Nonlinear Model Predictive Control of a Batch Polymerization Reactor

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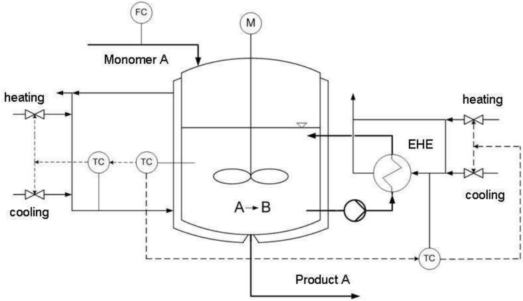
Batch Polymerization Reactor

- Monomer is fed into the reactor and it turns into a polymer via a very exothermic chemical reaction.

The reactor consists of :

- Jacket
- External Heat Exchanger (EHE)



- We can use both to control the temperature inside the reactor.

Mathematical Model

- Mass balances for the water, monomer and product of the process $(\mathbf{m}_w, \mathbf{m}_m, \mathbf{m}_p)$:

$$\dot{\mathbf{m}}_w = \dot{\mathbf{m}}_f w_{w,f}$$
$$\dot{\mathbf{m}}_m = \dot{\mathbf{m}}_f w_{m,f} - k_{r_1} m_{m,r} - k_{r_2} m_{awt} \frac{\mathbf{m}_m}{m_{ges}}$$
$$\dot{\mathbf{m}}_p = k_{r_1} m_{m,r} + \rho_1 k_{r_2} m_{awt} \frac{\mathbf{m}_m}{m_{ges}}$$

where

$k_{r_1} = k_0 \exp(\frac{-E_a}{R(T_r+273.15)})(k_{u_1}(1 - \frac{\mathbf{m}_p}{\mathbf{m}_p+\mathbf{m}_m}) + k_{u_2} \frac{\mathbf{m}_p}{\mathbf{m}_p+\mathbf{m}_m})$,
$k_{r_2} = k_0 \exp(\frac{-E_a}{R(T_{ek}+273.15)})(k_{u_1}(1 - \frac{\mathbf{m}_p}{\mathbf{m}_p+\mathbf{m}_m}) + k_{u_2} \frac{\mathbf{m}_p}{\mathbf{m}_p+\mathbf{m}_m})$
are reaction ratio inside reactor and EHE, respectively.

$m_{ges} = \mathbf{m}_w + \mathbf{m}_m + \mathbf{m}_p$ corresponds to the total mass,
$m_{m,r} = \mathbf{m}_m - \mathbf{m}_m \frac{m_{awt}}{m_{ges}}$ is current amount of monomer inside of the reactor,
$k_k = (\mathbf{m}_w k_{ws} + \mathbf{m}_m k_{ms} + \mathbf{m}_p k_{ps})/m_{ges}$ denotes the heat transfer coefficient of the mixture inside the reactor.

Mathematical Model

- Energy balances for the reactor, mixture in EHE, coolant leaving EHE, jacket and vessel $(\mathrm{T}_r, \mathrm{T}_{ek}, \mathrm{T}_{awt}, \mathrm{T}_j, \mathrm{T}_s)$:

$$\dot{\mathrm{T}}_r = \frac{1}{c_{p,r} m_{ges}} (\dot{\mathrm{m}}_f c_{p,f} (T_f - \mathrm{T}_r) + \Delta H_r k_{r_1} m_{m,r} - k_k A(\mathrm{T}_r - \mathrm{T}_s) - \dot{m}_{awt} c_{p,r} (\mathrm{T}_r - \mathrm{T}_{ek}))$$

$$\dot{\mathrm{T}}_{ek} = \frac{1}{c_{p,r} m_{awt}} (\dot{m}_{awt} c_{p,w} (\mathrm{T}_r - \mathrm{T}_{ek}) - \alpha(\mathrm{T}_{ek} - \mathrm{T}_{awt}) + k_{r_2} \mathrm{m}_m m_{awt} \frac{\Delta H_r}{m_{ges}})$$

$$\dot{\mathrm{T}}_{awt} = (\dot{\mathrm{m}}_{awt,kw} c_{p,w} (\mathrm{T}_{awt}^{in} - \mathrm{T}_{awt}) - \alpha(\mathrm{T}_{awt} - \mathrm{T}_{ek}))/(c_{p,w} m_{awt,kw})$$

$$\dot{\mathrm{T}}_j = \frac{1}{c_{p,w} m_{m,kw}} (\dot{m}_{m,kw} c_{p,w} (\mathrm{T}_j^{in} - \mathrm{T}_j) + k_k A(\mathrm{T}_s - \mathrm{T}_j))$$

$$\dot{\mathrm{T}}_s = \frac{1}{c_{p,s} m_s} (k_k A(\mathrm{T}_r - \mathrm{T}_s) - k_k A(\mathrm{T}_s - \mathrm{T}_j))$$

