Model-based Control and Optimization for Grade Transitions in Polyethylene Solution Polymerization Process

Jun Shi[1], Intan Hamdan[2], Lorenz T. Biegler[1]

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

[2]The Dow Chemical Company

Background and Motivation

LLDPE Solution Polymerization[1]

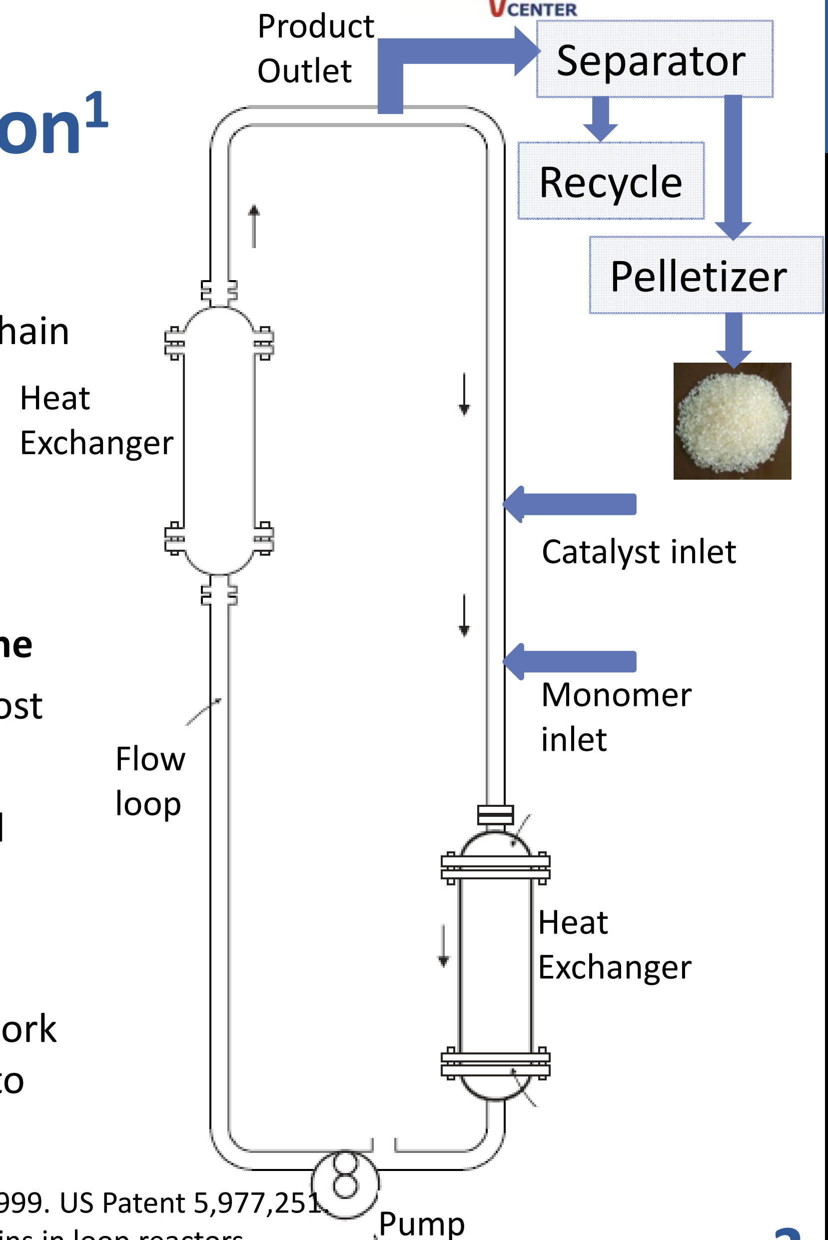
- Linear low-density polyethylene (LLDPE)
- Made by copolymerization of ethylene with longer-chain olefins (octene, butene, hexene, propylene)
- Long loop with heat exchangers
- Continuous operation with multiple feed positions

Current Practice

- Different grades produced in **a single production line**
- **Frequent grade transitions** due to high inventory cost
- **Model-based control** applied to calculate setpoint
- **PID** controller for flowrate and temperature control
- Hard to implement complex transitions

Objectives:

Develop a model based control and optimization framework to minimize **transition time** and **offgrade products,** and to increase **flexibility** in production wheel



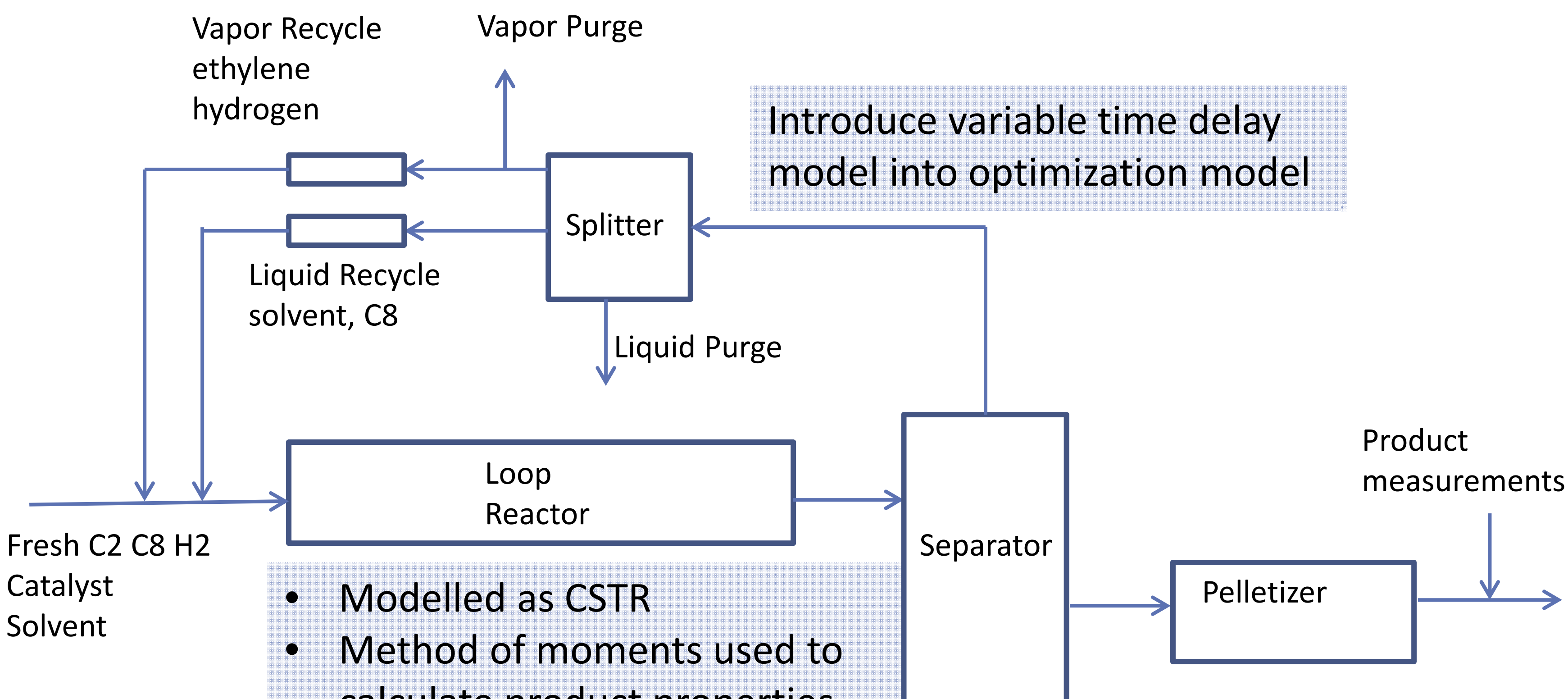
1. Che I Kao et al. Non-adiabatic olefin solution polymerization, November 2 1999. US Patent 5,977,251.
2. J.J. Zacca and W.H. Ray. Modelling of the liquid phase polymerization of olefins in loop reactors. Chemical Engineering Science, 48(22):3743–3765, 1993.

