Constrained NMPC for Maximizing production in polymerization processes

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Outline

- Connections with fast systems
- Problem statement
- The parametrized NMPC solution
- Model uncertainty
- Simulation results
- Experimental results
- Computation time

Connections with *fast systems*

- Low dimensional control parametrization is a key issue in deriving *fast NMPC formulations*
- Sampling time for the measurement acquisition is $\sim 10\ s$
- Emergence of *Nano-reactors on ship*.

Simplified model of the LAGEP's prolymerization reactor

$$\begin{aligned}
\dot{N}^T &= F \\
\dot{N} &= F - R_p(N^T, N, T, V) \\
\dot{T} &= \frac{1}{\rho_m V C_p}\Big[(-\Delta H)R_p + UA(T_j - T) + Q_{feed}(T, F)\Big] \\
\dot{V} &= \frac{MW_m}{\rho_m} \cdot F \qquad [u = (F, T_j)^T \text{ is the control input}]
\end{aligned}$$

- N^T Total number of monomers
- N Number of remaining monomers
- F Input flow rate
- R_p Reaction rate
- T Temperature
- T_j Jacket temperature
- V Volume of the reaction zone.

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$$

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\begin{aligned}
R_p &= \mu \cdot V \cdot k_{p0} e^{-EA/(RT)} \cdot M(N^T, N) \\
M(N, N^T) &= \begin{cases} \frac{(1-\phi_p^p)\rho_m}{MW_m} & \text{if} \quad \Gamma(N^T, N) \geq 0 \\ \frac{N}{MW_m\left(\frac{N^T - N}{\rho_p} + \frac{N}{\rho_m}\right)} & \text{otherwise} \end{cases} \\
\Gamma(N^T, N) &= \frac{MW_m}{\rho_m} N - \frac{1 - \phi_p^p}{\phi_p^p}\Big[\frac{MW_m}{\rho_m}(N^T - N)\Big] \geq 0 \\
Q_{feed}(T, F) &= F \cdot C_{p,feed}(T_{feed} - T)
\end{aligned}
$$

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$$
\begin{aligned}
\dot{x} &= f(x, u) \\
x &= \begin{pmatrix} N^T & N & T & V \end{pmatrix}^T \\
u &= \begin{pmatrix} F & T_j \end{pmatrix}^T
\end{aligned}
$$

$$\begin{aligned}\dot{N}^T &= F\\ \dot{N} &= F - R_p(N^T, N, T, V)\\ \dot{T} &= \frac{1}{\rho_m V C_p}\Big[(-\Delta H)R_p + UA(T_j - T) + Q_{feed}(T, F)\Big]\\ \dot{V} &= \frac{MW_m}{\rho_m}\cdot F \qquad [u = (F, T_j) \text{ is the control input}]\end{aligned}$$

Control objective

$$\max_{(F(\cdot),T_j(\cdot))\in\mathcal{U}} \left[\int_0^{t_f} R_p(\tau)d\tau\right]$$

Constraints

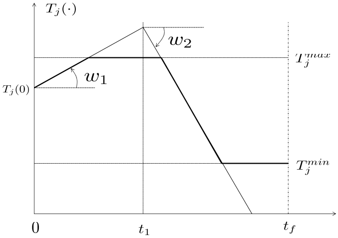
$F \in [0, F_{max}]$	Maximum flow rate
$(T_j, T) \in [T_j^{min}, T_j^{max}] \times [T^{min}, T^{max}]$	Admissible temperature ranges
$\lvert\dot{T}_j\rvert \le \dot{T}_j^{max}$	Thermal inertia of the jacket
$Q_R := (\Delta H)\cdot R_p \le Q_R^{max}$	Maximum allowed heat production.

