Team 02:

PolyBioScaffold

Final Design Report

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Calvin COLLEGE Engineering

Executive Summary

This report details the research and design decisions and calculations for the detailed design of a chemical process to produce medical-grade polycaprolactone (PCL) on a large scale. These include the constraints on the project as well as decisions about reactor type, catalyst system, and separation methods. Engineering considerations, market factors, and design norms all influenced the results of this report. The medical grade polycaprolactone will be sold for $410 per kg, an economically profitable rate with an internal rate of return of 78% over 20 years.

A batch reactor was chosen carry out the polymerization reaction of the monomer caprolactone to PCL, because the PCL product needs a molecular weight of 75,000 g/mol, which translates into a viscosity of approximately $3x10^6$ cP at the reaction temperature. Batch reactors are typically best for slow, highly viscous reaction systems. To reduce costs and promote stewardship of resources, the team designed the separations process to be continuous, thus eliminating most startup energy use for the separation units. Holding tanks were designed to join the batch reactor to the continuous separations process.

The primary use of the polycaprolactone will be in PCL-bioactive-glass composite, which can be used in medical procedures such as bone or cartilage repair. As a result, the biocompatibility and purity of the product was of utmost importance. Phenyllithium was determined to be the optimum initiator, for a system in which neither a solvent nor a traditional catalyst was needed. Separation and solidification methods included adsorption, falling strand devolatilization, extrusion, cooling, and pelletizing.

Table of Contents

Table of Figures

Table of Tables

1. Introduction

The objective of this senior design project was to develop a preliminary chemical process design that would allow for mass production of medical-grade polycaprolactone (PCL) to be used in a PCL-bioactive-glass composite scaffold for *in vivo* cartilage regrowth. We developed a process design that covers the equipment and chemicals used to produce PCL from its monomer caprolactone. Due to the theoretical nature of the project, computer simulations and hand calculations were used throughout.

1.1 Project Description

1.1.1 Problem Definition

Polycaprolactone can be created from ε-caprolactone, a 7-membered cyclic ester and member of the lactone family, when introduced to a catalyst or initiator. Figure 1 shows the basic reaction of caprolactone to polycaprolactone (PCL). PCL is depicted by its repeat unit, many of which would link together to form a long chain.

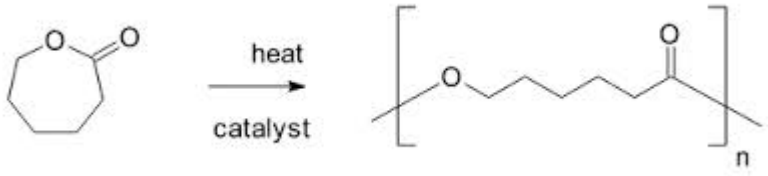

Figure 1: Reaction for manufacturing polycaprolactone [3]

Researchers have found composites containing polycaprolactone and a bioactive glass to possess properties similar to cartilage and the ability to bond to surfaces within the body such as bone [6][10]. The composite may be formed through various processes, including electrospinning, salt-leaching, and thermally induced phase separation [11]. Although the bioactive glass is currently used in bone grafts on some occasions, the composite, with its mechanism for osseointegration and variety of potential uses, is still being analyzed [12]. Technological advancements and current needs in human-tissue engineering present great potential for the manufacturing of medical-grade PCL for use in this composite, which was be the primary focus of this initiative.

The current processes for production of medical-grade polycaprolactone are relatively small scale since currently medical applicability is limited. However, the potential for increased medical-grade polycaprolactone demand due to the technological advancements previously presented exposes an unfulfilled niche in the manufacturing industry. Economies of scale provide a basis for understanding

why small-scale manufacturing incurs higher capital and operating costs per unit manufactured. On the other hand, large-scale manufacturing capitalizes on diminishing marginal costs and increased production efficiency. Although the ability to create polycaprolactone of sufficient grade has existed for years, the optimized process for doing so with high capacity has yet to be fully established [1]. The large-scale manufacturing of PCL, and, in turn, the PCL-bioactive-glass composite, improves the accessibility of cartilage replacement alternatives and decreases the overall expense of these procedures.

1.1.2 Solution

The process consists of two distinct segments: the reaction and the separation. The reaction can be executed using various combinations of solvents, catalysts, and initiators requiring different reaction times and temperatures. A relatively simple initiator, phenyllithium, can modify the environment to encourage a ring-opening mechanism to be performed on the cyclic caprolactone. The process is known to be coordination-deprotonation-insertion for phenyllithium. The monomer inserts into the bond formed between the lithium and carbonyl group of the caprolactone. This is unlike the mechanism of living polymerization that would be performed by an anionic catalyst. The insertion process (for a general rare-earth metal) is shown in Figure 2.

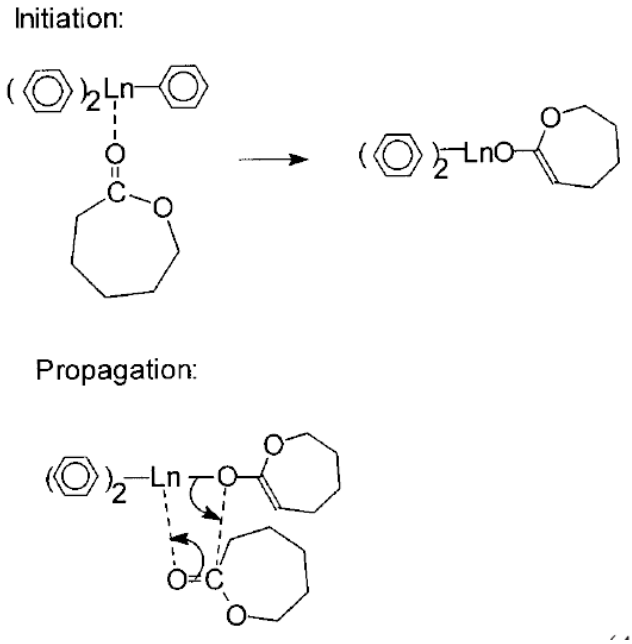

Figure 2: Synthesis of polycaprolactone from caprolactone initiated by a rare-earth phenyl compound

Various other catalysts and initiators were considered for executing the polymerization. However, most potential catalysts were rejected for one of four reasons. They were either too complex, and therefore, too

expensive, they reacted to form polymer in low yields or with high polydispersity, they required a significantly longer reaction time, or they were not biocompatible for the end use of the product. Past experiments and industrial data indicated that tin (II) octoate was one of the optimal catalysts for the polymerization [2] [12], however, this catalyst had to be rejected due to incompatibility with *in vivo* use. Therefore, phenyllithium, in a stabilizing solution of dibutyl ether, was chosen to carry out the polymerization of caprolactone [5]

The phenyllithium system described above has a reaction time of 2.5 hours in a batch reactor with a conversion of approximately 50% and a polydispersity index of 1.28 [3]. Polydispersity index is a distribution of polymer molecular weights. The reaction produced polymers with an average molecular weight of 75,000 g/mol, which is within the appropriate range for medical uses of a PCL-bioglass compound. The reaction temperature is carried out at 180^{o}C which is higher than the melting point of PCL, so it is considered liquid in the reactor. Due to its pyrophoric character, phenyllithium must be shipped in airtight drums and charging to the process will proceed through nitrogen-purged piping and valves. Benzene is created during the reaction, which will need to be separated out along with the dibutyl ether carrier. This separation will take place within the reactor, as these compounds are gases at the reaction temperature. These compounds will be vented as the reaction proceeds.

After the reaction is complete, the polymer is separated from the remaining monomer and volatiles. The separation techniques used in the process include granulated activated carbon (GAC) adsorption, falling-strand devolatilization, and melt extrusion. GAC adsorption is used to purify nitrogen purged from the reactor with benzene and dibutyl ether impurities. The falling-strand devolatilizer and hot melt extruder separate the remaining monomer from the lithium and PCL. The monomer is returned to a holding tank to be reused in the next batch reaction, to save raw material costs. A diagram of the process may be seen in Section 5.1 and details about each section of the process are provided in Section 6.

1.1.3 Constraints

For the intended use in tissue engineering, the PCL required the following characteristics: mechanical properties similar to human cartilage, biocompatibility, and ease of sterilization. Research confirmed the biocompatibility of PCL and, with a molecular weight between 50,000 and 100,000 g/mol, is mechanically similar to human cartilage [11] [12]. The method of combining the PCL and the bioactive glass impacts the characteristics of biocompatibility, sterilization, and mechanical-compatibility. Further, biomedical applications demand a high-purity polymer due to the various health hazards that arise with tissue repair. These hazards can include, but are not limited to, introduction of foreign material or

remaining starting material impurities in the composite. Any significant amount of leftover impurities could result in sickness, infection, inflammation, or other reactions to the foreign material. Cost and economic feasibility analysis were conducted to ensure that the required purities can be met at a reasonable expense. The economic analysis is presented in Section 7 of the report.

The volume of PCL produced and the economic feasibility of the process depended on the market for the PCL-glass-composite and its potential uses in tissue engineering. Based on current processes and PCL demand, we concluded that a batch reactor would produce a sufficient supply of PCL most efficiently. Batch reactors also provide better control over the extent of polymerization. Again, the proposed system was designed to produce 10,000 kg of composite material (8,000 kg of PCL) per year. However, the option to oversize the continuous separations process remains, as this would provide room for increased demand and increased production. The designed process is intended to be sold to and implemented in an existing specialty chemicals or polymer processing plant, due to the expected low demand, and its economic feasibility was analysed accordingly.

1.1.4 Market

The intended market for the medical-grade PCL product is any client with specific demands that could require a composite-based cartilage replacement. This client will likely be a composite manufacturer who will combine the PCL with bioactive glass and then 3D print the necessary scaffold for the patient. This client has the responsibility of coordinating between the doctor and the polymer manufacturer to ensure that the patient receives the correct scaffold. Therefore, the polymer manufacturer's responsibility is providing the client with highly pure, medical-grade polycaprolactone. The necessary purity of this polymer will be discussed later in the report.

The PCL-glass composite enables improved cartilage regrowth and a potentially longer lifetime than the current prosthetic options. Polycaprolactone has various other uses outside the medical field, such as hot-melt glue or an additive for many resins. However, due to the purity and quality of the process and polymer being developed, the use of the proposed product remains in the medical field for tissue engineering and scaffold implementation. If it is desired, potential minor modification of this design could be performed to create lower-grade PCL, such as industrial grade or food grade product, however, this additional analysis was not performed. Similar process designs typically involve a patent process, so that companies interested in implementing the design would be required to pay an agreed amount of money to use the patented design. The exact size of the market has not been determined yet since this is emerging technology, so we set a reasonable estimate of 8,000 kg of PCL produced per year, of the millions of

cartilage replacements in the US per year. It was decided that this technology will probably not be suitable for all replacements, so it was estimated that less than 10% of these surgeries would involve implementation of the composite. This helped to better estimate the feasibility of this technology, even considering a relatively small market.

1.1.5 Scope

As previously discussed, the main focus of this project was the development of an optimal process for manufacturing medical-grade polycaprolactone from ε-caprolactone. Due to a lack of materials, equipment, and time, experimental data that is typically obtained in the lab was instead researched and gathered from others' prior experiments and applied to the circumstances and conditions of this system as appropriate. Again, the potential to look at other applications of polycaprolactone exists, however, to reduce complexity and maintain feasibility of a detailed design, these alternative applications were not analyzed. The combination of PCL and bioactive glass was also determined to be outside of the scope of this project, since this step would likely be performed at another facility specializing in composite manufacturing.

1.1.6 Background

Discovery of the PCL-bioactive-glass composite occurred during research for artificial cartilage-replacement alternatives. Initially, researchers considered bioactive glass as a sole component for cartilage replacement. However, it was soon realized that bioactive glass itself also embodied undesired qualities, such as brittleness and a tendency to fracture when implemented in high-stress environments like knees or hips [1]. These complications stimulated much of the further research that lead to the final PCL-containing composite. After various alternatives were developed and rejected, researchers found a polymer that could be combined with the bioactive glass to better resemble the qualities of actual cartilage. This was polycaprolactone. When combined with bioactive glass, the composite exhibited new characteristics highly desired in cartilage-replacement materials [1]. Not only did the developed composite increase in its rigidity and flexibility, it also was able to bond to surfaces like bone and encouraged cartilage regrowth [1] [11].

1.2 Team Members

1.2.1 Kyle Disselkoen

Kyle was born and raised in Cedar Rapids, Iowa. He is a double major in chemical engineering and chemistry and will attend Stanford for a PhD in inorganic chemistry. He has been a summer research assistant at Calvin College, Vogel Paints, and Michigan State University.

1.2.2 Jenna Sjoerdsma

Jenna Sjoerdsma grew up in the small town of Ayden, North Carolina. She studied chemical engineering at Calvin and plans to attend graduate school at Notre Dame to complete a PhD in Chemical Engineering. She interned at Vertellus Specialties, Inc. in Zeeland, MI.

1.2.3 Benjamin Tomaszewski

Benjamin Tomaszewski was raised in the small, victorian port city of Manistee, MI. He is currently completing his senior year of chemical engineering at Calvin College and desires to work in the pharmaceutical or petroleum industry after graduation in May 2017. He has interned as a chemical engineer for a small startup company called CASEQ Technologies, as well as at Pfizer in Kalamazoo, Michigan.

1.3 Advisors

1.3.1 Primary Faculty Advisor: Jeremy VanAntwerp, PhD

Jeremy VanAntwerp is a chemical engineering professor at Calvin College. He attended Michigan State University for his undergraduate degree and received his doctorate in chemical engineering from University of Illinois, Urbana-Champaign. Professor VanAntwerp offered the team guidance, technical information, and access to resources throughout the entire course of the project.

1.3.2 Primary Industry Advisor: Phil Brondsema, PhD

Phil Brondsema is a Global Product Steward with Celanese. He holds a doctorate in chemistry and has worked in polymer manufacturing for many years. His contacts and knowledge in the field of polymerization were invaluable.

1.3.3 Chemistry Faculty Advisor: Chad Tatko, PhD

Chad Tatko is a chemistry professor at Calvin College. He attended Wheaton College for his undergraduate degree and received his doctorate in organic chemistry from the University of North Carolina Chapel Hill. He provided the team with chemistry and biocompatibility insights.

1.3.4 Secondary Industry Advisor: Bobby Deck

Bobby Deck is a Process Technology Fellow with Celanese. He provided excellent advice on the separations process steps, from personal experience working with polymerization and devolatilization processes.

1.4 Senior Design

Our team consists of three senior chemical engineering students who completed a year-long project that functions as the capstone course for Calvin College. The project occurs in conjunction with a senior design class structured to guide students through the project. Senior design projects incorporate a wide range of classroom learning from technical engineering courses to other STEM courses to humanities courses like oral rhetoric. Calvin College is a private, Christian, liberal arts college with a flourishing engineering program of about 100 graduates per year in four concentrations: chemical, civil/environmental, computer/electrical, and mechanical engineering.

2. Project Management

2.1 Team Organization

The team used a collaborative work style, which provided an advantage through the work ethic and decision-making abilities of each individual. Each individual was able to recommend new ideas, changes, and improvements. Tasks were split equally, and major decisions were made as a group. For the majority of research and technical work, all team members participated, but one often took the lead. The assigned tasks below were lead by one individual with aid and input from one or both of the other team members.

Kyle Disselkoen

Kyle was the webmaster, in charge of developing and updating the project website. He also was primarily in charge of kinetics, energy balance, and economics research and calculations.