Outline

- **Background and Motivation**
- **Model Development**
  - Mass and heat balance equations
  - Moment model and polymer property correlations to predict product density and MI
  - ***Surrogate model*** to predict bubble point pressure
  - Recycle streams introduced as ***a variable time delay model***
- **Offline Dynamic Optimization**
  - Proposed new optimization framework – ***multistage optimization formulation***
  - Demonstrations: single-stage formulation vs. multistage formulation
- **Optimization under Uncertainty**
  - Concept of backoff
  - Approaches to obtaining backoffs
  - Case study on hypothetical problem
- **Online Implementation: Nonlinear Model Predictive Control + State Estimation**
- **Conclusions and Future Work**

Model Development

Process Flowsheet



Introduce variable time delay model into optimization model

- Modelled as CSTR
- Method of moments used to calculate product properties
- Data-driven surrogate VLE model for bubble point pressure monitoring

Offline Dynamic Optimization

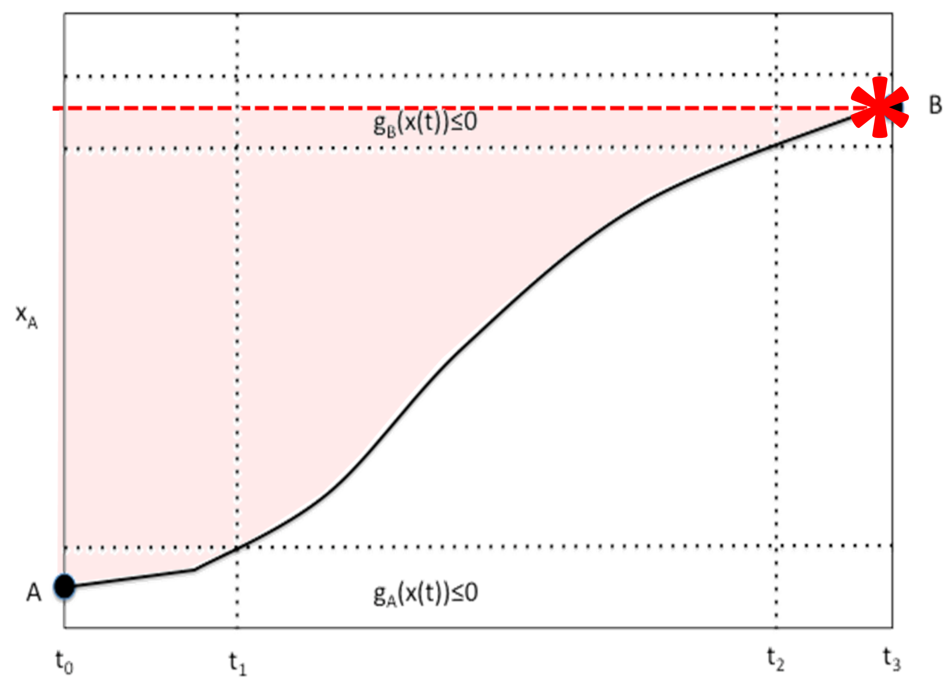
Single-stage Formulation

- **Objective function for obtaining optimal transition profile**

$$\min \int_0^{t_f} \left\| y(t) - y^* \right\|_Q^2 + \left\| u(t) - u^* \right\|_R^2 dt$$

  - y is a vector of output variables, u is a vector of manipulated variables.
  - Q and R are diagonal weighting matrices.