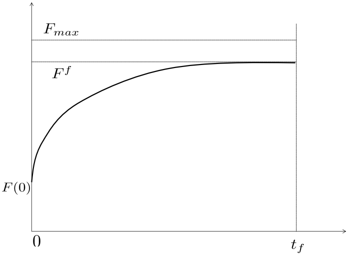
What is a good control parametrization

- Few number of decision variables
- Sufficiently rich to contain *good* solutions
- Structurally meeting constraints

Do not forget that :

Resulting Receding-Horizon closed-loop behavior is more rich than open-loop parametrization

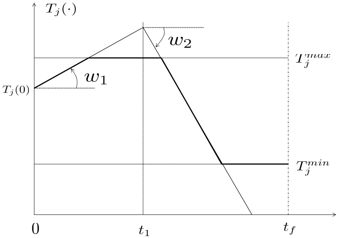


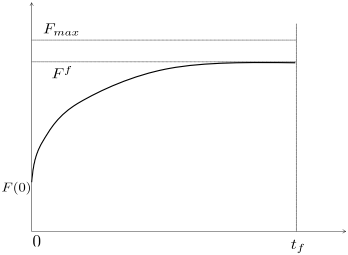


$$T_j(t) = Sat_{T_j^{min}}^{T_j^{max}}\left(T_j(0) + \int_0^t w(\tau)d\tau\right) \quad ; \quad F(t) = (F^f - F(0))\left(1 - e^{-\lambda t}\right) + F(0)$$

with the signal $w(\cdot)$ defined by :

$$w(t) := \begin{cases} w_1 & \text{if} \quad t < t_1 \\ w_2 & \text{if} \quad t \in [t_1, T_p] \end{cases}$$

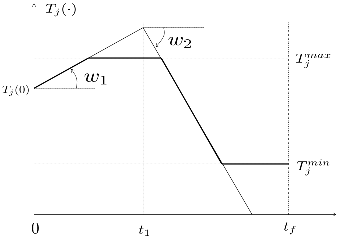


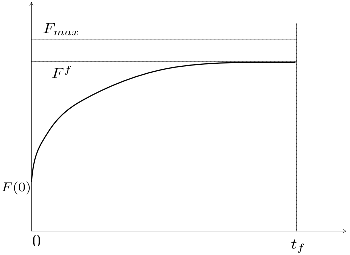


$$p := \begin{pmatrix} \frac{w_1}{\dot{T}_j^{max}} \\ \frac{w_2}{\dot{T}_j^{max}} \\ \frac{t_1}{t_f} \\ \frac{F^f}{F_{max}} \end{pmatrix} \in [-1,1]^2 \times [0,1]^2$$

Constraints structurally satisfied

$T_j \in [T_j^{min}, T_j^{max}]$
$|\dot{T}_j^{max}| = \dot{T}_j^{max}$
$F \in [0, F_{max}]$





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Constraints structurally satisfied

$T_j \in [T_j^{min}, T_j^{max}]$
$|\dot{T}_j^{max}| = \dot{T}_j^{max}$
$F \in [0, F_{max}]$

Remaining constraint to be handled

$Q_R := (\Delta H) \cdot R_p \leq Q_R^{max}$

Originally $$J(p) = \max_{(F(\cdot),T_j(\cdot))\in\mathcal{U}} \left[\int_0^{t_f} R_p(\tau)d\tau\right]$$

But $$R_p(\tau) = \dot{N}^T - \dot{N}$$

Therefore $$J(p) = N^T(t_f) - N(t_f)$$

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Modified cost function

$$J(p) = \left[1 - \frac{1}{\varepsilon}\max\left(0, \sup_{\tau\in[0,t_f]} \frac{Q_R(\tau) - Q_R^{max}}{Q_R^{max}}\right)\right]\left[N(t_f) - N^T(t_f)\right]$$

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The solution cannot violate the constraint by more than ε%.

To summarize

The original constrained problem is transformed into a 4-dimensional optimization problem to be solved on the hyper-cube $[-1, 1]^2 \times [0, 1]^2$.

