

Presented at the
World Batch Forum
North American Conference
Chicago, IL
May 16-19, 2004



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Model Predictive Control of Batch Temperature

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KEY WORDS

Adaptive Control, Model Predictive Control (MPC), Laguerre Identification, Control of batch reactors, Temperature Control

ABSTRACT

Control modules used for critical phases of reactor operation such as heating, cooling and reacting can be optimized using advanced process control technology to reduce batch cycle time. Temperature control of batch reactors is difficult for conventional Proportional-Integral-Derivative (PID) controllers due to the open loop instability of these processes coupled with the long time delays and large time constants. These dynamics are present on various reactor designs involving heating or cooling with jackets, internal coils, or recirculation loops through external heat exchangers. Model Predictive Control (MPC) provides an alternative to PID for use in these control modules to dramatically improve temperature set point tracking, improve product consistency, and reduce batch cycle time. This paper describes the design of an MPC controller that is built to specifically handle the dynamics found on batch reactors as well as the large process disturbances that occur due to exothermic reactions. The results of an application example will be discussed.

1. Introduction

PID based temperature control modules for batch reactors have a tendency to overshoot on target changes and are slow to correct on disturbances (see Fig. 1) due to the long dead times and the integrating characteristics of the reactor. Typically, operators use manual control or employ a number of ad hoc schemes to support the PID controller in the control modules used for the heating, cooling, and reacting phases of reactor operation. Such schemes include slow ramping of set points to avoid temperature over shoot and the use of sequential logic to force heating or cooling actuators to maximum or minimum levels under different conditions.

The advanced model predictive controller (MPC) described in the paper has the ability to model and control marginally stable processes with long time delays and long time constants found in batch reactor temperature control. The controller can incorporate the effect of measured disturbances and has a unique unmeasured disturbance cancellation scheme. Application results on a polyurethane reactor demonstrate improvements in batch consistency, reduced batch cycle times, and improved productivity. This paper will address the theory behind the MPC controller design and present the results achieved.

2. The Adaptive Predictive Control Strategy

Based on an original theoretical development by Dumont et al [1, 2] at the University of British Columbia, the controller was first developed for self-regulating systems. The design is an indirect adaptive controller based on an on-line identification of the process dynamics using a Laguerre orthonormal series representation together with a model based minimum variance predictive controller. This design was extended to handle systems that are open loop integrators with time delay and time constant. United States Patent # 6,643,554 describes the details of the algorithm. A brief overview of the modeling method is described in section 2.1.

The MPC controller features a unique strategy for rejection of unmeasured disturbances, such as those that occur on a reactor during stages of the batch that are exothermic or endothermic. Up to three measured disturbance variables are also included in the MPC controller so that temperature disturbances caused by known events such as chemical additions can be effectively rejected. The MPC controller has recently been expanded to handle multivariable control problems with system dimensions up to 48 inputs and 12 manipulated outputs.

The MPC controller has been applied to a wide variety of difficult control applications in many different industries and is available as a commercial software product. It can be easily connected to existing control systems using an OPC connection. Most applications of the controller require only about one week to implement.

2.1 Process Modeling using Laguerre Series Representation

Dumont et al [3] considered system identification based on Laguerre orthonormal functions. This method proved its simplicity when dealing with the representation of transient signals, closely resembling the Pade approximation for systems exhibiting dead time. Conceptually, this approach is

similar to using Fourier Series expansions to approximate periodic signals to produce a frequency spectrum representation for a signal. In this case, the basis function set is the cosine function at multiples of the base frequency. The frequency spectrum represents the identified weights of the Fourier series expansion. Just as it is now simple to obtain a frequency spectrum for a signal, the Laguerre method used in the MPC controller makes it easy to obtain a representation of the transient dynamics of the plant. This representation is the fundamental requirement to implement a model predictive controller. The Laguerre function, a complete orthonormal set in L_2 , has the following Laplace domain representation:

$$L_i(s) = \sqrt{2p} \frac{(s-p)^{i-1}}{(s+p)^i}, \quad i = 1, \dots, N \quad (1)$$

where:

i is the number of Laguerre filters ($i = 1, N$);

$p > 0$ is the time-scale;

$L_i(x)$ are the Laguerre polynomials.

