Robust Optimization for Grade Transitions In Polyethylene Solution Polymerization

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Background and Motivation

LLDPE Solution Polymerization\(^1\)

- Linear low-density polyethylene (LLDPE)
- Made by copolymerization of ethylene with longer-chain olefins (octene, butene, hexene, propylene)
- Long loop with heat exchangers
- Continuous operation with multiple feed positions

Current Practice

- Different grades produced in a single production line and grade transition takes a long time
- Hard to implement complex transitions
- Room for improvement

Objectives

Develop a model based control and optimization framework to minimize transition time and offgrade products

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Model Development

- CSTR with *data-driven surrogate VLE model*
- *Method of moments* for product property prediction
- *Variable time delay* for recycle streams
- Process constraints

Offline Dynamic Optimization

- Single stage optimization (single value target)
- *Multistage* optimization (specification bands)
To Lower Density and Higher MI

Comparison of MI Profile

- MI: 1 → 12 g/10min
- Multistage: Capable of minimizing the transition time and the off-grade product directly
- Faster transition in S2 reduces the transition time
- Oscillations within the band
- More than 50% reduction

**Optimal solution fails at unknown uncertainty level!**

![Graph showing MI profile comparison between baseline, single-stage, and multi-stage methods with transition time and duration of S2 metrics.](image)
Methodology

Concept of backoff

Original constraints
\[ f(x, u, p) \leq 0 \]

Updated inequality constraints
\[ f(x, u, \bar{p}) + b_c \leq 0 \]

Monte Carlo simulation to approximate \( b_c \)
- Assume the uncertainty \( p \) is in a range around its nominal value and it follows normal distribution \( N(p_0, \sigma^2) \)
- Assume 5% of \( p_0 \) is within \( 3\sigma \)
- \( m=200 \) in the following case study

Optimization w/ Nominal Uncertainty Level

Optimal input profiles

Monte Carlo simulation

State and output profiles

Data Processing
Approximate backoff \( b_c \)

Backoff \( b_c \)

Optimization w/ Backoff constraints

“Robust” optimal input profiles

Data Processing
Check the performance

Case study

Monte Carlo Optimization

Optimization w/ Nominal Uncertainty Level

Monte Carlo Simulation

Optimal input profiles

Data Processing

Approximate backoff $b$

Resulting state and output profiles

Backoff $b$

Optimization w/ Backoff constraints

Check the performance

"Robust" optimal input profiles

Density (200 runs)

Transition time longer than 2.7 hrs for $t$

MI (200 runs)

Density (g/cc)

MI (g/10min)

 MI (200 runs)

Transition time longer than 2.7 hrs for $t$

Density (g/cc)

MI (g/10min)

MI (200 runs)

Density (g/cc)

MI (g/10min)

Density (g/cc)

MI (g/10min)

Density (g/cc)

MI (g/10min)
Case study

Approximate backoff $b_c$

Optimization w/ Nominal Uncertainty Level

Monte Carlo simulation

Optimal input profiles

Resulting state and output profiles

Data Processing

Approximate backoff $b_c$

Optimization w/ Backoff constraints

“Robust” optimal input profiles

Data Processing

Check the performance

• Obtain standard deviation $\sigma$

• Add backoff constraints ($2.9 \sigma$) in the original optimization problem

Sample variance of MI varies over time

MI (200 runs)

Max standard deviation

Melt Index 0.61

Density 0.0002

Production rate 14.21

Reactor temp. 0.29

Ethylene conc. 0.01

Pb in reactor 0.02

VI (g/10min)

Melt Index (200 runs)

Sample variance of MI varies over time

0 0.5 1 1.5 2 2.5 3 3.5 4 4.5

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7
Case study

Optimization with backoffs

- Optimization w/ Nominal Uncertainty Level
- Monte Carlo simulation
- Optimal input profiles
- Resulting state and output profiles
- Optimization w/ Backoff constraints

Data Processing
- Check the performance
- "Robust" optimal input profiles

1. Oscillations within the band
2. Better control the propagation error

Graphs showing:
- Density (200 runs)
- MI (200 runs)

Comparing:
- Single-stage vs. multi-stage
- Multistage w/o backoffs vs. Multistage w/ time-varying backoffs

In min
- No violations
- Transition Time  Duration of S2
- Multistage w/o backoffs 39.1 33.6
- Multistage w/ time-varying backoffs 40.2 34.8

Density (g/cc)
- 0.86 to 0.91

MI (g/10min)
- 0.86 to 0.91

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<th>Density (g/cc)</th>
<th>MI (g/10min)</th>
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Significance

Developed a rigorous dynamic model for the process
• Built and integrated a surrogate VLE model
• Predicts accurately with reduced model complexity

Single-stage formulation vs. multistage formulation
• Takes specification bands into account
• Minimizes transition time and off-grade product directly
• Greatly reduces the transition time and the off-grade production

Robust optimization using backoff constraints
• Computationally tractable optimization with time-varying backoffs
• Robust transition policies
Potential Value and Future Work

Potential Value

• **Reduction** of transition time and off-grade product
• **Guided** complex transitions
• Increased **flexibility** in production wheel
• **Robust** offline transition policies

Future Work

• **Improve the performance** by tuning parameters and refining the model
• Apply **adjoint sensitivity formulation** for optimization under uncertainties
• Consider **online** optimization and model predictive control

*Thanks for your attention!*