Predictive Control for Continuous Stirred Tank Reactors

Ioana NASCU\textsuperscript{1,3,*}, Ioan NASCU\textsuperscript{2}, Wen-li DU\textsuperscript{1} and Sai GU\textsuperscript{3}

\textsuperscript{1}Key Laboratory of Advanced Control and Optimization for Chemical Processes, Ministry of Education, East China University of Science and Technology, Shanghai 200237, China

\textsuperscript{2}Department of Automation, Technical University of Cluj-Napoca, Romania

\textsuperscript{3}Department of Chemical and Process Engineering, University of Surrey, Guildford GU2 7XH, UK

*Corresponding author

Keywords: Predictive control, PID control, Chemical reactor, Process model.

Abstract. The paper focuses on the implementation of a model based predictive control (MBPC) method, for Continuous Stirred Tank Reactors. First, the modelling problem of a single irreversible exothermic reaction, taking place in a perfectly mixed continuously stirred tank reactor (CSTR) is presented. The dynamic model consists of differential material and energy balance equations. The control strategy is investigated and evaluated by performing simulations and analyzing the results. The disturbance rejection capacity of the control system (regulatory control performances) have been tested and compared with those obtained using a classical Proportional Integral Derivative (PID) based controller. The results show that this control strategy has good performances and can be efficiently used to control the CSTR.

Introduction

Chemical reactors are very important parts of chemical industry installations. The CSTR configuration is widely used in industrial applications and in wastewater treatment units. The processes that take place in these reactors are very complex because of the chemical and mass transformations with high quantities of heat exchanged. Many authors have extensively studied the model problem of an irreversible, exothermic reaction, taking place in a perfectly mixed continuously stirred tank reactor, and its extensions. The early literature was presented by Douglas \cite{1} and Razon and Schmitz \cite{2}, detailing the multiplicity and dynamic behavior of chemically reacting systems. Topics related to dynamics and control of chemical reactors, including Aspen Plus simulation, are presented by Luyben \cite{3}. It is very difficult to control this non-linear process. One of the main reasons of this difficulty in control is the uncertainty in chemical kinetics, multiple steady states and non-linear behavior.

MBPC techniques have been recognized as efficient approaches to improve operational process efficiency and profitability. MBPC is a general designation for controllers that make explicit use of a model of the plant to obtain the control signal by minimizing an objective function over a time horizon. This strategy allows dealing with multivariable and non-linear processes, as well as unusual behavior of processes. A great interest has been shown for this control techniques, resulting in many interesting scientific papers and books \cite{5-8}. Some examples of MPC strategies described in \cite{5} are: Generalized Predictive Control (GPC), Dynamic Matrix Control (DMC), Model Algorithmic Control (MAC) and Extended Prediction Self-Adaptive Control (EPSAC). EPSAC can be considered as a viable control solution for many applications \cite{9, 10}. A particularly challenging and interesting process to test the performance of EPSAC is a continuous stirred tank reactor. A comparison of different strategies to control the CSTRs is presented in \cite{11, 12}. This paper investigates the multivariable predictive control of a CSTR with cooling jacket. The input flow rate and the coolant flow rate are the manipulated variables. The product concentration and the reactor temperature are the controlled outputs.
Process Modeling

The main goal of this section is to determine the dynamic state behavior of an exothermic, perfectly mixed, continuous stirred tank reactor (Figure 1). An irreversible, single reactant, single product reaction was assumed according to the equation: A → B. The developed model is based on the following assumptions:

- level in the reactor will be considered constant, the CSTR operates at a constant volume;
- time delay introduced by the pipe transportation from the actuator to the reactor is neglected;
- cooling agent flow rate is considered high enough so that the temperature will remain constant along the jacket.

In the conditions given above, the variables used in Figure 1 can be explained as follows:

- \( q_i \) – input flow-rate (feed flow-rate) [m\(^3\)/s];
- \( q \) – output flow-rate, \( q_i = q \) (constant level in the reactor) [m\(^3\)/s];
- \( c_i \) – molar concentration of component A in the feed line [kmol/m\(^3\)];
- \( c \) – molar concentration of component A in residue (output line) [kmol/m\(^3\)];
- \( m_m \) – molecular mass [kg/mol];
- \( T_i \) – temperature of the input component [K];
- \( T \) – temperature of the reactor mixture [K];
- \( T_{ri} \) – input temperature of the cooling agent [K];
- \( T_r \) – cooling agent temperature in the jacket [K];
- \( V \) – volume of the mixture in the reactor [m\(^3\)].

