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On-Demand Block Copolymer Production System

Background

- Specialty block copolymers, such as block copolymers are often produced in smaller-scale continuous or batch plants. Have wide range of applications.
- Block copolymers are derived from two or more polymers and are arranged in long “blocks”.

General diblock copolymer structure

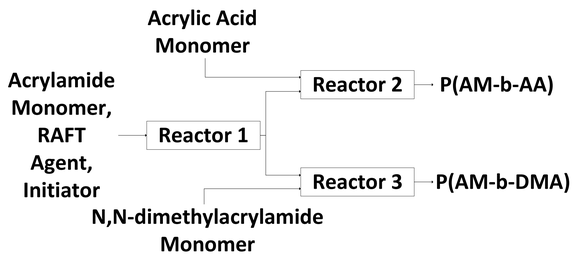
Project Objectives

- Design a modular and reconfigurable small-scale process that produces two different diblock copolymer products.
- Reaction must be in liquid phase with water solvent.

Design Considerations

- Reaction mechanism that maximizes production.
- Monomer, initiator, and chain transfer agent selection.
- Concentrations, stream flowrates, temperature, pressure.
- The type of reactor model, and their configurations.
- Pumping, Heat transfer, and pre-mixing.

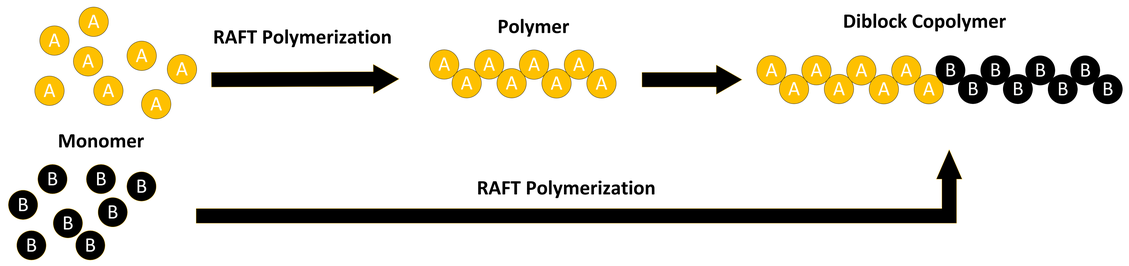
General Process Configuration



- RAFT agent is **4-((((2-Carboxyethyl)thio)carbonothioyl)thio)-4-cyanopentanoic acid**.
- Initiator selected is **4,4’-azobis (4-cyanopentanoic acid)**. Activates at 69˚C.

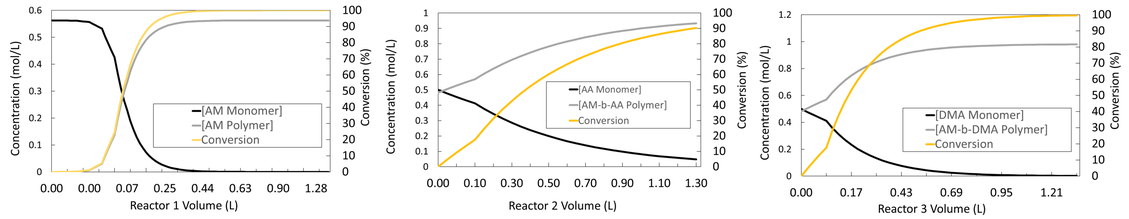
Details of Design

Reaction Mechanism



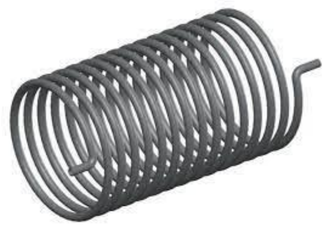
Reactor Design

- Modelled three reactors as isothermal plug flow tube reactors at 69˚C and 1 atm using MATLAB.

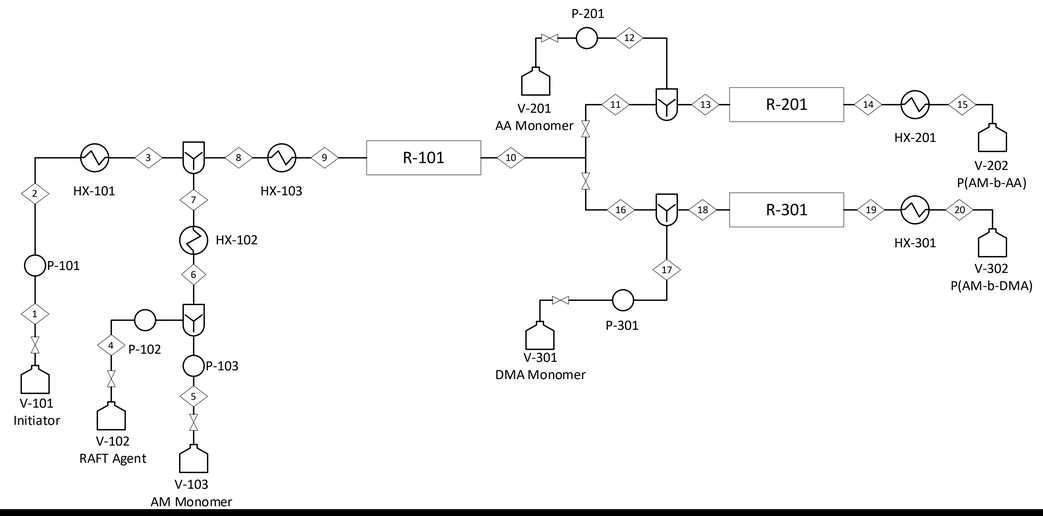


The following details were determined for each reactor:

- Reactor volume = **1.3 L**
- Length = **66.2 m**
- Inner Diameter = **0.005 m**
- Coiled reactor configuration to account for long length.
- Water bath heat exchanger will maintain isothermal conditions. Heat exchangers will also have this design.



Process Flow Diagram



Major Safety Considerations

- Acrylamide is a carcinogen.
  - *Limit exposure to chemical where possible.*
- Toxic gas release from runaway thermal reaction.
  - *Temperature control to maintain isothermal conditions*
- Chemicals potentially harmful to environment.
  - *Proper disposal and containment procedures required*.

Conclusions and Recommendations

Conclusions

- Designed a small-scale modular block copolymer production system, meeting requirements of scope.
- Poly(AM-b-AA) and poly(AM-b-DMA) produced at high conversions.

Recommended Improvements

- Signs of axial dispersion in reactor results effects model validity.
  - *Need to determine effect of axial dispersion on results.*
- Need to determine ideal post processing technique.
  - *Likely dialysis or precipitation.*
- Refine assumptions, kinetics, and configuration.

References

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