The reason for using the Laplace domain is the simplicity of representing the Laguerre ladder network, as shown in Fig. 1.

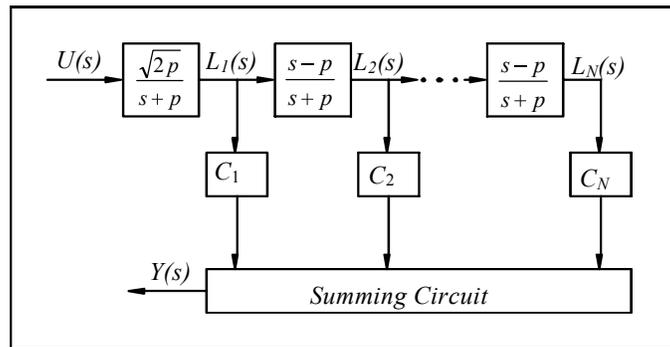


Figure 1: The Laguerre Ladder Network

This network can be expressed as a stable, observable and controllable state space form as:

$$l(k+1) = Al(k) + bu(k) \quad (2)$$

$$y(k) = c^T l(k) \quad (3)$$

where:

$l(k)^T = [l_1(k), \dots, l_N(k)]^T$ is the state of the ladder (i.e., the outputs of each block in Fig. 1);

$C_k^T(k) = [c_1(k), \dots, c_N(k)]$ are the Laguerre coefficients at time k ;

A is a lower triangular square ($N \times N$) matrix.

The Laguerre coefficients represent a projection of that plant model onto a linear space whose basis is formed by an orthonormal set of Laguerre functions. The above form is suitable to represent stable systems. The challenge is to overcome the integrating characteristic of the plant, as found on batch reactor temperature controls. In these circumstances, the approach taken was a factorization of the plant into its stable and marginally stable part (the presence of the integrator), considered known. This approach leads to a discrete time Single Input Single Output (SISO) controller that reads variation of the process variable (system output) $\Delta y(k)$ but provides control variable movements (system input) $u(k)$.

The same concept used in the plant identification is used to identify the process load (output disturbance) for measured feed forward variables. For unmeasured disturbances, an estimate of the load is made. This estimate is based on the observation that an external white noise feeds the disturbance model, resulting in a colored signal. The disturbance can be estimated as the difference between the plant process variable increment and the estimated plant model with the integrator removed. Using the plant and disturbance models we can then develop the Model Predictive Control (MPC) strategy.

2.2 The Predictive Control Strategy

The concept of predictive control involves the repeated optimization of a performance objective over a finite horizon extending from a future time (N_1) up to a prediction horizon (N_2) [4, 5]. Fig. 2. characterizes the way prediction is used within the MPC control strategy. Given a set point $s(k + l)$, a reference $r(k + l)$ is produced by pre-filtering and is used within the optimization of the MPC cost function. Manipulating the control variable $u(k + l)$, over the control horizon (N_u), the algorithm drives the predicted output $y(k + l)$, over the prediction horizon, towards the reference.