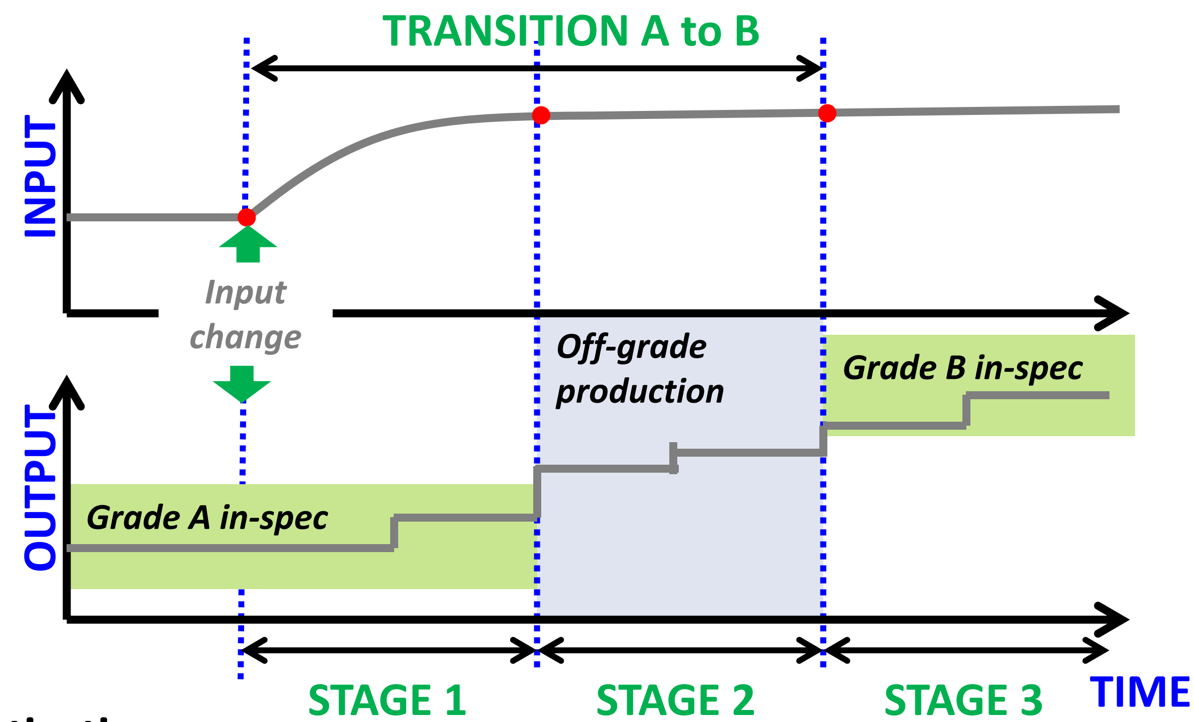
- **Simultaneous dynamic optimization**
  - **3-point collocation on finite elements** to discretize both controls and states
  - Over **130,000** variables and equations
  - Resulting NLP problem solved in GAMS



Dealing with Specification Bands[3]

Multistage Optimization

Target ± *Specification Band*
instead of *Target*



Motivation:

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

3. Nyström, R. H., Franke, R., Harjunkoski, I., & Kroll, A. (2005). Production campaign planning including grade transition sequencing and dynamic optimization. *Computers & chemical engineering*, *29*(10), 2163-2179.

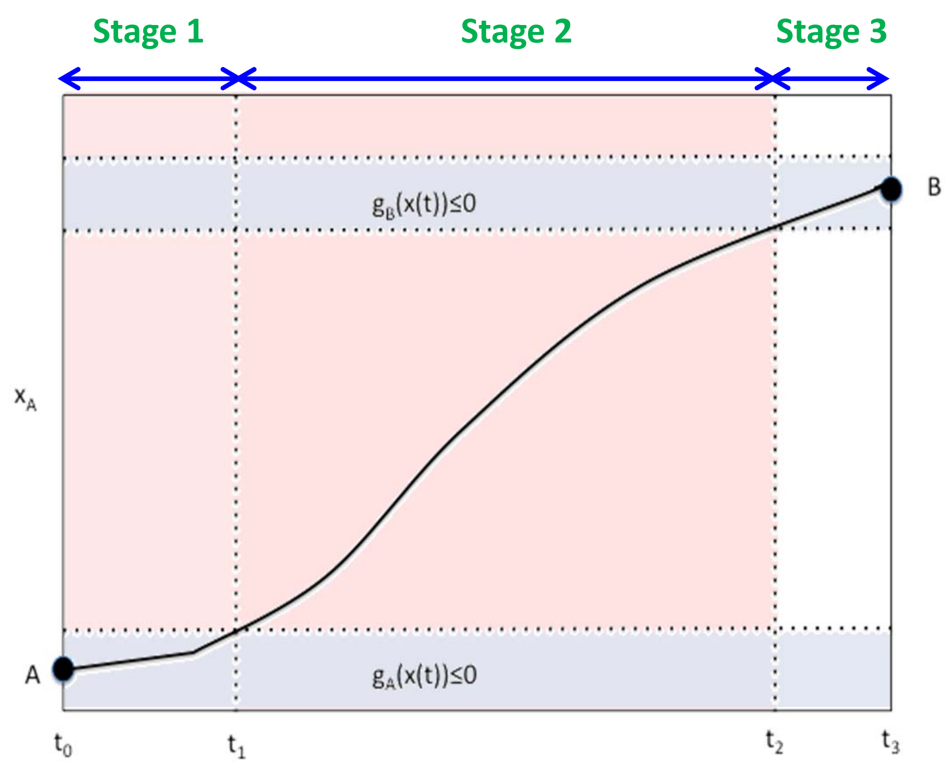
Dealing with Specification Bands

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



- Minimize a combination of **the off-spec product between t1 and t2** and **the transition time t2-t0**.
- Regularizing term to promote a smooth unique solution
- Moving finite element

To Lower Density and Higher MI

Comparison of Density Profile

Density transition: 0.908→ 0.864 g/cm ^{3}

MI transition: 1→12 g/10 min

Constant production level

*Kinetics from open literature

Baseline:

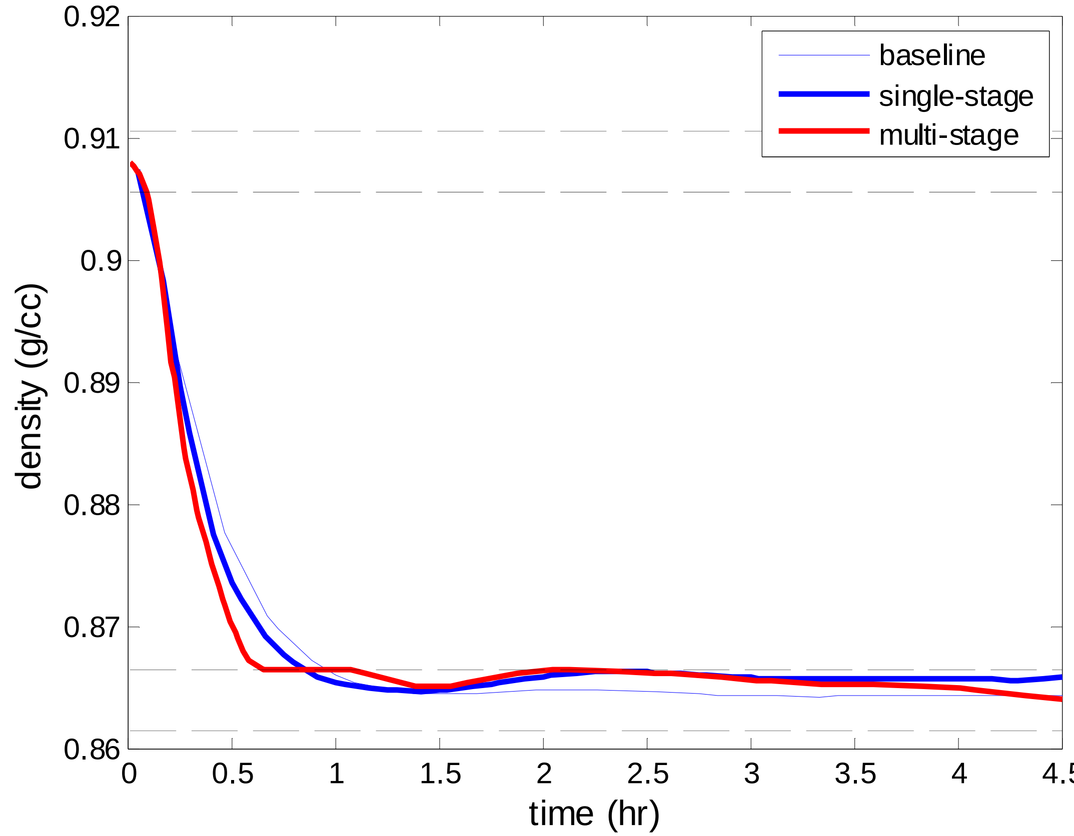
- Ramping all inputs at constant rates

Single Stage:

- Fast transition

Multistage:

- Faster transition in Stage 2
- Possible oscillations within the band



To Lower Density and Higher MI

Comparison of MI Profile

MI: 1 → 12 g/10min

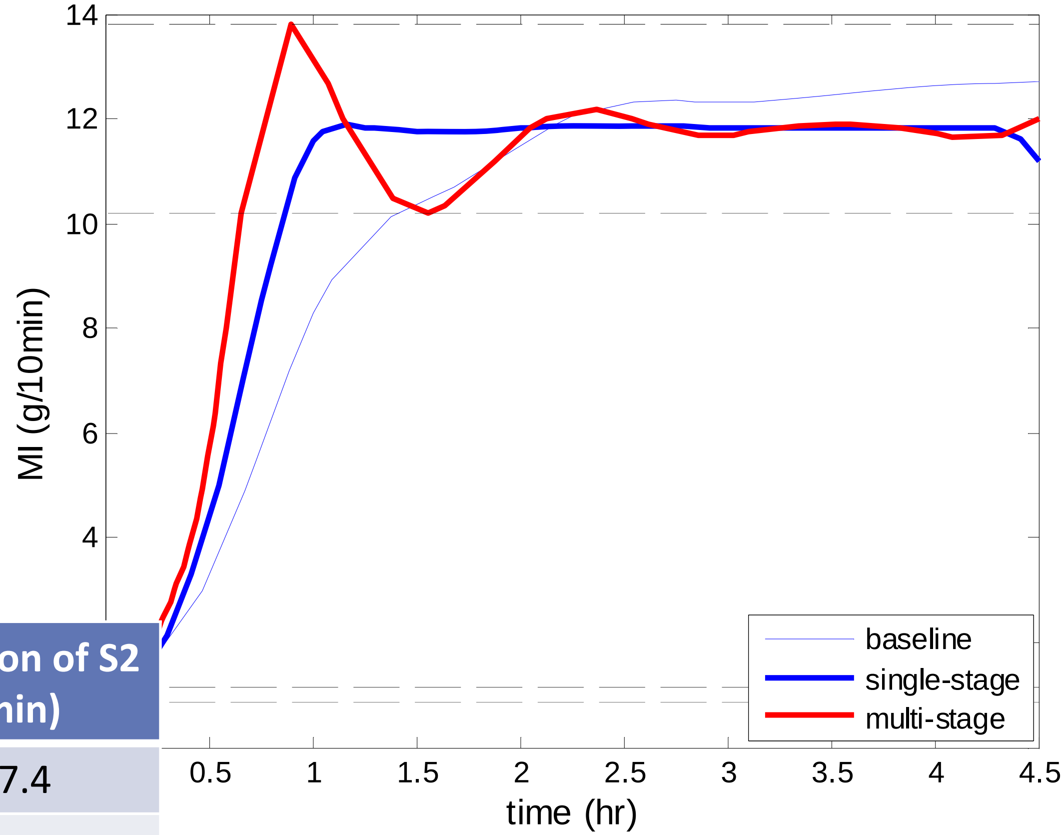
Multistage

- Capable of minimizing the transition time and the off-grade product directly

  → Economic objectives

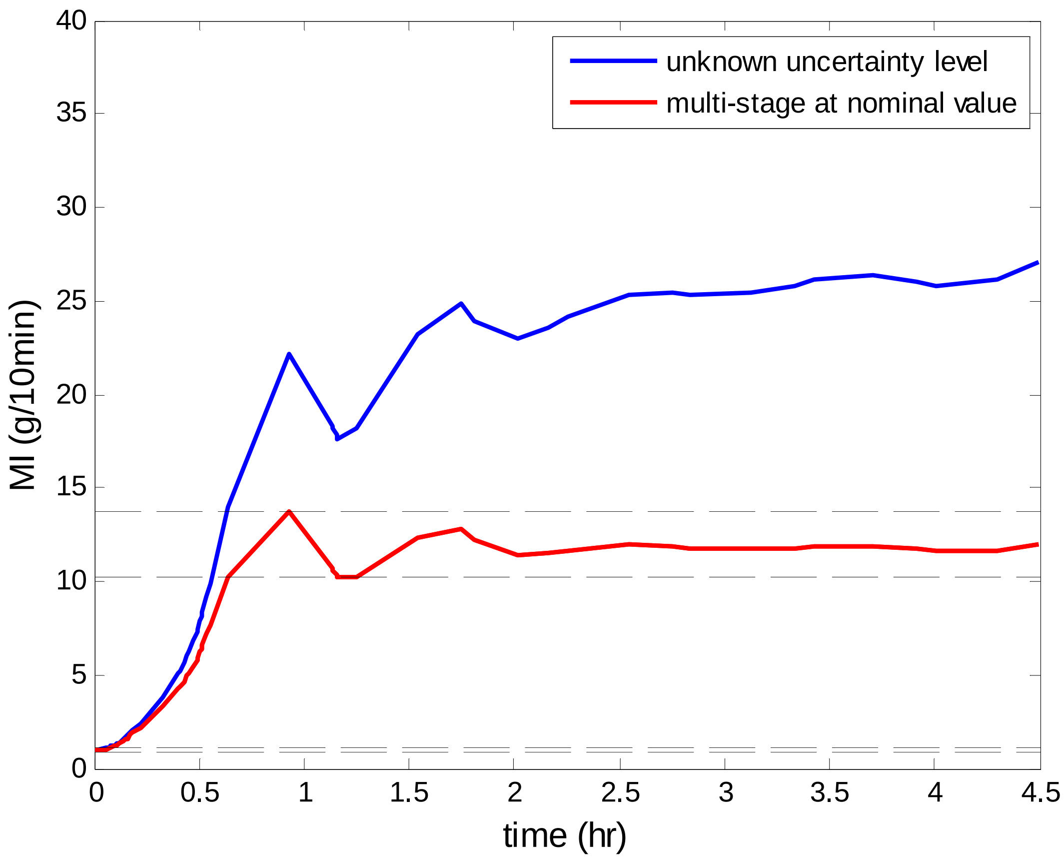
- Faster transition in S2 reduces the transition time
- Oscillations within the band
- **More than 50% reduction**

	Transition Time (min)	Duration of S2 (min)
Baseline	82.8	77.4
Single-stage	51.0	45.6
Multistage	39.1	33.6



Motivation

Optimal solution fails at unknown uncertainty level



Methodology

Concept of Backoff[4]

Original constraints

$$f(x,u,p) \leq 0$$

Updated inequality constraints

$$f(x,u,\bar{p}) + b_c \leq 0$$

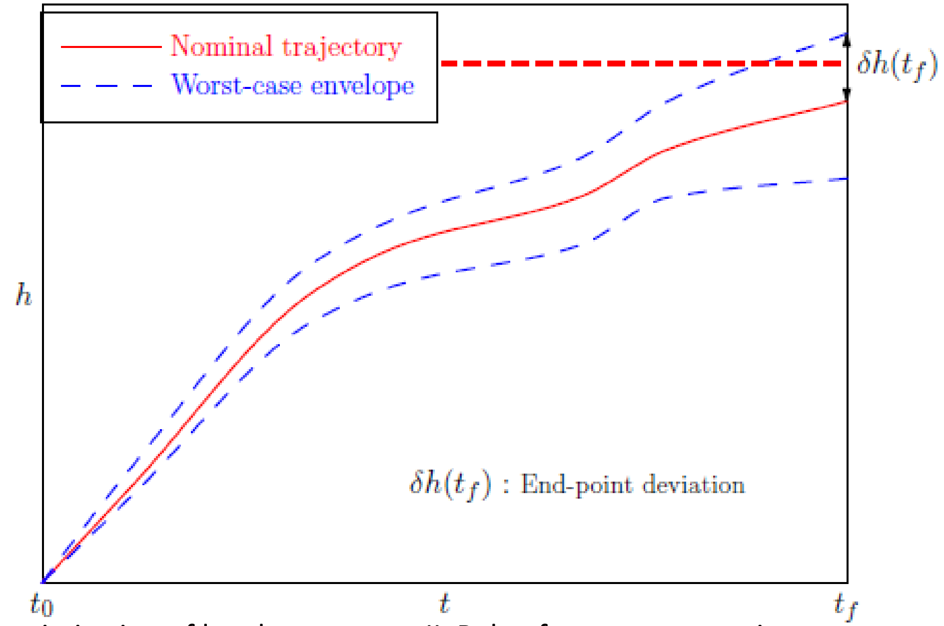
Nominal value

$b_c \geq 0$ backoffs required for constraint satisfaction in the presence of uncertainty

When $f(x,u,\bar{p}) + b_c = 0$,
$P[f(x,u,p) \leq 0] = c$

confidence level

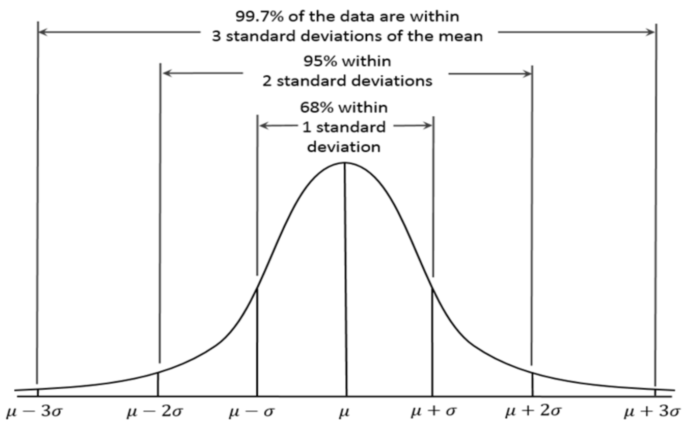
$c = 1$ worst case solution



4. Srinivasan, B., Bonvin, D., Visser, E., & Palanki, S. (2003). Dynamic optimization of batch processes: II. Role of measurements in handling uncertainty. *Computers & Chemical Engineering*, *27*(1), 27-44.

