QUARTERLY PROGRESS REPORT
March 2026 – May 2026

PROJECT TITLE: PLASTIC RECYCLING VIA REACTIVE MELT PROCESSING: ALIPHATIC POLYESTER RECOVERY

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Research Description:

Quantum chemistry calculations were conducted to examine the degradation mechanisms of polylactic acid (PLA). The goal was to identify how PLA chains cleave at the molecular level and to determine which bond-breaking mechanisms can reasonably explain degradation products observed experimentally by NMR and GC/MS. Chain-end concerted cleavage and beta-scission pathways were studied specifically on a five-monomer PLA model. We found that the chain-end beta-scission is kinetically unfavorable, producing a activation barrier of 140.6 kJ/mol and leading to chain fragmentation products.

Further investigation of the PLA degradation kinetics was undertaken using quantum calculations. During this time, much effort was placed into the mid chain transesterification degradation of PLA. Both reactants and products have been optimized, however the determination of the correct transition structure is still under completing. Additionally, preliminary work has begun to study the effect of Ti(IV), Zn(II), Sn(IV), and Ce(IV) on the stability of cyclic PLA structures.

Computational studies were conducted to investigate the effect of single water molecules on PLA oligomers with varying stereochemistry. Model compound studies have revealed insight to the possible mechanisms at play in peroxide-initiated PLA degradation. The context qualitative NMR has provided will be confirmed through other available testing methods that will segue into qualitative analysis.

Preparation is being made for experimental work on PLA synthesis. Synthesis methods have been modified based on literature reviews and will be tested to produce high MW PLA. Synthesized PLA will serve as the model material for future work involving architectural and mechanical upgrading, with the goal of mechanistic design and optimization for recycling of PLA via melt processing.

For Life Cycle Assessment (LCA), literature information for the remaining LCA scenarios were identified to support inventory definition. Mass and energy balances for the Technoeconomic Analysis (TEA) were

refined to improve transparency across each process step. Capital Investment, Utility costs, Working Capital, and Cost of Manufacturing were determined.

Work accomplished during this reporting period:

For this reporting period, we are starting to combine the computational investigation with those of model compound study to understand the degradation kinetics; conducting preliminary experiments on PLA synthesis for reaction profile and formulation design; and completing life cycle assessment and technoeconomic analysis, respectively.

Computational Study on Degradation Mechanism:

Degradation kinetics. A chain-end ester cleavage pathway was evaluated as a non-radical degradation mechanism, occurring near the terminal ester group.[1-3] The current transition-state search produced a plausible reaction coordinate from reactants to products, but the activation barrier is not yet finalized. This pathway is noteworthy because the mechanisms is similar to transesterification without producing radical products.

For chain-end beta-scission, we use a five-monomer PLA chain and evaluates scission of the backbone through a transition state that leading to fragmented products.[1-3] The final transition-state result gave an activation barrier of 140.6 kJ/mol. This barrier is lower than previously reported mid-chain alpha-scission barrier of 156.2 kJ/mol, but still kinetically unfavored. Further study includes building ONIOM and solvation model as well as conducting energy correction using ORCA software.[4, 5]

