.



This figure displays their decision fusion matrix.



This figure shows the distribution of parameter data.

VOCAB: (w/definition)

Lignins – organic polymers

	<p>Ensemble machine learning – multiple models working together</p> <p>Biclustering algorithm – grouping similar samples and features</p> <p>Decision fusion - Combining the outputs of multiple models to make one final decision</p> <p>Shallow learning - Machine learning models with few parameters and no deep layered structure.</p> <p>uniform manifold approximation - A dimension reduction technique</p> <p>Deep learning - Models made from multiple layers of neurons</p>
Cited references to follow up on	<p>Deep learning and knowledge-based methods for computer-aided molecular design—toward a unified approach: state-of-the-art and future directions</p> <p>A machine learning-based ensemble model for estimating diurnal variations of nitrogen oxide concentrations in Taiwan</p>
Follow up Questions	<p>How can these be applied to recycling?</p> <p>How can these methods be improved?</p>

Article #20 Notes: Prediction of Hansen Solubility Parameters with a New Group-Contribution Method

Source Title	Prediction of Hansen Solubility Parameters with a New Group-Contribution Method
Source citation (APA Format)	Stefanis, E., & Panayiotou, C. (2008). Prediction of Hansen solubility parameters with a new group-contribution method. <i>International Journal of Thermophysics</i> , 29(2), 568–585. https://doi.org/10.1007/s10765-008-0415-z
Original URL	https://link.springer.com/article/10.1007/s10765-008-0415-z
Source type	Journal Article
Keywords	Group-contribution method · Hansen solubility parameters
#Tags	
Summary of key points + notes (include methodology)	Solubility parameters are good metrics to understand how two substances will interact with each other. The Hildebrand Solubility parameter focuses mostly on nonpolar solvents. Hansen Solubility Parameters are a good way to combat this issue as they look at polarity and hydrogen bonding alongside dispersion forces. Past studies have looked at group contribution to predict HSPs with some success.

This study utilizes a mixture of first and second order groups to predict the parameters. A molecule can be represented as bunch of dominant and recessive conjugates. They looked at which conjugates most affect the standard enthalpy of formation. To find second order groups, they had to look at first order groups around them, figure out the possible configurations, and estimate bond energies. Then, they used regression analysis to determine which groups contributed most to the overall enthalpy of formation. With his informations they were able to create equations to predict the HSPs.

Research Question/Problem/ Need

How can group contribution be used to predict HSPs?

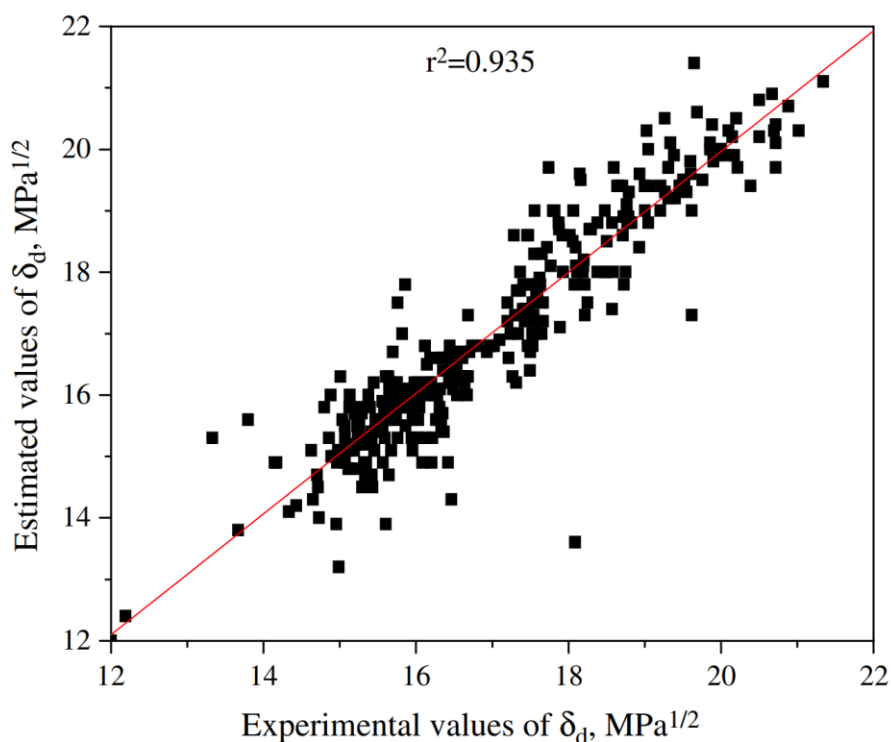
Important Figures

$$\delta_d = \left(\sum_i N_i C_i + W \sum_j M_j D_j + 17.3231 \right) \text{MPa}^{(1/2)} \quad (24)$$

$$\delta_p = \left(\sum_i N_i C_i + W \sum_j M_j D_j + 7.3548 \right) \text{MPa}^{(1/2)} \quad (25)$$

$$\delta_{hb} = \left(\sum_i N_i C_i + W \sum_j M_j D_j + 7.9793 \right) \text{MPa}^{(1/2)} \quad (26)$$

This explains how they were able to predict different HSPs.

