Model Based Parametric Controller for the Operation of an Experimental Reactor

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Abstract
The aim of this work is to demonstrate on a pilot-plant-scale partially simulated exothermic reactor the implementation and performance of novel parametric controllers, recently developed at Imperial College London. A first-principles model of the process is used and then the parametric controller for the plant model is derived. The controller is given by a set of piecewise affine functions of the manipulating variables, the reactor input flow and cooling jacket temperature, in terms of the controlled variables, the temperature and concentration of the reactor. These affine functions are stored on a computer, which is interfaced to the plant using PARAGON, 5.3. The on-line model-based control therefore reduces to simple affine function evaluations.

Keywords: Parametric Controller, Pilot Plant, Model Predictive Control, Parametric Programming

1. Introduction
Contrary to the conventional model-based control techniques, model predictive control (MPC) is particularly effective for a wide class of complex multivariable constrained processes. Model predictive control determines the optimal future control profile according to a prediction of the system behavior over a receding time horizon. The computation of the control actions is achieved by solving at each sampling time an online optimal control problem. The most profound reasons for the reluctance of many industries to adopt advance control for a wide variety of systems are: (i) the rigorous online computations involved in the MPC implementation, (ii) the unfavorable investment time required for testing and implementing these techniques, (iii) the high price of the necessary hardware and software involved in the controller operation and functioning and (iv) the complexity of the resulting controller structure that requires advanced and expensive operators training. However, the development of new type of advanced controllers the so-called model-based parametric controllers, can readily address these issues (ParOS, 2003). This control design technique moves off-line the rigorous calculations involved in MPC. It is based on newly proposed parametric programming algorithms, developed at Imperial College London (Pistikopoulos et al., 2000, 2002), which derive the explicit mapping of the optimal control actions in the space of the state measurements. Thus, a simple state feedback controller is derived that avoids the online optimization and preserves all the beneficial features of MPC. Nevertheless, this

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type of controllers has not yet been tested on a chemical process experimental set-up. In this paper, we report the implementation of the parametric controller on a pilot plant.

2. Pilot Plant PARSEX Reactor

The pilot plant, PARSEX (PARtially Simulated Exothermic) reactor at Imperial College London, has been devised for testing the performances of control algorithms (Kittisupakorn, 1995; Pinheiro and Kershenbaum, 1999). A schematic diagram of this plant is shown in Figure 1.

This plant consists of two main units: (i) a continuous well-stirred tank reactor of approximate volume 0.1 m$^3$ and (ii) a cooler with approximately 0.7 m$^2$ of heat transfer area. The reactor is charged with water and fed continuously with additional water; this represents the process stream in this PARSEX system. Fresh feed to the reactor is pumped from the feed tank via pump M12 at a measured and controlled flowrate through the valve V1. Heat from the process stream is exchanged with the cooling medium by recirculating the reactor contents through the external cooler via pump M6. The cooler is provided with efficient recirculation of cooling water by the pump M10 and fresh make-up water can be added. The temperature of the reactor, T14, is regulated by adjusting the cooling water temperature, T12. This cooling water temperature is controlled by the addition of fresh make-up cooling water through the control valve V5. No real reaction takes place in the system. The rate of heat evolution by chemical reaction is simulated by sparging live steam into the reactor, which is controlled by

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*Figure 1 Schematic diagram of the PARSEX reactor*
valve V3. Highly exothermic reactions can be experimentally simulated quite realistically in this setup.

The mathematical model of the PARSEX reactor, derived based on the first principles, is given below (Kittisupakorn, 1995):

\[
\frac{dC_a}{dt} = -R_1 + \frac{F}{V_r} (C_{a0} - C_a) \tag{1}
\]

\[
\frac{dT_r}{dt} = \frac{Q_r}{\rho_r C_{pr} V_r} + \frac{F}{V_r} \left( T_f - T_r \right) + \frac{U_r A_r (T_j - T_r)}{\rho_r C_{pr} V_r} \tag{2}
\]

\[
\frac{dT_j}{dt} = \frac{F_j}{V_j} \left( T_{cw} - T_j \right) - \frac{U_r A_r (T_j - T_r)}{\rho_r C_{pj} V_j} \tag{3}
\]

where,

\[R_1 = k_0 \exp \left( -\frac{E}{RT_r} \right) C_a, Q_r = (-\Delta H)R_1 V_r, C_a = \text{concentration of the reactant, kmol/m}^3,\]

\[C_{a0} = \text{nominal feed concentration, kmol/m}^3, T_r = \text{reactor temperature, K}, T_j = \text{jacket temperature, K}, T_{cw} = \text{cooling water temperature, K}, T_f = \text{feed temperature, K}, F = \text{feed flowrate, m}^3/\text{min}, F_j = \text{jacket flowrate, m}^3/\text{min}.\]

The states in this model are: \(C_a\) and \(T_r\).

