Optimization Strategies of an Emulsion Polymerization Reactor

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Introduction

Emulsion polymerization (EP) is :

- An important process for manufacturing water based polymers such as rubbers, coatings and adhesives.
- A free radical polymerization carried out under the heterogeneous condition.
- A mostly used process for latex production

Advantages:

- Easy control due to the physical state of kinetics
- High average molecular weight of product
- Less thermal and viscosity problems than bulk polymerization

Objectives:

Modeling and simulation of the process to determine:

- Monomer conversion
- Size and number of generated particles
- Molecular weight averages and distributions

Investigation of the model's Prediction for

- Batch reactor
- Semi-batch reactor
- Continuous stirred tank reactor (CSTR)

Optimization of the process to:

- Enhance the monomer conversion and product quality
- Stabilize the reactor operation

Reaction Mechanism

The model focuses on the behaviour of vinyl acetate :
High water solubility and significant desorption

Assumptions of model

- Negligible gel effect
- Less dominancy of termination reactions
- Importance of chain transfer reactions in controlling molecular weight averages
- Introduction of chain transfer to monomer as the first step in desorption process

Chemical Initiation : $S_2O_8^{-2} \xrightarrow{k_I} 2SO_4^{-\bullet}$

Chemical Initiation : $SO_4^{-\bullet} + M \xrightarrow{k_i} R_1^\bullet$

Propagation : $R_r^\bullet + M \xrightarrow{k_p} R_{r+1}^\bullet \quad r \geq 1$

Termination by Combination : $R_r^\bullet + R_s^\bullet \xrightarrow{k_{tc}} P_{r+s}$

Transfer to Monomer : $R_r^\bullet + M \xrightarrow{k_{fm}} P_r + R_1^\bullet$

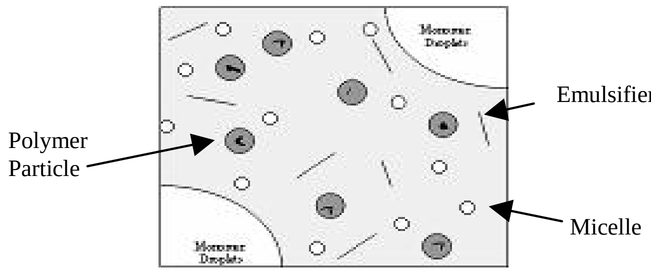
Transfer to Polymer : $R_r^\bullet + P_s \xrightarrow{k_{fp}} R_s^\bullet + P_r$

Transer to CTA : $R_r^\bullet + CTA \xrightarrow{k_{fcta}} P_r + CTA^\bullet$

Transfer to Inhibitor : $R_r^\bullet + MI \xrightarrow{k_{MI}} MI^\bullet + P_r$

Terminal Double Bond : $R_r^\bullet + P_m \xrightarrow{k_p^*} R_{r+m}^\bullet$

Emulsion Polymerization ⟹ Three stages



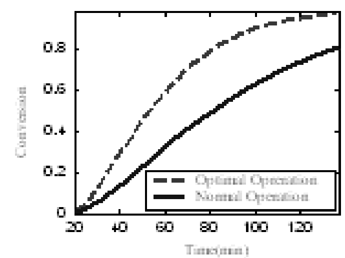
1- Optimization of Batch Reactor

- Effect of impurity on conversion

Normal Condition

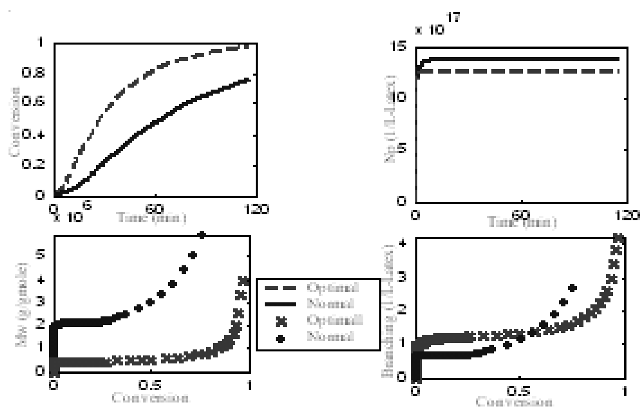
$$\begin{cases} T = 323.15 \quad K \\ I_F = 0.0022 \; mol/L \\ S_F = 0.0417 \; mol/L \\ IM = 200 \quad ppm \end{cases}$$

$$J_{min} = (\text{Conversion} - 1)^2$$



- Increasing the monomer conversion and average molecular weight

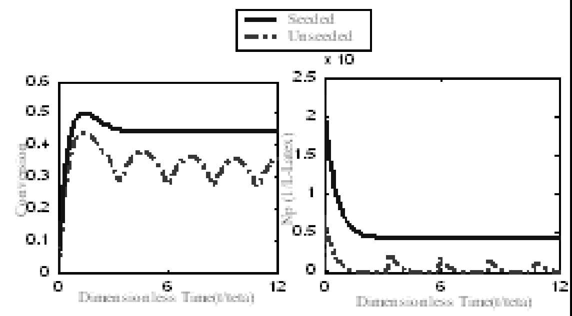
$$J_{min} = (\overline{M}w - 8\times10^6)^2 + (\text{Conversion} - 1)^2$$



2- Optimization of Continuous Reactor

- The oscillatory behavior due to periodic particle nucleation

Basic Remedy ⟹ Feeding a stream of seed particles



Emulsion Reactor Train Configuration

The first large reactor is preceded by a very small initial CSTR :

- Almost all of the initiator and emulsifier are fed to the first reactor
- Generation of most polymer particles can be entirely accomplished in the first reactor
- The second reactor will be used only for particle growth