Optimal Control Problem

Let define the vector of entire state and control input variable for each sampling time to be $x_k = \{\mathbf{m}_{w,k}, \mathbf{m}_{m,k}, \mathbf{m}_{p,k}, \mathbf{T}_{r,k}, \mathbf{T}_{ek,k}, \mathbf{T}_{awt,k}, \mathbf{T}_{j,k}, \mathbf{T}_{s,k}\}$ and $u_k = \{\dot{\mathbf{m}}_{f,k}, \mathbf{T}^{in}_{awt,k}, \mathbf{T}^{in}_{j,k}\}$, where $\dot{\mathbf{m}}_{f,k}, \mathbf{T}^{in}_{awt,k}, \mathbf{T}^{in}_{j,k}$ are the feed flow, coolant temperature at the inlet of the jacket, EHE. Now we can define an optimization program as follows:

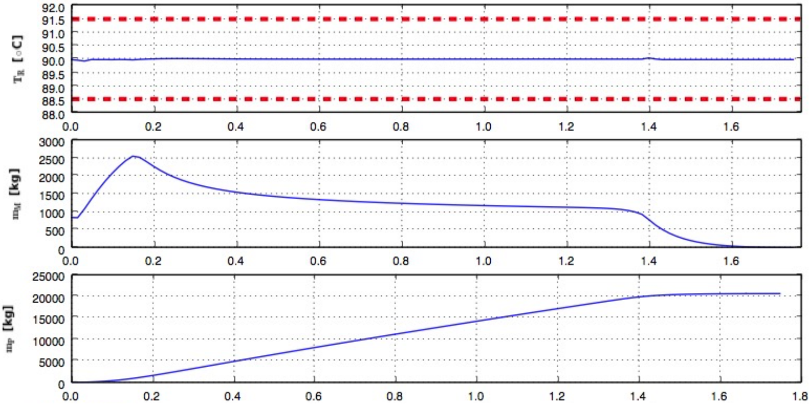
$$\min_{u} \sum_{k=1}^{N} -\mathbf{m}_{p,k} + \alpha \left|\mathbf{T}_{r,k} - T_{set}\right|^2$$

$$\begin{aligned} x_{k+1} &= f(x_k, u_k) \\ \underline{\mathbf{x}} \leq x_k &\leq \bar{\mathbf{x}} \\ \underline{\mathbf{u}} \leq u_k &\leq \bar{\mathbf{u}} \end{aligned}$$

where T_{set} is the desired reaction temperature to be ensured that the produced polymer has the required properties.

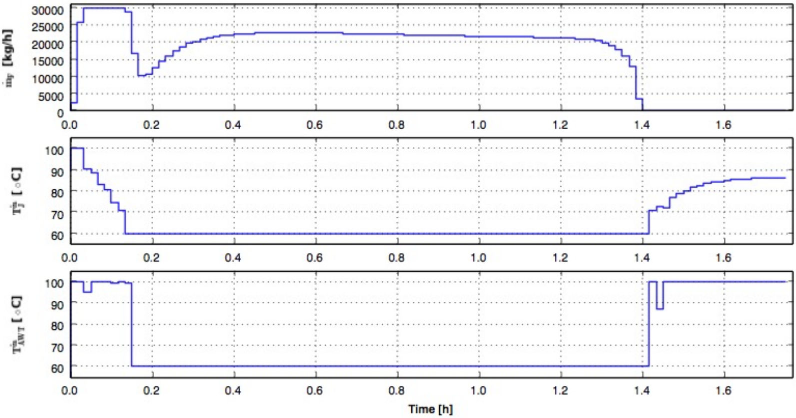
Simulation Study

State variables trajectory:



Simulation Study

Control variables trajectory:



Thanks!
Questions?