The jacket dynamics are fast enough to assume steady state behaviour in the jacket heat exchanger, i.e. \(\frac{dT_j}{dt} = 0\). The manipulating variable is \(T_j\) and the disturbance is \(F\).

For the current experimental setup, the model parameters considered are: \(U_r = 68.0\) kcal/\((\text{min.m}^2\ ^\circ\text{C})\), \(A_r = 0.7\ \text{m}^2\), \(C_{pr} = C_{pj} = 1.0\ \text{kcal/\text{kg}^\circ\text{C}}\), \(\rho_r = \rho_j = 1000\ \text{kg/m}^3\), \(k_0 = 3.43568 \times 10^6 \text{min}^{-1}\), \(E/R = 6215.7\ \text{K}^{-1}\), \(V_r = 0.24\ \text{m}^3\), \(V_j = 0.012\ \text{m}^3\), \(T_{cw} = 293.15\ \text{K}\), \(\Delta H = 8000\ \text{kcal/kmol}\) and \(C_{a0} = 31.29\ \text{kmol/m}^3\).

3. Derivation of the Explicit Model Based Control Law

This model is linearized about the steady-state values of \(T_r = 318.15\), \(C_a = 12.5\), and \(T_j = 313.15\) to obtain a discrete state space representation.

\[
\begin{cases}
    x_{1+1} = Ax_t + Bu_t + B_d d_t \\
    y_t = Cx_t
\end{cases}
\tag{4}
\]

subject to the following constraints:

\[
y_{\text{min}} \leq y_t \leq y_{\text{max}} \\
u_{\text{min}} \leq u_t \leq u_{\text{max}}
\tag{5}
\]
where \( x_t \in \mathbb{R}^n \), \( u_t \in \mathbb{R}^m \), and \( y_t \in \mathbb{R}^p \) are the state, input and output vectors respectively at time \( t \), subscripts \( \text{min} \) and \( \text{max} \) denote lower and upper bounds respectively. The state variables, \( x_t \), correspond to \((C_a - 12.5)\) and \((T_r - 318.15)\) and input variable, \( u_t \), correspond to the manipulating variable \( T_j \). The output variable \( y_t \) represents the measured variables \( T_r \) and \( C_a \) and \( d_t \) represents the input disturbance which is feed flow rate \( F \). The sampling time considered is 20 seconds. The discrete state-space matrices \( A, B, C \) and \( B_d \) are as follows:

\[
A = \begin{bmatrix}
0.9937 & -0.0226 \\
0.0036 & 0.9554
\end{bmatrix}, \\
B = \begin{bmatrix}
-0.0008 \\
0.0647
\end{bmatrix}, \\
C = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}, \\
B_d = \begin{bmatrix}
0.0523 \\
-0.0060
\end{bmatrix}
\]

The constraints imposed are: \( 10 \leq C_a \leq 15 \), \( 298.15 \leq T_r \leq 323.15 \) and \( 293.15 \leq T_j \leq 317.5 \). Model Predictive Control (MPC) problem is then posed as the following optimization problem:

\[
\begin{align*}
\min_{U} J(U, x(t)) &= x_t^T P x_t + \sum_{k=0}^{N_c-1} \left( y_{t+k|t}^T Q y_{t+k|t} + u_{t+k}^T R u_{t+k} \right) \\
\text{s.t.} & \quad y_{t+k|t} \leq y_{t+k|t}^{\max}, \quad k = 1, \ldots, N_c \\
& \quad u_{t+k|t} \leq u_{t+k|t}^{\max}, \quad k = 1, \ldots, N_c \\
& \quad x_{t+k|t} = x(t) \\
& \quad x_{t+k|t} = Ax_{t+k|t} + Bu_{t+k}, \quad k \geq 0 \\
& \quad y_{t+k|t} = Cx_{t+k|t}, \quad k \geq 0 \\
& \quad u_{t+k} = Kx_{t+k|t}, \quad N_u \leq k \leq N_f
\end{align*}
\] (6)