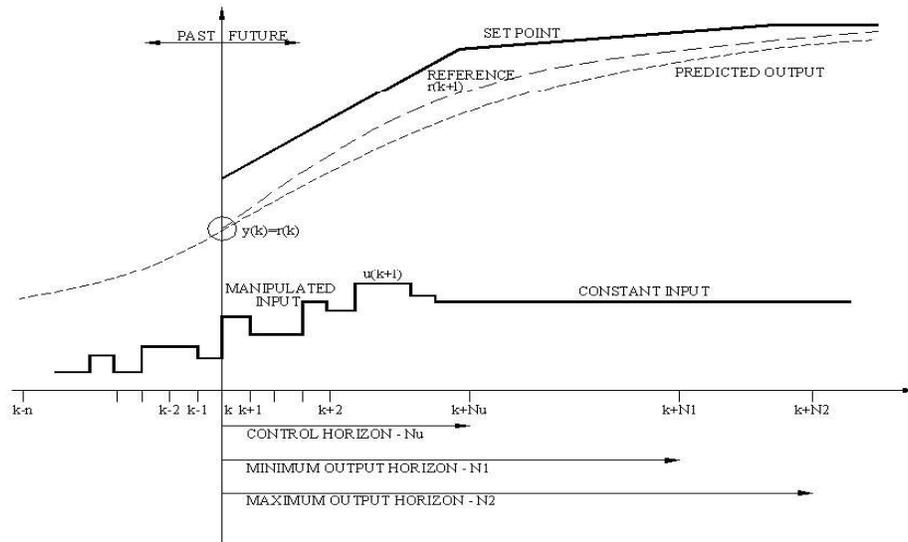


Figure 2: The MPC Prediction Strategy

In this paper, we deal with a simplified version of the MPC algorithm because we have to ensure real time implementation of the whole indirect adaptive scheme, based on a sampling time of 0.1 s. Predictive control is used instead of conventional passive state or output feedback control techniques due to its simplicity in handling varying time delays and non-minimum phase systems. The simplified version, i.e., minimum variance control, is characterized by the fact that the N_2 steps ahead output prediction

$y(k + N_2)$ is assumed to have reached the reference trajectory value $y_r(k + N_2)$. In other words, we can write:

$$y_r(k + N_2) = y(k + N_2) = y(k) + y_d(k + N_1) + y_{ff}(k + N_2) + C_k^T(l(k + N_2) - l(k)) \quad (4)$$

Making an essential assumption that the future command stays unchanged: $u(k) = u(k + 1) = u(k + N_2)$, then the N_2 steps ahead predictor becomes:

$$y(k + N_2) = y(k) + k^T l(k) + k_d^T l_d(k) + k_{ff} l_{ff}(k) + \beta_d u_d(k) + \beta_{ff} u_{ff}(k) + \beta u(k) \quad (5)$$

where:

$$\begin{aligned} k^T &= C_k (A^{N_2} - I) \\ k_d^T &= C_d (A_d^{N_2} - I) \\ k_{ff}^T &= C_{ff} (A_{ff}^{N_2} - I) \\ \beta &= C_k^T (A^{N_2} + \dots + I) b \\ \beta_d &= C_d^T (A_d^{N_2} + \dots + I) b_d \\ \beta_{ff} &= C_{ff}^T (A_{ff}^{N_2} + \dots + I) b_{ff} \end{aligned}$$

Note that here $u(k)$ is unknown, $u_d(k)$ (the estimated disturbance model input) is estimated and $u_{ff}(k)$ (measured disturbance model input) is measured. β^* is the sum of the first N_2 parameters of each corresponding system (i.e., plant, stochastic disturbance and deterministic disturbance, respectively).

As shown in Fig. 2, a first order reference trajectory filter can be employed to define the N_2 steps ahead set point for the predictive controller ($y_r(k + N_2)$):

$$y_r(k + N_2) = \alpha^{N_2} y(k) + (1 - \alpha^{N_2}) y_{sp} \quad (6)$$

Solving control equation (4) for the required control input $u(k)$ we have:

$$u(k) = \beta^{-1} (y_r(k + N_2) - (y(k) + k^T l(k) + k_d^T l_d(k) + k_{ff} l_{ff}(k) + \beta_d u_d(k) + \beta_{ff} u_{ff}(k))) \quad (7)$$

2.3 Indirect Adaptive Control Scheme

The indirect adaptive control scheme uses a modified recursive least square algorithm [6] to estimate the parameters of the models involved in control equation (4). Since the control is computed at each time instant, issues of stability and the convergence of the method become paramount. In [1] these issues are partially addressed. We have knowledge of the existence of the integrator both in the plant and in the disturbance models, therefore our option was to predict the evolution of the stable part of the plant only and then add the integrator directly in the control law.

3. Polyurethane Reactor

The production of one-shot soft foam polyurethane occurs in a batch reactor with stepwise addition of epoxides to a starter containing catalyst. The reactions resulting from both of these epoxide feeds are exothermic, causing need for continuous cooling during the reaction steps. Between addition steps, the temperature of the batch reactor is raised for an extended cookout stage. The reactor temperature control must have the capability to both heat and cool. A process schematic is shown in Fig. 3.