Monte Carlo simulation to approximate b_c

Assume uncertainty p follows normal distribution $\mathrm{N}(p_0, \sigma^2)$



Procedure

- Sample from $\mathrm{N}(p_0, \sigma^2)$
- Simulate m times with nominal optimal input
- Get an idea of how output varies with the change of uncertainty level to approximate b_c

Optimization w/ Nominal Uncertainty Level

↓ Optimal input profiles

Monte Carlo simulation

↓ State and output profiles

Data Processing
Approximate backoff b_c

↓ Backoff b_c

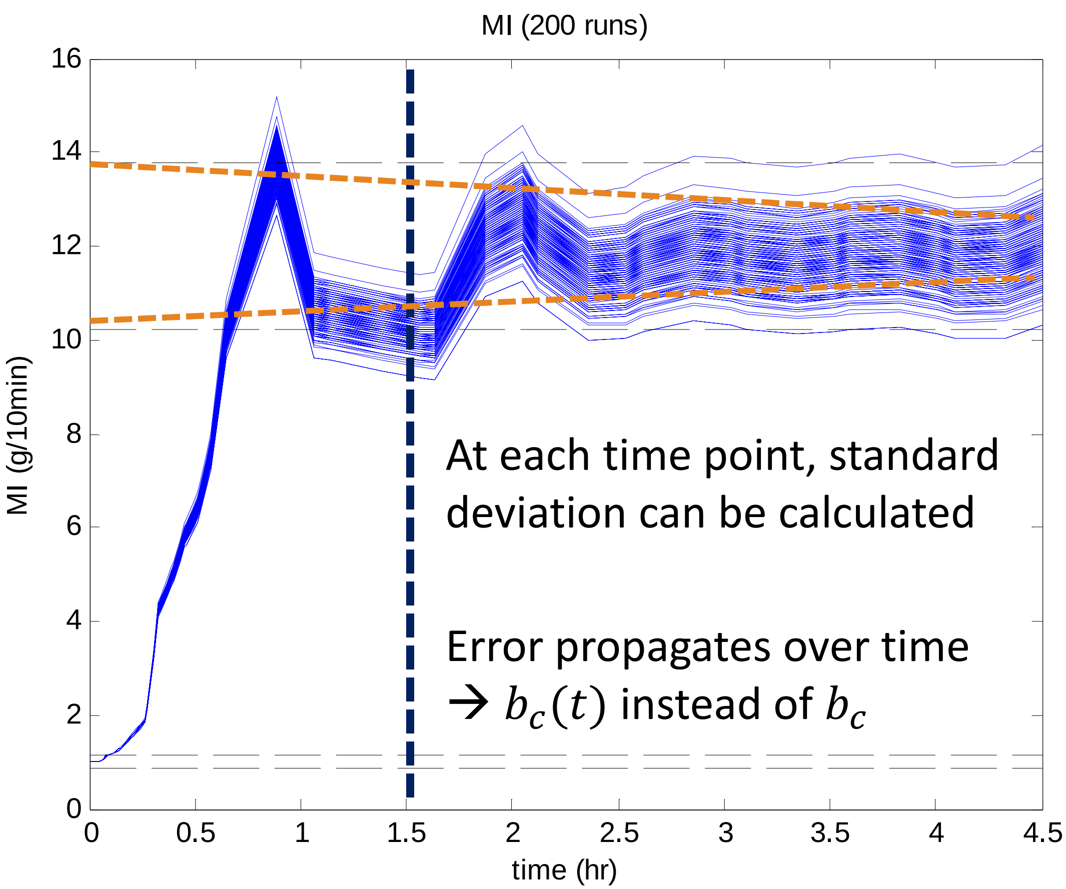
Optimization w/ Backoff constraints

↓ “Robust” optimal input profiles

Monte Carlo simulation
Check the performance

Case Study

Monte Carlo simulation: MI profiles



Optimization w/ Nominal Uncertainty Level

↓ Optimal input profiles

Monte Carlo simulation

↓ Resulting state and output profiles