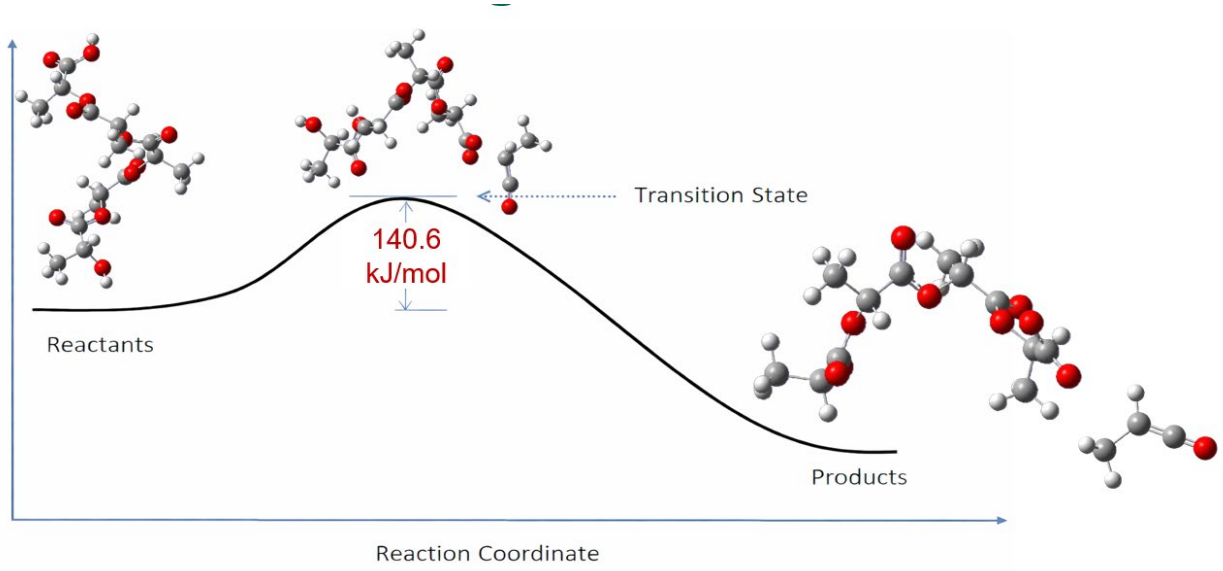

Figure 1. The calculated transition-state reveals an activation barrier of 140.6 kJ/mol for beta-scission at the end of a five-monomer PLA chain with fragmented products.

Emphasis has been placed on modeling the transition state for the mid chain transesterification of polylactic acid.

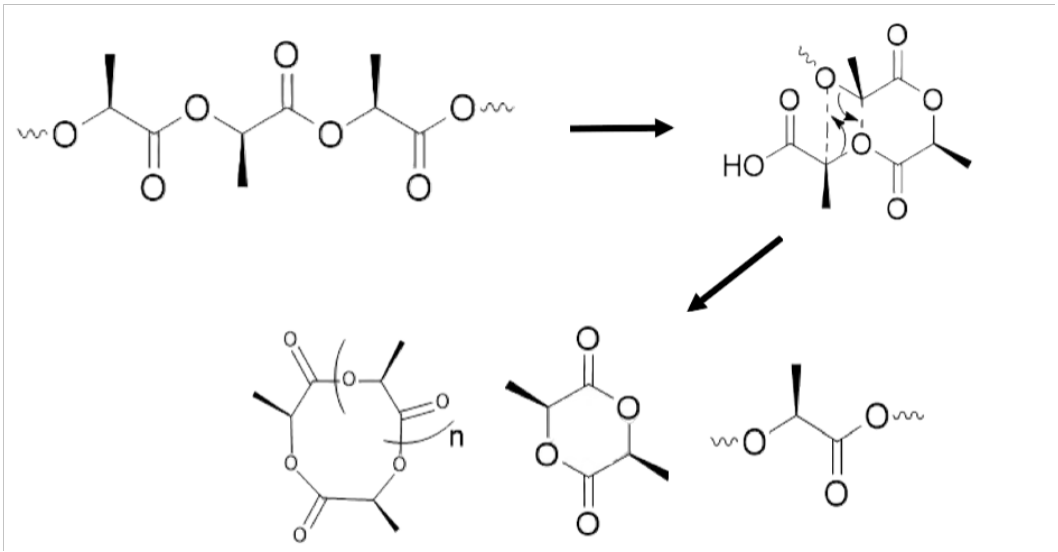

Figure 2. Mid chain transesterification of polylactic acid resulting in the formation of cyclic PLA.

In this reaction, this degradation mechanism, a lone pair of electrons on the PLA backbone attacks another site on the same PLA chain resulting in the formation of a cyclic PLA. For this system a 7-monomer linear PLA chain was modelled and optimized as the reactant; with the products being a 5-monomer cyclic PLA oligomer and a 2-monomer PLA linear chain. Optimized transition state is needed to quantify the kinetics and its feasibility to degrade PLA in molten state.

In previous reports, we evaluated the effect of metal ions on cyclic PLA with varying sizes and thermal stability. We now expand our scope to include additional metal ions i.e. Ti^{4+}, Zn^{2+}, Sn^{4+}, and Ce^{4+}. These ions were chosen due to good catalytic ability with PLA systems. Initial work has been done to model these ions within an 8-monomer cyclic PLA oligomer.

