Optimization For Grade Transitions In Polyethylene Solution Polymerization

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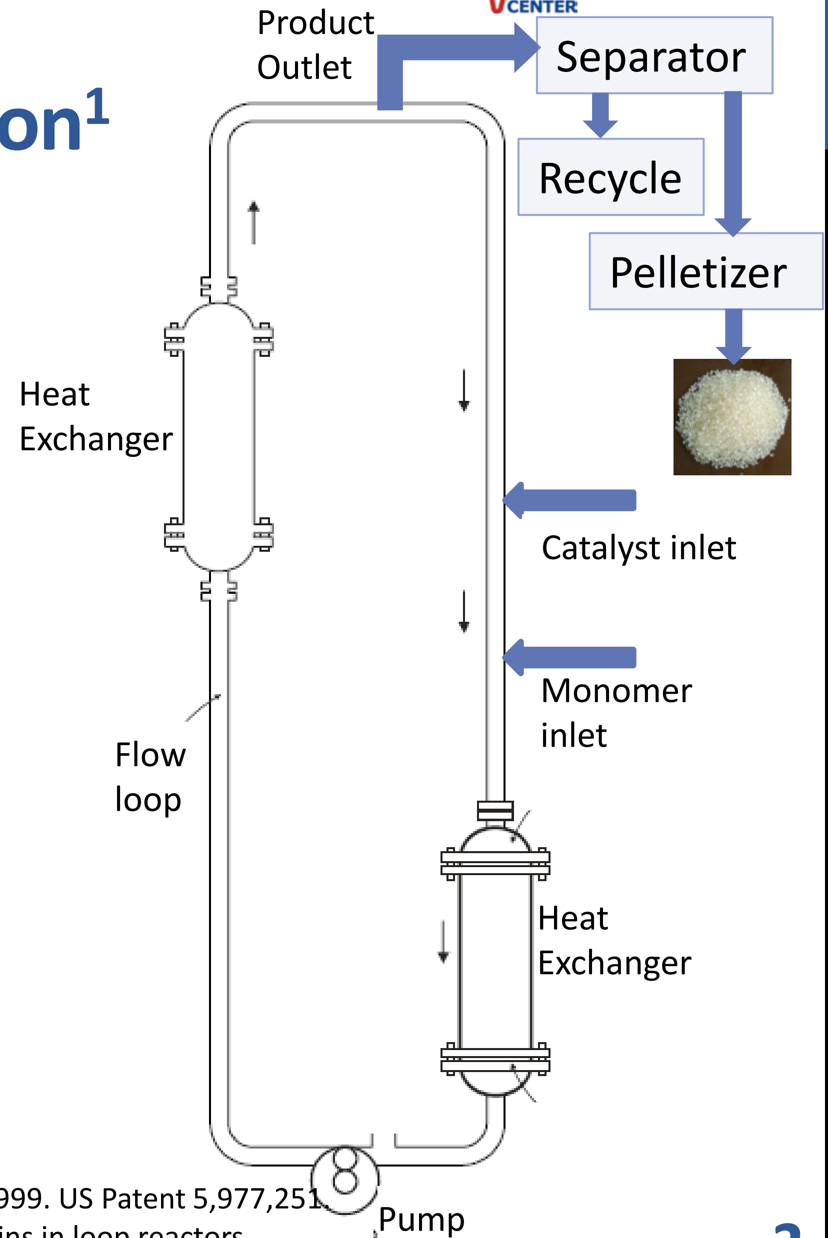
Background

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
- Multiple feed positions for:

  Ethylene, Comonomer, Catalyst, Solvent, Hydrogen



1. Che I Kao et al. Non-adiabatic olefin solution polymerization, November 2 1999. US Patent 5,977,251.
2. J.J. Zacca and W.H. Ray. Modelling of the liquid phase polymerization of olefins in loop reactors. Chemical Engineering Science, 48(22):3743–3765, 1993.

Project Overview

Motivation and Objectives

Current Practice

- Different grades produced in **a single production line**
- Grade transition takes **a long time**
- **PID** controller for flowrate and temperature control
- Hard to implement complex transitions; Room for improvement

