Optimization For Grade Transitions In Polyethylene Solution Polymerization

Jun Shi[1], Intan Hamdan[2],

Sarat Munjal[2], Lorenz T. Biegler[1]

[1]Center of Advanced Process Decision-making
Department of Chemical Engineering
Carnegie Mellon University

[2]The Dow Chemical Company

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

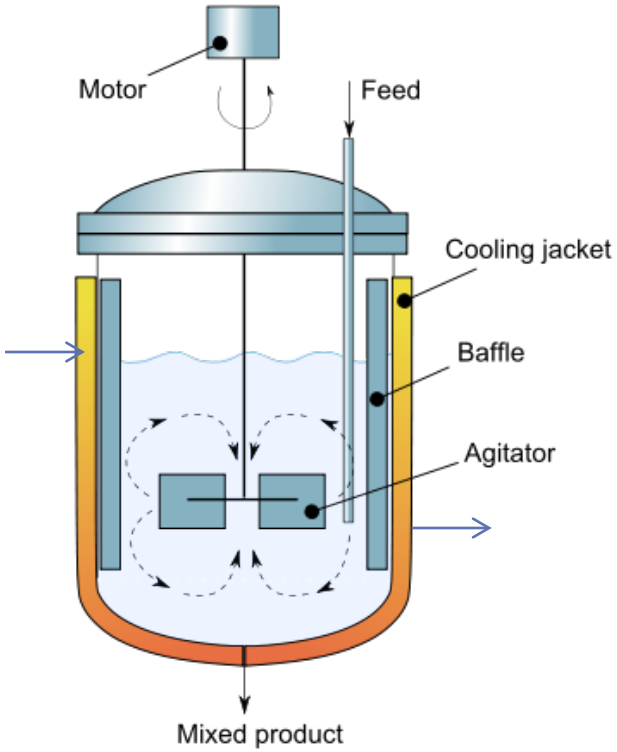
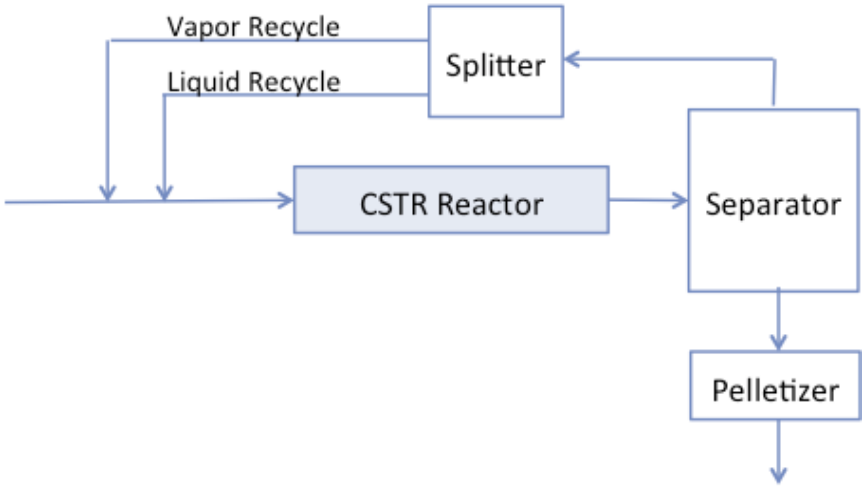


