The Chemies

“It’s not easy being green”

Project Proposal and Feasibility Study

Team 16
Mike Hall
Laura Hamilton
Dave Janke
Briley Lambert
Abstract

Team 16 will design and determine the economic feasibility of a pilot plant to produce poly(beta-hydroxybutyrate) also referred to as PHB. PHB is a biodegradable polymer that has previously only been made by a fermentation process. New catalysts have been discovered that now allow PHB to be created synthetically. The chemistry for this process is straightforward. The pilot plant is to produce 20,000kg of PHB annually. The toxicity of the starting reactants, highly exothermic reactions and poisoning of catalysts with air and water are all challenges that will be addressed in this project.
Table of Contents

1. Problem Statement
2. Project Objective
3. Christian Perspective
4. Alternative Solutions
5. Feasibility Study
6. Preliminary Design
7. Method of Approach
8. Task Breakdown with Time Schedule
9. Material Cost Estimates
10. Resources

Appendix A: Physical Properties Data
Appendix B: Determination of Rate Laws
Appendix C: Microsoft Project Timeline
Appendix D: Interview Notes with Professor Coates
1. Problem Statement

Due to the negative environmental impact of current non-biodegradable plastics, a biodegradable alternative is desirable. Poly(Beta-hydroxybutyrate) (PHB) is one such polymer. However, production of PHB has been economically unfeasible due to the high costs of growing the polymer in biological cells. The discovery of catalysts enabling a synthetic pathway to PHB by Dr. Geoffrey Coates of Cornell University has the potential to allow mass production of the polymer economically.

2. Project Objective

The objective of this project is to create a detailed design of pilot plant to produce 20,000kg of PHB annually and determine if this process is economically feasible on an industrial scale. The goals of this project are to have at least a 60% overall conversion, to ensure that the process is environmentally friendly, and to create a design that is cheaper than the fermentation process already in use.

3. Christian Perspective

Stewardship is the driving force behind this project. For decades, society has demonstrated poor stewardship by using billions of pounds of non-biodegradable plastics. These plastics adversely affect the environment in two ways. First, production of polymer products consumes fossil fuels and generates carbon dioxide, which may contribute to global warming. Second, many of these products are dumped into landfills and do not break down. Designing a process to produce biodegradable PHB solves both of these problems. Additionally, the catalytic process may allow better stewardship of money and
raw materials than current fermentation processes by eliminating costly bioreactors and polymer processing.

Safety is a primary concern in this process. Since all the reactants and intermediates are toxic, precautions must be taken to protect both plant workers and the surrounding community. Since the catalysts are relatively new, their health and environmental effects are not well known. These will have to be estimated from known effects of the metals in the catalysts and considered in the consumer use of the product. Due to the high selectivity and effectiveness of the catalysts, the reactions run essentially to completion and produce virtually no byproducts, greatly reducing the need to handle waste streams.

This design will fit well into the current American culture because it will allow consumers to continue using polymer products similar to those currently available. At the same time, it will allow them to be more environmentally responsible, which is an important issue for many Americans. Manufacturers will benefit because they can still use polymers in their products and packaging without worrying that the government will impose restrictions on polymer disposal. In short, this technology will allow society to take better care of God’s creation without making massive changes to its production or consumption habits.

4. Alternative Solutions

One alternative to this project is to use fermentation rather than a purely chemical synthesis. However, this approach has already been found economically unfeasible, except for boutique applications. Another alternative is to produce a copolymer of PHB
and PHV (poly-beta-hydroxyvalerate), which has better physical properties. This alternative will be considered as we proceed with the project.

5. Feasibility Study

For this process to be feasible we must have an in depth knowledge of the properties of our catalysts and final product. We have been in contact with Dr. Coates, the inventor of the catalysts used in our process. He answered many of our questions and mentioned other possible sources of information. These resources are listed in Section 10 below. While the process of synthetically producing this polymer has never been done before on an industrial scale, due to the concept of unit operations we are confident that a process can be developed.