Tempered water from a holding tank can be partially or completely passed through a process cooler before entering the heat exchanger, and steam can be also be directly injected into the heat exchanger. A single control output is sent to all three valves using a split range scheme: the process cooler flow valve (designated 02A) is 100% open at 3 mA and closed at and above 15 mA; the process cooler bypass valve (designated 02B) is completely closed at 4 mA and is fully open at and above 12 mA; and the steam addition valve (designated 02C) is closed until the 12 mA point and is fully open at 20 mA.

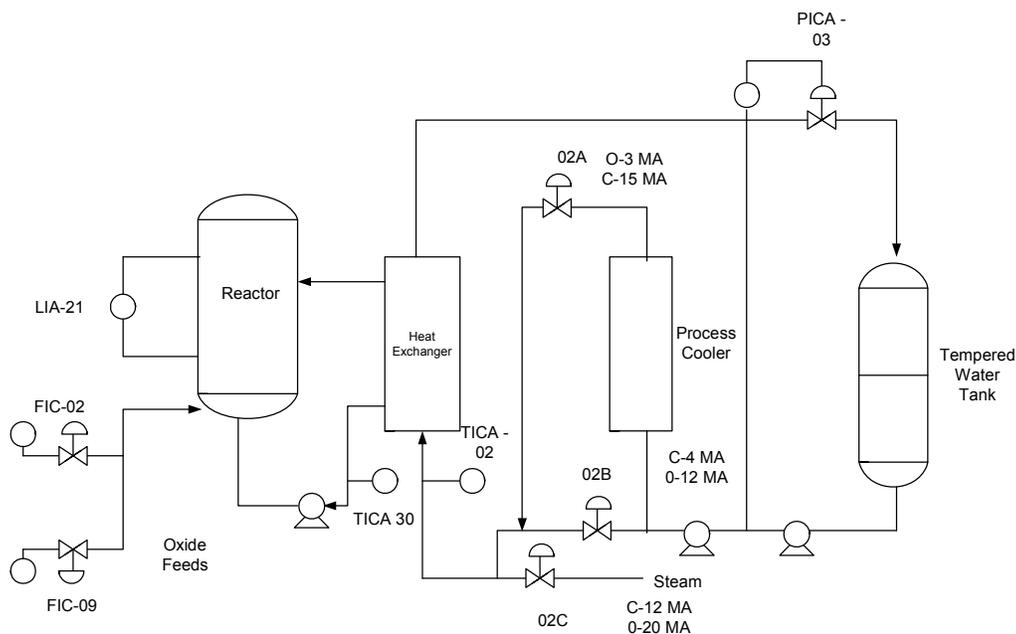


Figure 3: Batch Reactor Overview Schematic

The reactor temperature loop was chosen to be the focus of this project because:

- It is difficult to control using conventional PID technology;
- Better control will provide substantial economic benefits to the plant, i.e., more robust temperature control, increased product throughput, improved quality, and minimal process upsets;
- All required control elements are accessible via an OPC connection to the ABB Advant DCS;
- Historical data is readily available for establishing benchmark performance and validating the results;
- Existing instrumentation yields reliable and accurate information.

3.1 Performance on PID Control

Prior to MPC implementation, batch reactor temperature control was achieved through use of cascaded PID loops. An inner loop controlled the tempered water temperature with the three analog valves. It was set up with relatively high gain, moderately low reset, and no significant derivative term. The outer loop controlled the reactor temperature with high gain, very low reset, and a large amount of derivative. The typical reactor performance under the existing PID control is shown in Fig. 6. PID has difficulty when the target temperature changes.

The initial slow rise and overshoot creates delay during the start of the batch. The cookout phase represents a critical step in achieving desired product properties, but the PID control shows overshoot and does not maintain precise temperature control. The initial part of the cool down during the subsequent oxide feed step shows undershoot and overshoot of the temperature control. At the end of the oxide feed step there is an uncontrolled drop off in reactor temperature causing 30 minutes of idle time while PID regains temperature. The following step is a second cookout phase, which cannot begin until proper temperature is regained. A more advanced control strategy is needed to improve the process.