Jenna Sjoerdsma

Jenna functioned as the team organizer, keeping the team up-to-date on deadlines and arranging meetings. She was in charge of updating the material balance and the process flow diagram. She took the lead on research into viscosity and biological issues.

Benj Tomaszewski

Benj mastered the modeling and simulation program SuperPro and was tasked with the lead in modeling the process. He was also the primary member in contact with Professor Tatko on chemistry and biocompatibility issues.

3. Requirements

3.1 Biomedical Use

Biomedical application of any material demands high purity and biocompatibility, as well as significant testing to prove the feasibility of its application. Biocompatibility is highly important with cartilage and tissue repair or regrowth, which involves internal surgical binding and long-term service. The composite was proven to have properties similar to that of actual cartilage, which ensures that the cartilage will regrow and the scaffold will remain intact until the cartilage is fully regrown [6]. PCL slowly degrades into biocompatible molecules over three or four years [11], so that the regrowing cartilage may fully repair. The material had to also be easily sterilizable. Sterility is key in biomedical applications due to the health hazards that are present when introducing an outside substance into the body. Hazards must not only be recognized but analyzed, and the results of those hazards must be acknowledged and understood. If the product is not able to be sterilized easily, the chance of outside contaminants entering the body increases significantly, which could negatively impact the feasibility of the application. Sterility and biocompatibility were major considerations throughout the design process.

3.2 Deliverables

3.2.1 Project Proposal & Feasibility Study (PPFS)

A PPFS was completed during the first semester, alongside smaller tasks, such as system material balances, the project website, and an overall system process flow diagram (PFD). See section *3.2.4 Process Flow Diagrams* for more information on the PFD.

3.2.2 Posters

The team designed posters for Engineering Fridays at Calvin, one in the fall semester and one in the spring. These posters were geared toward future engineering students and their parents and intended to display the progress made on the project. For Senior Design Night, two final posters were designed, showcasing the team's work and the final design. The main poster may be viewed in the Engineering Building during the 2017-2018 school year, and both the main poster and the PFD poster may be seen on the team's website, the link to which is in section 3.2.3 Website.

3.2.3 Website

The team website contains the documents submitted throughout the year, a project overview, and details about the team members and Calvin engineering. The URL for the website is http://engr.calvinblogs.org/16-17/srdesign02/.

3.2.4 Process Flow Diagram (PFD)

Several iterations of the PFD were completed throughout the course of the year, as the process was updated and optimized. The final version (Figure 3) shows the main reaction, separation, and solidification operating units, as well as auxiliary equipment such as pumps and condensers.

3.2.5 Final Design Report

The intent of this final design report is to demonstrate the procedure for designing a process to produce 8,000 kg of medical-grade polycaprolactone per year. The report details key design decisions and considerations that were made during the optimization of the process. The final report was delivered to the team's advisor, Professor VanAntwerp, on May 10, 2017.

4. Design Criteria

4.1 Economics

One of the primary concerns of this project is to determine whether the proposed design will be economically feasible. This will depend on how efficiently the polymer and composite can be manufactured, as well as on how much of the composite the market will sustain. The market for medical-grade PCL is rather small, making competitiveness in this market difficult. Currently, no market exists for the composite, as it has only been produced at bench-scale. Thus, if the composite can be produced at large scale, it will be competing only with traditional methods of cartilage replacement.

4.2 Product Grade

Due to the biomedical applications of the PCL, the polymer product must be of medical-grade or quality. Medical-grade polymers typically must have very low impurities, (i.e. < 1%), including residual monomer and initiator. To achieve this quality of material, industry implements good manufacturing practices (GMPs), sometimes called current GMPs or cGMPs. In the United States, the FDA's Center for Drug Evaluation and Research (CDER) sets GMPs [8].

For our project, the product grade particularly drove the design of the separations process. The high purity required meant that multiple stages of rigorous separation techniques needed to be used to reach the impurity levels listed in Table 1.

Table 1. Maximum impurity levels for in-process chemical properties in final PCL product

Name of Impurity	**Maximum Allowable Level**	**Data Source**
Caprolactone (Monomer)	2000 ppm	[30]
Lithium	900 ppm	[19]
Benzene	2 ppm	[29]
Dibutyl Ether	5000 ppm	[29]

4.3 Environmental Impact

According to BASF, caprolactone is a skin, eye, and lung irritant and a potential carcinogen [18]. Caprolactone should not be released to the environment without proper authorization. With large-scale

manufacturing, it is likely that purged material will have to be sent to a processing facility due to the environmental hazards of purging large amounts of the reagents.

Phenyllithium, as an initiator, will be used in relatively small amounts (about a 200:1 monomer-to-initiator ratio). We do not expect phenyllithium to be released into the environment. If it was, it would be a safety hazard as it is pyrophoric.The small amount of lithium that results from the initiation process will be contained in the final product polymer, so it will also not be released.

Dibutyl ether and benzene will be vented from the reactor and enter a GAC adsorber. The effluent from the adsorber will still contain a small amount of both chemicals, which must meet EPA and OSHA guidelines.

Most of the materials used in this process are relatively low hazards to the environment in small quantities. Recycling the materials as much as possible decreases the amount of processing that is required for purged material. Outside processing should be minimal since material will only be purged if accumulation begins to occur; most of the feed materials can be reused.

Since energy usage is also a significant concern, we considered how to minimize the environmental impact of keeping much of our process equipment at elevated temperatures. Using high pressure steam at the same temperature as the heat source for all of the process units allowed for the design of a single trunk line of steam entering the process and another exiting to a large boiler. Limiting the number of boilers needed for the process reduces energy usage.

4.4 Marketability

The market for PCL is not as extensive as more common polymers such as PCV or PCP, and with a rather low demand for the substance, the process would likely not draw much interest. Throughout the late 1970s and early 1980s, the market for PCL increased dramatically due its “rheological and viscoelastic properties” [11]. However, newer polymers soon out-competed and replaced PCL, and the market for polycaprolactone subsided. In the past decade, newly developed applications for PCL and similar substances caused the market to expand, and a resurgence of PCL use occurred.

Creating a process and supplier that can make medical-grade PCL, and then use that product to manufacture cartilage replacement composites would allow the company to operate in their own market. Rather than buying more expensive medical-grade polymer, they could manufacture their own from

cheaper starting materials. Using that product in creating a cartilage replacement composite, rather than selling the polymer to an intermediate manufacturer would then allow them to maximize profit since they would be selling the composite material themselves. Running both manufacturing processes themselves would increase upfront and operation costs, but this would be balanced by selling the composite material themselves, rather than just selling the polymer to a composite manufacturer. The market for a cartilage-replacement composite like this also a sole or primary supplier, so being the primary supplier for this composite would make it difficult for competitors to grow. The main competition for this composite, then, would be prostheses. However, prostheses typically only last about 10 years before surgery is necessary again. If the composite can increase this replacement time, or be a one-time surgery, just that development alone would give people an incentive towards the product.

The preliminary design for this plant proposes to produce 8,000 kg per year of polycaprolactone, which will be combined with bioactive glass to form a composite. Caprolactone was assumed to have a purchase price of $1.35 per lb [39]. Phenyllithium is $20 per liter when purchased in bulk but since the monomer:initiator ratio is so low, the cost is not prohibitive [40]. Medical grade polycaprolactone is worth significantly more than its raw material precursors. Section 7 provides more information regarding the economic dimension of the design.

4.5 Design Norms

The design norms of stewardship, integrity, caring, and justice served as further design criteria for this project [15]. Due to the call to stewardship of the earth and its resource, the design limits use of hazardous chemicals and reduce waste by recycling where possible. The norms of integrity, caring, and justice called for a design that would produce an end product safe for biomedical use and that was capable of performing as claimed.

As stewards of the earth, engineers are responsible to all current and future inhabitants of the environment. Engineering involves decisions that are scaled such that a single decision can have a measurable impact on the environment in ways that daily habits do not. We considered the environmental impact of our project directly alongside the minimization of costs and the maximization of revenue.

Our product will have integrity and be a just product if it meets or exceeds expectations given by the medical-grade designation and functions reliably despite adverse circumstances. A knee or hip replacement should not cause undue pain to the recipient and should allow them to fruitfully interact with society in ways that were not possible before the surgery.

The impetus for our project was a focus on caring for those in need of a hip or knee replacement. Given the millions of surgeries occurring per year in the United States, it is clear that an improvement in surgical technique would have a significant impact on the health and well-being of the population of the US. A PCL-bioactive-glass composite has the potential to improve surgeries substantially.

5. Process Overview

5.1 Process Flow Diagram (PFD)

Our overall system for manufacturing polycaprolactone consists of two main sections: a batch reactor and a continuous separation process.[1] The two sections are joined with a holding tank. Both the reactor and the holding tank must undergo a nitrogen purge to prevent the contents from contacting air or water, which would react with the pyrophoric initiator. The purge vent on these systems contains nitrogen as well as the other volatiles in the system, namely benzene and dibutyl ether. The outlet of this vent stream is sent through an activated carbon adsorber, which removes the benzene and dibutyl ether to levels safe for release into the environment.

From the reactor effluent holding tank, the polymer-monomer mixture is sent to a falling-strand devolatilizer and then a hot melt extruder to evaporate off the monomer and remaining light impurities. The monomer pulled off in these separation units is recycled, condensed, and sent to another holding tank. The hot polymer product from the extruder is sent to a water bath for cooling and then through a pelletizer. The pellets are then dried in a low heat, dehumidified air dryer. A diagram of this overall system is shown in Figure 3 and descriptions of the units in shown may be found in Tables 2 and 3.

[1] Design specifications and decisions are explained further in Section 6 “Process Design” for each piece of the process.

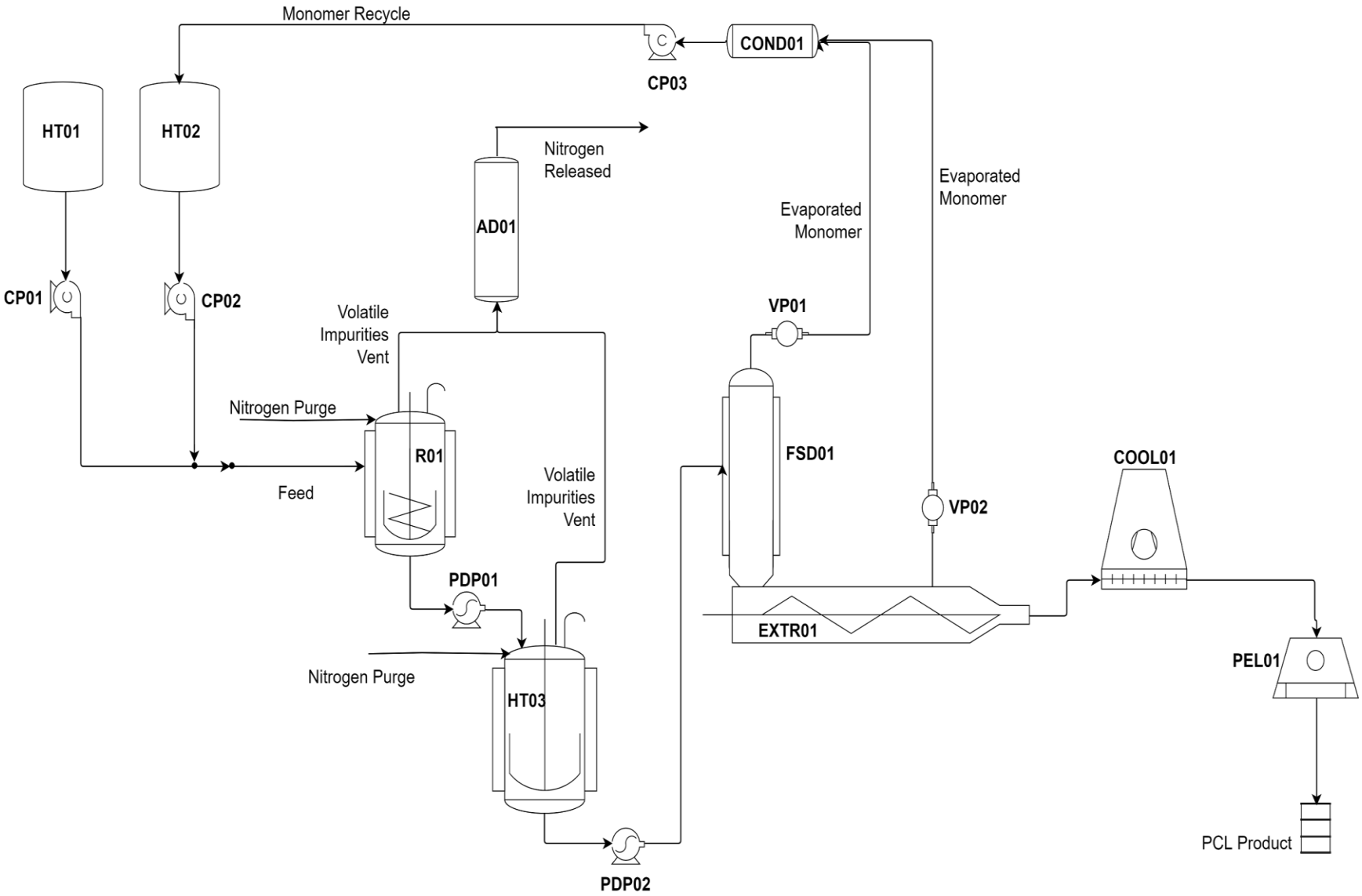

Figure 3. Process flow diagram (PFD), including reaction and separation processes

Table 2. Names and descriptions of main process equipment

Name of Unit	Description	Size
AD01	Granular Activated Carbon (GAC) Adsorber	400 lb canister
COND01	Condenser for Monomer Recycle	5 m^2 surface area
COOL01	Cooling Table	10 m
EXTR01	Hot Melt Extruder	15 Nm/cm^3
FSD01	Falling-Strand Devolatilizer	16 m^3
HT01	Fresh Monomer Holding Tank	6.25 m^3
HT02	Recycled Monomer Holding Tank	6.25 m^3
HT03	Reactor Effluent Holding Tank	6.25 m^3
PEL01	Pelletizer	10 kW motor
R01	Batch Reactor	1.5 m^3

Table 3. Names and descriptions of auxiliary process equipment [2]

Name of Unit	Description
CP01	Centrifugal Pump on HT01
CP02	Centrifugal Pump on HT02
CP03	Centrifugal Pump on COND01
PDP01	Positive Displacement Pump after R01
PDP02	Positive Displacement Pump after HT03
VP01	Vacuum Pump on FSD01
VP02	Vacuum Pump on EXTR01

5.2 Energy Balance

5.2.1 Heat Transfer

To perform an energy balance on the proposed system, the energy consumption for each piece of equipment was calculated. It was assumed that the reactor would operate isothermally at 180 degrees

[2] Pump sizing is given in Table 6.

celsius. Therefore, two stages of energy transfer were assumed for the reactor: heating of reactants and maintaining reactor temperature. Heat capacities of the reactants were used for determining the energy needed for heating the contents to 180 degrees celsius. Values for thermal conductivities, convective heat transfer coefficients, jacket thicknesses, and insulation thicknesses were assumed based off of textbook problems. These values can be found in Table 4.

Table 4. Assumed values for necessary heat transfer parameters for process tanks.