The recent development of the catalysts in our process means that limited data is available. We will acquire all the relevant data that is available, but some estimation will be necessary over the course of our design. This will be based on similar processes and materials, mathematical estimate techniques, and application of our engineering knowledge.

For the reasons described above, the synthetic route we have chosen is chemically feasible. The purpose of our project is to determine if our process is economically practical for developing this plastic industrially, which has not been feasible in the past. Unfortunately we will not be able to determine this until much later in the project. Factors that still need to be determined are cost of catalysts, level environmental safety precautions required due to toxic initial reactants, amount of separation equipment
required to obtain desired purity, and other considerations. The initial reactants are cheap and readily available. Since we are only designing a pilot plant, equipment costs will be much less expensive than an actual plant due to the smaller size.

Since propylene oxide is more than twice as expensive as polypropylene, the plastic most similar to our polymer, the cost for our biodegradable plastic will not be competitive with polypropylene. However, we may be able to charge a premium for our plastic due to its environmentally friendly properties. Thus our goal is to be cheaper than PHB produced by fermentation methods, rather than competitive with polypropylene.

6. Preliminary Design

As of now we have many “black boxes” within our process flow diagram. See Figure 1 for the preliminary PFD. Due to the toxicity of the reactants and the sensitivity of the catalyst to air and water, the design of reactor 1 is difficult. To give maximum conversion of propylene oxide, we are currently considering a spray column reactor, where propylene oxide containing dissolved catalyst is sprayed through a high pressure CO atmosphere. Since the reaction takes approximately an hour, we will need to recycle the liquid several times to give the necessary residence time in the reactor. In this design we have to determine if a CO recycle is necessary, or if we can simply charge the reactor with CO, then add CO as it is used up in the reaction.

Another reactor we have considered is a bubble column, where CO is bubbled through liquid propylene oxide with the catalyst. This design allows adequate time to react without as much recycle, but has higher levels of propylene oxide present, which could be more of a safety risk if the reactor leaked. With a bubble column reactor, CO is the
limiting reactant, so the propylene oxide will not be as fully converted. This would mean higher separation costs. A distillation column will be used to separate the reactor effluent to produce a nearly pure \(\beta\)-butyrolactone product stream. The propylene oxide removed by the column will be recycled back into the feed stream. The bottoms product of \(\beta\)-butyrolactone will be mixed with catalyst 2 and added to a small reactor to form \(\beta\)-hydroxybutyrate. We currently plan to use a continuous stirred tank reactor for this step, but we will consider other options in the detailed design. The polymerization of \(\beta\)-hydroxybutyrate will occur in the extruder, which will produce PHB pellets as our final product.

From articles by Professor Coates reaction conditions and rate laws were determined. The initial conditions for the first reaction are 50°C and 880 psi. The rate law for reaction 1 was calculated as

\[
\text{rate} = k \times [\text{catalyst 1}] \times [\text{propylene oxide}] \tag{1}
\]

where \(k = 23.7 \text{ dm}^3/\text{mol-hr}\)

The second reaction also must be at a temperature of 50°C. The rate law for the second reaction is

\[
\text{rate} = k \times [\text{catalyst 2}] \times [\beta\text{-butyrolactone}] \tag{2}
\]

where \(k\) can be described by

\[
Ae^{-\frac{E}{RT}}
\]

\[
A = 2.8 \times 10^9 \text{ dm}^3/\text{mol-hr}
\]

\[
E = 743 \text{ J/mol}
\]

\[
R = \text{universal gas constant}
\]

\[
T = \text{temperature (K)}
\]
7. Method of Approach

Decisions by our team are made by simple consensus. When we need to decide between alternatives, such as deciding what project to do, we discuss the options as a group, until a majority agrees on a decision. Since our group is small and gets along well, disagreements have been rare. Delegation has been done by strength. Certain team members are better at certain aspects of the design process (HYSYS, rate laws, Polymath, etc.) and work in those areas has naturally fallen along those lines. As the project progresses, however, more work will be delegated due to time constraints and to maintain equality of labor. Much of the process equipment that needs to be designed has not been addressed in our previous classes. To address this issue we are going to create teams of two who will become “experts” on specific pieces of equipment used in our design. This will increase the productivity of our group.