Effect of added water.

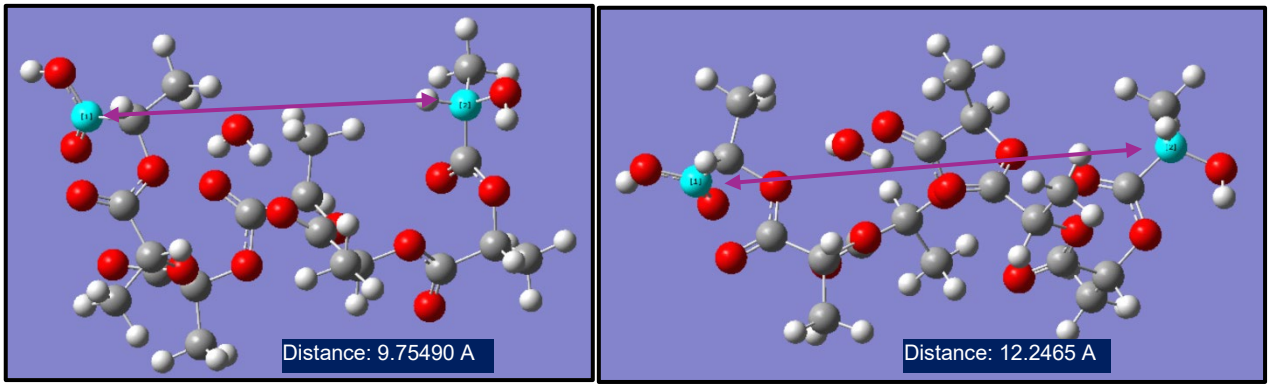

Figure 3. An optimized PLA oligomer (7-monomer-mix-b_1) before (left) and after (right) hydrogen-bonding with a water molecule. A hydrogen bond was formed and a 25.1% increase in end-to-end length was observed (measured along the longest Carbon-Carbon chain).

As summarized in Table 1, a significant difference has been observed between linear isomers of mixed chirality compared to those of homogeneous chirality. Mix-a and Mix-b refer to mixed-chirality PLA oligomer isomers containing alternating L- and D-lactic acid repeat units along the same chain. They differ by the sequence of the L and D stereocenters along the oligomer backbone. In contrast, the L- and D-

isomers represent homogeneous-chirality oligomers, where a single oligomer has either all L units or all D units. Mix-a and Mix-b isomeric structures increased in end-to-end distance (Fig. 3) while L and D isomers decreased the distance by approximately 1–32% relative to the corresponding solvated oligomer without water molecules. Overall, these findings indicate the significance of stereochemistry on affecting the interaction of water molecules with PLA oligomer structure.[6, 7]

Table 1. Percent change in end-to-end distance of linear PLA oligomers after interaction with one water molecule, organized by stereochemical isomer type.

Linear PLA	L-isomer	D-isomer	Mixed-a-isomer	Mixed-b-isomer
3 monomer	10 % decrease	7.14 % decrease	TBD	1% increase
4 monomer	TBD	3% decrease	4% increase	-
5 monomer	31.7% decrease (2H)	2.6% decrease	20% increase	7.4% increase
6 monomer	10% decrease	11 % decrease (2H)	TBD	-
7 monomer	7 % decrease (2H)	TBD	TBD	25.1% increase
8 monomer	TBD	16.5% decrease	15% increase	-
9 monomer	22.8% decrease	TBD	4.4% increase	31.2% increase

Note entries marked "(2H)" indicate structures in which the water molecule formed two hydrogen bonds with the PLA oligomer. All other listed structures formed one hydrogen bond with the water molecule. TBD indicates values that are to be determined.