Thermal Conductivity of Stainless Steel (W/m K)	Thermal Conductivity of Insulation (W/m K)	Convective Heat Transfer Coefficient to Inside (W/m k)	Convective Heat Transfer Coefficient to Outside (W/m k)	Thickness of Jacket (m)	Thickness of Outside Insulation (m)
20	0.064	5,680	11.4	0.005	0.02

These same parameters were used in the energy calculations for the reactor, holding tank after the reactor, and condenser. The energy necessary for heating of the reactor (before and during the reaction) can be found in Table 5.

Table 5. Energy values for heat transfer before and during reaction.

Energy from Steam to Reactor Before Reaction (kJ/hr)	Energy from Steam to Reactor During Reaction (kJ/hr)
303,000	33,500

The necessary steam flow rate for achieving this heat transfer is 2.4 kg/s and 0.26 kg/s, respectively. This steam flow rate was calculated based on a temperature change of 15 degrees celsius in the steam. High pressure steam was selected as the heating fluid due to the high temperature required for maintaining a viscous polymer.

The energy necessary for maintaining a holding tank temperature of 180^{o}C is 44,800 kJ/hr, which demands a steam flow rate of 0.35 kg/s. Again, this assumes a 15^{o}C change in the steam temperature.

The condenser uses ambient-temperature[3] water to lower the temperature of the recovered monomer below its boiling point of 252°C. The required amount of energy to be removed from the monomer is about 20,300 kJ/hr, which will require a water flow rate of approximately 0.06 kg/s. This assumed a temperature increase of 25°C in the water.

5.2.2 Electricity

The energy balance also required calculations for electricity consumption by the extruder, cooling table, pelletizer, and various pumps that are used. Three types of pumps are used in the process, which include two high-viscosity positive displacement pumps, two vacuum rotary vane pumps, and three liquid centrifugal pumps. The specifications for these pumps can be found in Table 6.

Table 6: Specifications for the three types of pumps implemented in the proposed design

Type of Pump	Maximum Power (HP)	Efficiency	Electricity Consumption (kW)	Capacities
High viscosity positive displacement pump, lobe	3	0.6	3.73	50 gal/min
Vacuum rotary vane pump	30	0.5	37.3	min pressure: 0.3 bar, 600 ft^3 per min
Liquid centrifugal pump	8	0.85	9.94	max pressure: 39 psi, 200 gal/min

The electricity consumption by the cooling table and extruder was 10 kW and 108 kW, respectively, which were determined based on the specifications for this equipment found in user manuals. The electricity value for the extruder incorporated assumptions about efficiency (about 65%) and percent torque (about 80%). The cooling table was assumed to have an efficiency of about 75%. These specifications can be found in section 6.4.2 for the extruder and section 6.4.3 for the cooling table and pelletizer.

[3] Approximated as 25°C. Ambient temperature will change with the seasons and the geographic location of the plant.

5.3 Modeling and Simulation

Given the limited kinetic data available for the complex polymerization process, Microsoft Excel was used to model the reaction (see section 6.2.2). The length of polymer chains was modeled at various reaction times appropriate to the catalyst data available. SuperPro was used for modeling the separations portion of the process. SuperPro is a process simulation program capable of modeling both continuous and batch processes, but cannot model polymerization reactions. For modeling the separation within the reactor, a flash was used, which sent the overhead vapors of the reaction to a GAC adsorption unit to be purified before release. This was done under batch conditions since a batch reactor was chosen. The purification of the PCL product was modeled as a continuous process to reduce energy usage required for startup and shutdown. The devolatilization that occurred within the extruder was modeled as a flash prior to the extruder since SuperPro does not contain devolatilization extruders.

6. Process Design

6.1 Monomer and Initiator

Supplementary tables from a review of the various methods of producing PCL detail over 100 catalysts and initiators that can successfully induce the polymerization of caprolactone to polycaprolactone [3]. Project constraints were applied to the list to eliminate most of the possible catalysts. Overly complex catalysts would be too expensive for large scale production of PCL. Catalysts that did not produce high yields would require additional expensive separation processes to separate unreacted monomer from the polymer product. Many catalysts did not produce a polymer product with a molecular weight or polydispersity index within the project constraints. Lastly, availability of the catalyst on a large scale was considered.

The team originally planned to use tin (II) octoate as the catalyst, with toluene as the solvent and butyl alcohol as the initiator. However, tin is not biocompatible and proved too difficult and expensive to separate from the polymer, so the supplementary tables of catalysts and initiators were reviewed once more with the added criteria of biocompatibility. Phenyllithium was chosen as the optimum catalyst option, though it functions as an initiator, not as a catalyst. The reaction with phenyllithium does not require a solvent, so the team chose not to use any solvent to reduce the separation and recycling needed in the process. However, phenyllithium must be transported in dibutyl ether, so a small amount of dibutyl ether also had to be separated out of each batch of PCL. Phenyllithium is also a pyrophoric chemical, meaning that it spontaneously combusts when it contacts oxygen in air. Special handling requirements due to this are discussed in subsequent sections.

Phenyllithium break apart into benzene and lithium; however, it is still a more biocompatible choice than most of the catalyst options, because the benzene can be removed with relative ease due to its low boiling point. Lithium, in low doses, is safe for consumption and is, in fact, used in medications to treat manic depressive disorders. Research into lithium dosages showed that the amount of lithium in the final product would be safe for implantation in the human body without any separation steps to remove the lithium. The long-term daily dose for lithium medications is 900-1200 mg per day [19]. The team's final PCL product would contain only about 300 mg of lithium per kg of PCL. A typical implant would contain well under a kilogram of PCL and would be implanted for up to three years before degradation completed. So, the amount of lithium released into the human body on a daily basis could be expected to be at least a full order of magnitude smaller than the recommended pharmaceutical dosage. Since ingested chemicals do not necessarily impact the body in the same way that implanted chemicals would, the team also researched the absorption and excretion pathways of lithium to determine how reliably

information on oral dosages would compare to implantation dosages. This research showed that ingested lithium is almost exclusively absorbed into the blood, as opposed to being directly excreted through either the urinary or renal tracts [20]. Lithium in an implant would also be taken up in the blood before any form of excretion could occur, so it was determined that the oral pharmaceutical dosages of lithium could be used to determine safe levels of lithium in the PCL for implantation.

6.2 Reactor

6.2.1 Reactor Design and Materials

Broadly, reactors can be categorized by how material is processed, either in batches (batch reactor) or in a continuous flow (continuous stirred-tank reactor, CSTR, or plug flow reactor, PFR). Batch reactors tend to be used for smaller quantities of material or for slow reactions with viscous products. Flow reactors often have better mixing and can accommodate high reactant concentrations. Dr. Brondsema recommended using a batch reactor for the polycaprolactone polymerization process given the benefits above. The designed process is for a relatively small quantity of polycaprolactone, and the molten polymer is very viscous so it would be difficult to keep the product flowing in a continuous flow reactor.

The reactor is to be constructed of stainless steel to avoid metallic impurities entering the final product and to prevent any side-reactions from occurring with the reactor. Stainless steel is the typical material of construction for pharmaceutical and medical-grade process units.

Due to the high viscosity of the polymer, a helical-ribbon agitator blade was determined to be optimal [21]. An anchor paddle was combined with the helical-ribbon blade to scrape the sides of the reactor vessel and prevent charring of the polymer due to the high heat of the jacketed reactor sides. The agitator blade must also be stainless steel.

When the process is implemented, the energy draw on the agitator may be correlated with viscosity, and thus with molecular weight, to determine quickly when the reaction is complete. This would allow for repeatable quality in terms of polymer molecular weight. A high energy draw alarm could also be used to determine if the reaction has proceeded too far and the polymer become too viscous. If not caught in time, this could cause the polymer to completely solidify in the reactor, which would essentially ruin the reactor. If an over-polymerization is caught in time, a chemical quench or an inert solvent, such as toluene, may be used to stop it. A chemical quench would be the preferred method, since a quenched

batch might still be saved. A batch flooded with toluene would have to be sent to waste handling, but the reactor would be preserved.[4]

6.2.2 Kinetics

The initiator phenyllithium was chosen for its biocompatibility and other favorable properties. However, there is not a large amount of published data on the compound performing the ring-opening polymerization of caprolactone. Specifically, there is not time-dependent kinetic data for the process. In lieu of this data, the data for tin(II)-octoate provided a basis for kinetic analysis of the reaction.

The polydispersity values for ideal addition polymerization were calculated. Equations 1 and 2 were used to calculate the distribution and the number average polymer length [9]. The instantaneous concentration of the monomer is related to the initial concentration $[M]_0$ (mol/L), the time constant τ (min), a rate constant k (L/mol·min), and the initial concentration of the initiator $[A]_0$ (mol/L). The concentration of the growing polymer $[AM]_j$ (mol/L) is also a function of the number of monomer units j.

$$[M](\tau) = \frac{[M]_0}{1 + k\tau[A]_0} \qquad \text{Equation 1}$$

$$[AM_j](\tau) = \frac{[A]_0(k\tau[M])^j}{(1 + k\tau[M])^{j+1}} \qquad \text{Equation 2}$$

A kinetics graph of the natural log of the concentration ratio of monomer versus time is shown below [4]. The initial concentration of monomer and initiator was also provided. This allowed us to calculate a rate constant k in [L/mol·min] from the slope of the graph (Fig. 4, below) of line #1.

[4] Acknowledgements to Phil Brondsema for his expert advice and ideas on these topics.

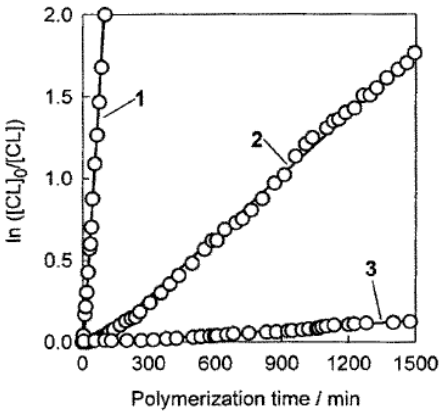

Fig. 4. Kinetics of polymerization of ε-caprolactone (CL) initiated with tin octoate ($Sn(Oct)_2$) followed dilatometrically. Conditions: $[CL]_0 = 2.0\ mol \cdot L^{-1}$, $[(Sn(Oct)_2)]_0 = 0.05\ mol \cdot L^{-1}$, THF solvent, 80 °C; (1) added butyl alcohol (BuOH), $[BuOH]_0 = 0.10\ mol \cdot L^{-1}$, (2) no additive, (3) added 2-ethylhexanoic acid (OctH), $[OctH]_0 = 6.5 \cdot 10^{-3}\ mol \cdot L^{-1}$

First, Equation 1 was used to determine the concentration of monomer as a function of time. Then Equation 2 was used to plot the concentration of the growing polymer chain at various lengths, as shown in Figure 4.

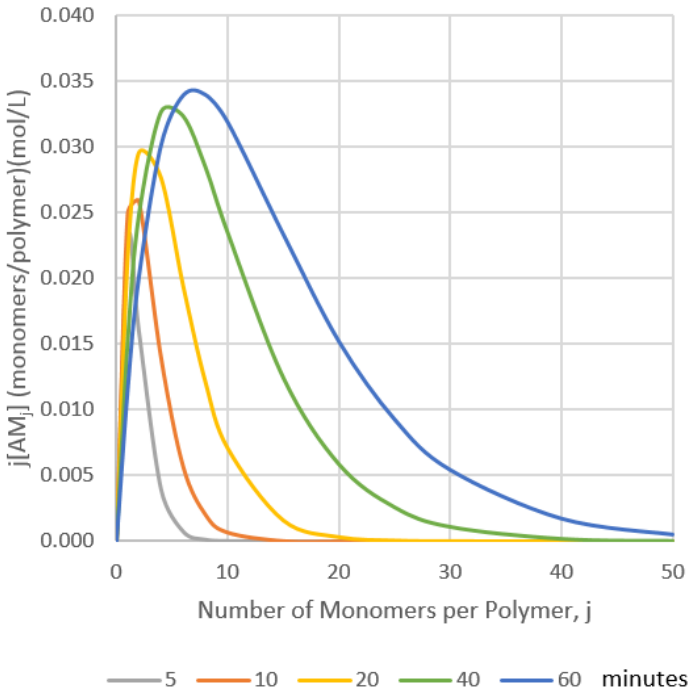

Figure 5. Weight distribution ($j[AM_j]$) as a function of the number of monomers per polymer (j), with time of reaction as a parameter

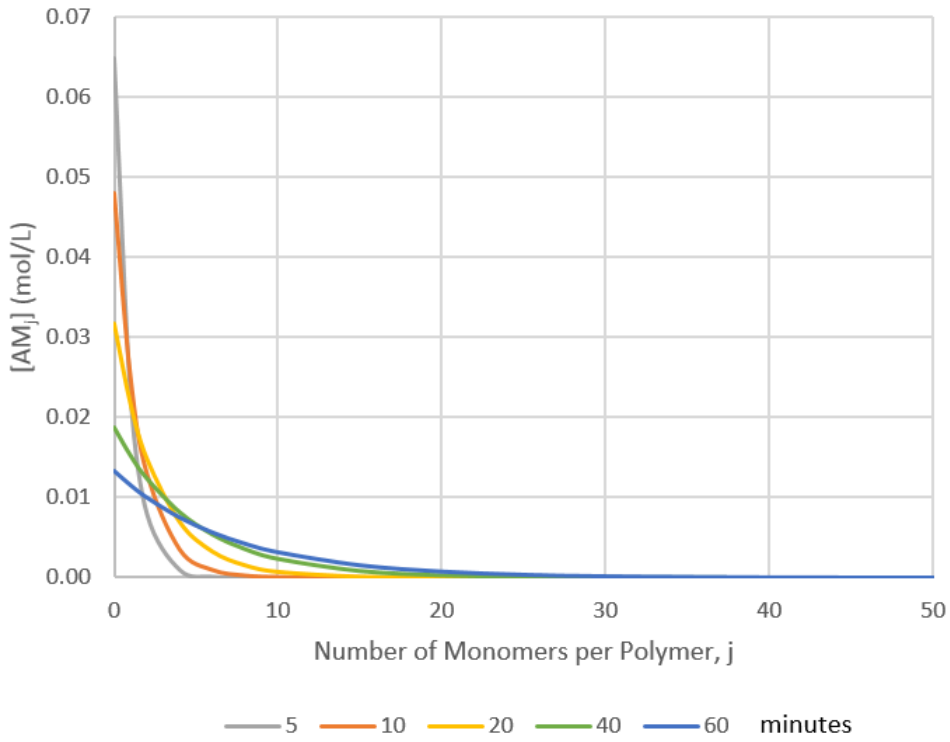

Figure 6. Concentration of polymer of length j ($[AM_j]$) as a function of the number of monomers per polymer (j), with time of reaction as a parameter

6.2.3 Removal of Volatiles

The nitrogen purge on the reactor also allowed for the removal of some volatiles during the reaction. Since the optimum reaction temperature of 180ºC was well above the boiling points of both benzene (80ºC) and dibutyl ether (142ºC), both components would be in the vapor phase in the reactor.

Table 7. Normal boiling points (at 1 atm) of components to be separated from PCL product

Component	Normal Boiling Point
Benzene (initiator product)	80.1 ºC
Dibutyl ether (initiator carrier)	142.4 ºC
ε-caprolactone (monomer)	253 ºC

The release vent on the nitrogen purge could then also be used to purge benzene and dibutyl ether. This stream needed to be cleaned of volatiles before it could be released, so it was run through a granular activated carbon (GAC) adsorber to remove the benzene and dibutyl ether to acceptable levels for

environmental release. The EPA requires that no more than 2 weight percent benzene be in the stream emitted to the environment and that the overall amount of organic volatiles released be 5 weight percent or less [28].