Figure source: http://en.wikipedia.org/wiki/Continuous_stirred-tank_reactor

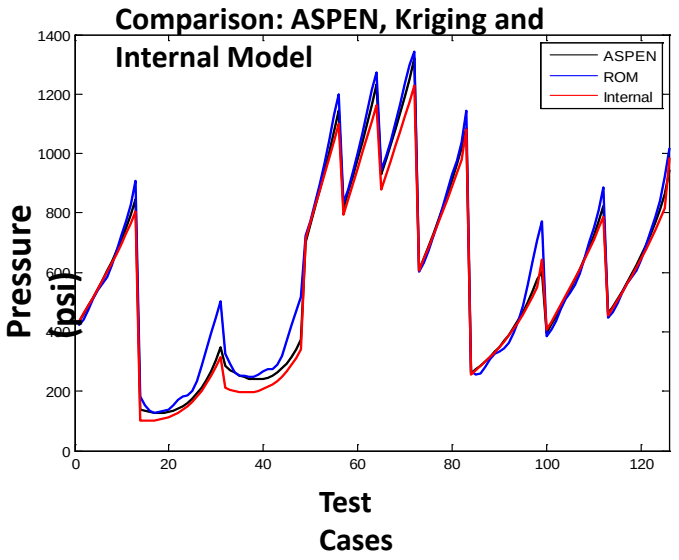
Process Model Development

Assumptions and Components

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

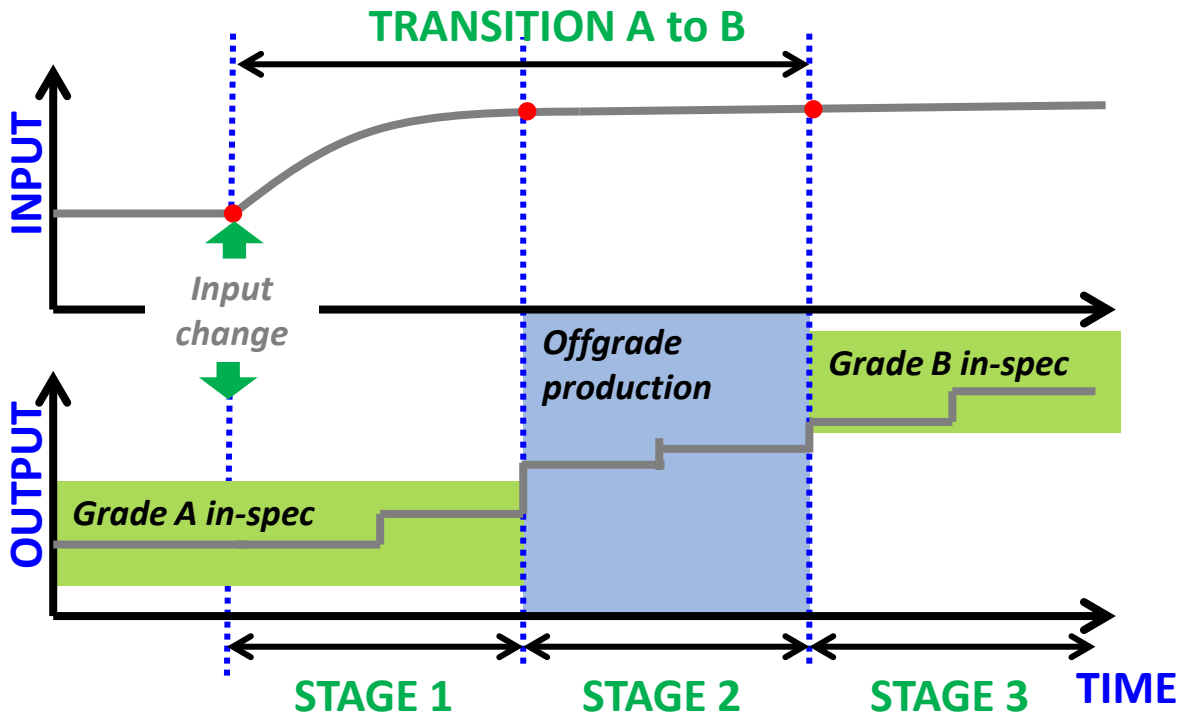


- **The model has five parts**
- Mass and heat balance
- Moment model
- *Surrogate model for VLE*
- *Recycle time delay model*
- *Process constraints*



Dealing with Specification Band

Multistage Optimization

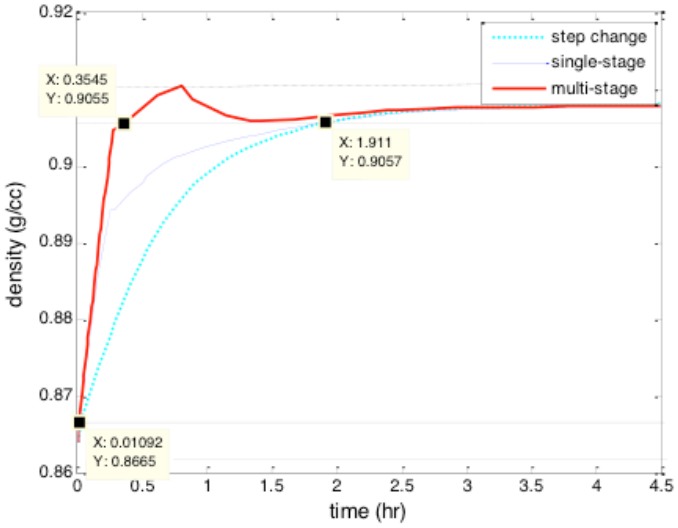


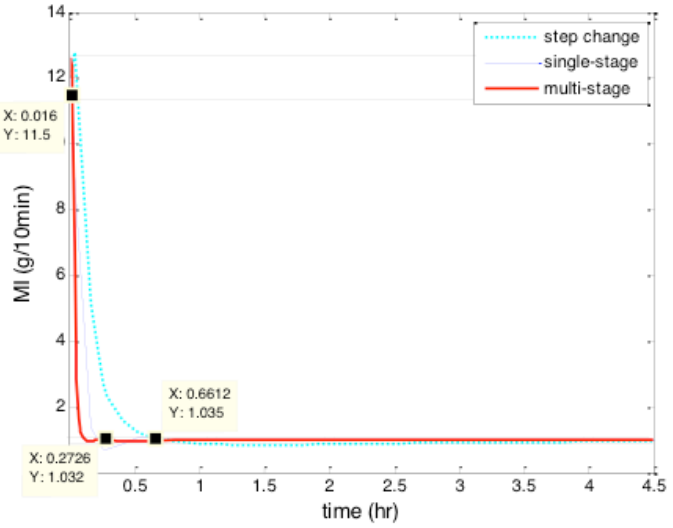
Motivation:

- 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





	Transition Time	Duration of Stage 2
Multistage	21.3 min	20.3 min
Single-stage	114.7 min	113.7 min

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