Optimization For Grade Transitions In Polyethylene Solution Polymerization

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Dynamic Optimization Models
Grade Transition for LLDPE

- Continuous Stirred-Tank Reactor (CSTR) (represents two actual processes)
- Assume perfect mixing
- Three types of variables: $F_1, F_2, F_h, F_c$
  - Manipulated variables
    - Ethylene, comonomer, hydrogen and catalyst feed flowrates
    - Inlet temperature of cooling media
  - Output variables
    - Product properties: MI and density
    - Process requirement: ethylene conversion and reactor temperature
  - State variables
    - Concentrations and moments
- Method of moments
  - predict product properties from state variables

Reactions:
- Chain initialization
- Chain propagation
- Chain transfer
- Site deactivation

Figure source: http://en.wikipedia.org/wiki/Continuous_stirred-tank_reactor
Process Model Development
Assumptions and Components

• Perfect mixing
• Chain Initiation,
• Chain Propagation,
• Chain Transfer,
• Site Deactivation.

• The model has five parts
• Mass and heat balance
• Moment model
• Surrogate model for VLE
• Recycle time delay model
• Process constraints

Comparison: ASPEN, Kriging and Internal Model
Dealing with Specification Band
Multistage Optimization

Motivation:

• In-spec product is qualified for sale.

• Specification band should be taken into account when calculating off-grade.

Nystrom et al, Computers & Chemical Engineering 29 (2005) 2163-2179
Results and Analysis

<table>
<thead>
<tr>
<th>Transition Time</th>
<th>Duration of Stage 2</th>
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</thead>
<tbody>
<tr>
<td>Multistage</td>
<td>21.3 min</td>
</tr>
<tr>
<td>Single-stage</td>
<td>114.7 min</td>
</tr>
</tbody>
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Fast transition in S2
Oscillations within the specification band

The multistage solution

- A faster transition to reach the boundary of the second band
- More oscillations within the specification band
- Better performance