For an irreversible, exothermic reaction taking place in a perfectly mixed continuously stirred tank reactor presented in Figure 1, we can adopt the nonlinear mathematical model:

\[
\begin{align*}
V \frac{dc(t)}{dt} &= q(t) \cdot c_i(t) - q(t) \cdot c(t) - V \cdot k_0 \cdot e^{-E/RT(t)} \cdot c(t) \\
\rho V c_p \frac{dT(t)}{dt} &= \rho q(t)c_p [T_i(t) - T(t)] - k_T A_T \left[ T(t) - T_r(t) \right] + (-\Delta H) V k_0 e^{-E/RT(t)} c(t) \\
\rho V_m c_{pr} \frac{dT_r(t)}{dt} &= \rho_r q(t)c_{pr} [T_{ri}(t) - T_r(t)] + k_T A_T \left[ T(t) - T_r(t) \right]
\end{align*}
\]

(1)

In this paper, the base case parameters for irreversible exothermic reaction taken from [3] are considered: preexponential factor \( k_0 = 30750000 \) [s\(^{-1}\)], activation energy \( E = 69710 \) [kJ/kmol], reactor volume \( V = 7 \) [m\(^3\)], jacket volume \( V_m = 1.6 \) [m\(^3\)], reactant density \( \rho = 801 \) [kg/m\(^3\)], coolant density \( \rho_r = 1000 \) [kg/m\(^3\)], reactant specific heat \( c_p = 3.137 \) kJ/(kg.K), coolant specific heat \( c_{pr} = 4.183 \) [kJ/(kgK)], reactor heat transfer area \( A_T = 32 \) [m\(^2\)], heat transfer coefficient \( k_T = 851 \) [W/m\(^2\)K], heat of reaction \((-\Delta H) = 69710 \) [kJ/kmol], gas constant \( R = 8.314 \) [kJ/(kmolK)].
Control Strategy

The Extended Prediction Self-Adaptive Control approach of MBPC [4] is a control strategy that use the process model for on-line computing the process output predictions and optimizing control actions. For a process with 2 inputs/ 2 outputs (MIMO), the process output is modeled as:

\[ y_i(t) = x_i(t) + n_i(t), \quad i = 1, 2 \]  

(2)

The disturbance \( n_i(t) \) includes all effects in the measured output \( y_i(t) \) which do not come from the model outputs \( x_i(t) \) and can be modeled as a colored noise process, \( n_i(t) = e_i(t)C_i(q-1)/D_i(q-1) \), in which \( e_i(t) \) is white noise. The filter \( C_i(q-1)/D_i(q-1) \) can be used to improve the quality of the control performances, by supplying information to the controller about the type of disturbances [4].

The model output \( x_i(t) \) represents the effect of the control inputs \( u_j(t) \), for \( j=1,2 \), on the process output \( y_i(t) \) and is also a non-measurable signal given by the generic dynamic model:

\[ x_i(t) = f[x_i(t-1), x_i(t-2),..., u_j(t-1), u_j(t-2),...], \quad i = 1, 2, j = 1, 2 \]  

(3)

The prediction is based on the process model (11), and the process output predicted values are:

\[ y_i(t+k|t) = x_i(t+k|t) + n_i(t+k|t), \quad i = 1, 2 \]  

(4)

for \( k = N_{i1},..., N_{i2} \), where \( N_{i1} \) and \( N_{i2} \) are the minimum and the maximum prediction horizons for each \( i \)-output of the process. The process output prediction is based on the measurements available at sampling instant \( t \), and future values of the input signals. Linear EPSAC strategy considers the future process response as being the result of two effects:

\[ y_{iopt}(t+k|t) = y_{ibase}(t+k|t) + y_{iopt}(t+k|t), \quad i = 1, 2 \]  

(5)

The first component \( (y_{ibase}(t+k|t)) \) contains the effect of past control \( \{u_i(t-1), u_i(t-2),...\} \), effect of basic future control sequence \( (u_{ibase}(t+k|t)) \), and effect of predicted disturbances \( (n_i(t+k|t)) \). The second component \( (y_{iopt}(t+k|t)) \) is the effect of the optimizing future control actions: \( \delta u_i(t+k|t) = u_i(t+k|t) - u_{iba}(t+k|t) \), \( k=0,...,N_{ai}-1 \). The design parameters \( N_{ai} \) are called the control horizons. The prediction horizons \( N_{ai} \) could be different for the two outputs and the control horizons \( N_{ai} \) could be different for the two inputs.