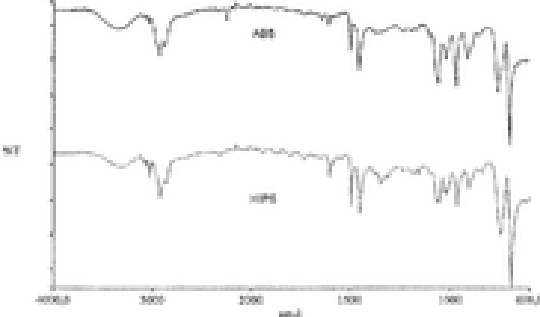


	This figure shows their approximations vs the expected values.
VOCAB: (w/definition)	<p>UNIFAC groups - universal factorial groups used for modeling non ideal solutions</p> <p>First-order groups – basic functional groups</p> <p>second-order groups – subtle chemical differences based on environment</p> <p>ABC framework - A - hydrogen-bond donors, B - hydrogen-bond acceptors, C - non-polar / dispersive interactions</p> <p>dominant conjugate – drives interaction (stronger forces)</p> <p>Recessive conjugate - adjusts to driver</p>
Cited references to follow up on	<p>L. Constantinou, E. Stefanis, C. Panayiotou, V. Vassiliades, A. Afantitis, G. Melagraki, O. Markopoulou, in Proceedings of 22nd European Symposium on Applied Thermodynamics (ESAT) (Elsinore, Denmark, 2006), pp. 316–321</p> <p>E. Stefanis, L. Constantinou, C. Panayiotou, Ind. Eng. Chem. Res. 43, 6253 (2004)</p>
Follow up Questions	<p>How can this work be applied to machine learning?</p> <p>Is there a chemical reason why their model works well?</p> <p>Why is there error when the values are low?</p>

Patent #1 Notes: Method for recycling plastic materials and use thereof

Article notes should be on separate sheets

Source Title	Method for recycling plastic materials and use thereof
Source citation (APA Format)	Maeurer, A., Schlummer, M., & Beck, O. (2012, March 20). Method for recycling plastic materials and use thereof.
Original URL	https://patents.google.com/patent/US8138232B2/en
Source type	Patent
Keywords	Recycling; solvent; precipitation
#Tags	
Summary of key points + notes (include methodology)	One fifth of recycled electronic material in the EU is plastic. This plastic is highly contaminated by substances such as brominated flame-retardant additives. There are many different kinds of polymers in this waste which need to be separated. Past research uses dissolution and precipitation;

	<p>however, since the composition of the mixture is sometimes unknown, more than one type of polymer can dissolve and be precipitated at once. The researchers decide to look at how to separate mixtures of two or more polymers. They decided to add a solvent that at least one polymer was soluble in. Then, they added a precipitant in to precipitate out a solvent form the system. From there, they can separate the polymers based on the separation of phases. The polymers are based on polystyrene. Costs of this can stay low due to recirculating solvent. The preferred temperature was room temperature, but higher ones were acceptable. Some components can be separated with density screening. The claims reiterate the parts mentioned in the description.</p>
Research Question/Problem/Need	<p>How can mixtures of polymers be separated?</p>
Important Figures	 <p>This figure shows infrared spectroscopy.</p>
VOCAB: (w/definition)	<p>brominated flame-retardant additive – brominated chemicals that stop the spread of flame dioxin formation – toxic components from incomplete combustion Rheological – flow and deformation, ex. viscosity Sedimentation – particles settling out of a liquid Fourier transform infrared spectrum - shows bonding</p>
Cited references to follow up on	<p>Uddin, M. A.; Bhaskar, T.; Kaneko J.; Muto A.; Sakata, Y.; Matsui, T. (2002) “Dehydrohalogenation during pyrolysis of brominate flame retardant containing high impact polystyrene (HIPS.Br) mixed with polyvinylchloride (PVC), Fuel 81, pp. 1819-1825</p> <p>(Mäurer, A., Schlummer, M. (2004) “Good As New. Recycling plastics from WEEE and packaging waste”, Waste Management World, May-June 2004, pp. 33-43</p>
Follow up Questions	<p>How can this be applied to other kinds of polymers? How does this differ from processes like STRAP? What other ways can waste mixtures be separated?</p>