3.2 Reactor Temperature Control Strategy

In this closed batch reactor, dynamics are changing dramatically as reactor level is increasing. Analysis of the batch data reveals that at the beginning of a batch, process dead time and the process time constant for the temperature loop are each about N seconds (process response details are represented in relative terms due to confidentiality concerns for this process). The plant gain is estimated at about Y . At the end of the batch, the dead time and time constant are closer to $6*N$ seconds and the gain is less than $0.2*Y$. Dead time and time constant are 6 times longer at the end compared to the beginning of a batch, and the gain changes by factor of 5. One set of controller parameters cannot be used for temperature control from the beginning to the end of a batch. Fig. 4 shows estimated process dynamics at different reactor fill levels.

During a batch, a significant amount of oxidizer 1 and oxidizer 2 are added at different times. When these events happen, the controller has to be aggressive and precise to keep the reactor temperature inside allowed limits. Various reactor temperature set point changes are also required during a batch.

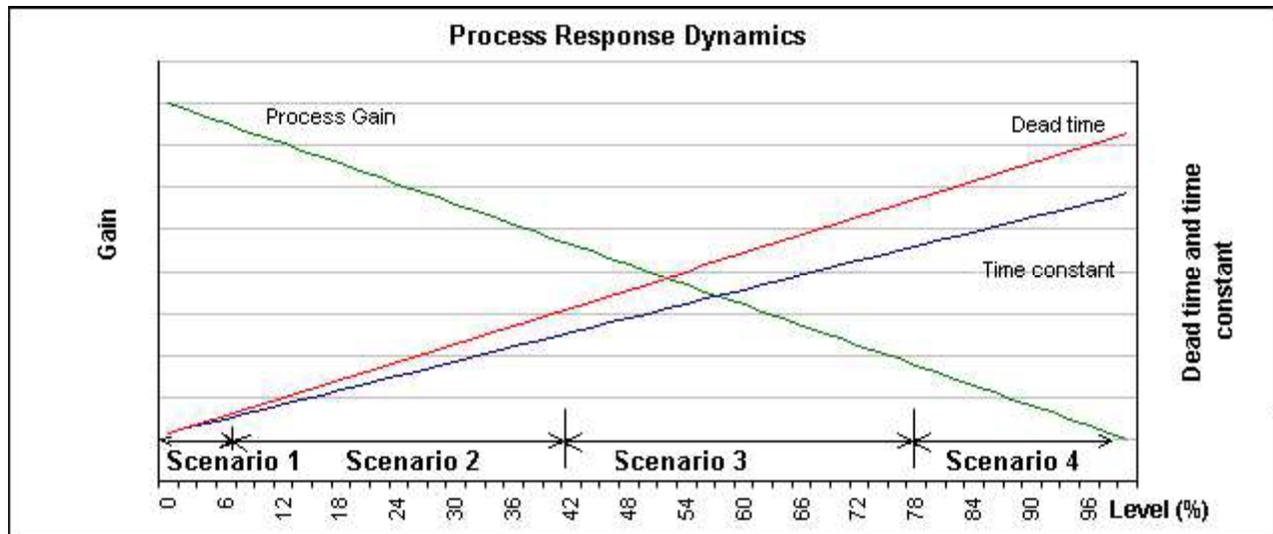


Figure 4: Reactor temperature dynamics as a function of reactor level

For the MPC controller, the batch sequence was divided into 4 sections. For each section, one set of process models (a “scenario”) was developed representing the best fit of the process dynamics for that section. Fig. 5 shows the implemented control strategy using four scenarios with the following parameters:

- Scenario 1 - Batch start, dead time of N seconds, time constant of N seconds, and a gain of Y .
- Scenario 2 – Initial Feed, dead time of $1.2*N$ seconds, time constant of $2*N$ seconds, and a gain of $0.75*Y$.
- Scenario 3 - Initial Cookout & Final feed, dead time of $3*N$ seconds, time constant of $3.6*N$ seconds, and a gain of $0.40*Y$.
- Scenario 4 - Final Cookout, dead time of $4*N$ seconds, time constant of $4*N$ seconds, and a gain of $0.20*Y$.