Data Processing
Approximate backoff b_c

↓ Backoff b_c

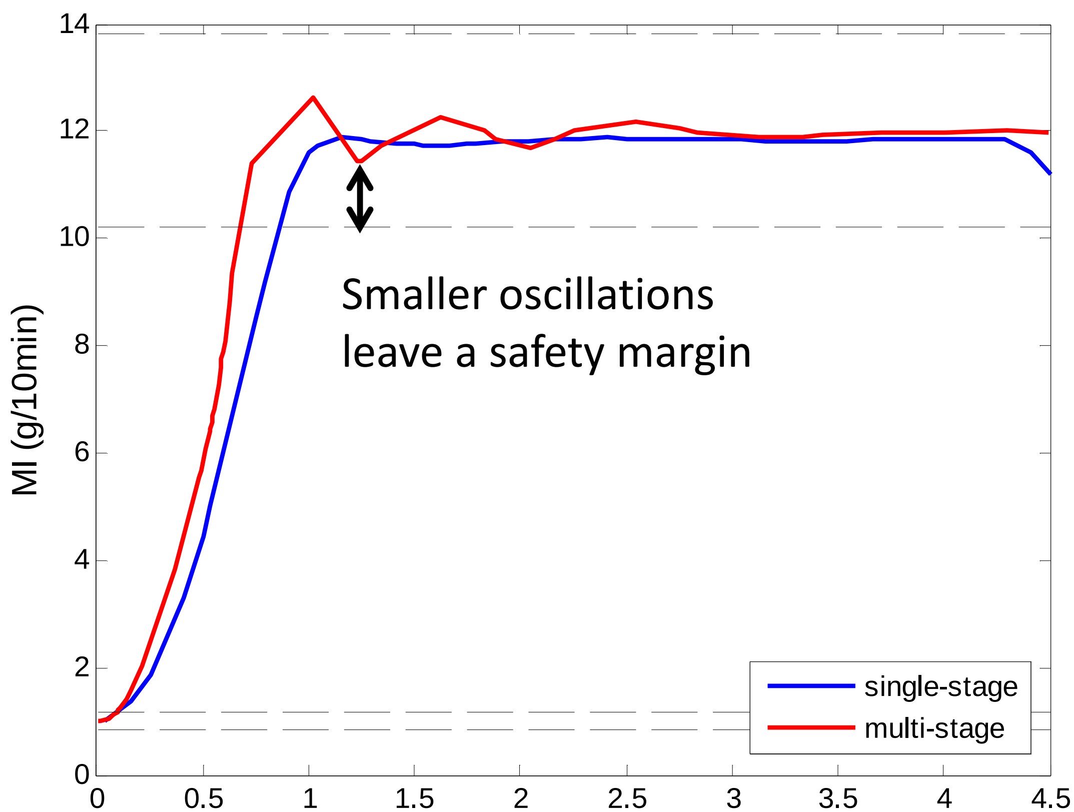
Optimization w/ Backoff constraints

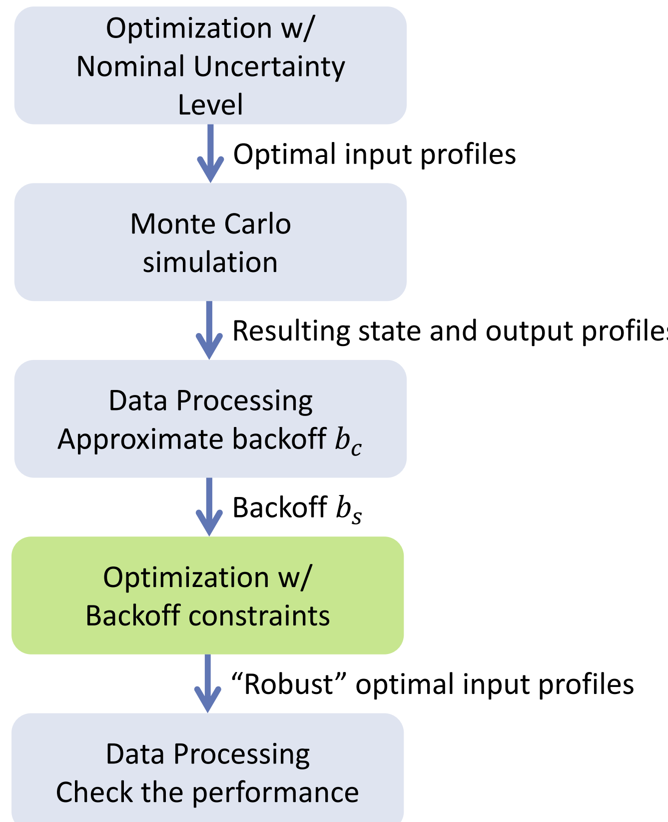
↓ "Robust" optimal input profiles

Data Processing
Check the performance

Case Study

Optimization with Time-varying Backoffs

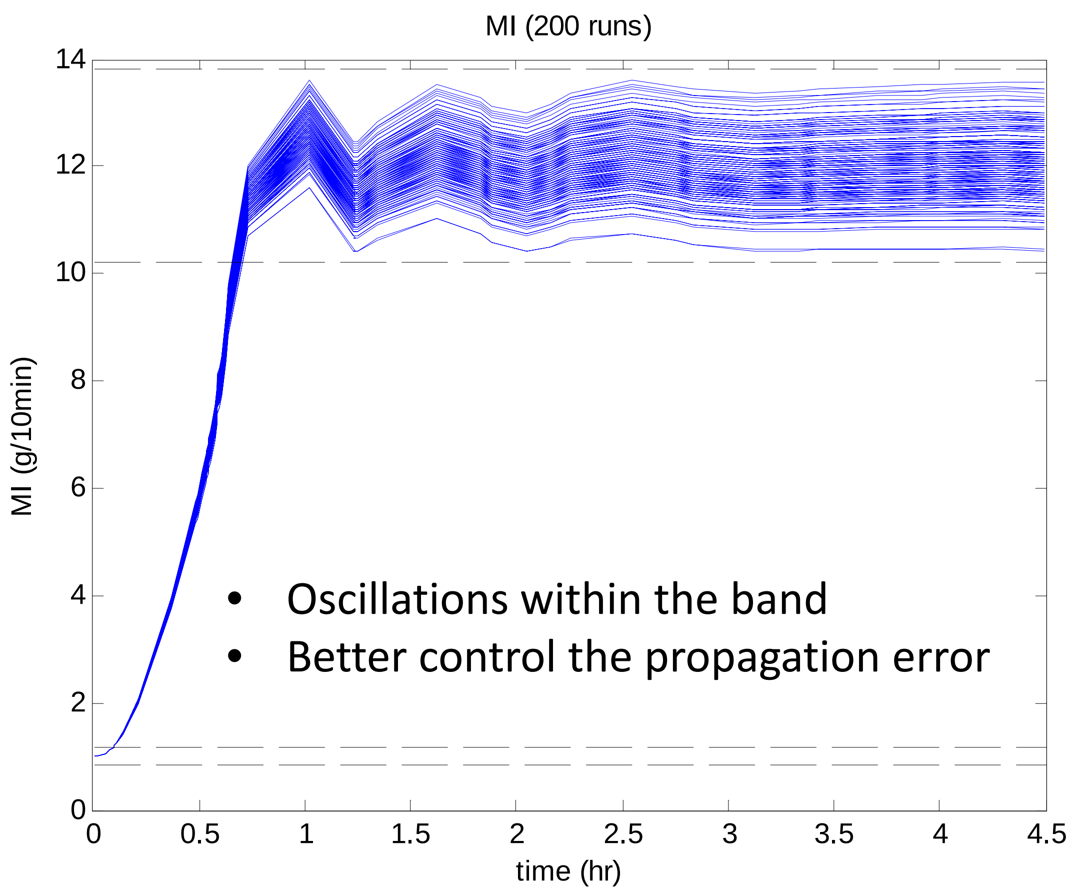




	Transition Time (min)	Duration of S2 (min)
Multistage w/o backoffs	39.1	33.6
Multistage w/ time-varying backoffs	40.2	34.8

Case Study

Performance under Uncertainty



- Oscillations within the band
- Better control the propagation error

Optimization w/ Nominal Uncertainty Level

↓ Optimal input profiles

Monte Carlo simulation

↓ Resulting 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

Online Implementation

Nonlinear Model Predictive Control (NMPC)

