Modelling and Simulation of ARGET ATRP of BMA solution in Continuous Stirred Tank Reactor

Faisal Sahul Hameed, (MASc) Supervisor: Dr. Ramdhane Dhib
Department of Chemical Engineering, Ryerson University

INTRODUCTION

ARGET ATRP (Activators Regenerayed by Electron Transfer Atom Transfer Radical Polymerization) has received widespread attention for its ability to improve upon the faults associated with the conventional ATRP method. In this project, mathematical models are developed for the CSTR version of this process. The simulation of the model provides some important insights into the system which can be used to control the process.

OBJECTIVES

- Develop a kinetic model of commercially available BMA undergoing ARGET ATRP in a continuous stirred tank reactor.
- Determine the steady state point of the system to study the dynamics.
- Develop a controller to control the ARGET ATRP process of BMA in CSTR.

PROCESS DESCRIPTION

1. (Reduction of deactivator species)
   \[ R_A^{\ddagger} + A + X \rightarrow X + A + R_A^{\ddagger} \]
2. (Activation of initiator)
   \[ I + M \rightarrow M + I \]
3. (Initiation)
   \[ I + M \rightarrow M + I \]
4. (Propagating, Where \(i\) is)
   \[ R_i + M \rightarrow M + R_i \]
5. (Termination)
   \[ R_i + R_j \rightarrow R_i + R_j \]
6. (Transfer)
   \[ M + R_A^{\ddagger} \rightarrow P_i + M \]
7. (Deactivation of Monomer Radical)
   \[ M + A \rightarrow X + A \]
8. (Activation of Dormant Monomer)
   \[ M + X \rightarrow X + A \]

ACKNOWLEDGMENT

NSERC and Department of Chemical Engineering, Ryerson University for financial support.

REFERENCES