Experimentation on Reaction Profile and Formulation Design:

Model compound study. Studies are underway to establish an understanding of the chemical reactions at play in PLA melt processing and reconcile with the mechanism inferred from quantum calculations. Current efforts have centered around a qualitative assessment of peroxide-initiated PLA degradation. Results from NMR spectra confirm that PLA does not exhibit self-initiated degradation under typical melt processing conditions, and that a peroxide initiator (Dicumyl Peroxide, DCP) is required for degraded species to appear. Furthermore, it was found that triol or plasticizer additives do not result in additional chemical structures and/or reactions. These findings have shifted attention into identifying the change in local chemical environments due to DCP-initiated PLA degradation as indicated by the appearance of new peaks along NMR spectra. (Fig. 4) 2D NMR measurements via Heteronuclear Single Quantum Coherence (HSQC) spectroscopy were used to determine that DCP-induced degradation results in exclusively hydroxyl end groups with evidence of transesterification occurring.

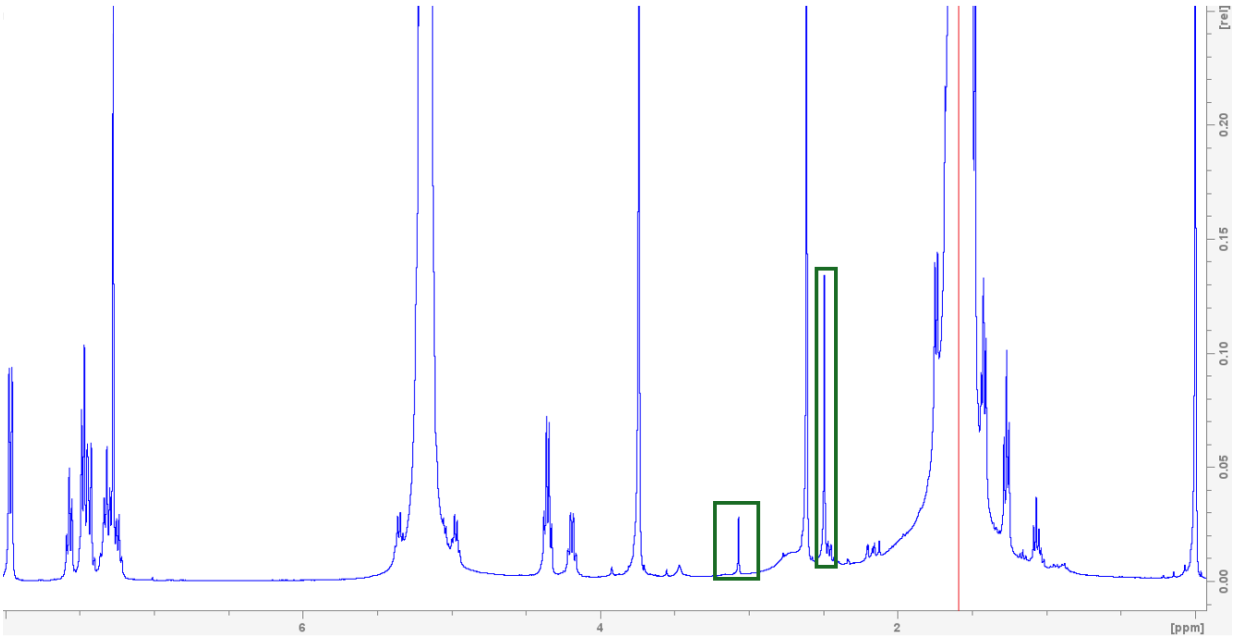

Figure 4. NMR spectrum of a PLA reacted with 2.5 wt. % Dicumyl Peroxide (DCP). The peaks squared in green are not associated with unreacted PLA structures, or structures found in DCP's degraded species, meaning they belong to newly formed chemical structures resulting from peroxide initiated degradation.

Model Polylactic Acid Synthesis.

Additional work has been done in preparation for the synthesis of PLA. As mentioned previously, the ring-opening polymerization (ROP) of lactide synthesis route as described in Kamber, N. E., et al 2007[8] was chosen, however slight modifications have been made to procedure based on an expanded literature study. These changes include increasing the incubation time to 180-200 C for 24-30 hours for bulk polymerization.[9] This will allow the synthesized PLA to have the desired high MW of about 100 Kg/mol.

