Unscented Kalman Filter based Nonlinear MPC of an Autoclave LDPE Reactor

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Introduction

- Most polymerization reactors exhibit highly nonlinear dynamics and can benefit from process control strategies that account for these features.
- Chemical processes usually operate at or close to constraints (e.g. product quality, environmental) and it is important that the controller is aware of them.
- Nonlinear model predictive control (NMPC) is an advanced control algorithm that *explicitly* considers nonlinear dynamics and plant constraints in its formulation.
- The goal of this work was to develop and demonstrate (simulation) an NMPC formulation for the control of temperature profile and polymer quality (molecular weight) in a high-pressure LDPE autoclave reactor.

Process Modeling

- Industrial LDPE autoclaves are usually long vessels with multiple initiator, monomer feed points along the reactor length.
- The reactor is usually assumed to be adiabatic because the thick reactor walls required to withstand high operating pressures more-or-less prevents heat transfer/loss.
- In this study, the LDPE autoclave is modeled as an adiabatic reactor with three well mixed zones.
- The reactor is divided such that a single pair of initiator, monomer feed streams enters each zone.
- Backmixing between adjacent zones is included to model imperfect mixing.
- Online measurements of temperature profile and molecular weight (i.e. controlled variables) are assumed available.
- Control inputs are the initiator (heating effect), monomer (cooling effect) feed rates.

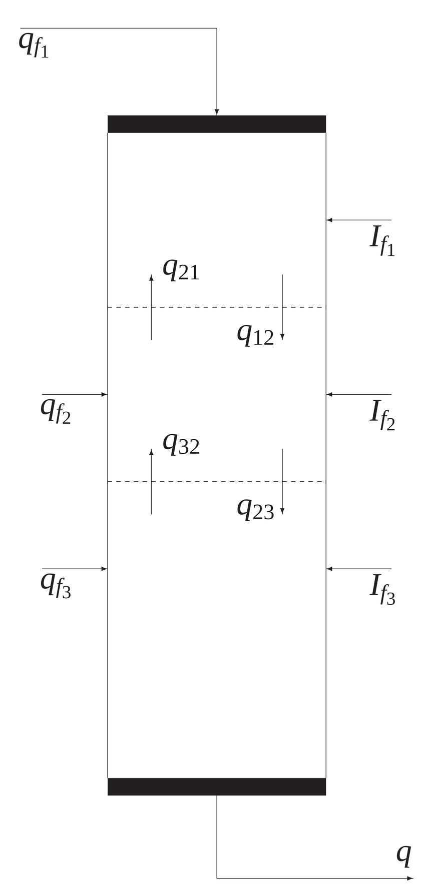

Figure: LDPE Reactor

Model Development

- Material, energy, and population balances were developed for all three reactor zones yielding a system of 21 ODEs with state vector

$$x = [\mathbf{I} \quad \mathbf{M} \quad \mathbf{M_t} \quad \mathbf{T} \quad \mu_\mathbf{0} \quad \mu_\mathbf{1} \quad \mu_\mathbf{2}]^T$$

  where, for example

$$\mathbf{T} = [T_1 \quad T_2 \quad T_3]$$

- The controlled outputs (z_k), measurements (y_k), and control inputs (u_k) used here are:

$$z_k = y_k = \left[\mathbf{T} \quad \overline{M}_w\right]^T \qquad u_k = [\mathbf{q_f} \quad \mathbf{I_f}]^T$$

  where,

$$\overline{M}_w = M_0 \left(\mu_{2_3}/\mu_{1_3}\right)$$

Controller Formulation

- NMPC is based on the repeated solution online of a finite-horizon optimal control problem at each sampling instance.
- The control algorithm can be divided into two different NLPs, (i) Regulator, and (ii) Target Calculator.

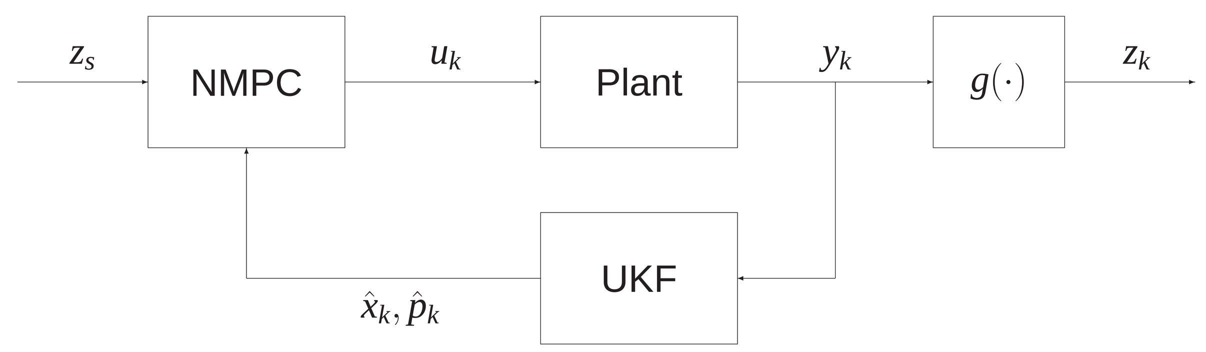

Figure: Schematic of the control structure

Regulator

- The regulator NLP calculates 'optimal' state, control profiles which minimize a given (usually) quadratic cost function.
- Only the first control input (u_j) is applied to the plant. The remaining state, control profile is used to initialize the next Regulator NLP.