NMPC considered for effective control of polymer properties[6]

- Strong nonlinearity of polymerization process
- Process constraints and bounds on variables
- Coupled controlled variables; multi-input-multi-output (MIMO) system

Nonlinear programming formulation for NMPC[7]

$$\begin{aligned} \min_{z_l, v_l} \quad & J_N := F(z_N) + \sum_{l=0}^{N-1} \psi(z_l, v_l) \\ s.t. \quad & z_{l+1} = f(z_l, v_l), l = 0, \ldots, N-1 \\ & z_0 = x(k), z_l \in \mathbb{X}, z_N \in \mathbb{X}_f, v_l \in \mathbb{U} \end{aligned}$$

- Given a **target trajectory**
- Make future predictions of model's behavior based on **plant model** + **state estimation**
- **Optimize over manipulated variables**

F, ψ - terminal and stage costs, z - state variables, z_0 - initial value,

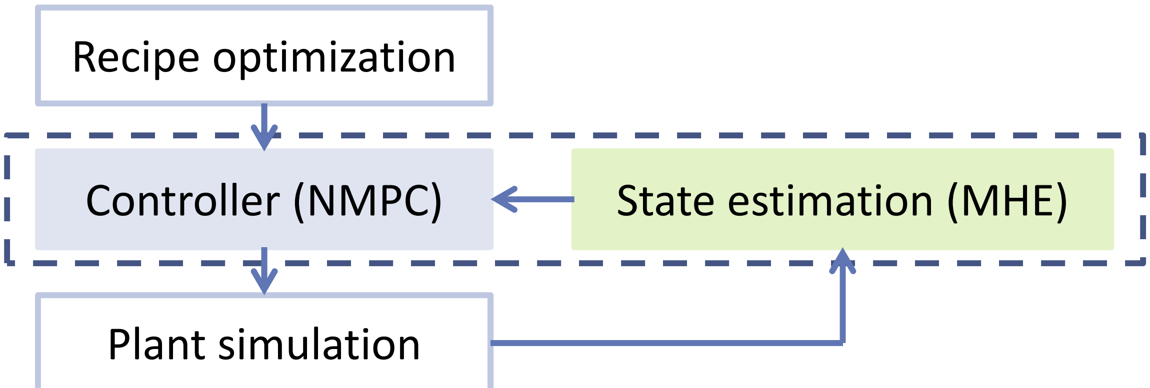
v - manipulated variables, $x(k)$ - measurement of state at t_k,

N - time horizon with N time steps

6. John R Richards and John P Congalidis. Measurement and control of polymerization reactors. Computers & chemical engineering, 30(10):1447–1463, 2006.
7. Victor M Zavala and Lorenz T Biegler. The advanced-step nmpc controller: Optimality, stability and robustness. Automatica, 45(1):86–93, 2009.

Online Implementation

Online Optimization Framework



MHE

- ***Similar model*** as solved in recipe optimization
- Optimization over ***states and parameters***
- Estimate states and parameters based on the data in the past

NMPC

- ***Similar model*** as solved in recipe optimization
- Optimization over ***manipulated variables***
- Determine controls to track setpoint

K K+1 K+2

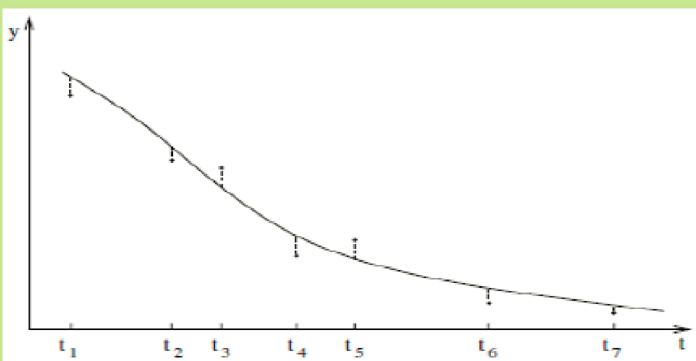
time

Expanding horizon LSE + Shrinking horizon NMPC[8]

- Good performance satisfying the product specification target despite initialization errors and measurement noises

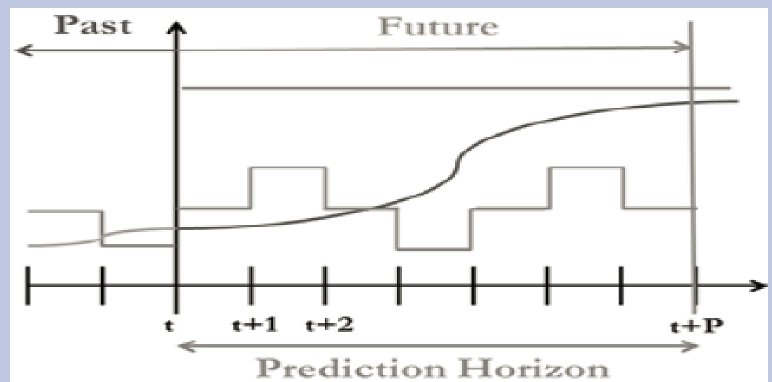
Expanding horizon LSE

- To determine current state and parameter estimates
- Over different control time intervals
- Minimize squared measurement errors and disturbance regularization



Shrinking horizon NMPC

- To minimize the overall horizon
- To track dynamic setpoint
- Penalty to end-point constraints



time

8. Jung, T. Y., Nie, Y., Lee, J. H., & Biegler, L. T. (2015). Model-based On-Line Optimization Framework for Semi-batch Polymerization Reactors.

Conclusions and Future Work

- **Model Development**
  - Mass and heat balance equations
  - Moment model and polymer property correlations to predict product density and MI
  - ***Surrogate model*** to predict bubble point pressure
  - Recycle streams introduced as ***a variable time delay model***
- **Offline Dynamic Optimization**
  - Proposed new optimization framework – ***multistage optimization formulation***
  - Demonstrations: Single-stage formulation vs. multistage formulation
- **Optimization under Uncertainty**
  - ***Monte Carlo simulation*** to obtain backoffs
  - Case study on hypothetical problem
- **Online Implementation: *eh*-LSE + *sh*-NMPC**

Questions?