With regards to PLA Synthesis, a Schlenk line is being assembled. This Schlenk line will ensure that the synthesis occurs under vacuum conditions and that the system is free from contaminants which can result in additional side reactions. The main Schlenk line has been completed, however we are still in the process of building an additional Schlenk line which will be used solely for PLA synthesis.

Another important instrument for PLA synthesis is the High-Performance Liquid Chromatography (HPLC) Instrument. This is a vital tool for confirming the MW distributions of the synthesized PLA via GPC. This is important since the synthesized PLA would need to have high MW and chain entanglements to represent commercial products. The HPLC has been set up and training has been completed. An SOP has also been created for this instrument. Training runs have also been performed however we are still in the process of learning to evaluate and interpret the results.

<u>Life Cycle Assessment on PLA End of Life Pathways</u>

The inventory for Scenario 3 (S-3) and the counterfactual scenario (Landfill) was investigated and discussed in what follows. The inventory definition for mechanical recycling (S-2) is under development. Note that for scenario 1 (S-1, i.e. reactive melt processing), preliminary results were presented in the previous report. (Fig. 5)

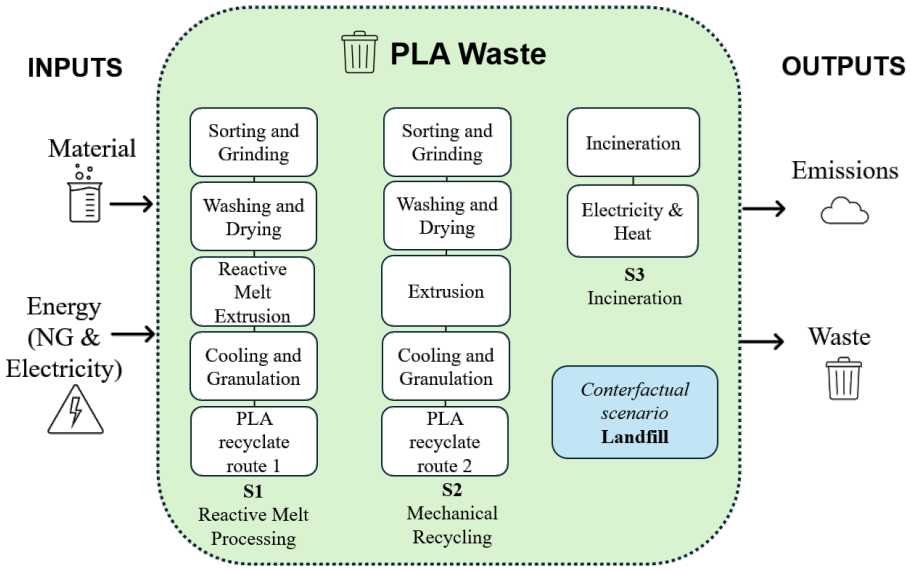

Figure 5. System boundary for Cradle to Gate of end-of-life PLA, considering 1 kg of waste PLA as the functional unit.

Incineration (S-3): When polylactic acid (PLA) is incinerated, CO_2 and H_2O are formed. In this work, PLA is assumed to be produced from corn starch, and not by fossil routes. As it is a renewable feedstock, the CO_2 released during the incineration can be considered similar to the CO_2 adsorbed from corn used to make PLA. This indicates that the released CO_2 from incineration will be denoted as biogenic carbon dioxide[10, 11]. The cut-off approach[12] was also considered, in which environmental burdens from material production (PLA) and waste generation are fully assigned to the original product, and recycling starts from waste treatment. Although there is no consensus regarding the assumption of biogenic carbon neutrality in the field, and studies diverge across different assumptions and considerations to take into account carbon credits[13], in this work, biogenic carbon neutrality is assumed and reflected in the results presented.

The thermal energy content of PLA (Ingeo NatureWorks), equal to 18.56 MJ/kg[14] was used as a reference for S-3. (Table 2) The amount of CO_2 released was adjusted by data provided by NatureWorks for burning Ingeo[14], which include the elemental analysis (C = 48.22 % avg.), and decomposition products (CO_2 = 2020 mg/g and H_2O > 260 mg/g), volatiles, semi volatiles and carbon monoxide were reported in quantities lower than 0.1 mg/g and were not added as emissions in the LCA inventory of this work.