6.2.4 Polymer Degradation

Charring and degradation of a polymer must be considered when exposing it to high temperatures. However, PCL undergoes no degradation until it reaches a temperature of approximately 350 ^{o}C [3]. No indication of charring was stated in the literature on PCL; since the team lacked the resources to test this, an assumption was made that no significant charring would occur below 350 ^{o}C. The melt extruder is the process unit operating at the highest temperature, and since it is operating at reduced pressure it will not operate about 300^{o}C.

6.3 Reactor Effluent Holding Tank

The effluent from the reactor must be pumped into a holding tank to join the batch reactor to the continuous separations process. This tank was designed to hold two batches of effluent, and thus has a volume of 6.5 m^3. To prevent the polymer-monomer mixture from solidifying in the tank, a jacketed tank design was chosen, with the temperature of the polymer maintained near 180^{o}C. The tank also has an anchor paddle agitator to scrap any polymer from the sides of the tank to prevent charring.

6.4 Separation Processes

To purify the PCL to medical-grade requirements, the polymer needed to be separated from the remaining monomer, initiator, and other impurities in the reactor effluent. The following separations and solids-handling operations were used: a falling-strand devolatilizer, a hot melt extruder, a cooling table, and a pelletizer. Like the reactor, all of the separation units needed to be made from stainless steel to prevent metallic impurities from entering the final product and to prohibit the process material from reacting with the equipment walls.

6.4.1 Falling Strand Devolatilizer

A falling strand devolatilizer (FSD) functions much like a flash, which is a large vertical tank run under vacuum pressure to pull off the lighter components as vapor. The advantage of the FSD over a simple flash was the ability of the FSD to handle, and effectively remove volatiles from, high viscosity substances [31]. An FSD schematic may be seen in Figure 7.

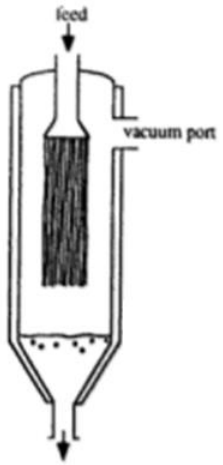

Figure 7. Schematic of a falling-strand devolatilizer [38]

The FSD, the first step of the separation process, served to evaporate off the about 94% of the unreacted monomer in the reactor effluent, by lowering the pressure of the mixture to 0.3 bar. The FSD brought the mass percent of monomer down from 50% to approximately 3%. The evaporated monomer was sent to a condenser to be cooled and recycled. The monomer-polymer mixture remaining in the bottom of the FSD was directly deposited into the extruder through a conical bottom with an auger to move the viscous material.

6.4.2 Hot Melt Extrusion

A twin-screw extruder was necessary to handle moving the highly viscous polymer after removal of the majority of the excess monomer in the falling-strand devolatilizer. The hot melt extruder was used to evaporate off more of the monomer, to reduce the monomer level to within the acceptable impurity limit of 2000 ppm monomer in the final PCL product. The monomer vapor from the extruder was collected above the extruder and sent to be condensed and recycled along with the vapor from the falling-strand devolatilizer.

The extruder was sized based on a polymer throughput and viscosity. Ensuring the twin-screw extruder can generate the necessary torque for extruding a high-viscosity polymer is a key aspect for sizing this piece of equipment. Pure PCL, with the required molecular weight of 80,000 g/mol and at the process temperature of 180^{o}C, has an approximate viscosity of three million centipoise. The throughput for the extruder was based on the initial demand of the PCL (about 8,000 kg/yr). However, it is likely for the demand for the composite and thus the PCL to increase over time, thus investing in a larger extruder from the beginning could be desirable. The recommended extruder would have specifications similar to the

Leistritz ZSE 50 MAXX extruder shown in Table 8 and detailed in Figure 8, with a max torque around 2000 N-m and a max screw speed of about 1200 rpm.

Table 8. Specifications for proposed extruder design [26]

ZSE 50 MAXX	
Screw diameter (mm)	51.0
Flight depth (mm, without tolerance)	10.1
OD/ID	1.66
maXXstandard-torque (Nm)	1,500
maXXtorque (Nm)	2,144
Screw speed (rpm)	300, 600, 900, 1,200
Weight (kg)	~ 4,200

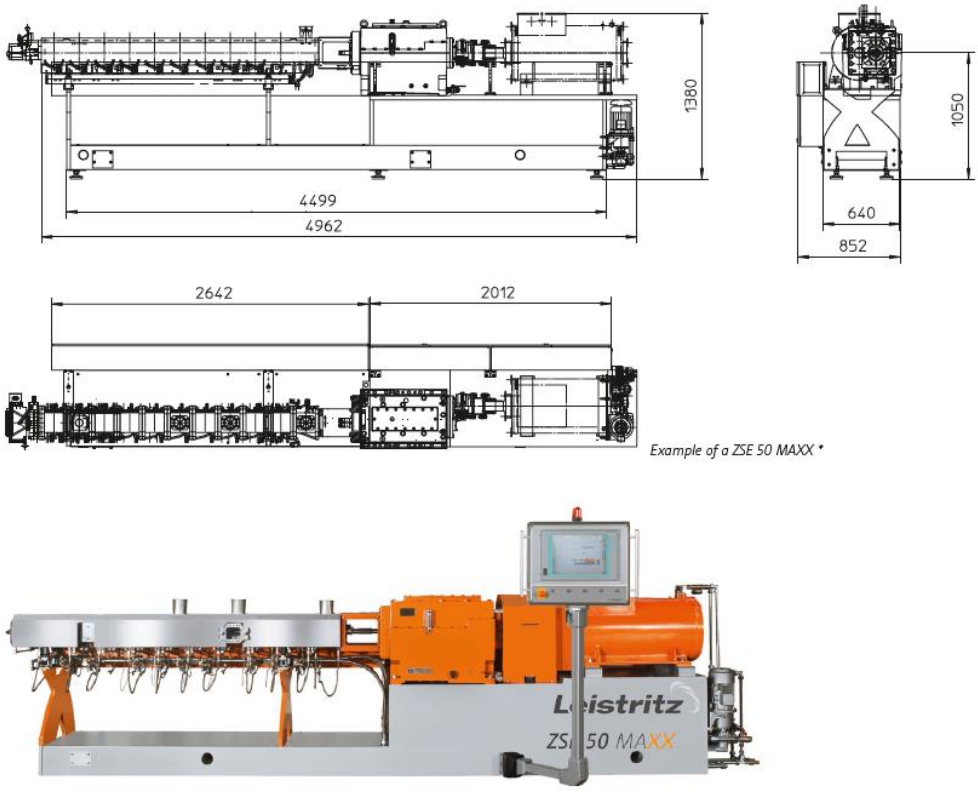

Figure 8. Schematic and picture of a feasible extruder for the proposed process [26]

6.4.3 Solidification

Due to PCL's low melting temperature of approximately 60°C, the extruder alone would not be effective at cooling the polymer sufficiently to produce evenly cut pellets. The output of the twin-screw extruder is a strand of PCL containing residual lithium from the catalyst. Polymers are typically cooled in a water

bath or with a spray of water, as it offers a higher heat capacity than cooled air. However, because lithium reacts vigorously with water, the PCL must be cooled with chilled, dehumidified air. The polymer will be extruded onto a cooling table similar to the one shown in Figure 9, although, as previously state, the proposed process will require air cooling rather than water.

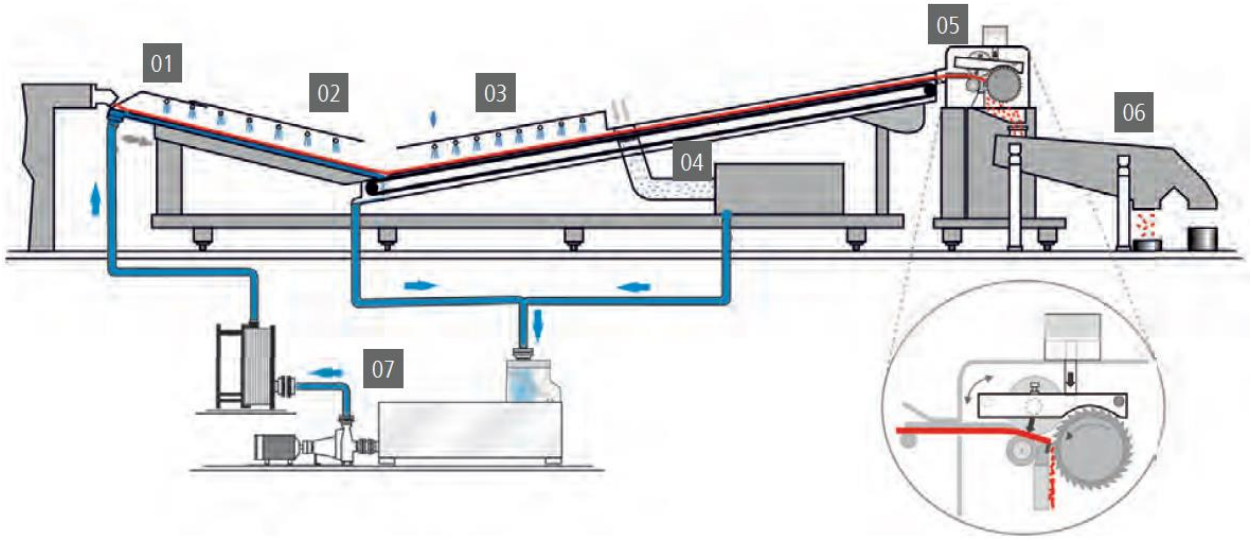

Figure 9. Process diagram of proposed cooling table/pelletizer, which features water-spray cooling rather than our proposed air-cooling method [27]

The cooling table will feed directly into the pelletizer, which cuts the cooled polymer strand into uniform pellets before packaging. Often, pelletizing would be performed in the same unit as the extruder, however, the incomplete cooling in the extruder due to the low melting temperature of PCL prevent this. Thus, a cooling-table-pelletizing combination unit was added to the process after the extruder. The technical data for this type of cooling table is shown in Table 9.

Table 9. Specifications for proposed cooling-table-pelletizer design [27]

Technical data:	JSG 200	JSG 300	JSG 400	JSG 600	JSG 900
Strand pelletizer:	PRIMO^{Plus}			M-ASG	
Operating width:	200 mm	300 mm	400 mm	600 mm	900 mm
Pelletizer motor power (depending on material type, pellet weight, and pellet size):	5.5-18.5 kW	7.5-22 kW	11-30 kW	15-45 kW	30-75 kW
Line speed:	50-150 m/min				
No. of strands (at 3 mm pellet diameter):	25	40	50	80	120
Length of strand guide section:	2, 3 or 4 m				
Length of conveyor belt:	3, 5 or 7 m				

Due to the relatively low throughput of our separations process (about 1 kg/min), a cooling-table-pelletizer combined unit similar to the JSG 200 is recommended. Again, increasing the equipment size to allow for increased demand in the scaffold may be a cost-effective consideration when implementing this process.

6.5 Clean Room

Since the PCL pellets are intended for medical application, the final processes of extrusion, cooling, and pelletizing will take place in an ISO Class clean room. This will ensure that the final product does not come in contact with contaminants that could harm the end-user. Only an ISO Class 5 or ISO Class 6 clean room will be required, because the pellets will undergo further purification during composite manufacturing. The particle content in ISO Class 5 and ISO Class 6 clean rooms is about 0.1-1.0% of a typical non-graded area, which will require implementation of high efficiency particulate air filters.[5]

6.6 Monomer Recycle

To reduce waste and expenses, the unreacted monomer remaining in the reactor effluent stream exiting the reactor was recycled as it was pulled off in the falling-strand devolatilizer and extruder. These recycled streams were sent through a condenser to fully liquefy the monomer so that it could be pumped back to the appropriate holding tank. No further separation was performed on the monomer recycle streams, as the amounts of benzene [5]and dibutyl ether in these recycled streams were minimal and any excess volatiles would be removed in the reactor and holding tank during the next batch.

6.7 Safety

Safety in chemical plants is incredibly important, not only for the well-being of employees but also for the productive and consistent operation of the plant. The plant design includes several common safety features, as well as a few that are more unique to this design. Federal law requires implementation of a wide range of safety procedures and consistent testing and upkeep of those features.

The process equipment operated at high temperatures will be equipped with temperature alarm systems that alert the operator of temperature irregularities. If the temperature deviation is significant enough, the control system will alter the fluid flow rate or temperature to change the temperature inside the vessel accordingly. Since the polymerization reaction is not strongly exothermic [25], there is not a significant

[5] Knowledge of ISO classification system obtained during internship at Pfizer in the summer of 2016.

risk of a runaway reaction. The more significant risk is a decrease in temperature leading to solidification of the polymer in one of the vessels which would be very difficult to clean out and keep the process operational. Pressurized vessels will also have high pressure alarms that operate in a similar manner to the temperature alarms.

Since phenyllithium is pyrophoric [23], additional materials handling procedures are set in place. Pyrophoric materials spontaneously combust when they contact air (specifically, oxygen) at or below 55^{o}C. In small quantities, Class D fire extinguishers are used to prevent such fires from burning further. All vessels holding phenyllithium, including the vessels that it is transported in, are flushed with nitrogen, an inert gas. The high purity nitrogen will come from a stream already available from the larger chemical plant. Backup containers of nitrogen will be in place in case of a situation where the standard stream of nitrogen is not available. Significant personal protective equipment will be used by any operators who are handling the pyrophoric material.

For the reactor, falling-strand devolatilizer, and effluent holding tank, pressure relief valves and rupture discs will be in place in case of an unexpected increase in pressure. Although this event is unlikely, it is important to have these valves in place to prevent an explosion of the entire vessel. At high pressure, a control system will open the pressure relief valves, which will vent to the GAC adsorber. The pressure rupture discs do not use a control system; they burst under a significantly elevated pressure, which for this process would be around 10 bar.

6.8 Waste Handling

The used carbon from the adsorber, which will contain benzene and dibutyl ether, will need to be treated as hazardous waste. It will be sent to a carbon reactivation facility, potentially the same facility that supplied the activated carbon, so the contaminants may be burned off and the vessel recharged.

7. Economics

7.1 Capital Costs

When considering the economic implications of building a chemical plant, it is important to consider both capital costs (one-time purchases of equipment) and operating costs (continual purchases of consumable goods). Of course, other economic realities like taxes, depreciation, loans, and market shifts must also be taken into account to fully understand the profitability of the design. First, the capital costs were estimated with tables and figures from Peters and Timmerhouse [22] and scaled to the present day using the CEPCI index [24].

Table 10 shows the estimated capital cost for each major piece of process equipment in the design. Because of the demands of pharmaceutical grade polymer processing, all of the equipment is made with stainless steel. This increases the price of equipment significantly compared to carbon steel, the most common material, but it is necessary for the process. The figures presented in Peters and Timmerhouse scaled costs of equipment by their most relevant metric, usually size. Sizes of equipment were based off the amount of material being processed, which was not as high as many chemical plants.

