Computational Control of Polymer Design

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Abstract

Achieving sequence-level controlled synthesis of polymers is of interest as this offers the potential of controlling material properties at a scale beyond current capacity. Increased control over resultant polymer compositions signify facilitating the exploration of polymer material function relationships; inherently intertwined to the chemical and physical properties present. We are developing a program able to predict the composition of polymers synthesized using CLRP as well as creating synthesis procedures to be executed by liquid handling robots. The program integrates CLRP chemistries to predict the resultant polymer compositions from user-defined parameters e.g. monomer reactivity ratios. The program can then utilize these inputs to generate a python script with synthesis procedures for liquid-handling robots to carry out the synthesis. Theoretical understandings of gradient-block copolymers are well developed yet, rarely applied in experimental plans due to its complexity; the automation of polymerization can facilitate including these on experimental plans. Implementing automation for polymer development/research increase productivity, and reproducibility thus, providing close control over polymer properties. The increased control over polymer compositions by the implementation of automation tools in polymer research may signify a stride toward achieving sequence-level controlled synthesis.

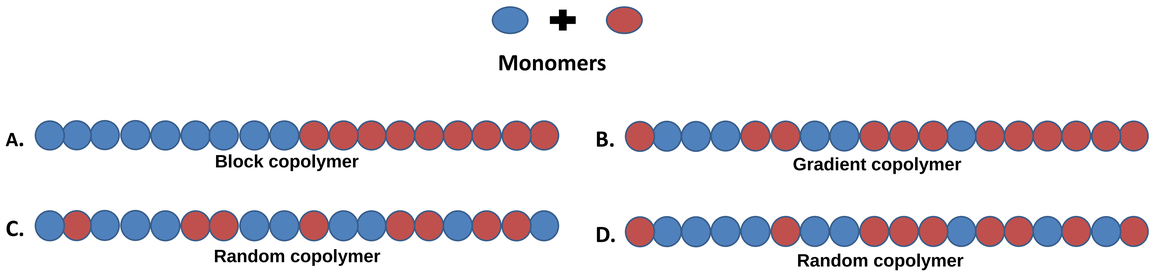

Figure 1: A & B are possible products from controlled polymerization, the composition of these polymers is more closely controlled. C & D are possible products from polymerization reaction that are not performed using a controlled polymerization method or (CLRP).

Background

- Polymers are often incorporated to new technologies thus, advancements in material science are fostered by elucidation of polymer properties.
- Before oxygen-tolerant CLPR, the use of automation tools was limited due to impracticability.
- Theoretical understandings of gradient-block copolymers are well developed yet, rarely applied in experimental plans due to its complexity .
- The program for polymer synthesis developed follows the avenue of Compositional Drift Simulator by Vincent Wu which employs the Mayo-Lewis and penultimate model of monomer addition.
- Transition to a fully automated polymer synthesis and post polymerization modification enhance control of polymer composition.

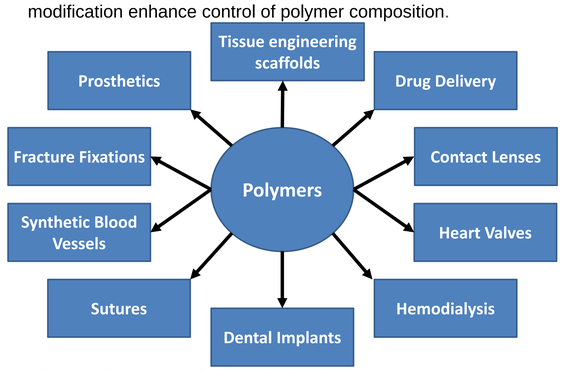

Figure 2: Examples of polymer applications in medicine

References

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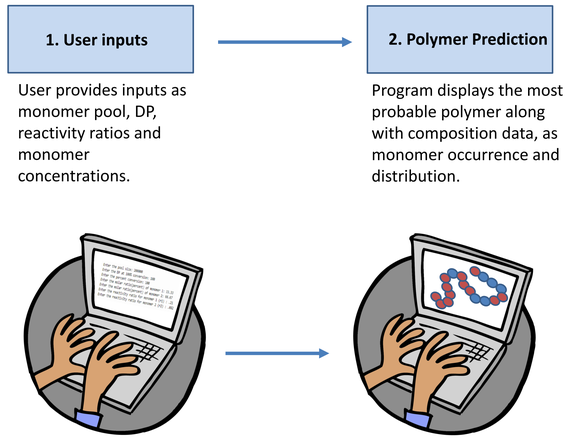
Methods: Program Overlook