Objectives

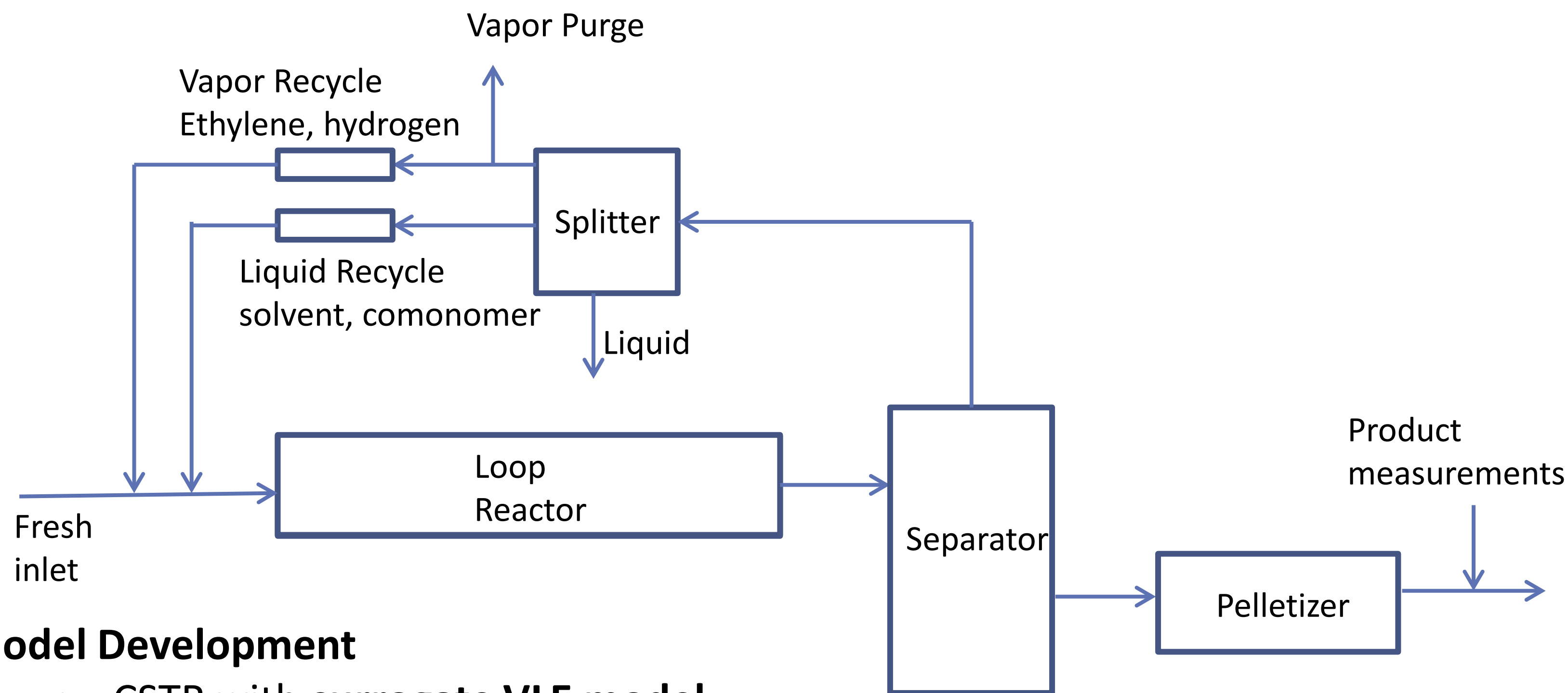
- Develop a model based control and optimization framework to
  - Minimize **transition time**
  - Minimize **offgrade products**

Potential Value

- **Reduction** of transition time
- **Guided** complex transitions
- Increased **flexibility** in production wheel

Project Progress

Model Development and Offline Optimization



Model Development

- CSTR with **surrogate VLE model**
- Method of moment for product property prediction
- *Recycle time delay model*
- *Process constraints*