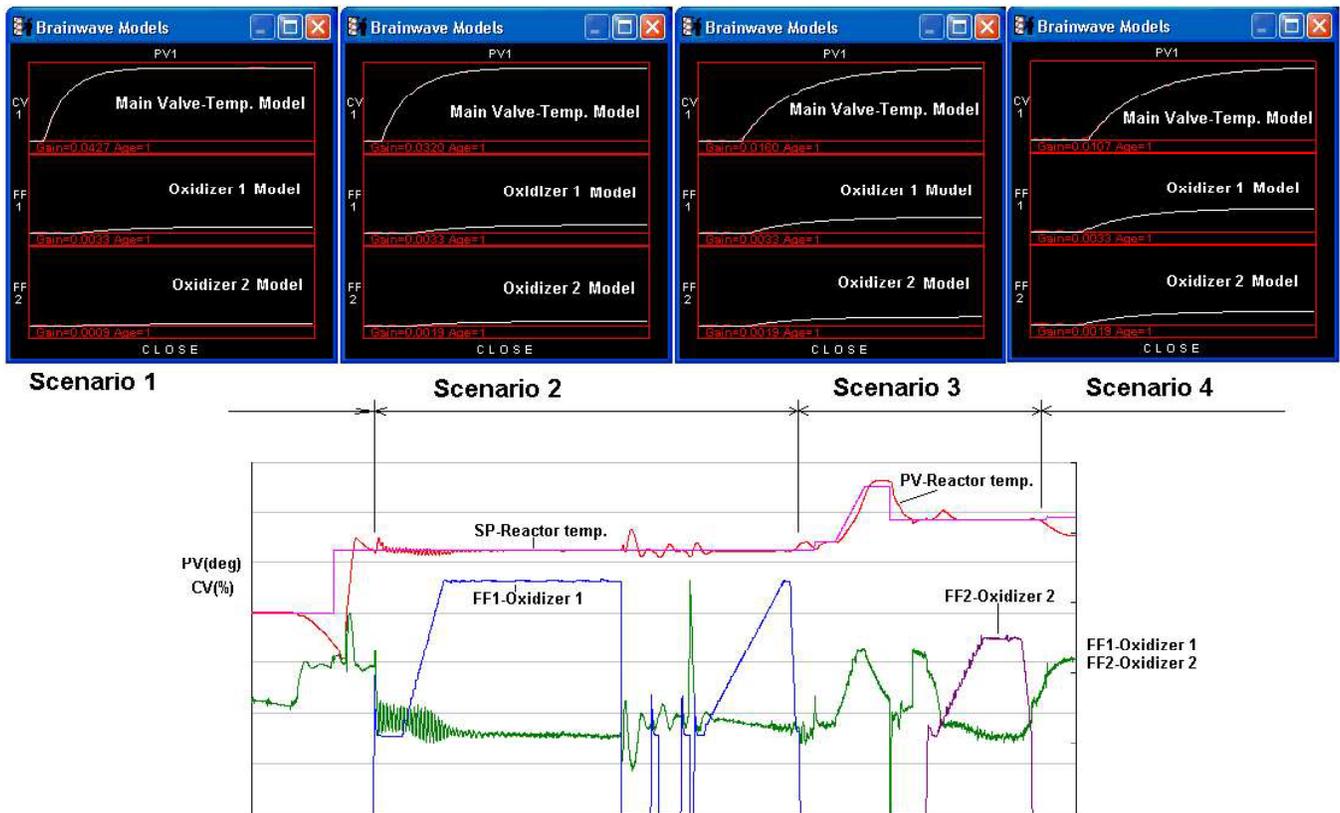


Figure 5: MPC model scenarios used in control strategy

3.3 Performance Analysis

The objective of the control was to reduce the time following the set point change after cookout from elevated temperature down to the feed temperature. The temperature must be stabilized as a permissive to allow the batch sequence to begin the oxidizer 1 feed step. Reducing the temperature settling time following the set point change would reduce the total batch time. A reduction of 15 minutes in batch cycle time would yield sufficient ROI to make the advanced control project attractive. As shown in Fig. 6, the time to stabilize the temperature after the set point change following the cookout phase under PID control was typically 60 minutes. Fig. 7 shows the MPC control, where two temperature SP changes are performed as well as holding reactor temperature during final feed. MPC control stabilized the reactor temperature in about 25 minutes, a reduction of 35 minutes compared to PID control. It should be noted that there was much less action applied to the valves as indicated by the CV position trend. This is expected to have the added benefit of reducing total energy requirements for steam and wear on the valves.