Table 10. Capital costs for process equipment

Equipment name	Cost (2017)
Fresh monomer holding tank	$ 75,000
Recycled monomer holding tank	$ 75,000
Jacketed batch reactor	$ 100,000
Jacketed post-reactor holding tank	$ 75,000
Falling strand devolatilizer	$ 120,000
Condenser	$ 40,000
GAC gas adsorber	$ 15,000
Hot melt extruder	$ 230,000
3 centrifugal pumps	$ 23,000
2 positive displacement pumps	$ 15,000
2 vacuum rotary vane pumps	$ 60,000
Post-reactor tank agitator	$ 75,000
Conical auger for flash vessel	$ 7,500
Pelletizer	$ 45,000
Cooling Table	$ 150,000
Total Purchased Cost	**$ 1,106,000**
TOTAL CAPITAL COST	**$ 3,010,000**

The Chemical Engineering Plant Cost Index (CEPCI) is a single number that changes over time to track changes in price for chemical engineering process equipment. It is chosen from a statistically random sample of various industries that use chemical processing units. For this project, an index of 541.7 (the average value for 2016) was used for all of the capital cost calculations.

In Table 11, the total purchased cost is simply the sum of all of the purchased costs of the equipment. The total capital cost is a more complicated calculation. Table 7 shows the additional costs associated with the unit operation equipment. Buying the equipment is not enough: it must be designed, installed, connected to piping, insulated, and wired with instrumentation and electricity. The percentages shown are percentages of the total purchased cost. Therefore, the total capital cost is the sum of the total purchased cost and the additional costs for each of the additional costs.

Table 11. Additional costs for process equipment

Additional costs	Percent of equipment cost
Installation	40%
Piping	66%
Electrical	10%
Insulation	8%
Instrumentation	13%
Engineering	30%
Biocompatibility Study	5%

The last entry in Table 11 is the biocompatibility study. This includes the purchase of biocompatibility data from another manufacturer as well as an in-house study to determine that the specific product produced is biocompatible. The FDA permits companies to perform a “read-across”, which is a risk assessment based on an existing study of a very similar material. An argument is developed based on the similarity to another company’s product. These are much less expensive and time-consuming than conducting the entire biocompatibility test alone.

7.2 Operating Costs

Operating costs for a chemical plant are due to a wide range of activities, many of which will be lumped together in larger categories (see Appendix Table A.2.10). The primary categories for operating costs are raw materials, utilities, and labor. For raw materials, our analysis showed that in a large chemical plant, nitrogen was very inexpensive at $0.21 per 100 cubic feet [32]. Even though the reactor is continually

purged with nitrogen over the course of the reaction, the nitrogen costs were not significant enough to be considered separately.

The utilities that are required for this design are high pressure steam, process water, and electricity. The high pressure steam is used to heat all of the vessels that are above room temperature. The process water is used to cool the condenser and the cooling table air stream. Electricity powers the pumps throughout the process, including the vacuum pumps on the extruder and the compressor that drives airflow through the nozzles on the cooling table. Given the cost of process water at $0.354 per GJ and the amount we need, the cost is not significant [33].

Table 12 shows the operating costs for this design. Labor was calculated to be $40 per hour (including benefits) [34], electricity at $0.06 per kWh, and high pressure steam at $17.70 per GJ [33]. Raw material prices were calculated from the ICIS website or scaled to those values if the costs were not available [35]. The "Other" category in the table covers costs for process water, nitrogen, shipping and handling, maintenance, etc.

Table 12. Annual operating cost categories and amounts

Annual Operating cost	**Total annual cost**	
High Pressure Steam	$	153,000
Electricity	$	4,000
Labor	$	40,000
Monomer	$	30,000
Initiator	$	10,000
Other	$	47,000
Total Annual Cost	**$**	**285,000**

7.3 Payback Period

The payback period is calculated using the capital outlay, operating expenses, and expected profits. To better model the economics, the after-tax cash flow (ATCF) model shows how taxes are paid and how capital equipment depreciates over time. Specifically, the General Depreciation System (GDS), set up by the Internal Revenue Service (IRS) applies well for chemical manufacturing plants. Operating profits are taxed using the federal income tax rates. The ATCF model takes these two into account and allows for the calculation of a payback period. The payback period is the amount of time it takes for an investment to recoup all of the money invested, i.e. to break even. Of course, the goal of any investment is to produce

profits so ideally the payback period will be short enough that the plant will operate for many years at a profit.

For our design, the IRS permits a GDS depreciation over 5 years for the category “Manufacture of Chemicals and Allied Products” [36]. In the tax analysis, a minimum annual rate of return (MARR) of 15% is used to compare the profitability of this venture to other possible projects. The MARR assumes that there are projects that can make a 15% return annually so this design needs to exceed that value to be economically feasible. Also since this design is assumed to be implemented by a relatively large chemical company, a federal income tax level of 35% will be used, which is the level for companies making more than $18,333,333 annually [36].

The bulk market price of medical grade polycaprolactone is not well defined because currently companies are only producing it on a kg scale. Vornia Bio-Inks sells the product for $3,800 per kg in lots of 1 kg each [37]. Since we are designing a bulk process, our polymer should sell for significantly less. Our calculations show that selling the polymer for $410 per kg is sufficient for a payback period of exactly one year [Table A.3.5]. This price is obviously significantly lower than the Vornia price (approximately an order of magnitude), which shows two things. First, the economy of scale is important in chemical processes. Second, pharmaceutical materials tend to have very high profit margins because the cost of the material is not a significant percentage of the total cost of the procedure.

If the polymer is sold at $410 per kg, and the expected lifetime of the process equipment is 20 years, the present worth of the process is just over $11 million and the internal rate of return (IRR) is 78%. Overall this analysis shows that if the market for bulk medical grade polycaprolactone is present, manufacturing it is an excellent investment. Even if costs are higher than expected, the IRR is very high so even with an increase in costs the process would remain economically feasible.

8. PCL-Glass Combination

Over a dozen documented methods of combining polymers with a bioactive glass exist [6]. The two methods that specifically use PCL are electrospinning [7] and salt-leaching [6]. The criteria for choosing a combination method would include the porosity of the composite, the maintenance of both PCL and glass properties, ease of purification, and scalability of the process from bench to industrial scale. The team performed preliminary research into combination methods but determined the design of a combination process to be outside of the scope of this project, since the PCL-glass combination step would likely be performed by a manufacturer specializing in composites.

9. Conclusion

This report details the initial research and design decisions for the detailed design of a chemical plant that can produce medical-grade polycaprolactone (PCL) on a large scale. These include the constraints on the project as well as decisions about reactor features, catalyst system, and separation methods. Key designs features of reactors, falling-strand devolatilizers, and extruders were presented, such as operation temperature and pressure and equipment materials of construction. Engineering considerations, market factors, and design norms all influenced the results of this report. The primary use of the polycaprolactone will be in PCL-bioactive-glass composite, which can be used in medical procedures such as bone or cartilage repair. The medical grade polycaprolactone will be sold for $410 per kg, an economically profitable rate. Combination methods for the PCL-bioactive-glass composite were researched to gain a better understanding of the requirements for the polycaprolactone. This composite production is intended to be executed by an outside party.

10. Acknowledgments

We would like to thank Professor Jeremy VanAntwerp for his knowledgeable support of the project and the team.

We would also like to thank Dr. Phil Brondsema for his enthusiasm for this project, his willingness to be a long-distance advisor, his countless ideas, his donation of $500 worth of reference books and textbooks, and his many helpful contacts at Celanese.

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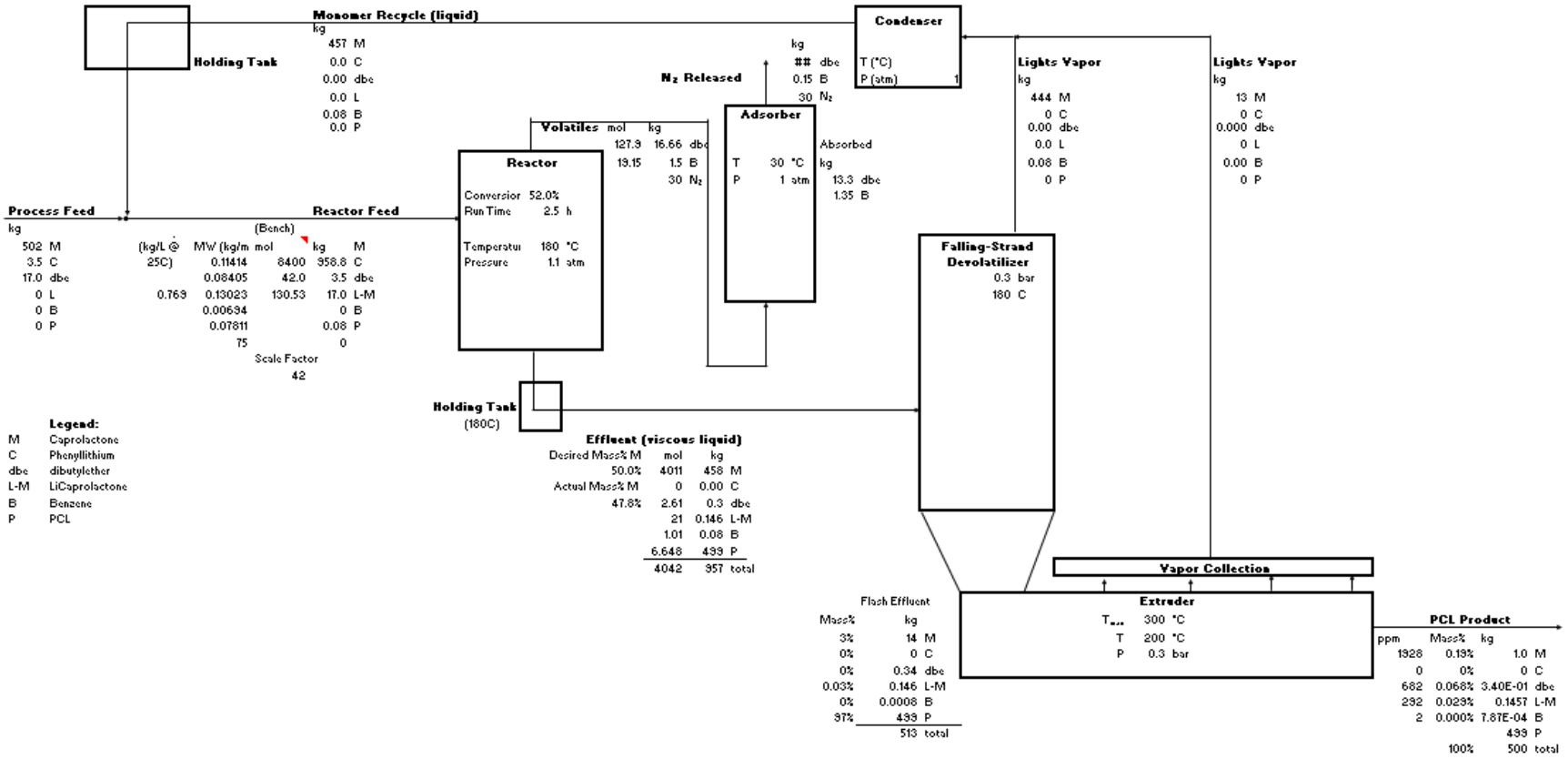
12. Appendix

A.1 PCL Process Material Balance



Material balance for PCL production process

A.2 Energy Balances

Table A.2.1. Volume calculations for each tank

VOLUME		
Density of Caprolactone	0.946	g/mL
Initial Mass Caprolcatone	958.8	kg
Total Volume Caprolactone	1013.5	L
Volume Reactor	1520.3	L
Volume Reactor	1.52	m3
Height Reactor	2.00	m
Diameter Reactor	1.00	m
Surface Area Reactor	6.28	m2
Volume Holding Tank	6.25	m3
Height Holding Tank	4.00	m
Diameter Holding Tank	2.50	m
Surface Area Holding Tank	31.4	m2

Table A.2.2. Sizing calculations for condenser

CONDENSER		
Flowrate Caprolactone	4003.9	mol
Temperature in	190.0	oC
Temperature out	170.0	oC
Average Temperature	453.15	K
Flowrate Caprolactone	76.17	kg/hr
Surface Area Inside	5.0	m2

Table A.2.3. Extruder operating conditions

EXTRUDER		
Temperature	200.0	oC
Pressure	0.30	bar

Table A.2.4. Energy consumption calculations for extruder

Extruder Motor			
Power	125	kW	
Percent Torque	0.75		
RPM fraction	0.67	running at 400 RPM with a max of 600 RPM	
Gearbox efficency	0.95		
kW applied	59.4	kW	
Total power	108.0	kW	

Table A.2.5. Energy consumption calculations for condenser

	air/min	HP required	Electricity Consumption (kW)	Capacity
Cooling Table	42.4	10	9.942666667	42.4 CFM @ 100-175 psi

Table A.2.6. Component data used for reactor and holding tank energy balances

Benzene is phase change		
HEAT of VAPORIZATION	Equation	
dibutylether (dbe)	61040.9	J/mol
Benzene (B) (or phenyllithium)	44335.7	J/mol
Caprolactone (M)	27430	J/mol
HEAT CAPACITIES (gas)		
dibutylether (dbe)	257.5	J/gmol K
Benzene (B) (or phenyllithium)	82.4	J/gmol K
N2	29.12	J/gmol K
Caprolactone (M)	191.3	J/gmol K
HEAT of REACTION		
Overall at 450 oC	10.8	kJ/mol
Temp Reactor in K	453.15	K
Temp Feed in K	298.15	K

Table A.2.7. Reactor, holding tank, and condenser energy balances.

Reactor During Reaction										
Power During Reaction (kW)	Outside Temperature (oC)	Initial Steam Temperature (oC)	Final Steam Temperature (oC)	Average Steam Temperature (oC)	Thermal Conductivity stainless (W/m K)	Thermal Conductivity insulation (W/m K)	Convective heat transfer coefficient inside (W /m k)	Convective heat transfer coefficient outside (W /m k)	Surface area of Reactor (m2)	Thickness of Jacket (m)
5.80	25	260	245	252.5	20	0.064	5678.3	11.36	6.28	0.005
Thickness of Insulation	Flowrate steam (mol/hr)	Flowrate steam (kg/s)	Heat Capacity Steam (J/mol K)	Sum of Resistances	T steam - T Environment	Q dot left side (kJ/hr)	Q dot reactor right side (kJ/hr)	Q dot calcd right side (kJ/hr)	Sum of Q dot right side	
0.02	52326.3	0.262	42.7	0.065	227.5	33515	20894.9	12620.1	33515.0	
Reactor Heating Up Before Reaction										
Power During Reaction (kW)	Outside Temperature (oC)	Initial Steam Temperature (oC)	Final Steam Temperature (oC)	Average Steam Temperature (oC)	Thermal Conductivity stainless (W/m K)	Thermal Conductivity	Convective heat transfer coefficient inside (W /m	Convective heat transfer coefficient outside (W /m	Surface area of Reactor (m2)	Thickness of Jacket (m)
80.58	25	260	245	252.5	20	0.064	5678.3	11.36	6.28	0.005
Thickness of Insulation	Flowrate steam (mol/hr)	Flowrate steam (kg/s)	Heat Capacity Steam (J/mol K)	Sum of Resistances	T steam - T Environment	Q dot left side (kJ/hr)	Q dot reactor right side (kJ/hr)	Q dot calcd right side (kJ/hr)	Sum of Q dot right side	
0.02	472626.1	2.37	42.7	0.065	227.5	302717	290097.3	12620.1	302717.4	
Holding Tank After Reactor										
Power During Reaction (kW)	Outside Temperature (oC)	Initial Steam Temperature (oC)	Final Steam Temperature (oC)	Average Steam Temperature (oC)	Thermal Conductivity stainless (W/m K)	Thermal Conductivity	Convective heat transfer coefficient inside (W /m	Convective heat transfer coefficient outside (W /m	Surface area of Reactor (m2)	Thickness of Jacket (m)
0	25	260	245	252.5	20	0.064	5678.3	11.36	31.4	0.005
Thickness of Insulation	Flowrate steam (mol/hr)	Flowrate steam (kg/s)	Heat Capacity Steam (J/mol K)	Sum of Resistances	T steam - T Environment	Q dot left side (kJ/hr)	Q dot reactor right side (kJ/hr)	Q dot calcd right side (kJ/hr)	Sum of Q dot right side	
0.02	69909.4	0.35	42.7	0.018	227.5	44777	0	44777.0	44777.0	
Condenser										
Power During Reaction (kW)	Outside Temperature (oC)	Initial Steam Temperature (oC)	Final Steam Temperature (oC)	Average Steam Temperature (oC)	Thermal Conductivity stainless (W/m K)	Thermal Conductivity	Convective heat transfer coefficient inside (W /m	Convective heat transfer coefficient outside (W /m	Surface area of Reactor (m2)	Thickness of Jacket (m)
0	25	25	50	37.5	20	0.064	5678.3	11.36	5.0	0.005
Thickness of Insulation	Flowrate steam (mol/hr)	Flowrate steam (kg/s)	Heat Capacity Steam (J/mol K)	Sum of Resistances	T steam - T Environment	Q dot left side (kJ/hr)	Q dot reactor right side (kJ/hr)	Q dot calcd right side (kJ/hr)	Sum of Q dot right side	
0.02	10798.9	0.054	75.2	0.081	12.5	-20302	-20856.9	555.3	-20301.6	

