Unscented Kalman Filter based Nonlinear MPC of an Autoclave LDPE Reactor
Noel C. Jacob and Ramdhane Dhib
Department of Chemical Engineering, Ryerson University

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.

Model Development

- Material, energy, and population balances were developed for all three reactor zones yielding a system of 21 ODEs with state vector
  \[ x = [I \ M \ 1 \ T \ \mu_1 \ \mu_2]^T \]
  where, for example
  \[ T = [T_1 \ T_2 \ T_3] \]
- The controlled outputs \( y_z \), measurements \( y_k \), and control inputs \( u_k \) used here are:
  \[ y_z = y_k = [T \ \mu_1 \ \mu_2]^T \]
  \[ u_k = [\mu_1 \ \mu_2]^T \]

State Estimation

- Unscented Kalman filtering (UKF) was employed to estimate states \( x_k \) and integrating disturbances \( \mu_k \) 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.

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](image)

Regulator

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

\[
\min_{\Delta u_k} \| y_k - z_k \|^2 + \sum_{k=0}^{P-1} \| y_k - z_k \|^2 + \| u_k - w_k \|^2 + \| \Delta u_k \|^2
\]

subject to:
\[
\begin{align*}
T_{k+1} &= f(T_k, \mu_k, q_k, q_0, 0.0) ; \\
\mu_{k+1} &= f(T_k, \mu_k, q_k, q_0, 0.0) ; \\
T_0 &= 210^\circ C ; \\
\mu_0 &= 210 \text{[min.]} ; \\
\eta_k & > 0 ; \\
\eta_k & < 1.04
\end{align*}
\]

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.

\[
\min_{\Delta u_k} \frac{1}{2} \Delta u_k^T R_1 \Delta u_k + \frac{1}{2} \Delta y_k^T R_2 \Delta y_k
\]

subject to:
\[
\begin{align*}
T_{k+1} &= f(T_k, \mu_k, q_k, q_0, 0.0) ; \\
\mu_{k+1} &= f(T_k, \mu_k, q_k, q_0, 0.0) ; \\
T_0 &= 210^\circ C ; \\
\mu_0 &= 210 \text{[min.]} ; \\
\eta_k & > 0 ; \\
\eta_k & < 1.04
\end{align*}
\]

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.](image)

Response with Plant-Model Mismatch

![Figure: Comparison of temperature profile (left) and weight-averaged molecular weight (right) responses to a sudden unmeasured +7°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.](image)

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.