$$\min_{\mathbf{x},\mathbf{u}} \|z_{j+P} - z_{t,j}\|^2_{\mathbf{P}} + \sum_{k=j}^{j+P-1} \|z_k - z_{t,j}\|^2_{\mathbf{Q}} + \|u_k - u_{t,j}\|^2_{\mathbf{R}} + \|\Delta u_k\|^2_{\mathbf{S}}$$

subject to:

$$x_{k+1} = f(x_k, u_k, p_k, 0, t_k), \;\; y_k = h(x_k, p_k, t_k), \;\; z_k = g(y_k)$$
$$x_L, u_L, \Delta u_L \leq x_k, u_k, \Delta u_k \leq x_U, u_U, \Delta u_U$$
$$u_k = u_{M-1} \quad \forall k = M, M+1, \ldots, P$$

Target Calculator

- The target calculator NLP identifies *steady-state* targets for the states, controls that satisfy, or (if impossible) approximately satisfy the controlled output setpoint.

$$\min_{x_{t,j}, u_{t,j}, \eta} \tfrac{1}{2}\eta^T Q \eta + q^T \eta + \tfrac{1}{2}\Delta u_{t,j}^T R \Delta u_{t,j}$$

subject to:

$$x_{t,j} = f(x_{t,j}, u_{t,j}, p_j, 0, t_j), \;\; y_{t,j} = h(x_{t,j}, p_j, t_j), \;\; z_{t,j} = g(y_{t,j})$$
$$z_{t,j} - \eta \leq z_s \leq z_{t,j} + \eta$$
$$x_L, u_L \leq x_{t,j}, u_{t,j} \leq x_U, u_U$$
$$\eta \geq 0$$

State Estimation

- Unscented Kalman filtering (UKF) was employed to estimate states $(\hat{x}_k)$ and integrating disturbances $(\hat{p}_k)$ from measurements.
- The UKF does not require Jacobians to be provided, unlike the extended Kalman filter (EKF), which makes its implementation very rapid, as Jacobians are hard to evaluate for polymerization models.
- Previous research has proven that UKF gives higher-order accuracy state estimates than EKF which has traditionally been used in chemical engineering.
- Unfortunately, due to space constraints, technical details on the UKF methodology are omitted here.

Simulation Results

- The finite-horizon optimal control problem was discretized using orthogonal collocation on finite elements (OCFE), and the resulting NLP was solved using the feasible-path GRG code CONOPT.
- Simulations to test the controller performance were performed in Matlab. The states, inputs, and outputs were transformed to a 'scaled-deviation' form to improve conditioning of the controller NLPs.
- The control interval chosen was 1min long. Prediction horizon $P = 6$ and control horizon $M = 4$ was found to give acceptable results.