The optimized output can be expressed as the cumulative effect of \( N_{ai} \)-impulses and a step:

\[ y_{opt}(t+k|t) = h_{i1}^f \delta u_i(t|t) + h_{i2}^f \delta u_i(t+1|t) + \cdots + h_{iN_{ai}+1}^f \delta u_i(t+N_{ai}-1|t) \]  

(6)

where \( h_{ik}^f \) are the unit impulse response coefficients and \( \delta u_i(t+k|t) \) the unit step response coefficients of the process \( i=1,2, j=1,2 \) and \( k= N_{i1},..., N_{i2} \). In brief, using (14) and (15), the key EPSAC-MPC equations can be expressed in matrix notation:

\[ Y = Y_{thease} + Y_{iopt} = \bar{Y}_1 + \sum_{j=1}^{N_{ai}} G_{ij} U_j \]  

(7)

where for \( i = 1, 2 \) and \( j = 1, 2 \):

\[ Y_i = [y_i(t + N_{i1}|t) \cdots y_i(t + N_{i2}|t)]^T \]

\[ \bar{Y}_i = [y_{ibase}(t + N_{i1}|t) \cdots y_{ibase}(t + N_{i2}|t)]^T \]

\[ U_j = [\delta u_j(t|t) \cdots \delta u_j(t + N_{ai} - 1|t)]^T \]

\[ G_{ij} = \begin{bmatrix} h_{N_{i1}}^{ij} & h_{N_{i1}+1}^{ij} & \cdots & h_{N_{i2}}^{ij} \\ h_{N_{i1}+1}^{ij} & h_{N_{i1}+2}^{ij} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ h_{N_{i2}+1}^{ij} & h_{N_{i2}+2}^{ij} & \cdots & \delta_{N_{i1}+N_{ai}+1}^{ij} \end{bmatrix} \]  

(8)

once the output is predicted, it is possible to optimize the control signal \( U \) by minimizing the cost function:

\[ J(U) = \sum_{k=0}^{N_{ai}} [r_1(t+k|t) - y_1(t+k|t)]^2 + \sum_{k=0}^{N_{ai}} [r_2(t+k|t) - y_2(t+k|t)]^2 \]  

(9)

where \( r \) is the reference trajectory for the controlled output and \( y \) is the measured process output .

Considering compound matrices \( G_1 = [G_{11}, G_{12}] \) and \( G_2 = [G_{21}, G_{22}] \) and the compound vector \( U = [U_1, U_2]^T \), it is possible to represent (18) in a quadratic cost index in \( U \):
\[ J(U) = U^T H U + 2 f^T U + c \]  
with \( H = G_1^T G_1 + G_2^T G_2, f = [-G_1^T (R_1 - \bar{Y}_1) + G_2^T (R_2 - \bar{Y}_2)], c = (R_1 - \bar{Y}_1)^T (R_1 - \bar{Y}_1) + (R_2 - \bar{Y}_2)^T (R_2 - \bar{Y}_2) \)

Minimizing \( J(U) \) with respect to \( U \), leads to the optimal (unconstrained) solution:

\[ U^* = -H^{-1} f \]  

The CSTR process is subjected to constraints and the calculation of the constrained control actions is approached as a constrained optimization problem (19) subject to linear inequality constraints \( AU < b \), with \( A \) a specified matrix and \( b \) a specified vector (both depending on the type of constraints). This is a standard, well-known optimization problem called quadratic programming and is solved using quadratic programming. Constrained optimization generally leads to better results than a simple clipping procedure [4].