8. Task Breakdown with Time Schedule

<table>
<thead>
<tr>
<th>Refined Task Specifications</th>
<th>Target Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Problem defined</td>
<td>completed 10/1</td>
</tr>
<tr>
<td>Project objectives specified</td>
<td></td>
</tr>
<tr>
<td>Design norms identified</td>
<td></td>
</tr>
<tr>
<td>First Presentation Delivered</td>
<td>completed 10/11</td>
</tr>
<tr>
<td>Compiled data sheets on chemicals used and reactions</td>
<td>11/8</td>
</tr>
<tr>
<td>Gathered data from literature</td>
<td>completed</td>
</tr>
<tr>
<td>Obtained JACS articles from Prof. Coates</td>
<td>completed</td>
</tr>
<tr>
<td>Search Metabolix website</td>
<td></td>
</tr>
<tr>
<td>Researched polymer processing</td>
<td></td>
</tr>
<tr>
<td>Kirk-Othmer</td>
<td>completed 11/23</td>
</tr>
<tr>
<td>Metabolix</td>
<td>completed</td>
</tr>
<tr>
<td>Modern Plastics</td>
<td>completed 11/23</td>
</tr>
<tr>
<td>Extruders</td>
<td></td>
</tr>
<tr>
<td>Separation considerations</td>
<td></td>
</tr>
</tbody>
</table>
Thermal processing
Compiled questions and contacted Professor Coates completed 10/27
Entered data obtained during teleconference completed 11/29

Developed a project budget completed 10/25

Completed Preliminary Equipment Design 12/15

<table>
<thead>
<tr>
<th>Reactor 1</th>
<th>Type</th>
<th>Size</th>
<th>Duty</th>
<th>Materials of construction</th>
<th>Flow rates</th>
<th>Composition</th>
<th>Temperature</th>
<th>Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reactor 2</th>
<th>Type</th>
<th>Size</th>
<th>Duty</th>
<th>Materials of construction</th>
<th>Flow rates</th>
<th>Composition</th>
<th>Temperature</th>
<th>Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Process flow diagram (PFD)
Separation units
Possible distillation
Possible filtration—microfiltration or gel
Processing equipment
Extruder
Heat exchangers
Size—area, tube size, # tubes
Duty
Materials of construction

HYSYS base case
Economic Analysis
Determined break-even price
Compared to alternative processing methods (Metabolix)

Second Presentation Delivered 12/6
Web Page Created 12/10
PPFS written and submitted 12/10
Charts and Illustrations
Problem Statement
Project objectives
Alternative Solutions
Feasibility Study
Detailed task specifications
Preliminary design
Method of approach
Christian perspective on project
Task breakdown and time schedule
Cost estimate for product productions

**Alternative designs considered**
- recycle streams
- heat recycles
- separation units
- temperature
- pressure
- composition
- solvent
- form of final product

**Process optimized**

**PFD Finalized**

**Detailed Design Completed**

- Reactor 1
  - Type
  - Size
  - Duty
  - Materials of construction
  - Flow rates
  - Composition
  - Temperature
  - Pressure

- Reactor 2
  - Type
  - Size
  - Duty
  - Materials of construction
  - Flow rates
  - Composition
  - Temperature
  - Pressure
  - process flow diagram (PFD)

separation units
possible distillation
possible filtration—microfiltration or gel
processing equipment
extruder
heat exchangers
size—area, tube size, # tubes
duty
materials of construction
P&ID
HYSYS case
Economic Analysis

Scale-up for preliminary full-scale plant completed  4/20

Economic analysis completed  4/30
Break-even price
Market comparison

Senior Design Night Presentation Given  5/8
Display materials prepared
Presentation Delivered

Final Presentation Delivered  5/10

Final Report Written and Submitted  5/15

9. Material Cost Estimates

Propylene oxide can be purchased in bulk for $.72/lb. Metabolix Inc. sells poly(beta-hydroxybutyrate) for $1/lb, using the fermentation process. Based on that price, our goal is to have a break-even price of less than $1/lb for our product.