R_p is involved in the model, the cost function and the constraints

$$\begin{aligned}
\dot{N}^T &= F \\
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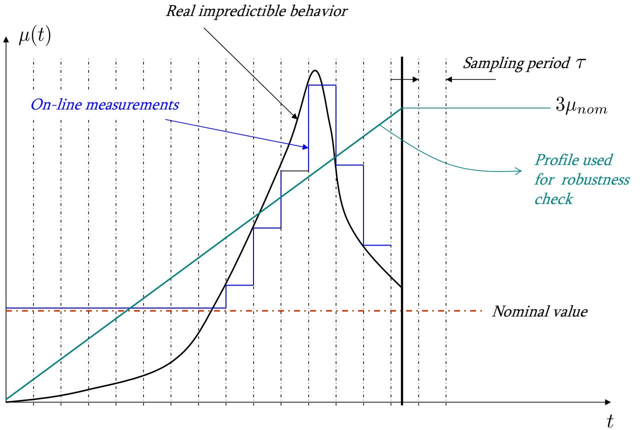
$$Q_R := (\Delta H) \cdot R_p \leq Q_R^{max}$$

$$\max_{(F(\cdot), T_j(\cdot)) \in \mathcal{U}} \Big[\int_0^{t_f} R_p(\tau) d\tau\Big]$$

$$R_p = \mu \cdot k_{p0} e^{-EA/(RT)} \cdot M(N, N^T)$$

Large variations of μ
with unknown dynamic
But good measurement



Typical Behavior of μ during the batch

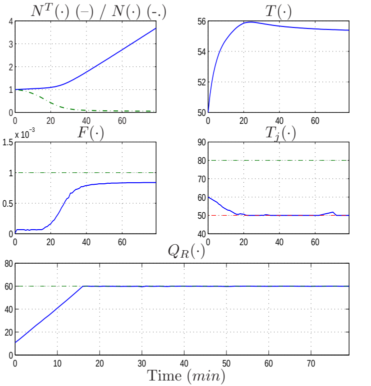


Fig. 3. Behavior of the closed loop system under the receding horizon feedback. $Q_R^{max} = 60$, $T_j^{max} = 80^o$, $T_j^{min} = 50^o$, $F_max = 0.001\ mol/s$. $\lambda = 1/10s^{-1}$. Sampling period $\tau_s = 1\ min$. $\varepsilon = 0.05$. Initial conditions $N(0) = N^T(0) = 1$, $T = 50^o$, $V(0) = 2$

Q_R^{max} taken equal to 60.

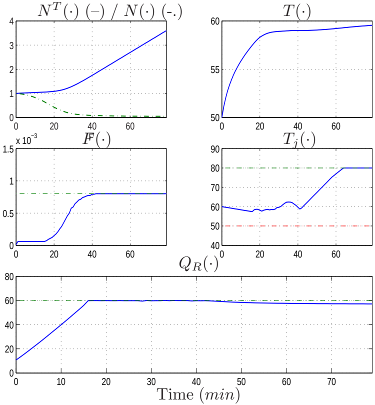


Fig. 4. Behavior of the closed loop system under the same conditions as Fig. 3 with a lower maximal allowable flow rate $F_{max} = 0.0008$. Note how the controller saturates the two control inputs in order to meet the control objective (remain close to the maximal allowable heat production $Q_R^{max} = 60$.

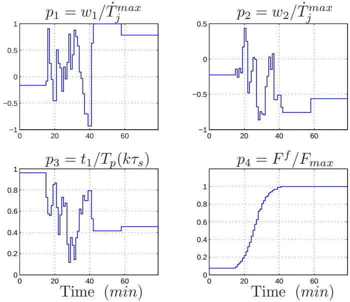
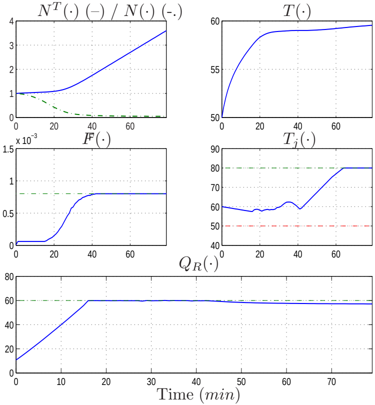


Fig. 5. Evolution of the optimal parameter vector $\hat{p}(k\tau_s) \in \mathcal{P} \in [-1,1]^2 \times [0,1]^2$ during the batch depicted on Fig. 4.