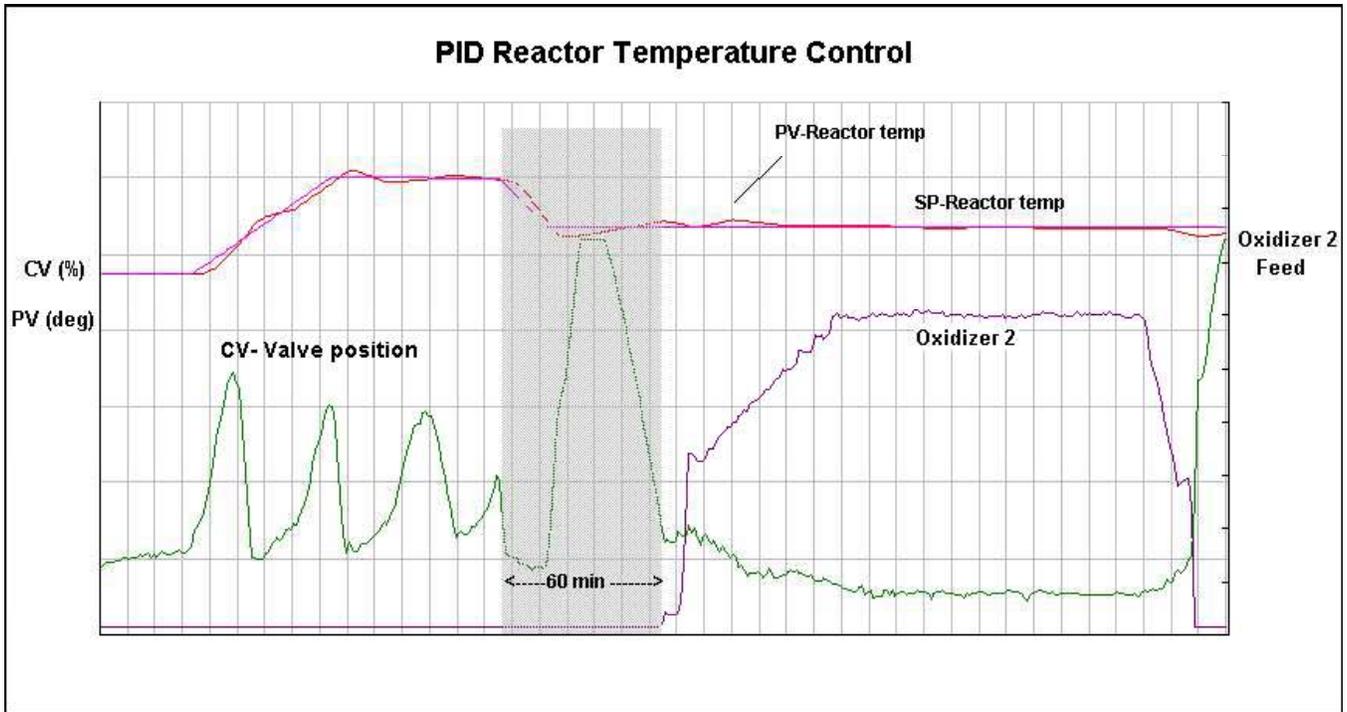


Figure 6: PID control

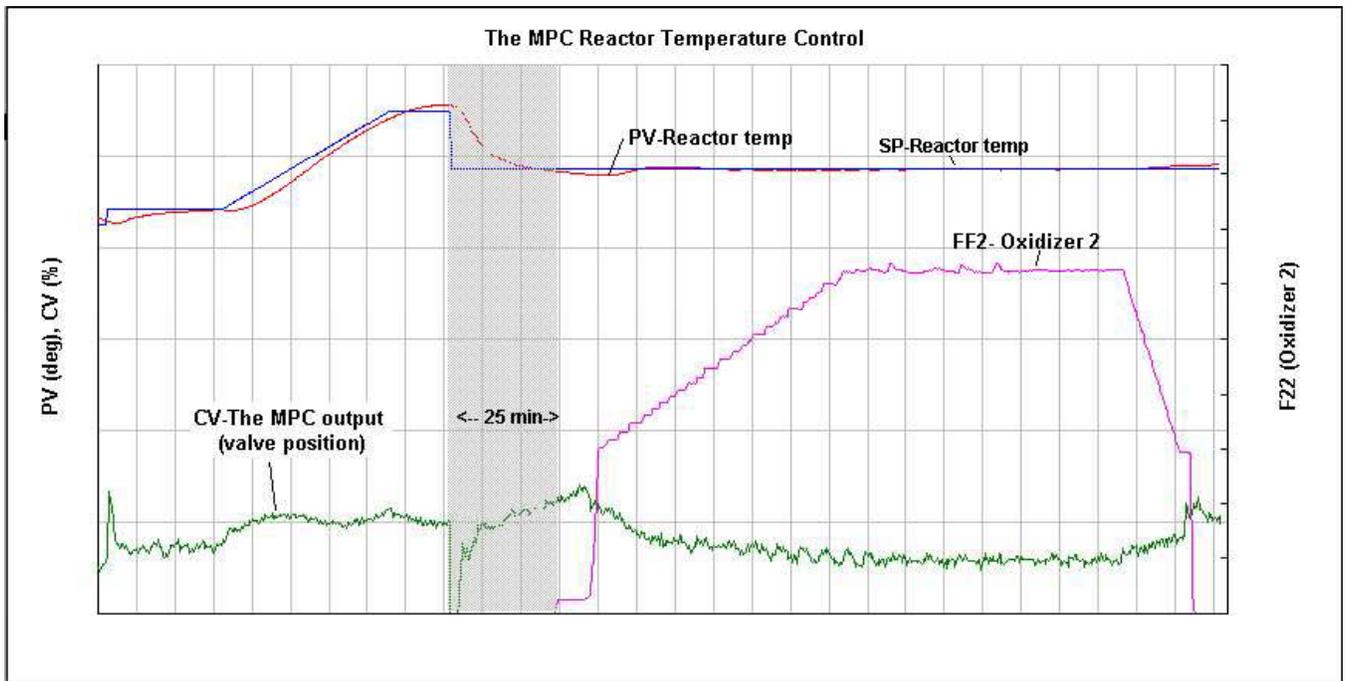


Figure 7: MPC control

4. Conclusions

Temperature control in closed batch reactors is difficult to achieve with conventional PID controllers due to the particular process dynamics of these systems. Such systems exhibit an integrating response compounded by long dead time and time constants that cannot be adequately handled with the PID control algorithm. These problems limit the performance of PID based control modules used for critical phases of reactor operation such as heating, cooling, and reacting. An advanced model-based predictive controller (MPC) developed for use on processes with these dynamics has been successfully applied to the batch reactor temperature control problem. The controller has achieved improvements in temperature control variability and enabled the use of control strategies that optimize production capacity of the reactor.

5. Acknowledgment

The authors gratefully acknowledge the assistance of Mr. Jay Cales of Bayer Corporation with the plant application and operating data presented in this paper. Many of the process details have been intentionally deleted to insure customer confidentiality.

6. References

- [1] C.C. Zervos and G.A. Dumont, "Deterministic adaptive control based on Laguerre series representation," *International Journal of Control*, Vol. 48(1), pp. 2333-2359, 1988.
- [2] C.C. Zervos, "Adaptive control based on orthonormal series representation," Ph.D. thesis, University of British Columbia, 1988.
- [3] G.A. Dumont and C.C. Zervos, "Adaptive control based on orthonormal series representation," *Proceedings of the 2nd IFAC Workshop on Adaptive Systems*, pp. 371-376, 1986.
- [4] D.W. Clarke and C. Mohtadi, "Properties of generalized predictive control," *Automatica*, 25(6):859-875, 6 1989.
- [5] D. Clarke, *Advances in Model-Based Predictive Control*, Oxford University Press, pp. 3-21, 1993.
- [6] G.C. Goodwin, M.E. Salgado and R.H. Middleton, "Exponential forgetting and resetting," *International Journal of Control*, a47(2):pp. 477-485, 1988.