10. Resources

3. Dr. Aubrey Sykes

6. *Modern Plastics* magazine


8. Dow Chemical properties sheet for Propylene Oxide


Appendix A: Physical Properties Data
### Table 1: Properties of Reactants, Catalysts, Intermediates, and Final Product

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS</td>
<td>CO</td>
<td>propylene oxide</td>
<td>4-methyl-2-oxetanone</td>
<td>PHB</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>carbon monoxide</td>
<td>epoxide</td>
<td>catalyst #1</td>
<td>l-butyrolactone</td>
<td>catalyst #2</td>
<td>poly((R)-l-hydroxybutyrate)</td>
</tr>
<tr>
<td></td>
<td>CAS Registry number</td>
<td>630-08-0</td>
<td>75-56-9</td>
<td>3068-88-0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>physical</td>
<td>molecular weight</td>
<td>28.01</td>
<td>58.08</td>
<td>86.09</td>
<td>1000 to &gt;1000000</td>
<td></td>
</tr>
<tr>
<td></td>
<td>boiling point (K)</td>
<td>81.63 K</td>
<td>207.9 K</td>
<td>110-118°C (24kPa), 71-73 (3.9kPa), 50-54 (1.3kPa)</td>
<td>unstable above 200°C</td>
<td></td>
</tr>
<tr>
<td></td>
<td>freezing point (K)</td>
<td>161.25 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>triple point (K)</td>
<td>67.95 K</td>
<td>161.22 K</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>critical temperature</td>
<td>134.45 K</td>
<td>488.2 K</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>critical pressure</td>
<td>34.9875 bar</td>
<td>54.40 bar</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>heat capacity</td>
<td>see NIST</td>
<td></td>
<td></td>
<td>see NIST</td>
<td></td>
</tr>
<tr>
<td></td>
<td>glass transition point</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-20 to 10°C</td>
</tr>
<tr>
<td></td>
<td>vapor pressure</td>
<td></td>
<td></td>
<td></td>
<td>Antoine see NIST</td>
<td></td>
</tr>
<tr>
<td></td>
<td>specific gravity</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.0555</td>
</tr>
<tr>
<td>thermodynamic</td>
<td>heat of reaction</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ΔH gas (kJ/mol)</td>
<td>-110.53</td>
<td>-94.68</td>
<td>na</td>
<td>-122.6</td>
<td>28.31</td>
</tr>
<tr>
<td></td>
<td>ΔH liquid (kJ/mol)</td>
<td>na</td>
<td></td>
<td>-122.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ΔvapH (kJ/mol)</td>
<td>28.31</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>mechanical</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>tensile strength</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>10 to 20 Mpa</td>
</tr>
<tr>
<td></td>
<td>ductile strength</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>200 to 600% elongation at break</td>
</tr>
<tr>
<td></td>
<td>elasticity</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>shear stress</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>shear strain</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H₂O vapor permeability</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>biodegradability</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>20-150 (g/m² day) 70 days in most environments including anaerobic</td>
</tr>
<tr>
<td>reaction #1</td>
<td>rate</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>k* catalyst1*PO</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>k_app (L/mol hr)</td>
<td>23.7 @23°C</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>reaction #2</td>
<td>rate</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A*e^(ERTn)<em>catalyst2</em>BBL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>A (L/mol min)</td>
<td>2.798*10⁹</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>E (J/mole)</td>
<td>743.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix B: Determination of Rate Laws
Pure Component Data:

<table>
<thead>
<tr>
<th></th>
<th>Pure Substrate</th>
<th>Pure Product</th>
<th>b-Butyrolactone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular Weight</td>
<td>58.08 g/mol</td>
<td>86.09 g/mol</td>
<td></td>
</tr>
<tr>
<td>Density @23°C, 1 atm</td>
<td>0.8 g/ml</td>
<td>1.0555 g/ml</td>
<td></td>
</tr>
<tr>
<td>Concentration</td>
<td>13.7741 mol/l</td>
<td>12.26043 mol/l</td>
<td></td>
</tr>
<tr>
<td>Molar Volume</td>
<td>0.0726 l/mol</td>
<td>0.081563 l/mol</td>
<td></td>
</tr>
</tbody>
</table>

