Quality Control of Polymer Production Processes


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Introduction

- Polymer plant operation
  - Grade transition
  - Maximizing production
  - Safe operation of reactor

- Quality control for the objectives

- On-line soft sensing and optimal grade changeover control
Prospective Control System

Production Planning

Polymerization Rate Control
Concentration Ratio Control
Pressure Control

Optimal Changeover Operation
Reaction Temp. Control
Material Feed Rate Control
Reactor Level Control

Product Quality Control
Online Property Sensor
Process Monitoring

Product Blending Planning

Polymerization Reactor Control System

Product Blending and Storing Scheduling

Catalyst Processing → Polymerization Reactor → Separation → Extruder → Blending Storing

POSTECH
Needs for Quality Modeling

Micro-scale

- **Low-Order Structure**
  - Chain Branching
  - LCB
  - SCB
  - Stereoregularity
  - Isotactic
  - Sindiotactic
  - Atactic

- **Distributed Parameter**
  - MWD
  - PSD
  - CCD

- **High-Order Structure**
  - Morphology
  - Molecular Mobility
  - Crystal Structure

- **Polymer Properties**
  - Melt Index
  - Density
  - Shear Viscosity
  - Melting Point

- **End-User Properties**
  - Color
  - Mechanical property
  - Strength
  - Electrical property

 Macroscale

- **Catalyst Processing**
- **Polymerization Reactor**
- **Separation**
- **Extruder**
- **Blending Storing**

Process&Plant

- **Residence Time Distribution**
Basic Structure of Inferential System

1. **Mechanistic model** derived from first principles
2. **Empirical model** derived from lab. data
3. **Black box model** by neural nets & statistical methods
An Examples of Three Kinds Model

- **Mechanistic model** *(McAuley & MacGregor, 1991)*

\[
\ln(MI_i) = 3.5 \ln \left( k_0 + k_1 \frac{[H_2]}{[C_2]} + k_2 \frac{[C_3]}{[C_2]} + k_3 \frac{[C_4]}{[C_2]} + k_4 \frac{[R]}{[C_2]} \right) + k_5 \left( \frac{1}{T} - \frac{1}{T_0} \right)
\]

\[
\frac{d MI_c(t)^{-0.286}}{dt} = \frac{1}{\tau(t)} MI_i(t)^{-0.286} - \frac{1}{\tau(t)} MI_c(t)^{-0.286}
\]

- **Empirical model** *(Watanabe et. al., 1993)*

\[
\log(MI_i) = \beta + \alpha_1 \log \left( \frac{[H_2]}{[C_2]} \right) + \alpha_2 \log \left( \frac{[H_2]}{[C_2]} \right) + \alpha_3 \log \left( \frac{[C_3]}{[C_2]} \right) + \alpha_3 \log \left( \frac{[C_4]}{[C_2]} \right)
\]

\[
+ \alpha_4 \log[R] + \alpha_5 \log[T]
\]

\[
\frac{d \log(MI_c(t))}{dt} = \frac{1}{\tau(t)} \log(MI_i(t)) - \frac{1}{\tau(t)} \log(MI_c(t))
\]

- **Neural net model** *(Koulouris, 1995)*

\[
MI_i^{-0.286} = \text{Wave} - \text{Net} \left( \frac{[H_2]}{[C_2]} \frac{[C_3]}{[C_2]} \frac{[C_4]}{[C_2]} \frac{[R]}{[C_2]} \right)
\]

\[
\left[ \frac{[H_2]}{[C_2]} \frac{[C_3]}{[C_2]} \frac{[C_4]}{[C_2]} \frac{[R]}{[C_2]} \right]
\]
MI Estimation by Models

- Mechanistic model
- Regression model
- Neural net model
MI Estimation with EKF

Estimation by mechanistic model with EKF

Estimation by regression model with EKF
Risk of Extrapolation

Mechanistic model

Regression model

Neural net model

Learning data
Grade Changeover Operation

1. Not time but grade optimal operation
2. Runaway reaction
Control System

- Iterative open-loop optimization
  - A new optimal trajectory is recomputed
  - The first input action is implemented at every new measurements

- Combination of FF&FB controllers
  - A optimal trajectory is pre-calculated of both MV & CV
  - MV is introduced to the plant in a FF manner
  - CV is deviated from the desired optimal trajectory, FB controller is activated to compensate the deviation
Results of Control

Manual operation
Control is activated
Optimal Blending

Reactor control is not good enough to satisfy the customer’s demands

MILP Problem
Blending Optimization Result

a) Blending operation by operator

b) Optimal Blending

c) Optimal Blending and tank assignment

d) Optimal Blending and assignment with 2 steps prediction
Conclusion

- Integration of process control, sensing and optimization is indispensable
- Most important factor is quality modeling