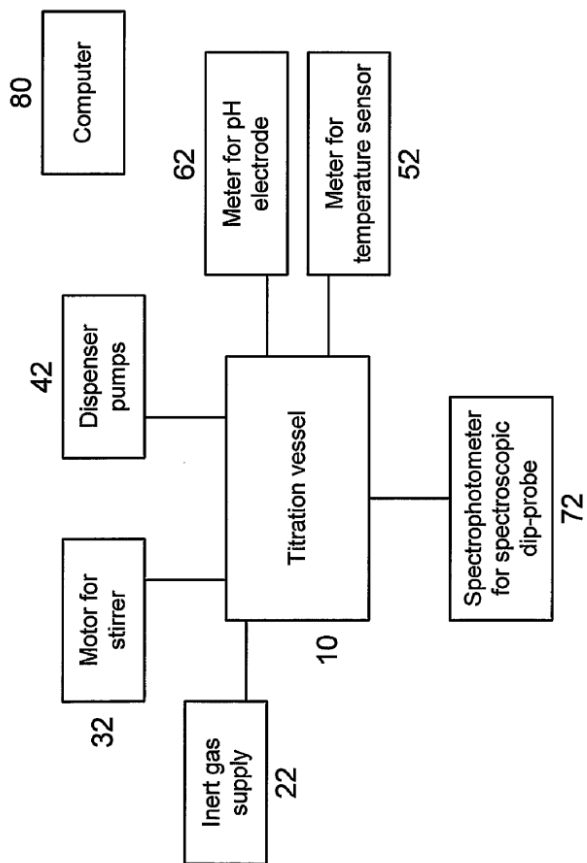
Patent #2 Notes: Method for determining solubility of a chemical compound

Article notes should be on separate sheets

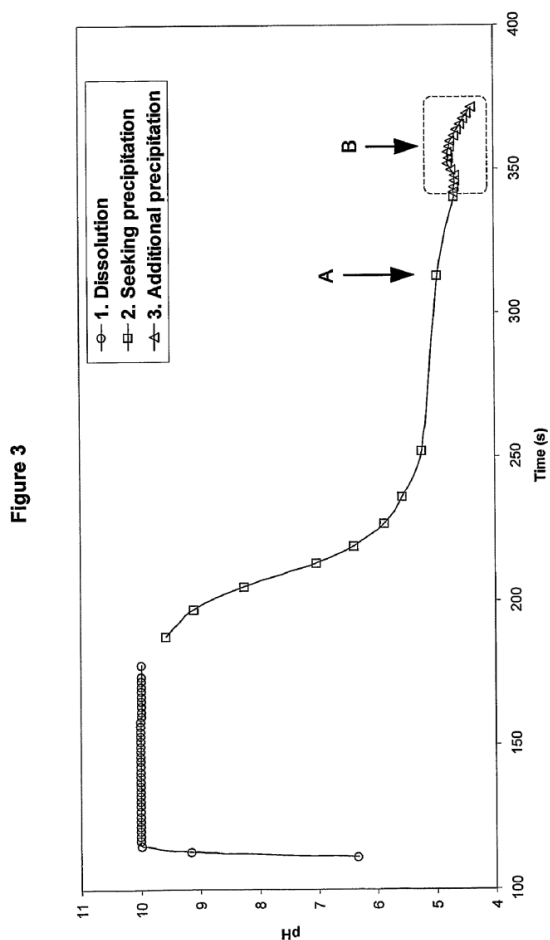
Source Title	Method for determining solubility of a chemical compound
Source citation (APA Format)	Stuart, M., & Box, K. J. (2010, May 25). Method for determining solubility of a chemical compound.
Original URL	https://patents.google.com/patent/US7723119B2/de
Source type	Patent
Keywords	Solubility Parameters; chemistry; pH
#Tags	
Summary of key points + notes (include methodology)	<p>Understanding the solubility of a substance is important for its use. Traditional methods do not fully encompass all attributes of solubility. The project proposes a methodology to determine solubility. The steps are as follows:</p> <ol style="list-style-type: none"> 1. preparing a close to saturated solution of the chemical compound with solid of the chemical compound present 2. measuring the pH of the test solution at regular intervals until a consistent rate of pH change is obtained, and then measuring the slope of the consistent rate of pH change 3. adding a known base or acid titrant to the test solution to adjust the pH slope 4. repeating above steps until the measured pH slope changes sign 5. determining the solubility of the compound as the concentration of the compound in solution when the measured pH slope is interpolated to 0 <p>The solution is saturated when it is at equilibrium and no more solute can dissolve. Super saturated solutions can occur when the pH is changed rapidly before all the particles can precipitate out. Then, the solution is titrated to determine the pH. It starts out in the dissolution stage where titrant is added until the substance dissolves. Then, in the seeking precipitation stage, the solution is titrated until precipitation occurs. Then, they adjust super or sub saturated solutions with titrant until they deviate from equilibrium.</p>
Research Question/Problem/Need	How can pH be used to create a method to determine solubility?

Important Figures

Figure 2



This figure shows their process visually.



This is an example titration graph with phases marked out.

VOCAB: (w/definition)

Phenols – hydroxyl group attached to aromatic group
 Amines – derived from ammonia
 Pyridines – rings with a single N
 spectroscopic dip probe - measure spectral properties like precipitate
 Spectrophotometer - light a substance absorbs at specific wavelengths

Cited references to follow up on

Physiochemical Properties of Prostaglandin F20, (Tromethamine Salt): Solubility Behavior, Surface Properties, and Ionization Constants: Journal of Pharmaceutical Sciences, 1973, 62: pages 1680-5

pH-metric Solubility. 1. Solubility-pH Profile from Bjerrum Plots. Gibbs Buffer and pKa in the Solid State: Pharm Pharmacol Commun 1998, 4: pages 165-178

Follow up Questions

How can pH related work be applied to environmental issues?
 Would changing pH change solubility of polymers?