Another important aspect of incineration is to generate electricity counted as the yield or energy recovery. Beigbeder et al.[15] studied a similar case, and the average value of European incinerators was considered (13 %). Islam et al. [16] assumed that 49 % of the PLA's heating value could be recovered (from which 29 % was considered as electricity and 71 % steam). Electricity generation efficiency was also assumed to be similar as those works using landfill gas, due to lack of data.[17] Here we assume 35 % of the PLA heating value could be recovered and assigned as electricity generation. The energy needed for incineration was assumed to be supplied by municipal solid waste[16].

Table 2. Inventory for scenario 3: incineration of waste PLA.

Material/ Energy source	Amount	Unit	Reference
Inputs			
Waste PLA	1	kg	This work
Municipal Solid Waste Incineration for energy	8.35	MJ/kg	[16]

Outputs			
Electricity	6.5	MJ/kg	This work
CO_2 biogenic	2.02	kg CO_2/kg PLA	Calculated from[14]
NO_X	1 x 10^{-4}	kg/kg PLA	Calculated from[14]
Water	0.26	kg/kg PLA	Calculated from[14]

Counterfactual scenario (Landfill): Considering the biogenic carbon present in biobased products, it might be noted that as the landfill ages, the decomposed carbon generates primary CH_4 and CO_2 (landfill gas, LFG). Therefore, it is important to distinguish the pathways involved in the production of these gases. Fugitive methane emissions might be noteworthy, as it has a high global warming potential and must be computed in the environmental impacts of landfilling. Kim et al.[18] reported pathways assuming decomposable carbon atoms will form landfill gas, or/and non-decomposed carbon atoms will be sequestered in the landfilled digestate (Fig. 6).

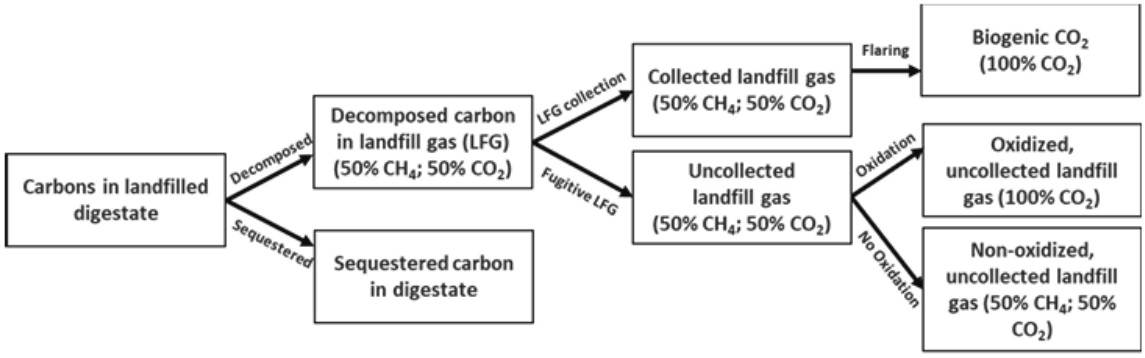

Figure 6. Carbon atoms contained in the landfilled digestate (Source: Kim et al.[18]).

Biodegradability of polymers, such as PLA, depends on the molecular structure. Amorphous structures usually emit methane in landfill conditions, while semi-crystalline PLA is difficult to hydrolyze and degrade[19]. As discussed by Benavides et al.[19], biodegradation of PLA is not usually present in landfills, and adjusting conditions (e.g., an increase in temperature) might be needed to accelerate the rate of hydrolysis of PLA. Assuming similar LFG collection efficiency (59 %), oxidation factor (36%), and CH_4 concentration (50 vol%)[20] as those of Fig. 2, our inventory for this scenario is described in Table 3.

Table 3. Inventory for counterfactual scenario.

Material/ Assumption	Amount	Unit	Reference
Inputs			
Waste PLA	1	kg	This work
Carbon Elemental	48.22	% avg	[14]
Degradable Organic Carbon	50	%	Assumption[20]
Outputs			
CO_2 biogenic	0.21	kg	Calculated based on the assumption
CH_4 biogenic	0.032	kg	Calculated based on the assumption

Technoeconomic Analysis for Development of PLA Recycling Technology:

Mass balances were determined considering the losses from each step due to dust formation or material hold up. Energy balances were defined mainly based on the mass flow rates and energy requirement

equations for each piece of equipment needed, as defined for plant design and economics. The results for energy balance can be found in Table 4 [21, 22].