where \( U = \left[ u_t, \ldots, u_{t+N_u-1} \right] \) \( Q \) and \( R \) are constant, symmetric and positive definite matrices, \( P \) is obtained by the solving Riccati equation, \( N_y \geq N_u \), \( N_f \), \( N_c \) and \( N_u \) are prediction, control and constraint horizons respectively and \( K \) is some feedback gain. Traditionally, problem (6) is solved repetitively at each time \( t \) for the current measurement \( x(t) \) and the vector of predicted state variables, \( x_{t+k|t}, \ldots, x_{t+k|t} \) at time \( t+1, \ldots, t+k \) respectively and corresponding control actions \( u_{t+k|t}, \ldots, u_{t+k|t-1} \) are obtained.

In the proposed approach, the equalities in formulation (6) are eliminated by making the following substitution:

\[
x_{t+k|t} = A^k x(t) + \sum_{j=0}^{k-1} A^j B u_{t+k-1-j}
\] (7)

Problem in (6) is then reformulated as the following Quadratic Program (QP):
\[
\begin{align*}
\min_U & \quad \frac{1}{2} U^T H U + x^T (t) F U + \frac{1}{2} x^T (t) Y x(t) \\
\text{s.t.} & \quad GU \leq W + Ex(t)
\end{align*}
\]  
(8)

where, \( U = \left[ u_1^T, \ldots, u_{s+t}^T \right]^T \in \mathbb{R}^s \), \( s = mN_u \), is a vector of optimization variables, \( H \) is a symmetric and positive definite matrix and \( H, F, Y, G, W, E \) are obtained from \( Q, R \) and (6) and (7). The QP problem in (8) and now be formulated as a multiparametric quadratic program (mp-QP) (Dua et al., 2002):

\[
V_z(x) = \min_z \frac{1}{2} z^T Hz
\]

\( s.t. \quad Gz \leq W + Sx(t),
\]  
(9)

where, \( z = U + H^{-1} F^T x(t), z \in \mathbb{R}^s, S = E + GH^{-1} F^T \). This mp-QP is solved (Pistikopoulos et al. 2002) by treating \( z \) as the vector of optimization variables and \( x \) as the vector of parameters to obtain \( z \) as an explicit function of \( x \). Such a controller is known as parametric controller. The following values were considered for deriving the control law, \( Q = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, R = [0.0020] \) and \( N_f = 10 \).

4. Results and Discussion

The parametric control law is derived consisting of 19 critical regions, i.e. by partitioning the space of state variables, in which a unique explicit expression in terms of state variables is defined. The critical regions are shown in Figure 2. For example, region 2, is defined by the following state inequalities: 27.7161 \( C_a \) – 0.05 \( T_r \leq 399.937, -0.401913 \( C_a \) – 9.83647 \( T_r \leq -3130.55, -0.401913 \( C_a \) \leq -4.02391, 0.401913 \( C_a \) + 9.83647 \( T_r \) \leq 3152.63, while its associated control function for the first time interval \( T_f(1) \) is given by:

\[ T_f(1) = -0.443395C_a -10.8517T_r + 3771.17 \]

These 19 control laws were stored on a computer, which is interfaced to the pilot plant using software PARAGON, 5.3. The control law is executed and the performance of the controller is shown in Figure 3. The oscillations around the set point, \( T_r = 318.15 \), are observed due to the presence of disturbances and nonlinearity. As shown in Figure 3, the parametric controller works and brings the state to the desired steady state set point starting from a nonsteady state point. The performance of PI controller is also shown. Note that the parametric controller incorporates the model of the plant and the system constraints and it is easy to implement on a software and hardware platform. Another key advantage of the parametric controller is that a complete road-map of all the possible scenarios is available a priori and one does not have to rely on the convergence of an on-line optimizer.
5. Concluding Remarks

This study indicates that advanced model-based parametric controllers are a profound candidate for industrial applications since (i) they incorporate in their structure the model of the plant and the system constraints and (ii) they are simple to use and easy to implement on a software or a hardware platform. The current work includes addressing the issue of presence of disturbances by: (i) including integral penalty to avoid off-set and (ii) implementing explicit robust model predictive control techniques to guarantee constraint satisfaction (Sakizlis et al., 2004). These implementations will be carried out by storing the affine functions on a microprocessor for controlling the plant.

References

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