Table A.2.8. Final energy balance values for reactor and condenser

Power During Heating Up		
Time	3600	sec
Power	80.6	kW
Power During Reaction		
Time	9000	sec
Power	5.80	kW
Power of Condensing Monomer		
Time per batch	21600	sec
Power	-5.79	kW

Table A.2.9. Energy balance on the 3 types of pumps

PUMPS					
Pump Description	HP	Efficiency	Electricity Consumption (kW)	Capacity	
High viscosity positive	3	0.6	3.73	50 gal/min	
Vacuum rotary vane pump	30	0.5	37.29	.03 bar min pressure, 18 ft3 per min	
Liquid centrifugal pump	8	0.85	9.94	200 gal/min, 39 max psi	

Table A.2.10. Final annual cost calculations based on electricity, utilities, labor, and starting materials

Utility	Units	Number of Units	Cost per Unit	Total Annual Cost
High Pressure Steam	GJ	8644	$ 17.70	$ 153,001.14
Electricity	kWh	67937	$ 0.06	$ 4,076.24
Process Water	GJ	0	$ 0.35	$ 0.00
Labor (3 operators)	hr of labor	1000	$ 40.00	$ 40,000.00
Raw Monomer	lb	22088	$ 1.35	$ 29,892.84
Initiator	L	491	$ 19.96	$ 9,802.52
Nitrogen	cubic feet	100000	$ 0.0021	$ 210.00
			Final Summed Annual	$ 279,504.79

A.3 Tax and Profitability Analysis

Table A.3.1 General Tax Information

Lifetime (years)	20
GDS recovery period	5
Income Tax Rate	35%
After tax MARR	15%

Table A.3.2 General Profitability Information

Annual Expenses	284000
Necessary Annual Income	3280000
kg Polycaprolactone/year	8000
Cost per kg	$410

Table A.3.3 After Tax Cash Flow Spreadsheet for 20 Year Lifetime

Year	BTCF	5-year	Deduction	BV sub k	Taxable Income	Cash Flow Income Tax	ATCF
0	$ (3,010,000)	Rate	$ -	$ 3,010,000	$ -	$ -	$ (3,010,000)
1	$ 3,280,000	0.2	$ 602,000	$ 2,408,000	$ 2,678,000	$ (937,300)	$ 2,342,700
2	$ 3,280,000	0.32	$ 963,200	$ 1,444,800	$ 2,316,800	$ (810,880)	$ 2,469,120
3	$ 3,280,000	0.192	$ 577,920	$ 866,880	$ 2,702,080	$ (945,728)	$ 2,334,272
4	$ 3,280,000	0.1152	$ 346,752	$ 520,128	$ 2,933,248	$ (1,026,637)	$ 2,253,363
5	$ 3,280,000	0.1152	$ 346,752	$ 173,376	$ 2,933,248	$ (1,026,637)	$ 2,253,363
6	$ 3,280,000	0.0576	$ 173,376	$ -	$ 3,106,624	$ (1,087,318)	$ 2,192,682
7	$ 3,280,000	0	$ -	$ -	$ 3,280,000	$ (1,148,000)	$ 2,132,000
8	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
9	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
10	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
11	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
12	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
13	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
14	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
15	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
16	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
17	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
18	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
19	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000
20	$ 3,280,000				$ 3,280,000	$ (1,148,000)	$ 2,132,000

Table A.3.4 Economic Benchmarks of the Design

PW	$11,062,000
AW	$1,767,000
IRR	78%

Table A.3.5 One Year Payback Period Determination of Price

Capital Investment	$ (3,010,000)
1 Year Operating	$(284,000.00)
1 Year Revenue	$ 3,294,000
kg Polycaprolactone/year	8000
Cost per kg	$ 410.00

A.4 Safety Data Sheets (SDSs) for Process Chemicals

Benzene

Material Safety Data Sheet
Benzene MSDS

Section 1: Chemical Product and Company Identification

Product Name: Benzene

Catalog Codes: SLB1564, SLB3055, SLB2881

CAS#: 71-43-2

RTECS: CY1400000

TSCA: TSCA 8(b) inventory: Benzene

CI#: Not available.

Synonym: Benzol; Benzine

Chemical Name: Benzene

Chemical Formula: C6-H6

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Benzene	71-43-2	100

Toxicological Data on Ingredients: Benzene: ORAL (LD50): Acute: 930 mg/kg [Rat]. 4700 mg/kg [Mouse]. DERMAL (LD50): Acute: >9400 mg/kg [Rabbit]. VAPOR (LC50): Acute: 10000 ppm 7 hours [Rat].

Section 3: Hazards Identification

Potential Acute Health Effects:
Very hazardous in case of eye contact (irritant), of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion. Inflammation of the eye is characterized by redness, watering, and itching.

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. The substance is toxic to blood, bone marrow, central nervous system (CNS). The substance may be toxic to liver, Urinary System. Repeated or prolonged exposure to the substance can produce target organs damage.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention immediately.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention if symptoms appear.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 497.78°C (928°F)

Flash Points: CLOSED CUP: -11.1°C (12°F). (Setaflash)

Flammable Limits: LOWER: 1.2% UPPER: 7.8%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances:
Highly flammable in presence of open flames and sparks, of heat. Slightly flammable to flammable in presence of oxidizing materials. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available. Explosive in presence of oxidizing materials, of acids.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog.

Special Remarks on Fire Hazards:
Extremely flammable liquid and vapor. Vapor may cause flash fire. Reacts on contact with iodine heptafluoride gas. Dioxygenyl tetrafluoroborate is as very powferful oxidant. The addition of a small particle to small samples of benzene, at ambient temperature, causes ignition. Contact with sodium peroxide with benzene causes ignition. Benzene ignites in contact with powdered chromic anhydride. Virgorous or incandescent reaction with hydrogen + Raney nickel (above 210 C) and bromine trifluoride.

Special Remarks on Explosion Hazards:
Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction

of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed. Be careful that the product is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

Precautions:
Keep locked up.. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as oxidizing agents, acids.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits:
TWA: 0.5 STEL: 2.5 (ppm) from ACGIH (TLV) [United States] TWA: 1.6 STEL: 8 (mg/m3) from ACGIH (TLV) [United States] TWA: 0.1 STEL: 1 from NIOSH TWA: 1 STEL: 5 (ppm) from OSHA (PEL) [United States] TWA: 10 (ppm) from OSHA (PEL) [United States] TWA: 3 (ppm) [United Kingdom (UK)] TWA: 1.6 (mg/m3) [United Kingdom (UK)] TWA: 1 (ppm) [Canada] TWA: 3.2 (mg/m3) [Canada] TWA: 0.5 (ppm) [Canada]Consult local authorities for acceptable exposure limits.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor:
Aromatic. Gasoline-like, rather pleasant. (Strong.)

Taste: Not available.

Molecular Weight: 78.11 g/mole

Color: Clear Colorless. Colorless to light yellow.

pH (1% soln/water): Not available.

Boiling Point: 80.1 (176.2°F)

Melting Point: 5.5°C (41.9°F)

Critical Temperature: 288.9°C (552°F)

Specific Gravity: 0.8787 @ 15 C (Water = 1)

Vapor Pressure: 10 kPa (@ 20°C)

Vapor Density: 2.8 (Air = 1)

Volatility: Not available.

Odor Threshold: 4.68 ppm

Water/Oil Dist. Coeff.: The product is more soluble in oil; log(oil/water) = 2.1

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility:
Miscible in alcohol, chloroform, carbon disulfide oils, carbon tetrachloride, glacial acetic acid, diethyl ether, acetone. Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Heat, ignition sources, incompatibles.

Incompatibility with various substances: Highly reactive with oxidizing agents, acids.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity:
Benzene vapors + chlorine and light causes explosion. Reacts explosively with bromine pentafluoride, chlorine, chlorine trifluoride, diborane, nitric acid, nitryl perchlorate, liquid oxygen, ozone, silver perchlorate. Benzene + pentafluoride and methoxide (from arsenic pentafluoride and potassium methoxide) in trichlorotrifluoroethane causes explosion. Interaction of nitryl perchlorate with benzene gave a slight explosion and flash. The solution of permanganic acid (or its explosive anhydride, dimaganese heptoxide) produced by interaction of permanganates and sulfuric acid will explode on contact with benzene. Peroxodisulfuric acid is a very powferful oxidant. Uncontrolled contact with benzene may cause explosion. Mixtures of peroxomonsulfuric acid with benzene explodes.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Absorbed through skin. Dermal contact. Eye contact. Inhalation.

Toxicity to Animals:
WARNING: THE LC50 VALUES HEREUNDER ARE ESTIMATED ON THE BASIS OF A 4-HOUR EXPOSURE. Acute oral toxicity (LD50): 930 mg/kg [Rat]. Acute dermal toxicity (LD50): >9400 mg/kg [Rabbit]. Acute toxicity of the vapor (LC50): 10000 7 hours [Rat].

Chronic Effects on Humans:

CARCINOGENIC EFFECTS: Classified A1 (Confirmed for human.) by ACGIH, 1 (Proven for human.) by IARC. MUTAGENIC EFFECTS: Classified POSSIBLE for human. Mutagenic for mammalian somatic cells. Mutagenic for bacteria and/or yeast. DEVELOPMENTAL TOXICITY: Classified Reproductive system/toxin/female [POSSIBLE]. Causes damage to the following organs: blood, bone marrow, central nervous system (CNS). May cause damage to the following organs: liver, Urinary System.

Other Toxic Effects on Humans:
Very hazardous in case of inhalation. Hazardous in case of skin contact (irritant, permeator), of ingestion.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans:
May cause adverse reproductive effects (female fertility, Embryotoxic and/or foetotoxic in animal) and birth defects. May affect genetic material (mutagenic). May cause cancer (tumorigenic, leukemia)) Human: passes the placental barrier, detected in maternal milk.

Special Remarks on other Toxic Effects on Humans:
Acute Potential Health Effects: Skin: Causes skin irritation. It can be absorbed through intact skin and affect the liver, blood, metabolism,and urinary system. Eyes: Causes eye irritation. Inhalation: Causes respiratory tract and mucous membrane irritation. Can be absorbed through the lungs. May affect behavior/Central and Peripheral nervous systems (somnolence, muscle weakness, general anesthetic, and other symptoms similar to ingestion), gastrointestinal tract (nausea), blood metabolism, urinary system. Ingestion: May be harmful if swallowed. May cause gastrointestinal tract irritation including vomiting. May affect behavior/Central and Peripheral nervous systems (convulsions, seizures, tremor, irritability, initial CNS stimulation followed by depression, loss of coordination, dizziness, headache, weakness, pallor, flushing), respiration (breathlessness and chest constriction), cardiovascular system, (shallow/rapid pulse), and blood.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are less toxic than the product itself.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:
Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Benzene UNNA: 1114 PG: II

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
California prop. 65: This product contains the following ingredients for which the State of California has found to cause cancer, birth defects or other reproductive harm, which would require a warning under the statute: Benzene California prop. 65 (no significant risk level): Benzene: 0.007 mg/day (value) California prop. 65: This product contains the following ingredients

for which the State of California has found to cause cancer which would require a warning under the statute: Benzene Connecticut carcinogen reporting list.: Benzene Connecticut hazardous material survey.: Benzene Illinois toxic substances disclosure to employee act: Benzene Illinois chemical safety act: Benzene New York release reporting list: Benzene Rhode Island RTK hazardous substances: Benzene Pennsylvania RTK: Benzene Minnesota: Benzene Michigan critical material: Benzene Massachusetts RTK: Benzene Massachusetts spill list: Benzene New Jersey: Benzene New Jersey spill list: Benzene Louisiana spill reporting: Benzene California Director's list of Hazardous Substances: Benzene TSCA 8(b) inventory: Benzene SARA 313 toxic chemical notification and release reporting: Benzene CERCLA: Hazardous substances.: Benzene: 10 lbs. (4.536 kg)

Other Regulations:
OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200). EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada):
CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F). CLASS D-2A: Material causing other toxic effects (VERY TOXIC).

DSCL (EEC):
R11- Highly flammable. R22- Harmful if swallowed. R38- Irritating to skin. R41- Risk of serious damage to eyes. R45- May cause cancer. R62- Possible risk of impaired fertility. S2- Keep out of the reach of children. S26- In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. S39- Wear eye/face protection. S46- If swallowed, seek medical advice immediately and show this container or label. S53- Avoid exposure - obtain special instructions before use.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 0

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/10/2005 08:35 PM

Last Updated: 05/21/2013 12:00 PM

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Caprolactone

SIGMA-ALDRICH sigma-aldrich.com

SAFETY DATA SHEET

Version 3.5
Revision Date 06/22/2015
Print Date 04/18/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : ε-Caprolactone

Product Number : 167363
Brand : Aldrich

CAS-No. : 502-44-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Eye irritation (Category 2A), H319

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal word Warning

Hazard statement(s)
H319 Causes serious eye irritation.

Precautionary statement(s)
P264 Wash skin thoroughly after handling.
P280 Wear eye protection/ face protection.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313 If eye irritation persists: Get medical advice/ attention.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula : $C_6H_{10}O_2$

Molecular weight	:	114.14 g/mol
CAS-No.	:	502-44-3
EC-No.	:	207-938-1

Hazardous components

Component	Classification	Concentration
Hexan-6-olide		
	Eye Irrit. 2A; H319	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Consult a physician.