**Simulation Results**

The assessment of the developed control strategy is done through numerical simulation in MATLAB/SIMULINK environment. The nonlinear model of the CSTR given by equations (7) was used to simulate the process dynamics. In the EPSAC algorithm the prediction of the process output is based on the linearized process model. The steady state values for the input variables are: \( q_0 = 4.72 \) [m\(^3\)/h], \( c_{i0} = 8.01 \) [kmol/m\(^3\)], \( T_{i0} = 294 \) [K], \( q_{r0} = 6 \) [m\(^3\)/h], \( T_{ri0} = 298 \) [K]. The steady state values for the process outputs are: \( T_{r0} = 357.98 \) [K], \( T_0 = 386.38 \) [K], \( c_0 = 0.1879 \) [kmol/m\(^3\)]. The temperature of the reactor mixture (T) and the output concentration of reactant in residue (c) are considered as controlled outputs. The feed flow rate (q) and the coolant flow rate (qr) are considered as the manipulated inputs, the other inputs being considered as disturbances. The maximum feed flow rate value is limited to 10m\(^3\)/h and the maximum coolant flow rate value is limited to 15m\(^3\)/h. For the simulation scenarios a constant setpoint is considered. Different aspects of input disturbances effects and the effect of some tuning parameters (prediction horizons and controller sampling period) have been investigated. Regulatory performances during simulation tests when a step disturbance with an amplitude equal to 10% of the steady state value \( c_{i0} \), at \( t=2h \) is considered on the \( c_i \) input.
In Figure 2, left plots, the performances of the multivariable EPSAC controller and the PI controllers designed by pole placement technique are compared. The EPSAC controller design parameters are $N_{u1} = N_{u2} = 1$, $N_{11} = N_{12} = 1$, $N_{21} = N_{22} = 10$, $T_s = 5s$. PI controllers parameters are: $k_p = -1.46$, $k_i = -3.65$, for the temperature controller and $k_p = 32$, $k_i = 98$, for the concentration controller. EPSAC control and PI control shows similar performances for the controlled output $c$ but for the controlled output $T$ the time to reject the disturbance was shorter and maximum deviation of process variable from set point smaller for the EPSAC controller. Certainly, PID controllers can also be tuned to be faster and more aggressive, but this will push the control loops to an oscillatory response. The next simulation scenario was performed to test the control system capability to deal with model uncertainties. For this purpose, the CSTR operating point is moved away from the previous nominal operating point but the controllers design parameters are preserved from the previous case. The new steady state values for the input/output variables are: $q_i^0 = 1.58 \ [\text{m}^3/\text{h}]$, $c_i^0 = 8.01 \ [\text{kmol/m}^3]$, $T_i^0 = 294 \ [\text{K}]$, $q_r^0 = 6 \ [\text{m}^3/\text{h}]$, $T_r^0 = 298 [\text{K}]$, $T_i^0 = 319.52 [\text{K}]$, $T^0 = 329.4 [\text{K}]$, $c^0 = 2.04 \ [\text{kmol/m}^3]$. The results are presented in Figure 2, right plots. It can be noticed that the performances obtained using EPSAC are similar to that obtained in the previous operating point, but the performances obtained with PID are considerably deteriorated.

Summary

In this paper, the multivariable EPSAC constrained control algorithm used to maintain a specified conversion rate and temperature of a single reactant, single product, irreversible non-linear CSTR has been evaluated. Mathematical modelling of the CSTR was done using mass and heat balances. Regulatory performances have been tested and compared with those obtained using a classical PID based controller. The simulation results, considering the nominal operating point, as well as other operating conditions, show that the designed MBPC control strategy performs good performances in dealing with process disturbances and exceeds the performance of traditional PID control.

Acknowledgement

This work was supported by National Natural Science Fund of China (61890933, International (Regional) Cooperation and Exchange Project (61720106008, National Science Fund for Distinguished Young Scholars (61725301) and Fundamental Research Funds for the Central Universities (222201917006).

References

[1] J.M. Douglas, Process Dynamics and control, Prentice Hall, Vol 1, 1972.
[2] L.F. Razon, R.A. Schmitz, Multiplicities and instabilities in chemically reacting systems. A Review, Chemical Engineering Science, 42(5), pp. 1005, 1987.
[3] W. Luyben, Chemical Reactor Design and Control. John Wiley & Sons. Inc., Hoboken, New Jersey, USA, 2007.
[4] R. De Keyser, Model Based Predictive Control, Invited Chapter, in UNESCO Encyclopedia of Life Support Systems (EoLSS), Eolss Publishers Co Ltd, Oxford, 2003, pp. 30.
[5] E.F. Camacho, C. Bordons, Model Predictive Control, Springer, 2nd Ed., 2007.
[6] S.J. Qin, and T.A. Badgwell, A survey of Industrial model predictive control technology, Control engineering practice, 11(7), 733-764, 2003
[7] C.E. Garcia, D.M. Prett, and M. Morari, Model predictive control: Theory and Practice a survey, Automatica, 25, no. 3, pp. 1753-1758, 1989.
[8] J.M. Maciejowski, Predictive control with constraints, Prentice Hall, 2002.
[9] Ioana Nașcu, Ioan Nașcu, Improving Activated Sludge Wastewater Treatment Process Efficiency Using Predictive Control, Advances in Technology Innovation (AITI), Vol. 3 No. 2 2018.

[10] L. Tamas, I. Nascu, R. De Keyser, The NEPSAC Nonlinear Predictive Controller in a Real Life Experiment, 11th International Conference on Intelligent Engineering Systems INES 2007, pp. 229.

[11] S. Allwin, N.S. Biksha, S. Abirami, H. Kala, Comparison of Conventional Controller with Model Predictive Controller for CSTR Process, International Journal of Advanced Research in Electrical, Electronics and Instrumentation Engineering. 2014, 3(9): 11934–11941.

[12] A.D. Shakib Joo, A Comparison of Different Control Design Methods for the Linearized CSTR Temperature Model, Journal of Electrical and Computer Engineering Innovat. 2013, 1(2): 107–114.