Table 4. Energy requirement for plant operation of scenario 1 (i.e. reactive melt processing with 1041.7 kg/h) considering only biodegradable plastic.

Process	Energy requirement (kW)	Notes	Reference for power calculation
Transportation	0.033	Conveyor belt	[22]
Grinding	118.5	Rotary cutter and hammer mill	[22]
Washing	136.6	Pumps and propeller	[22]
Drying	122.4	Rotary dryer and fluid bed	[23]
Extrusion	808.0	Screw diameter of 92 mm	[24]

Table 5. Mass balance description for scenario 1 (1041.7 kg/h) considering only biodegradable plastic.

Stage	Mass flow (kg/h)	Losses (%)
Input material	1041.7	0
Output of grinding step	1014.6	2.6[25]
Output of washing step	1004.5	1.0
Output of drying step	1004.5	0
Output of extruder	904.01	10
Output of cooling tank	885.93	2
Output of rotary dryer	885.93	0
Output of hammer mill	868.2	2

* Note that losses except the losses from grinding step are considered assumptions of this work.

Capital Investment: The Chemical Engineering Plant Cost Index (CEPCI) for 2024 (CEPCI= 800), served as the basis for cost calculations. Fixed Capital Investment (FCI) was obtained by adding 18 % of the Total Bare Module to account for contingency and fees. The equation below was used in updating the cost of the equipment from a past date to year 2024:

$$C_2 = C_1 * \frac{I_2}{I_1} \quad \text{Eq.1}$$

where C represents Purchased Cost, I stand for Cost Index. During construction, 60 % of the FCI was allocated to the first year and 40 % to the second year, with land costs (assumed at 2 % of FCI) incurred before construction.

Utilities cost Electricity, steam, and fuel were the main utilities used. The efficiencies and updated costs are based on the U.S. Energy Information Administration to estimate the utilities cost.

Working capital: A plant life of 15 years and a construction period of 2 years was assumed. The working capital was calculated as:

$$Working\ capital = A * C_{RM} + B * FCI + C * C_{OL} \quad \text{Eq.2}$$

where A, B, and C are 0.1 to weight the raw material costs (C_{RM}), Fixed Capital Investment (FCI), and cost of operating labor (C_{OL}), respectively. Cost of operating labor was determined by multiplying the total number of operators needed to run the plant all year round (8322 h/year) by the annual wage of a chemical plant operator. Here annual wage of $66,910 was used.

Cost of Manufacturing: The cost of manufacturing excluding depreciation (COM_d) was calculated below by Eq. 3.

$$COM_d = 0.18 * FCI + 2.76 * C_{OL} + 1.23 * (C_{UT} + C_{WT} + C_{RM}) \quad \text{Eq. 3}$$

Where C_{UT} is the cost of utilities, C_{WT} is the waste treatment costs, and C_{RM} is the raw materials costs. A summary of the preliminary results for scenario 1 can be found in Table 6.

Table 6. Preliminary economic results and assumptions for scenario 1 (1041.7 kg/h) considering only biodegradable plastic.

Variable	Results	Description
Total Equipment Cost	$ 1,050,126	
Total Module Cost	$ 2,010,000	Including contractor fees and contingency
Total Grass Roots Cost	$ 2,810,00	Consider that 50 % of the bare module cost represents auxiliary costs
Lang Factor	3.1	Solid processing plant
Lang Factor Cost	$ 3,300,000	Updated with Lang Factor
Annual Utility Cost (C_{UT})	$ 255,000	Considering efficiencies of machines
FCI	$ 2,810,000	18 % of the Total Bare Module to account for contingency and fees
C_{RM}	$ 0	Assuming the waste PLA will not be purchased and is on-site
C_{OL}	$1,472,020	Follow the description above
C_{WT}	$ 0	Assuming the pretreatment is made on-site
Working capital	$ 30,000,00	Calculated using Eq.2
COM_d	$ 4,882,225	Calculated using Eq. 3

* Results are subject to revision and continuous improvement as the study progresses.