In case of eye contact
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.
Storage class (TRGS 510): Combustible liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection
Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: Nature latex/chloroprene
Minimum layer thickness: 0.6 mm
Break through time: 60 min
Material tested:Lapren® (KCL 706 / Aldrich Z677558, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: clear, liquid Colour: colourless
b)	Odour	bitter almond
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	Melting point/range: -2.14 °C (28.15 °F) at 1,013 hPa (760 mmHg) Freezing point/ range: -25.14 °C (-13.25 °F) at 1,013 hPa (760 mmHg)
f)	Initial boiling point and boiling range	98 - 99 °C (208 - 210 °F) at 3 hPa (2 mmHg)
g)	Flash point	109 °C (228 °F) - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapour pressure	0.01 hPa (0.01 mmHg) at 20 °C (68 °F)
l)	Vapour density	3.94 - (Air = 1.0)
m)	Relative density	1.076 g/cm3
n)	Water solubility	1 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - completely soluble
o)	Partition coefficient: n-octanol/water	log Pow: 0.32 at 20 °C (68 °F)
p)	Auto-ignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	No data available

9.2 Other safety information

Relative vapour density	3.94 - (Air = 1.0)

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Strong oxidizing agents, Strong bases

10.6 Hazardous decomposition products

Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 4,290 mg/kg

Inhalation: No data available

LD50 Dermal - Rabbit - male - 6,400 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Irritating to eyes.
(OECD Test Guideline 405)

Respiratory or skin sensitisation
in vivo assay - Mouse
Result: negative
(OECD Test Guideline 429)
Remarks: No data available

Germ cell mutagenicity
Chromosome aberration test in vitro
Chinese hamster fibroblasts
Result: negative

Carcinogenicity

IARC:	No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
ACGIH:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
NTP:	No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA:	No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
No data available

No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: MO8400000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	LC50 - Poecilia reticulata (guppy) - 280 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 204 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	ErC50 - Desmodesmus subspicatus (green algae) - 2,616 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Hexan-6-olide	502-44-3	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Hexan-6-olide	502-44-3	

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Eye Irrit.	Eye irritation
H319	Causes serious eye irritation.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 3.5 Revision Date: 06/22/2015 Print Date: 04/18/2017

Dibutyl Ether

Material Safety Data Sheet
Butyl ether MSDS

Section 1: Chemical Product and Company Identification

Product Name: Butyl ether

Catalog Codes: SLB1741, SLB3232

CAS#: 142-96-1

RTECS: EK5425000

TSCA: TSCA 8(b) inventory: Butyl ether

CI#: Not available.

Synonym:

Chemical Formula: C8H18O

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Butyl ether	142-96-1	100

Toxicological Data on Ingredients: Butyl ether: ORAL (LD50): Acute: 7400 mg/kg [Rat]. DERMAL (LD50): Acute: 10000 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:
Hazardous in case of skin contact (irritant), of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator).

Potential Chronic Health Effects:
CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. Repeated or prolonged exposure is not known to aggravate medical condition.

Section 4: First Aid Measures

Eye Contact:
Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. WARM water MUST be used. Get medical attention.

Skin Contact:
In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.

Inhalation:
If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek medical attention.

Ingestion:
Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Loosen tight clothing such as a collar, tie, belt or waistband. Get medical attention if symptoms appear.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 194°C (381.2°F)

Flash Points: CLOSED CUP: 37°C (98.6°F).

Flammable Limits: LOWER: 1.5%

Products of Combustion: These products are carbon oxides (CO, CO2).

Fire Hazards in Presence of Various Substances: Flammable in presence of open flames and sparks.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable liquid, soluble or dispersed in water. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use alcohol foam, water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Absorb with an inert material and put the spilled material in an appropriate waste disposal.

Large Spill:
Flammable liquid. Keep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, sand or other non-combustible material. Do not touch spilled material. Prevent entry into sewers, basements or confined areas; dike if needed.

Section 7: Handling and Storage

Precautions:

Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes.

Storage:
Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protection:
Splash goggles. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Liquid.

Odor: Not available.

Taste: Not available.

Molecular Weight: 130.23 g/mole

Color: Not available.

pH (1% soln/water): Not available.

Boiling Point: 141°C (285.8°F)

Melting Point: -95.2°C (-139.4°F)

Critical Temperature: Not available.

Specific Gravity: 0.769 (Water = 1)

Vapor Pressure: 0.6 kPa (@ 20°C)

Vapor Density: 4.48 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility: Very slightly soluble in cold water.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances: Not available.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Not available.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
Acute oral toxicity (LD50): 7400 mg/kg [Rat]. Acute dermal toxicity (LD50): 10000 mg/kg [Rabbit].

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans:
Hazardous in case of skin contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

DOT Classification: CLASS 3: Flammable liquid.

Identification: : Dibutyl ether UNNA: UN1149 PG: III

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: Butyl ether Florida: Butyl ether Massachusetts RTK: Butyl ether New Jersey: Butyl ether TSCA 8(b) inventory: Butyl ether

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada): CLASS B-2: Flammable liquid with a flash point lower than 37.8°C (100°F).

DSCL (EEC):
R10- Flammable. R36/38- Irritating to eyes and skin.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 3

Reactivity: 0

Personal Protection: h

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 3

Reactivity: 1

Specific hazard:

Protective Equipment:
Gloves. Lab coat. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

Created: 10/09/2005 04:28 PM

Last Updated: 05/21/2013 12:00 PM

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Lithium

Material Safety Data Sheet
Lithium MSDS

Section 1: Chemical Product and Company Identification

Product Name: Lithium

Catalog Codes: SLL1456

CAS#: 7439-93-2

RTECS: OJ5540000

TSCA: TSCA 8(b) inventory: Lithium

CI#: Not available.

Synonym:

Chemical Name: Not available.

Chemical Formula: Li

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call: 1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Lithium	7439-93-2	100

Toxicological Data on Ingredients: Lithium LD50: Not available. LC50: Not available.

Section 3: Hazards Identification

Potential Acute Health Effects:
Extremely hazardous in case of skin contact (corrosive, irritant, sensitizer), of eye contact (irritant), of ingestion, of inhalation. The amount of tissue damage depends on length of contact. Eye contact can result in corneal damage or blindness. Skin contact can produce inflammation and blistering. Inhalation of dust will produce irritation to gastro-intestinal or respiratory tract, characterized by burning, sneezing and coughing. Severe over-exposure can produce lung damage, choking, unconsciousness or death. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

Potential Chronic Health Effects:
Extremely hazardous in case of skin contact (corrosive, irritant, sensitizer), of eye contact (irritant), of ingestion, of inhalation. CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available. The substance is toxic to lungs, the nervous system, mucous membranes. Repeated or prolonged exposure to the substance can produce target organs damage. Repeated exposure of the eyes to a low level of dust can produce eye irritation. Repeated skin exposure can produce local skin destruction, or dermatitis. Repeated inhalation of dust can produce varying degree of respiratory irritation or lung damage. Repeated or prolonged inhalation of dust may lead to chronic respiratory irritation.

Section 4: First Aid Measures

Eye Contact: Check for and remove any contact lenses. Do not use an eye ointment. Seek medical attention.

Skin Contact:
If the chemical got onto the clothed portion of the body, remove the contaminated clothes as quickly as possible, protecting your own hands and body. Place the victim under a deluge shower. If the chemical got on the victim's exposed skin, such as the hands : Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

Serious Skin Contact:
Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.

Inhalation: Allow the victim to rest in a well ventilated area. Seek immediate medical attention.

Serious Inhalation:
Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

Ingestion:
Do not induce vomiting. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: Flammable.

Auto-Ignition Temperature: 179°C (354.2°F)

Flash Points: Not available.

Flammable Limits: Not available.

Products of Combustion: Some metallic oxides.

Fire Hazards in Presence of Various Substances: Not available.

Explosion Hazards in Presence of Various Substances:
Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:
Flammable solid. SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray or fog. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion.

Special Remarks on Fire Hazards: Not available.

Special Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

Small Spill: Use appropriate tools to put the spilled solid in a convenient waste disposal container.

Large Spill:
Corrosive solid. Flammable solid that, in contact with water, emits flammable gases. Stop leak if without risk. Do not get water inside container. Do not touch spilled material. Cover with dry earth, sand or other non-combustible material. Use water spray to reduce vapors. Prevent entry into sewers, basements or confined areas; dike if needed. Eliminate all ignition sources. Call for assistance on disposal.

Section 7: Handling and Storage

Precautions:
Keep container dry. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing material. Do not breathe dust. Never add water to this product In case of insufficient ventilation, wear suitable respiratory equipment If you feel unwell, seek medical attention and show the label when possible. Avoid contact with skin and eyes Keep away from incompatibles such as oxidizing agents, acids, moisture.

Storage:
Flammable materials should be stored in a separate safety storage cabinet or room. Keep away from heat. Keep away from sources of ignition. Keep container tightly closed. Keep in a cool, well-ventilated place. Ground all equipment containing material. Keep container dry. Keep in a cool place.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:
Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:
Splash goggles. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:
Splash goggles. Full suit. Vapor and dust respirator. Boots. Gloves. A self contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid. (Metal solid.)

Odor: Not available.

Taste: Not available.

Molecular Weight: 6.94 g/mole

Color: Silver-white

pH (1% soln/water): Not available.

Boiling Point: 1336.5°C (2437.7°F)

Melting Point: 180.5°C (356.9°F)

Critical Temperature: Not available.

Specific Gravity: 0.534 (Water = 1)

Vapor Pressure: Not applicable.

Vapor Density: Not available.

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: Not available.

Ionicity (in Water): Not available.

Dispersion Properties: Not available.

Solubility: Not available.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Not available.

Incompatibility with various substances:
Extremely reactive or incompatible with oxidizing agents, acids, moisture. The product reacts violently with water to emit flammable but non toxic gases.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Evolves hydrogen on contact with water.

Special Remarks on Corrosivity: Not available.

Polymerization: No.

Section 11: Toxicological Information

Routes of Entry: Eye contact. Inhalation. Ingestion.

Toxicity to Animals:
LD50: Not available. LC50: Not available.

Chronic Effects on Humans: The substance is toxic to lungs, the nervous system, mucous membranes.

Other Toxic Effects on Humans: Extremely hazardous in case of skin contact (corrosive, irritant, sensitizer), of ingestion, of inhalation.

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: Not available.

Special Remarks on other Toxic Effects on Humans: Not available.

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation:
Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

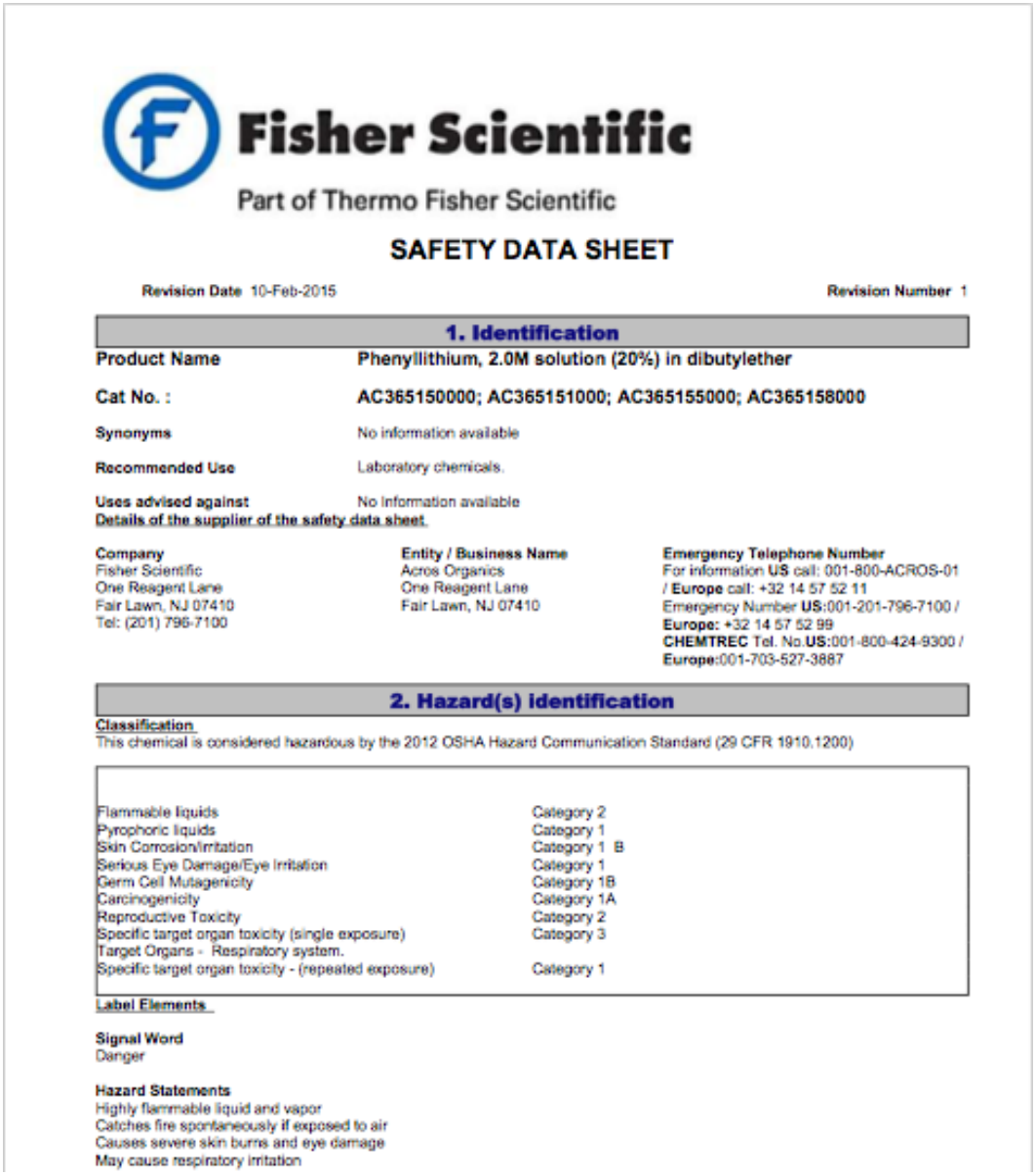
Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Section 14: Transport Information

Phenyllithium



Fisher Scientific

Part of Thermo Fisher Scientific

SAFETY DATA SHEET

Revision Date 10-Feb-2015 **Revision Number** 1

1. Identification

Product Name Phenyllithium, 2.0M solution (20%) in dibutylether

Cat No. : AC365150000; AC365151000; AC365155000; AC365158000

Synonyms No information available

Recommended Use Laboratory chemicals.

Uses advised against No information available

Details of the supplier of the safety data sheet

Company
Fisher Scientific
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Entity / Business Name
Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number
For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99
CHEMTREC Tel. No.**US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification
This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Pyrophoric liquids	Category 1
Skin Corrosion/Irritation	Category 1 B
Serious Eye Damage/Eye Irritation	Category 1
Germ Cell Mutagenicity	Category 1B
Carcinogenicity	Category 1A
Reproductive Toxicity	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	
Specific target organ toxicity - (repeated exposure)	Category 1

Label Elements

Signal Word
Danger

Hazard Statements
Highly flammable liquid and vapor
Catches fire spontaneously if exposed to air
Causes severe skin burns and eye damage
May cause respiratory irritation

May cause genetic defects
May cause cancer
Suspected of damaging fertility
Causes damage to organs through prolonged or repeated exposure

Precautionary Statements
Prevention
Obtain special instructions before use
Do not handle until all safety precautions have been read and understood
Use personal protective equipment as required
Do not breathe dust/fume/gas/mist/vapors/spray
Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Use only outdoors or in a well-ventilated area
Keep away from heat/sparks/open flames/hot surfaces. - No smoking
Keep container tightly closed
Ground/bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting/equipment
Use only non-sparking tools
Take precautionary measures against static discharge
Do not allow contact with air
Keep cool
Response
Immediately call a POISON CENTER or doctor/physician
Inhalation
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Skin
Wash contaminated clothing before reuse
IF ON SKIN: Immerse in cool water/wrap with wet bandages
Eyes
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
Ingestion
IF SWALLOWED: Rinse mouth. DO NOT induce vomiting
Fire
In case of fire: Use CO2, dry chemical, or foam for extinction
Storage
Store locked up
Store in a well-ventilated place. Keep container tightly closed
Store contents under inert gas
Disposal
Dispose of contents/container to an approved waste disposal plant
Hazards not otherwise classified (HNOC)
Toxic to aquatic life with long lasting effects
Reacts violently with water
Unknown Acute Toxicity
.? % of the mixture consists of ingredients of unknown toxicity.