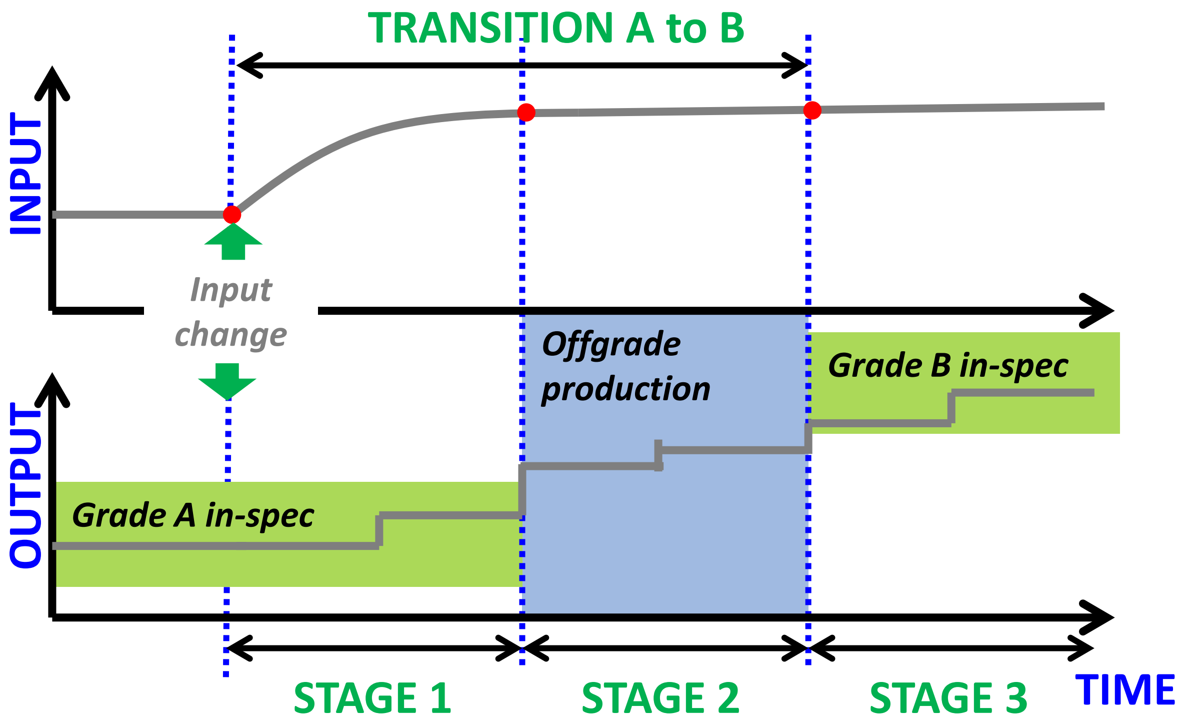
Offline Dynamic Optimization

- Single stage optimization $\min \int_0^{tf} \|x(t) - x^*\|^2{}_Q + \|u(t) - u^*\|^2{}_R \, dt$
- *Multistage optimization*

Dealing with Specification Bands

Multistage Optimization

$\rho^* = 0.9 \pm 0.0025 g/cm^3$
instead of $\rho^* = 0.9\ g/cm^3$



Motivation:

- In-spec product is qualified for sale.
- Specification band should be taken into account when calculating off-grade.

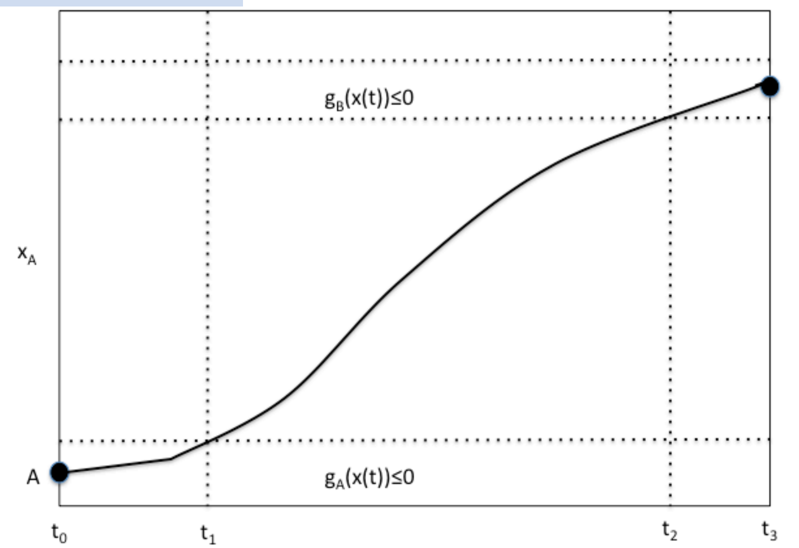
3. Nystrom et al, Computers & Chemical Engineering 29 (2005) 2163-2179

Dealing with Specification Bands

Multistage Optimization

Min (Off-spec + Trans. Time + Regularizing Term)

s.t.
- Dynamic model
- Grade A in-spec in Stage1
- Grade B in-spec in Stage3
- Continuity between stages
- Initial and Final Conditions



- **3 stages**:
  in-spec of A, out-of-spec and in-spec of B.

- Minimize a combination of **the off-spec product between t1 and t2** and **the transition time t2-t0**. A regularizing term that promotes a smooth unique solution.

- Application of 3-point collocation on 18 finite elements over 4.5 hours
- An NLP problem with over 63000 equations and over 63000 variables
- Simultaneous dynamic optimization with moving finite element

Case Studies

Grade Transitions between Two Grades

Operation conditions for two different grades[4]

		Meaning	Units	Grade A	Grade B
Properties	**MI**	Melt index	g/10min	1.0	12.0
	Conversion	Ethylene conversion rate		0.980	0.850
	Density	Product density	g/cm^3	0.908	0.864
Manipulated Variables	**Tji**	Inlet cooling water temp	°C	133.37	131.36
	F2	Ethylene inlet flow	L/s	3.43	3.26
	F8	Comonomer inlet flow	L/s	0.18	1.30
	FH	Hydrogen inlet flow	L/s	$3.38*10^{-4}$	$5.37*10^{-4}$
	Fc	Feed catalyst	L/s	$0.93*10^{-2}$	$2.65*10^{-2}$
	Fs	Solvent inlet flow	L/s	0.167	0.158

For each transition, step change simulation is performed as a baseline

- Typical way to perform grade transitions; May go to infeasible region

Specification bands: $\pm 0.0025 g/cm^3$ for density, $\pm 5\%$ for melt index.