Program Flowchart



Determination of Polymer Composition

1. The number of chains (N) in the polymer is calculated by dividing the monomer pool by the degree of polymerization.

$$N = \frac{pool\ size}{DP}$$

2. The chains are populated by monomers using the Mayo-Lewis equation to determine the first polymer in each chain.

$$\frac{d[M_1]}{d[M_2]} = \frac{(r_1[M_1]^2 + [M_2])}{(r_2[M_2]^2 + [M_1])}$$

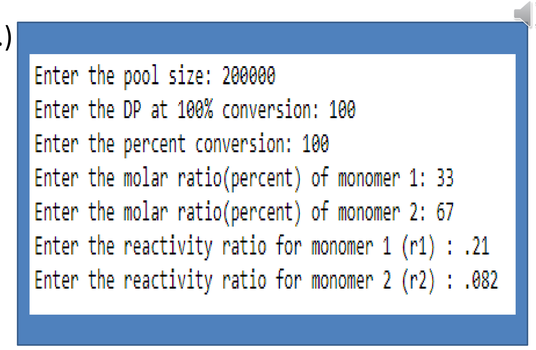
3. The probability of a monomer(2) being added to a propagating chain depending on the terminal monomer(1) of the chain is calculated.

$$P(2|1) = \frac{k_{12}[M_1]}{\sum_x k_{1x}[M_x]}$$

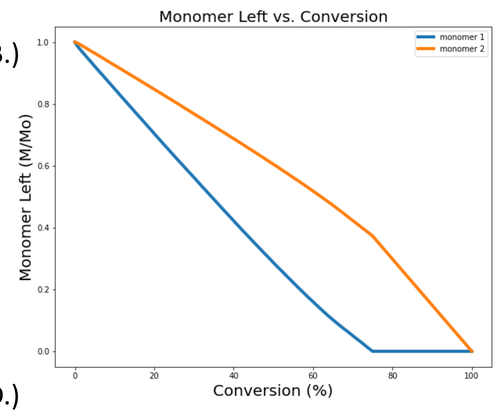
4. Monomers are added until the pool is converted to the percentage the user previously specified.

Results

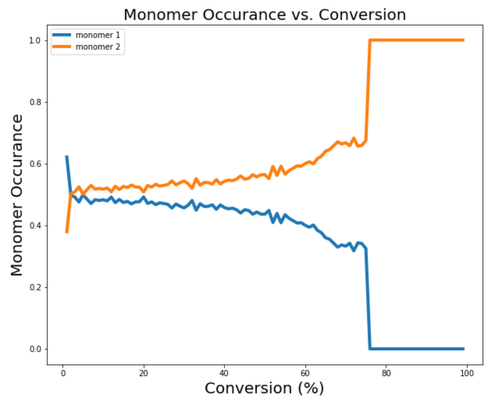
A.)



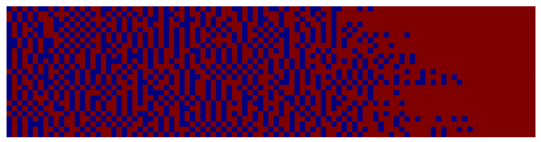
B.)



C.)



D.)

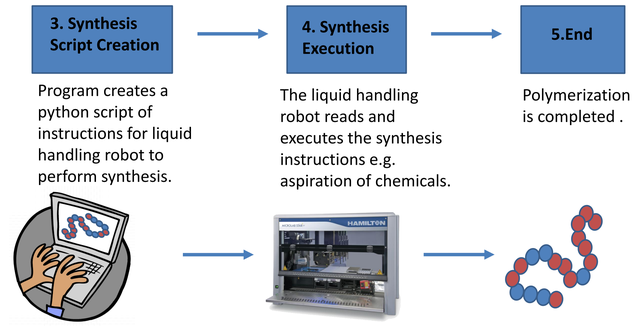


A.) User-input menu with polymer composition determination parameters provided.
B.) Unique monomers left with respect to monomer pool conversion.
C.) Shows the probability of finding a monomer along the polymer chain with respect to monomer pool conversion.
D.) Visual representation of monomer composition of 25 polymer chains.

Future Direction

The program is still under development we hope to accomplish the following in our next steps:

- Incorporate additional chemistries from literature to enhance the prediction of polymer compositions such as further exploration of steric hinderance effects.
- Enable the program to create python scripts for liquid handling robots to execute the polymer synthesis.
- Pass the synthesis instructions to a Hamilton MLSTARlet liquid handling robot to perform the polymer synthesis.
- Enable program to carry out synthesis and postpolymerization modifications as one single process.



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