3. Composition / information on ingredients

Component	CAS-No	Weight %
Butyl ether	142-96-1	65-80

Lithium, phenyl-	591-51-5	10-25
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	na	2.5-5
Biphenyl	92-52-4	1-2.5
Benzene	71-43-2	0.1-1

4. First-aid measures

Eye Contact Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Immediate medical attention is required.

Inhalation Remove from exposure, lie down. Move to fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration. Immediate medical attention is required.

Ingestion Do not induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. Call a physician immediately. If possible drink milk afterwards.

Most important symptoms/effects Breathing difficulties. Causes burns by all exposure routes. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Dry chemical.

Unsuitable Extinguishing Media No information available

Flash Point 20 °C / 68 °F
Method - No information available

Autoignition Temperature 185 °C / 365 °F
Explosion Limits
Upper No data available
Lower No data available
Sensitivity to Mechanical Impact No information available
Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical
Flammable. Contact with water liberates toxic gas. Water reactive. Produce flammable gases on contact with water.

Hazardous Combustion Products
Carbon monoxide (CO) Carbon dioxide (CO_2)
Protective Equipment and Precautions for Firefighters
As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
3	4	0	W

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment.

Environmental Precautions See Section 12 for additional ecological information. Avoid release to the environment. Collect spillage.

Methods for Containment and Clean Up Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not let this chemical enter the environment.

7. Handling and storage

Handling Do not breathe dust. Do not breathe vapors or spray mist. Do not get in eyes, on skin, or on clothing. Take precautionary measures against static discharges. Use only in area provided with appropriate exhaust ventilation. Handle under inert gas, protect from moisture. Use explosion-proof equipment. Use only non-sparking tools. Use only under a chemical fume hood.

Storage Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat and sources of ignition. Store in freezer. Protect from moisture. Never allow product to get in contact with water during storage. Store under an inert atmosphere.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH
Biphenyl	TWA: 0.2 ppm	(Vacated) TWA: 0.2 ppm (Vacated) TWA: 1 mg/m³ TWA: 0.2 ppm TWA: 1 mg/m³	IDLH: 100 mg/m³ TWA: 0.2 ppm TWA: 1 mg/m³
Benzene	TWA: 0.5 ppm STEL: 2.5 ppm Skin	(Vacated) TWA: 10 ppm Ceiling: 25 ppm (Vacated) STEL: 50 ppm (Vacated) Ceiling: 25 ppm TWA: 10 ppm TWA: 1 ppm STEL: 5 ppm	IDLH: 500 ppm TWA: 0.1 ppm STEL: 1 ppm

Component	Quebec	Mexico OEL (TWA)	Ontario TWAEV
Biphenyl	TWA: 0.2 ppm TWA: 1.3 mg/m³	TWA: 0.2 ppm TWA: 1.5 mg/m³ STEL: 0.6 ppm STEL: 4 mg/m³	TWA: 0.2 ppm
Benzene	TWA: 1 ppm TWA: 3 mg/m³ STEL: 5 ppm STEL: 15.5 mg/m³	TWA: 1 ppm TWA: 3.2 mg/m³ STEL: 5 ppm STEL: 16 mg/m³	TWA: 0.5 ppm STEL: 2.5 ppm Skin

Legend

ACGIH *- American Conference of Governmental Industrial Hygienists*
OSHA *- Occupational Safety and Health Administration*
NIOSH IDLH: *The National Institute for Occupational Safety and Health Immediately Dangerous to Life or Health*

Engineering Measures Use explosion-proof electrical/ventilating/lighting/equipment. Ensure that eyewash stations and safety showers are close to the workstation location.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Liquid
Appearance	Dark brown
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	No data available
Boiling Point/Range	140 - 143 °C / 284 - 289.4 °F
Flash Point	20 °C / 68 °F
Evaporation Rate	No information available
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	No information available
Relative Density	0.850
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	185 °C / 365 °F
Decomposition Temperature	No information available
Viscosity	No information available
Molecular Formula	C6 H5 Li
Molecular Weight	84.05

10. Stability and reactivity

Reactive Hazard Yes

Stability Reacts violently with water. Moisture sensitive. Air sensitive. Pyrophoric: Spontaneously flammable in air.

Conditions to Avoid Keep away from open flames, hot surfaces and sources of ignition. Exposure to air. Incompatible products.

Incompatible Materials Acids, Water, Alcohols, oxygen, Carbon dioxide (CO2)

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO_2)

Hazardous Polymerization No information available.

Hazardous Reactions None under normal processing.

11. Toxicological information

Acute Toxicity

Oral LD50 Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Dermal LD50 Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Vapor LC50 Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.
Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Butyl ether	7400 mg/kg (Rat)	10 mL/kg (Rabbit)	Not listed

Biphenyl	2140 mg/kg (Rat)	5010 mg/kg (Rabbit)	Not listed
Benzene	810 mg/kg (Rat) 1800 mg/kg (Rat)	8200 mg/kg (Rabbit)	44.66 mg/L (Rat) 4 h

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity May cause cancer.

Component	CAS-No	IARC	NTP	ACGIH	OSHA	Mexico
Butyl ether	142-96-1	Not listed	Not listed	Not listed	Not listed	Not listed
Lithium, phenyl-	591-51-5	Not listed	Not listed	Not listed	Not listed	Not listed
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	na	Not listed	Not listed	Not listed	Not listed	Not listed
Biphenyl	92-52-4	Not listed	Not listed	Not listed	Not listed	Not listed
Benzene	71-43-2	Group 1	Known	A1	X	A2

Mutagenic Effects May cause heritable genetic damage

Reproductive Effects Possible risk of impaired fertility.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system
STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and delayed Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

Endocrine Disruptor Information No information available

Component	EU - Endocrine Disrupters Candidate List	EU - Endocrine Disruptors - Evaluated Substances	Japan - Endocrine Disruptor Information
Biphenyl	Group III Chemical	Not applicable	Not applicable

Other Adverse Effects The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information.

12. Ecological information

Ecotoxicity
Do not empty into drains.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Butyl ether	Not listed	30.1 - 34.7 mg/L LC50 96 h	EC50 = 63.0 mg/L 5 min	Not listed
Biphenyl	1.28 mg/L EC50 = 3 h	1.4 - 1.6 mg/L LC50 96 h 4.3 - 5.1 mg/L LC50 96 h 1.17 - 1.81 mg/L LC50 96 h 1.65 - 2.29 mg/L LC50 96 h	EC50 = 1.89 mg/L 30 min EC50 = 3.20 mg/L 5 min EC50 = 3.30 mg/L 15 min	0.63 - 0.85 mg/L EC50 48 h
Benzene	29 mg/L EC50 = 72 h	70000 - 142000 µg/L LC50 96 h 22330 - 41160 µg/L LC50 96 h 28.6 mg/L LC50 96 h 22.49 mg/L LC50 96 h 5.3 mg/L LC50 96 h 10.7 -	Not listed	10 mg/L EC50 = 48 h 8.76 - 15.6 mg/L EC50 48 h

		14.7 mg/L LC50 96 h		

Persistence and Degradability No information available
Bioaccumulation/ Accumulation No information available.

Mobility No information available.

Component	log Pow
Butyl ether	3.21
Biphenyl	4.09
Benzene	1.83

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Component	RCRA - U Series Wastes	RCRA - P Series Wastes
Benzene - 71-43-2	U019	-

14. Transport information

DOT Not regulated
TDG Not regulated
IATA
- **UN-No** 2924
- **Hazard Class** 3
- **Subsidiary Hazard Class** 8
- **Packing Group** II

IMDG/IMO
- **UN-No** 2924
- **Hazard Class** 3
- **Subsidiary Hazard Class** 8
- **Packing Group** II

15. Regulatory information

International Inventories

Component	TSCA	DSL	NDSL	EINECS	ELINCS	NLP	PICCS	ENCS	AICS	IECSC	KECL
Butyl ether	X	X	-	205-575-3	-		X	X	X	X	X
Lithium, phenyl-	X	-	X	209-720-1	-		X	X	X	-	-
Biphenyl	X	X	-	202-163-5	-		X	X	X	X	X
Benzene	X	X	-	200-753-7	-		X	X	X	X	X

Legend:
X - Listed
E - Indicates a substance that is the subject of a Section 5(e) Consent order under TSCA.
F - Indicates a substance that is the subject of a Section 5(f) Rule under TSCA.
N - Indicates a polymeric substance containing no free-radical initiator in its inventory name but is considered to cover the designated polymer made with any free-radical initiator regardless of the amount used.
P - Indicates a commenced PMN substance
R - Indicates a substance that is the subject of a Section 6 risk management rule under TSCA.
S - Indicates a substance that is identified in a proposed or final Significant New Use Rule
T - Indicates a substance that is the subject of a Section 4 test rule under TSCA.
XU - Indicates a substance exempt from reporting under the Inventory Update Rule, i.e. Partial Updating of the TSCA Inventory Data Base Production and Site Reports (40 CFR 710(B).
Y1 - Indicates an exempt polymer that has a number-average molecular weight of 1,000 or greater.
Y2 - Indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule.

U.S. Federal Regulations

TSCA 12(b) Not applicable

SARA 313 Not applicable

Component	CAS-No	Weight %	SARA 313 - Threshold Values %
Biphenyl	92-52-4	1-2.5	1.0
Benzene	71-43-2	0.1-1	0.1

SARA 311/312 Hazardous Categorization

Acute Health Hazard	Yes
Chronic Health Hazard	Yes
Fire Hazard	Yes
Sudden Release of Pressure Hazard	No
Reactive Hazard	Yes

Clean Water Act Not applicable

Component	CWA - Hazardous Substances	CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants
Benzene	X	10 lb	X	X

Clean Air Act Not applicable

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
Biphenyl	X		-
Benzene	X		-

OSHA Occupational Safety and Health Administration
Not applicable

Component	Specifically Regulated Chemicals	Highly Hazardous Chemicals
Benzene	5 ppm STEL 0.5 ppm Action Level 1 ppm TWA	-

CERCLA
Not applicable

Component	Hazardous Substances RQs	CERCLA EHS RQs
Biphenyl	100 lb	-
Benzene	10 lb	-

California Proposition 65 This product does not contain any Proposition 65 chemicals

Component	CAS-No	California Prop. 65	Prop 65 NSRL	Category
Benzene	71-43-2	Carcinogen Developmental Male Reproductive	6.4 µg/day 13 µg/day	Developmental Carcinogen

State Right-to-Know

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Butyl ether	X	X	X	-	X
Biphenyl	X	X	X	X	X
Benzene	X	X	X	X	X

U.S. Department of Transportation

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security
This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Canada
This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations (CPR) and the MSDS contains all the information required by the CPR

WHMIS Hazard Class
B2 Flammable liquid
F Dangerously reactive material
E Corrosive material
D2A Very toxic materials

16. Other information

Prepared By
Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Revision Date 10-Feb-2015
Print Date 10-Feb-2015
Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS)

Disclaimer
The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

End of SDS

Polycaprolactone

SIGMA-ALDRICH sigma-aldrich.com

SAFETY DATA SHEET

Version 4.7
Revision Date 06/25/2014
Print Date 04/18/2017

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : Polycaprolactone

Product Number : 440744
Brand : Aldrich

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : 6-Caprolactone polymer

Formula : $(C_6H_{10}O_2)_n$

No ingredients are hazardous according to OSHA criteria.
No components need to be disclosed according to the applicable regulations.

4. FIRST AID MEASURES

4.1 Description of first aid measures

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration.

In case of skin contact
Wash off with soap and plenty of water.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
no data available

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides

5.3 Advice for firefighters
Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information
no data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Avoid dust formation. Avoid breathing vapours, mist or gas.
For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Provide appropriate exhaust ventilation at places where dust is formed.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place.

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
General industrial hygiene practice.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection
Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection
Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure
Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: crystalline Colour: beige
b)	Odour	no data available
c)	Odour Threshold	no data available
d)	pH	no data available
e)	Melting point/freezing point	Melting point/range: 60 °C (140 °F)
f)	Initial boiling point and boiling range	no data available
g)	Flash point	no data available
h)	Evapouration rate	no data available
i)	Flammability (solid, gas)	no data available
j)	Upper/lower flammability or explosive limits	no data available
k)	Vapour pressure	no data available
l)	Vapour density	no data available
m)	Relative density	1.145 g/mL at 25 °C (77 °F)

n)	Water solubility	no data available
o)	Partition coefficient: n-octanol/water	no data available
p)	Auto-ignition temperature	no data available
q)	Decomposition temperature	no data available
r)	Viscosity	no data available
s)	Explosive properties	no data available
t)	Oxidizing properties	no data available

9.2 Other safety information
no data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
no data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
no data available

10.4 Conditions to avoid
no data available

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
Other decomposition products - no data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
no data available

Inhalation: no data available

Dermal: no data available

no data available

Skin corrosion/irritation
no data available

Serious eye damage/eye irritation
no data available

Respiratory or skin sensitisation
no data available

Germ cell mutagenicity
no data available

Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a

carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity
no data available

no data available

Specific target organ toxicity - single exposure
no data available

Specific target organ toxicity - repeated exposure
no data available

Aspiration hazard
no data available

Additional Information
RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity
no data available

12.2 Persistence and degradability
no data available

12.3 Bioaccumulative potential
no data available

12.4 Mobility in soil
no data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

no data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)
Not dangerous goods

IMDG
Not dangerous goods

IATA
Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components
SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
No SARA Hazards

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
2-Oxepanone, homopolymer	-	

New Jersey Right To Know Components

	CAS-No.	Revision Date
2-Oxepanone, homopolymer	-	

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

HMIS Rating

Health hazard:	0
Chronic Health Hazard:	
Flammability:	0
Physical Hazard	0

NFPA Rating

Health hazard:	0
Fire Hazard:	0
Reactivity Hazard:	0

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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DOT Classification: CLASS 4.3: Material that emits flammable gases on contact with water.

Identification: : Lithium : UN1415 PG: I

Special Provisions for Transport: Not available.

Section 15: Other Regulatory Information

Federal and State Regulations:
Pennsylvania RTK: Lithium Massachusetts RTK: Lithium TSCA 8(b) inventory: Lithium

Other Regulations: OSHA: Hazardous by definition of Hazard Communication Standard (29 CFR 1910.1200).

Other Classifications:

WHMIS (Canada):
CLASS B-6: Reactive and very flammable material. CLASS E: Corrosive solid.

DSCL (EEC):
R14- Reacts violently with water. R35- Causes severe burns. R43- May cause sensitization by skin contact.

HMIS (U.S.A.):

Health Hazard: 3

Fire Hazard: 4

Reactivity: 2

Personal Protection: j

National Fire Protection Association (U.S.A.):

Health: 3

Flammability: 4

Reactivity: 2

Specific hazard:

Protective Equipment:
Gloves. Synthetic apron. Vapor and dust respirator. Be sure to use an approved/certified respirator or equivalent. Wear appropriate respirator when ventilation is inadequate. Splash goggles.

Section 16: Other Information

References: Not available.

Other Special Considerations: Not available.

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