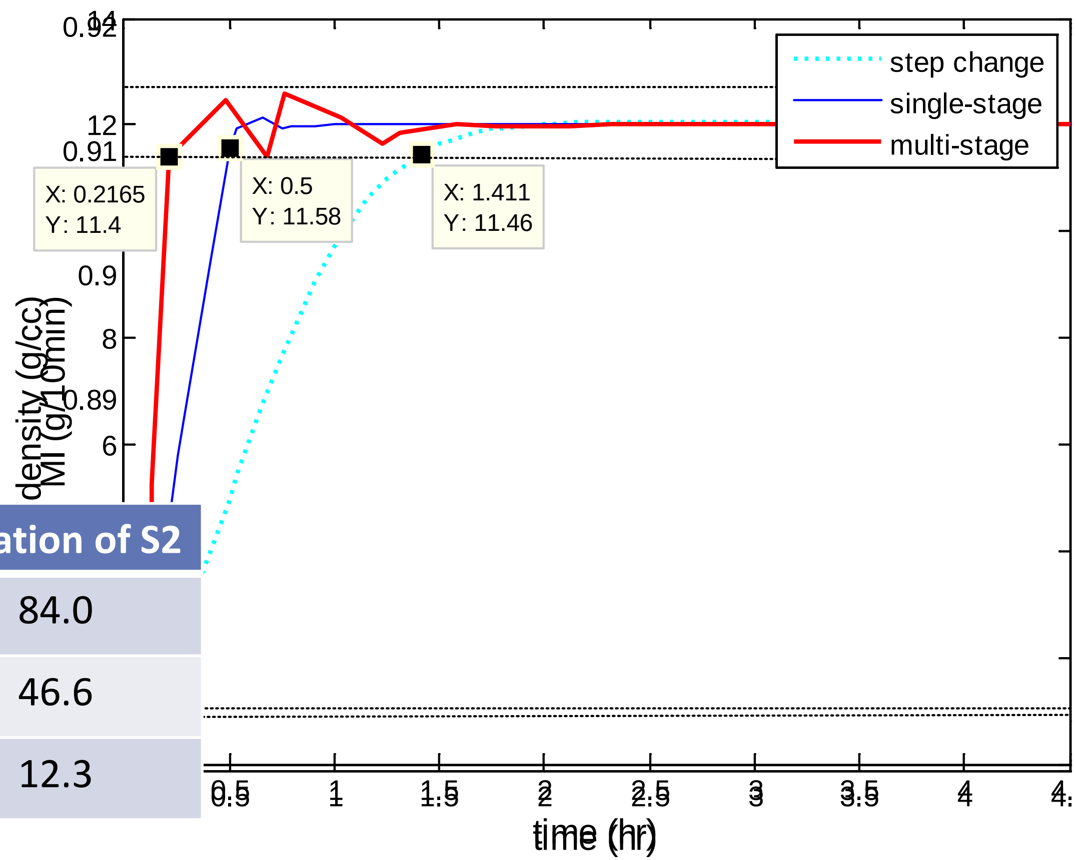
4. J.J. Zacca and W.H. Ray. Modelling of the liquid phase polymerization of olefins in loop reactors. Chemical Engineering Science, 48(22):3743–3765, 1993.

To Lower Density and Higher MI

Comparison of Output Profiles

The multistage solution

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



in min	Trans. Time	Duration of S2
Step change	84.7	84.0
Single-stage	47.3	46.6
Multistage	13.0	12.3

Novelty

Built and integrated a surrogate VLE model

- Accurate predictions with reduced model complexity

Single-stage formulation

- A common approach in dynamic optimization of grade transitions
- But, not minimizing transition time or off-grade product directly.
- Also, single value target is not practical.

Multistage formulation

- Specification bands are considered in some studies where integrated scheduling and dynamic optimization problem is solved.
- Takes specification bands into account
- Capable of minimizing transition time and off-grade product directly
- Has better performance (greatly reduces the transition time and the off-grade product)

Potential Value and Future Work

Potential Value

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

Future Work

- With accurate model and constraints we obtained, the resulting optimal transition profiles can be used as optimal trajectories.
- The performance can be further improved by tuning parameters and refining the model.
    - Identifying all the constraints and evaluating the solutions are necessary
- Online optimization and control issues will be considered in next step.
    - Computational time should be lowered if repeated optimization runs are performed during the process
    - Uncertainties/disturbances need to be taken into account