Experimental Conditions:

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>50 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>880 psi CO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 mol % Catalyst</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.137741 [cat] mol/l</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 time (hr)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>95 yield (%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.95 Conversion</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Assumptions:

[CO]=constant
[CO]=[CO]sat
Volume is independent of [Cat], [CO]
Volume change is linear function of conversion

Equations:

\[ \frac{d[Ca]}{dt} = ra \]

Rate = \( K \times [cat] \times [PO] \times [CO] \)

\( K \times [CO] = K \text{ apparent} \ l/(mol \ hr) \)

Standard reaction equations were used in an equation solver to calculate the rate constant for the reaction at constant temperature. (23 C)

Solved using Polymath Differential Equation Solver:

Kapp = 23.7
### POLYMATH Results

**No Title** 12-01-2004, Rev5.1.233

#### Calculated values of the DEQ variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>initial value</th>
<th>minimal value</th>
<th>maximal value</th>
<th>final value</th>
</tr>
</thead>
<tbody>
<tr>
<td>t</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Na</td>
<td>13.774105</td>
<td>0.6807639</td>
<td>13.774105</td>
<td>0.6807639</td>
</tr>
<tr>
<td>Nb</td>
<td>0</td>
<td>0</td>
<td>13.093341</td>
<td>13.093341</td>
</tr>
<tr>
<td>rhoA</td>
<td>0.8</td>
<td>0.8</td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>rhoB</td>
<td>1.0555</td>
<td>1.0555</td>
<td>1.0555</td>
<td>1.0555</td>
</tr>
<tr>
<td>MwA</td>
<td>58.08</td>
<td>58.08</td>
<td>58.08</td>
<td>58.08</td>
</tr>
<tr>
<td>MwB</td>
<td>86.09</td>
<td>86.09</td>
<td>86.09</td>
<td>86.09</td>
</tr>
<tr>
<td>MrhoA</td>
<td>0.0726</td>
<td>0.0726</td>
<td>0.0726</td>
<td>0.0726</td>
</tr>
<tr>
<td>MrhoB</td>
<td>0.0815632</td>
<td>0.0815632</td>
<td>0.0815632</td>
<td>0.0815632</td>
</tr>
<tr>
<td>K</td>
<td>23.676734</td>
<td>23.676734</td>
<td>23.676734</td>
<td>23.676734</td>
</tr>
<tr>
<td>V0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>X</td>
<td>0</td>
<td>0</td>
<td>0.950576</td>
<td>0.950576</td>
</tr>
<tr>
<td>v</td>
<td>0.0726</td>
<td>0.0726</td>
<td>0.0811202</td>
<td>0.0811202</td>
</tr>
<tr>
<td>V</td>
<td>1</td>
<td>1</td>
<td>1.1173588</td>
<td>1.1173588</td>
</tr>
<tr>
<td>Ca</td>
<td>13.774105</td>
<td>0.6092617</td>
<td>13.774105</td>
<td>0.6092617</td>
</tr>
<tr>
<td>Cb</td>
<td>0</td>
<td>0</td>
<td>11.718117</td>
<td>11.718117</td>
</tr>
<tr>
<td>Ccato</td>
<td>0.137741</td>
<td>0.137741</td>
<td>0.137741</td>
<td>0.137741</td>
</tr>
<tr>
<td>Ccato</td>
<td>0.137741</td>
<td>0.132738</td>
<td>0.137741</td>
<td>0.132738</td>
</tr>
<tr>
<td>Ra</td>
<td>44.92091</td>
<td>1.7782648</td>
<td>44.92091</td>
<td>1.7782648</td>
</tr>
</tbody>
</table>

#### ODE Report (RKF45)

**Differential equations as entered by the user**

1. \( \frac{d(Na)}{dt} = -Ra*V \)
2. \( \frac{d(Nb)}{dt} = Ra*V \)