Response to Polymer Grade Change

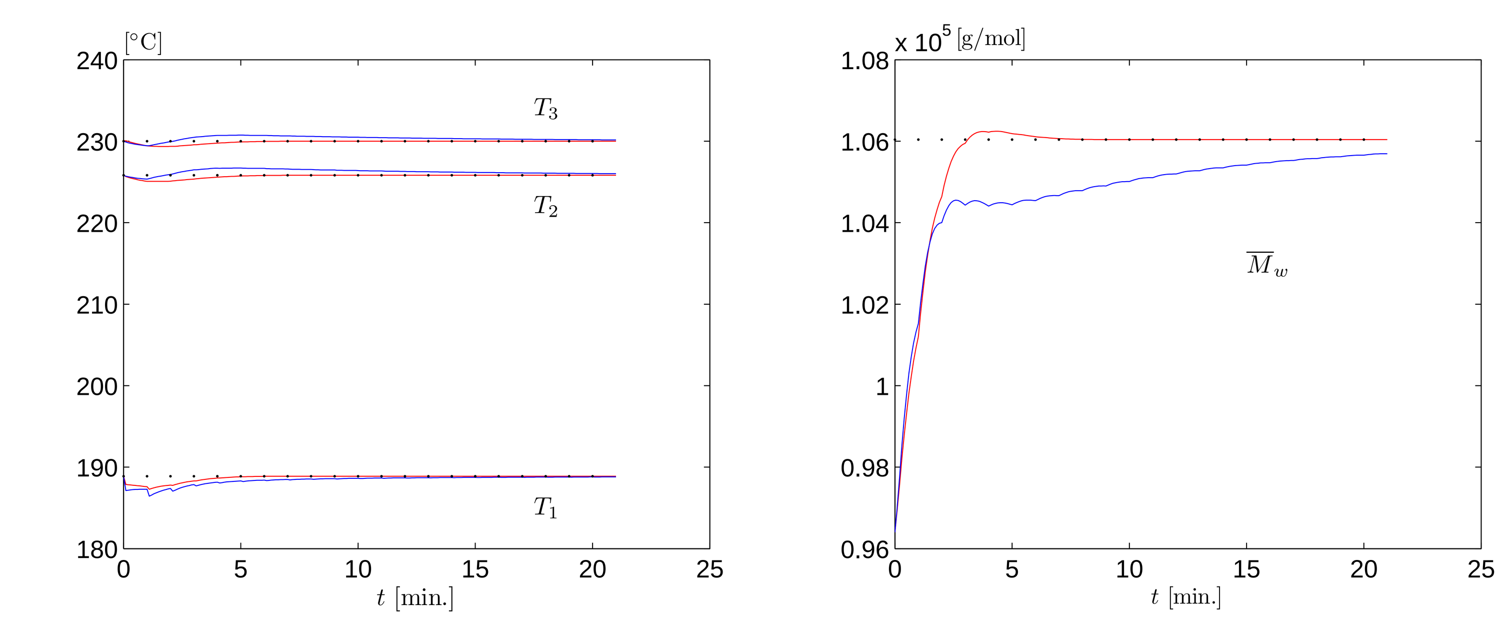

Figure: Comparison of temperature profile (left) and weight-averaged molecular weight (right) responses to a polymer grade change for NMPC (red) and linear MPC (blue) controllers. Note: No setpoint change to the temperature profile.

Response with Plant-Model Mismatch

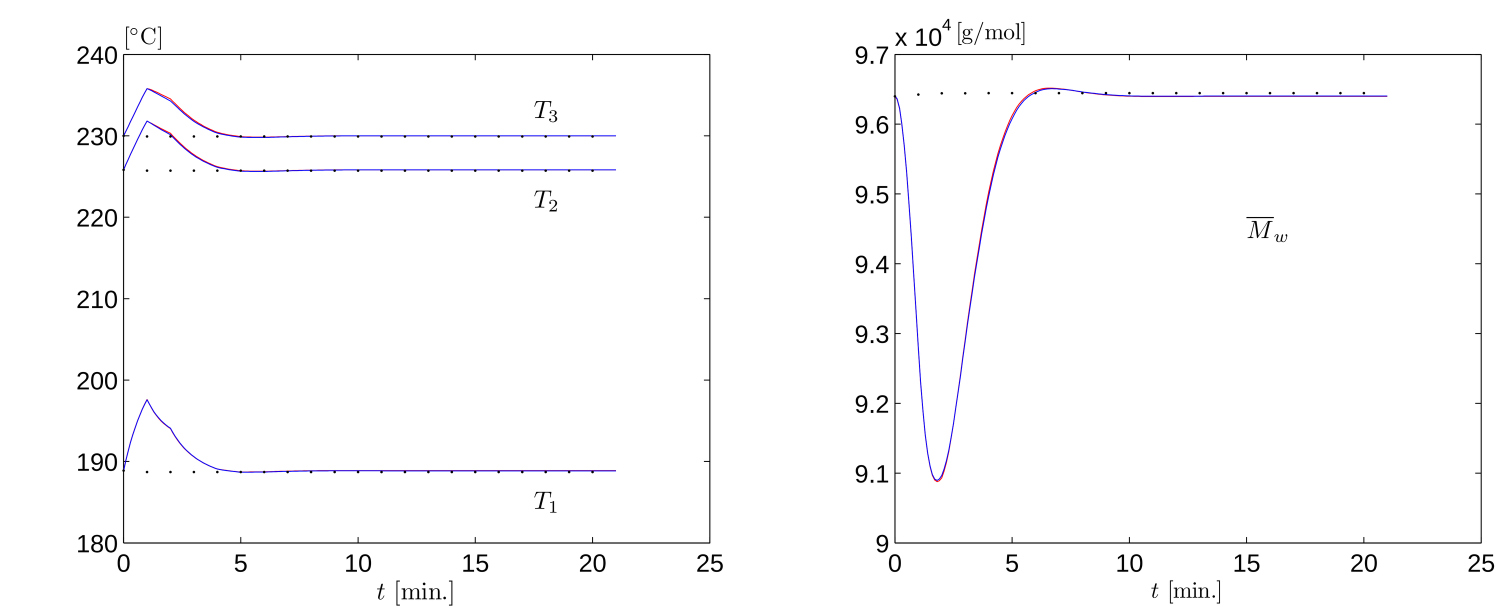

Figure: Comparison of temperature profile (left) and weight-averaged molecular weight (right) responses to a sudden unmeasured $+7\,^\circ$C rise in feed temperature for the nominal (red) and plant-model mismatch (blue) cases. The mismatch used here was a $+5\%$ increase to some rate constants in the 'internal' nonlinear model.

Conclusions

- NMPC was shown to be superior to linear MPC in polymer grade change situations, though the difference is more subtle for regulatory control (results not shown here).
- The results also show that the NMPC controller performs well even in the presence of reasonable plant-model mismatch.

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