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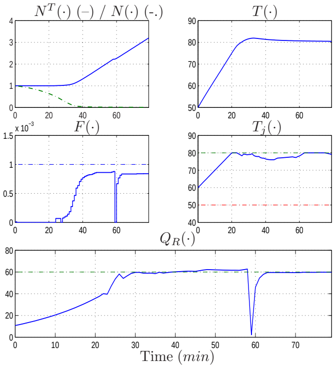


Fig. 6. Behavior of the closed loop system under the same conditions as Fig. 3 with the model uncertainty on the concentration of radicals given by (21). Case where $\psi_f = 2$, namely, the value of μ in (5) increases linearly from μ_{nom} to $3 \cdot \mu_{nom}$ during the reaction time interval $[0, T_{batch}]$. The dynamics of μ is unknown to the controller but current values are accessible to measurement according to section 2.2.

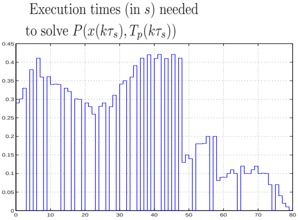


Fig. 7. The computation times needed to solve the four dimensional optimization problem at each sampling instant of the scenario depicted in Fig. 6. The upper bound of the execution times (say 0.5 s) is to be compared to the sampling period $\tau_s = 60$ s.

Nedler Mead simplex algorithm limited to 100 iterations

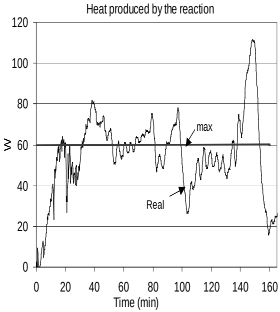


Fig. 8. Experimental validation of the controller. The heat produced by the reaction with a maximal constraint at 60 W

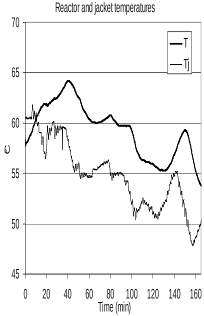


Fig. 9. Experimental validation of the controller. Reactor and jacket temperatures

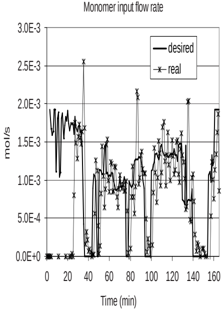
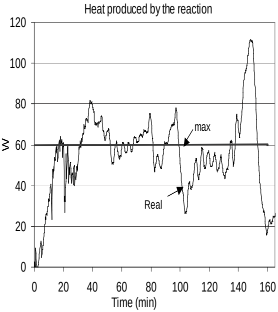


Fig. 10. Experimental validation of the controller. Controlled monomer flow rate and the reaction rate



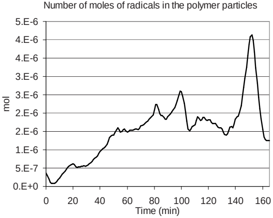


Fig. 12. Experimental validation of the controller. Number of moles of radicals in the polymer particles (μ)

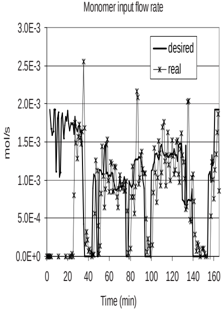


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Fig. 10. Experimental validation of the controller. Controlled monomer flow rate and the reaction rate

Conclusion & future work

- Oversimplified model
- Fast computation enabling use in miniaturized reactors
- *Ready-to-use* scheme with more sophisticated models

Future work

- Deriving dynamic model for μ
- Copolymerization reactors