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TAG meetings:

The 2nd TAG meeting was held on April 22nd at 2 pm. The full list of members is found at the website link. We were pleased to have many TAG members be able to join. The website will be updated soon to reflect the meeting took place and the slides will be uploaded there.

Future Tasks:

Computational Study on Degradation Mechanism:
Degradation kinetics. The next stage for kinetic study will focus on completing the transition-state search for both transesterification and concerted chain-end breakage mechanism, which has not yet been completed. Further refinement includes building the ONIOM model and energy correction via high-level theory using ORCA software. Additionally, there will be continued efforts to evaluate the effect of the new metal ions on the stability of cyclic PLA oligomers

Effects of water. Further investigation of the effect of water molecules on stereochemistry, specifically ring isomers. Additional data will be generated to quantify hydrogen-bonding effects along the PLA backbone. Results are currently in the preliminary stage.
2. Energy correction of linear isomers via ORCA

Experimentation on Reaction Profile and Formulation Design:
Model compound study. Employment of other testing procedures, such as GCP and GC/MS, are to be conducted in parallel with closer inspection of PLA transesterification Quantum chemistry calculations. Experience in these procedures will allow for determination of which results are indicators of degradation extent and rate.

Model Polylactic Acid Synthesis. Next steps for the model PLA Synthesis include completing the secondary Schlenk line which will be used solely for PLA synthesis. Additionally, the HPLC test runs will be interpreted and confirmed with HPLC technician to ensure all data is accurate and machine is fully operational. Another HPLC technician will be brought on-site to help set-up and perform training on for the Light Scattering component on the HPLC.

Reactants have been purchased for ROP PLA synthesis procedure. Once these arrive and Schlenk line has been completed, PLA synthesis procedures will begin and synthesized PLA will be characterized using conventional analytical measurements (GPC, NMR, FTIR).

Life Cycle Assessment on PLA End of Life Pathways:
The next steps include refining preliminary LCA results for all scenarios and evaluate carbon intensity and performing sensitivity analysis on key variables.

Technoeconomic Analysis for Development of PLA Recycling Technology:
The next steps include generating results for the remaining scenarios, including documentation of governing equations and underlying assumptions; calculating and interpreting Net Present Value (NPV), Payback Period, Return on Investment (ROI), and Cash Flow Diagram; as well as preforming sensitivity analysis on key process variables.

METRICS REPORTING

1. Summarize input provided by the TAG during this period.

   We recently completed our 2nd TAG meeting. As mentioned above, we had many TAG members attend. After ~ 40 min presentation, TAG members asked several questions, which helped us refine the explanations and scope of work. We anticipate also receiving feedback via email.

2. List research publications resulting from THIS Hinkley Center project. Has your project been mentioned in any research and/or solid waste publication/newsletters/magazines/blogs, etc.?

   None.

3. List research presentations resulting from (or about) THIS Hinkley Center project. Include speaker presentations, TAG presentations, student posters, etc.

   The work was presented at AICHE and mentioned at the FLA&WMA conference as part of an invited talk on a previous Hinkley project. Several abstracts have been submitted.

4. List who has referenced or cited your publications from this project. Has another author attributed your work in any publications?

   None.

5. How have the research results from THIS Hinkley Center project been leveraged to secure additional research funding? What additional sources of funding are you seeking or have you sought? Please list all grant applications and grants and/or funding opportunities associated with this project. Indicate if additional funding was granted.

   Multiple (pre)proposals on plastic upcycling and/or degradation mechanism are pending and in preparation. One is to NSF, one to EREF, and others to DOE as well as relevant industries.

6. What new collaborations were initiated based on THIS Hinkley Center project? Did any other faculty members/researchers/stakeholders inquire about this project? Are you working with any faculty from your institution or other institutions?

   None.

7. How have the results from THIS Hinkley Center funded project been used (not will be used) by the FDEP or other stakeholders? (1 paragraph maximum). Freely describe how the findings and implications from your project have been used to advance and improve solid waste management practices.

   None.

PICTURES: The most recent pictures have been uploaded to the website (linked above).