**Explicit equations as entered by the user**

1. \( \text{rhoA} = 0.8 \) g/ml
2. \( \text{rhoB} = 1.0555 \) g/ml
3. \( \text{MwA} = 58.08 \) g/mol
4. \( \text{MwB} = 86.09 \) g/mol
5. \( \text{MrhoA} = \frac{1}{(\text{rhoA} \times 1000/\text{MwA})} \) l/mol
6. \( \text{MrhoB} = \frac{1}{(\text{rhoB} \times 1000/\text{MwB})} \) l/mol
7. \( \text{Nao} = 13.774101468 \) mol
8. \( K = 23.67673355 \) l/(mol*hr)
9. \( V0 = \text{MrhoA} * \text{Nao} \) l
10. \( \text{Cao} = 1/\text{MrhoA} \) mol/l
11. \( X = (\text{Nao} - \text{Na})/\text{Nao} \) mol/mol
12. \( V = V^*(\text{Na} + \text{Nb}) \) l/mol
13. \( \text{V} = \text{V}^* (\text{Na} + \text{Nb}) \) l
14. \( \text{Ca} = \text{Na}/\text{V} \) mol/l
15. \( \text{Cb} = \text{Nb}/\text{V} \) mol/l
16. \( \text{Ccato} = 0.137741047 \) mol/l
17. \( \text{Ccato} = \text{Ccato}/\text{V0}/\text{V} \) mol/l
18. \( \text{Ra} = K^*\text{Ca}^*\text{Ccato} \) Mol/(l*hr)

**Independent variable**

- **variable name:** t
  - **initial value:** 0
  - **final value:** 1
Determination of Equilibrium constant at 23 degrees C

The rate constant for the reaction of β-butyrolactone to poly-β-hydroxybutyrate was determined from this graph from Dr. Coates paper on Single-Site-Diiminate Zinc Catalysts. The equation given for the line of best fit was used to calculate the value of k as shown in the calculations at left.

The slope of the fit line gives the reaction order. The y-intercept is a function of the rate constant. Algebraic manipulation of basic equations gives us the rate constant.

\[ y = 0.826 + 1.02x \]
\[ y = \ln(k_{app}) \]
\[ X = \ln(Zn) \]
\[ \ln(k_{app}) = 0.826 + 1.02 \ln(Zn) \]
\[ k_{app} = e^{0.826 + 1.02 \ln(Zn)} \]

Because the order of the rate law must be reasonable: 1.02=1

\[ k_{app} = e^{0.826 \ln(Zn)} \]
\[ k_{app} = e^{0.826}(Zn) \]

\[ \frac{k_{app}}{(Zn)} = e^{0.826} \]
\[ r = k_{app} \cdot \text{BBL} \]
\[ r = k \cdot \text{BBL} \cdot (Zn) \]
\[ k = \frac{k_{app}}{(Zn)} \]
\[ k := 0.826 \]
\[ k = 2.284 \frac{1}{\text{mole} \cdot \text{min}} \]
The temperature dependance of the rate constant for the reaction of β-butyrolactone to poly-β-hydroxybutyrate was determined. From kinetic data in Dr. Coates paper on Single-Site-Diiminate Zinc Catalysts. The line of best fit of a graph of 1/T vs ln(k) gives us the constants in the temperature dependant rate law.

Data:

<table>
<thead>
<tr>
<th>entry</th>
<th>M/I</th>
<th>Temp (°C)</th>
<th>Temp (K)</th>
<th>time (min)</th>
<th>Lactone (mol/l)</th>
<th>Catalyst (mol/l)</th>
<th>Conversion</th>
<th>k (calculus)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>200</td>
<td>23</td>
<td>296</td>
<td>70</td>
<td>2.45</td>
<td>0.01225</td>
<td>0.91</td>
<td>2.80809984</td>
</tr>
<tr>
<td>2</td>
<td>220</td>
<td>50</td>
<td>323</td>
<td>20</td>
<td>2.45</td>
<td>0.011136364</td>
<td>0.97</td>
<td>15.7437293</td>
</tr>
<tr>
<td>3</td>
<td>220</td>
<td>75</td>
<td>348</td>
<td>5</td>
<td>2.45</td>
<td>0.011136364</td>
<td>0.94</td>
<td>50.5265598</td>
</tr>
<tr>
<td>4</td>
<td>400</td>
<td>23</td>
<td>296</td>
<td>150</td>
<td>2.45</td>
<td>0.006125</td>
<td>0.91</td>
<td>2.62089318</td>
</tr>
<tr>
<td>5</td>
<td>1000</td>
<td>23</td>
<td>296</td>
<td>480</td>
<td>2.45</td>
<td>0.00245</td>
<td>0.94</td>
<td>2.39235605</td>
</tr>
<tr>
<td>6</td>
<td>2000</td>
<td>23</td>
<td>296</td>
<td>720</td>
<td>2.45</td>
<td>0.001225</td>
<td>0.9</td>
<td>2.6106407</td>
</tr>
<tr>
<td>14</td>
<td>150</td>
<td>23</td>
<td>296</td>
<td>30</td>
<td>2.45</td>
<td>0.016333333</td>
<td>0.67</td>
<td>2.26257678</td>
</tr>
</tbody>
</table>

For Temperature dependence of k \[ y = -6178.7x + 21.752 \]
\[ R^2 = 0.9926 \]

Manipulation of basic equations:

\[ y = -6178.7x + 21.752 \]
\[ x = \frac{1}{T} \]
\[ y = \ln(k) \]
\[ \ln(k) = -6178.7 \cdot \frac{1}{T} + 21.752 \]
\[ k = A \cdot e^{-\frac{E}{R \cdot T}} \]
\[ \ln(k) = \left( -\frac{E}{R \cdot T} \right) + \ln(A) \]

\[ \frac{-E}{R} = -6178.7 \frac{1}{K} \]
\[ R = 8.3144 \frac{J}{molK} \]
\[ E = 743.1 \frac{J}{mole} \]
\[ \ln(A) = 21.752 \]
\[ A = 2.79810^9 \frac{1}{molmin} \]

Rate = \( A \cdot e^{-E/(R \cdot T)} \cdot [\text{catalyst}] \cdot [\text{BBL}] \)
Appendix C: Microsoft Project Timeline
<table>
<thead>
<tr>
<th>ID</th>
<th>Task Name</th>
<th>Milestone</th>
<th>Progress</th>
<th>Rolled Up Task</th>
<th>Rolled Up Milestone</th>
<th>Rolled Up Progress</th>
<th>External Tasks</th>
<th>Group By Summary</th>
<th>Deadline</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Problem Defined</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Project objectives specified</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Design norms identified</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>First Presentation Delivered</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Compiled data sheets on chemicals used and reactions</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Gathered data from literature</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Obtained JACS articles from Prof. Coates</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Search Metabolix website</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Researched polymer processing</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>Compiled data sheets on chemicals used and reactions</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>Gathered data from literature</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>Obtained JACS articles from Prof. Coates</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>Search Metabolix website</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>Researched polymer processing</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>42</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>43</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>44</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>46</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>47</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>48</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>49</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>51</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>52</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>53</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>54</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>58</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>59</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>61</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>62</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>63</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>66</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>67</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>68</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>69</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>71</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>72</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>73</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>74</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>75</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>76</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>77</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>78</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>79</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>81</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>82</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>83</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>84</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>86</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>87</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>88</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>89</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>91</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>92</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>93</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>94</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>95</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>96</td>
<td>Reactor 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>97</td>
<td>Reactor 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>98</td>
<td>separation units</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>99</td>
<td>possible distillation</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>possible filtration—microfiltration or gel</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101</td>
<td>processing equipment</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>102</td>
<td>extruder</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>103</td>
<td>heat exchangers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>104</td>
<td>Economic Analysis</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>105</td>
<td>Completed Preliminary Equipment Design</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix D: Interview Notes with Professor Coates
**Thermodynamic data for both reactions (ΔH rxn)**

Carbonylation - calculate it from bonds broken/made

Both are exothermic, irreversible reactions

Reaction 2 is VERY exothermic

**Kinetic data for both reactions (specific rate constant, activation energy, raw data)**

(No specific answer from Prof. Coates)

Data from JACS journal articles should be enough for our design.

