Project Brief

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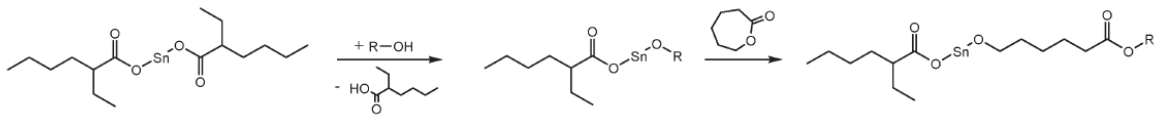
Objective

The objective of this project is to develop a process that can produce polycaprolactone (PCL) on a large-scale. The primary use of the polycaprolactone will be a PCL-silica bio-active glass, which can be utilized in medical procedures such as bone or cartilage repair. The intended project will discuss the various options that exist for a detailed plant design, and establish a optimal design that produces PCL satisfactory for utilization in biomedical materials. A stretch goal for the project is a design for the production of the PCL-bioactive-glass composite itself. Economic and practical applications will be analyzed in developing a plant design. Other small design goals include a detailed economic analysis based on real-world characteristics and detailed equipment designs - such as a reactor, separation process, heat exchangers, and pumps. Optimal reaction mechanisms include catalysts, so the proposed system includes a catalysis reactor. Since the product will be a polymer, the separation process (also known as polymer devolatilizion) will likely include a combination of screen filters and distillation.

Chemistry



Scheme 23 Initiation steps of the ROP of ε-CL initiated by an alcohol and catalysed by tin(II) octoate according to Kowalski *et al.*[83]

The tin catalyst reacts with the alcohol initiator to form a tin ester, which then reacts with the monomer caprolactone in ring-opening polymerization to form a long chain. This long chain reacts with another molecule of monomer to increase the chain length in the propagation step. The chain has the potential to form a cyclic polymer or a straight chain, but cannot branch. Currently we are planning to use buytl alcohol as the initiator in THF solvent. A paper by Kowalski et al. provides kinetic data for the reaction. Low initial concentrations of the tin octoate are necessary to limit the amount of tin in the polymer chains, allowing for biocompatibility.

Constraints

For the intended use in tissue engineering, the PCL must have the following characteristics: mechanical properties similar to human tissue, biocompatibility, and ease of sterilization. Research has shown that the PCL is biocompatible and, with a molecular weight between 50,000 and 100,000, is mechanically similar to human tissue. The method of combining the PCL and the bioactive glass will also impact the characteristics of biocompatibility, sterilization, and mechanical-compatibility. Potential combination methods include salt-leaching, electrospinning, polymer impregnation in glass scaffold, infiltration of polymer foams via slurry-dipping, and freeze-drying. Further, the biomedical application will demand a high polymer purity in comparison to other applications due to the various health hazards that arise with tissue repair. Cost analysis and economic feasibility will be conducted to ensure that the required purities can be met at a reasonable expense.

The volume of PCL produced and the economic feasibility of the process will depend on the market for the PCL-glass-composite and its potential uses in tissue engineering. The current and potential uses will also impact whether a batch or flow process will be developed, which is still in the research phase. Based on current processes, we predict that a batch system will produce a sufficient supply of PCL most efficiently.