**Physical Property data** Get other properties from Aldrich catalog or Metabolix website.

<table>
<thead>
<tr>
<th>Component</th>
<th>Co-Al catalyst</th>
<th>β-butyrolactone</th>
<th>Zn catalyst</th>
<th>PHB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiling point</td>
<td>Decomposes at 100°C</td>
<td></td>
<td>decomposes</td>
<td>NA</td>
</tr>
<tr>
<td>Freezing point</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat capacity</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Glass transition point</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>0°C</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solubility</td>
<td>Organics</td>
<td>Organics</td>
<td>Organics</td>
<td>CHCl3, Ethyl Acetate</td>
</tr>
<tr>
<td>Critical Temp.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Critical Pressure</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Viscosity</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Registry number</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Contact CEO of Metabolix Jim Barber

**Properties of PHB**

Is it available in many different grades or just one? See Metabolix (done)

To which grade(s) of polypropylene is it most similar? isotactic

What are its mechanical properties: tensile strength, ductile strength, elasticity, shear stress, shear strain?

Brittle
See Metabolix (done)

How fast does the polymer break down (biodegradation)?

Depends on conditions; needs heat, H2O and bacteria specifics from Metabolix

Similar to cotton

What compounds are produced when it breaks down? CO2, H2O

Can we buy some PHB for testing and display?

Metabolix, Archer Daniels Midland

**Catalysts**

Could the catalyst be made into a solid particle? yes

Is the catalyst degraded in the reaction? If so, can it be regenerated? Not degraded

How did you separate the catalyst from the desired product?

Vacuum distillation

Turnover of 10000-20000 molecules/ molecule of catalyst

Would the catalysts work on molecules of the opposite chirality to form (S)-PHB? yes

Would (S) PHB degrade as well as (R) PHB?
Probably not, since degradation is biological.

What is the method for synthesizing each catalyst?
See JACS articles

What is the approximate cost of each catalyst? (For economic analysis of the process)
Estimate from reagents. Prof. Coates said he would be interested in this info.

Process

Reaction 1 – β-lactone synthesis

Does 1 mol% Co mean 1 mol% of the catalyst? Yes

What were the concentrations of CO and epoxide?
No solvent necessary (neat)
CO pressure 6 atm to 800 psi

How was the CO introduced? gas

How was the R-BBL separated from the catalyst?
Distillation or silica gel filtration

Are there any byproducts of the reaction?
Trace isomerization (S)-BBL
BBL is toxic, so we want to drive the reaction to 100% conversion (no equilibrium)

What percentage of S-BBL will compromise the properties of the final polymer?
No answer

Reaction 2 – PHB

Is benzene-d6 solvent critical to the process, or would benzene work just as well?
Wouldn’t need any solvent
Pre-polymerize a bit and put it into an extruder.

What was the concentration of the BBL in benzene solution?
Use toluene or no solvent at all

Is the catalyst air or water sensitive?
Yes pretty much everything in this process is air and water sensitive, need to run under \( \text{N}_2 \)

Is acid quenching necessary? What does it do?
Possibly not if the concentration of catalyst is low.

Can the catalyst be recovered?
Yes, the ligand can be recovered, but it would need to be remetallated. Recommended using slower, cheaper catalyst and leaving it entrained in the plastic.
Are there any byproducts of the reaction?

Some monomer

Do you have any more data on the polymerization of (R)-BBL? Does it behave in the same way as rac-BBL?

(R)-BBL behaves essentially the same way as racemic, except that the optically pure type has a tendency to precipitate out.

Specifically: catalyst 1a, M/I 200-220, Temperature 23-50°C, conversion ≥ 90%

Contact Scheckman at Procter & Gamble They have a process to make polymer from monomer.