Advanced Control of Batch Reactor Temperature

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ABSTRACT

This paper describes the application of an advanced model predictive adaptive controller to the problem of batch reactor temperature control. Although a great deal of work has been done to improve reactor throughput using batch sequence control, the control of the actual reactor temperature remains a difficult problem for many operators of these processes. Temperature control on these systems is difficult for conventional Proportional-Integral-Derivative (PID) controllers because the response is characterized by an open loop integrator with long delay and time constant. Temperature control is important as many chemical reactions are sensitive to temperature for formation of desired products and reaction rates can be highly temperature dependent. The applications discussed in this paper include a PVC reactor and an Ethoxylated fatty acid reactor. In each case, the variability of the reactor temperature was reduced by 60% or more. Improved temperature control permitted operation at higher reaction temperatures with higher sustained feed rates of reactants and catalysts while remaining within product temperature limits. Batch cycle times were reduced by as much as 35% due to the higher sustained reaction rates. The applications demonstrate the attractive economics for optimization of batch reactors with model predictive controls and highlight the opportunity for tremendous improvements in batch consistency, reduced batch cycle times, and improved productivity.

1. INTRODUCTION

Control of processes that involve the heating and cooling of a closed batch reactor can be a real problem for conventional Proportional-Integral-Derivative (PID) based loop controllers, due to the reduced stability margins proved for these applications. These processes exhibit long dead times and time constants and have an integrating response due to the closed nature of the reactor. In order to keep reactor temperatures within product limits, operators of these systems typically resort to ad hoc PID controller override schemes and slow temperature set point ramp rates in the batch sequences to deal with the poor temperature control achieved with the PID controller.

Various indirect adaptive control schemes have been applied on batch polymerization reactors by a number of researchers [1-4]. In general these methods us a black box approach to determine the relationship between the manipulated variable (CV) and the process variable (PV). These methods do not use any information about the detailed chemical or physical process occurring in the system. The main reason for this approach is the difficulty in obtaining an analytical model and the number of unknowns in the raw feed materials.

The advanced controller 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. The field application results presented in this paper demonstrate that reactor temperature control can be dramatically improved using model predictive control technology. The improved reactor temperature control results in tremendous improvements in batch consistency, reduced batch cycle times, and improved productivity. This paper will address the theory behind the controller design and present results achieved on a PVC reactor and an Ethoxylated fatty acid reactor.

2. THE ADAPTIVE PREDICTIVE CONTROL STRATEGY

Based on an original theoretical development by Dumont et al [5, 6], the controller was first developed for self-regulating systems. This controller was credited by various users with several features, among which we can mention: the reduced effort required to obtain accurate process models, the inclusion of adaptive feedforward compensation, the ability to cope with severe changes in the process etc. All these features together with recognized need in industry made the authors of this paper consider further development of the control strategy for a controller capable of dealing with integrating systems with delay in the presence of unknown output disturbances. The result of these investigations was an indirect adaptive controller based on an on-line identification of the process dynamics using an orthonormal series representation together with a model based minimum variance predictive controller.

Process Modeling using Laguerre Series Representation

Dumont et al [7] considered the 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. The Laguerre function, a complete orthonormal set in L_2, has the following Laplace domain representation:

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

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.

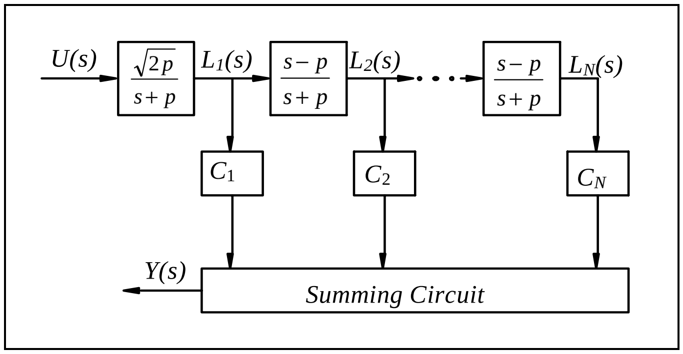

Fig. 1: The Laguerre Ladder Network

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:

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

$C_k^T(k) = \left[c_1(k), \quad ... \quad, c_N(k)\right]$ are the Laguerre coefficients at time *k*;

A is a lower triangular square (N x 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. 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 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). In this case the major difference is that the controller does not have access to the disturbance model input. This issue is addressed in a stochastic manner that provides an estimate of the load. The development is based on the observation that an external white noise feeds the disturbance model, resulting in a colored signal. This signal 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 develop the Model Based Predictive Control (MBPC) strategy.

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) [8, 9]. Fig. 2. characterizes the way prediction is used within the MBPC 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 MBPC 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.

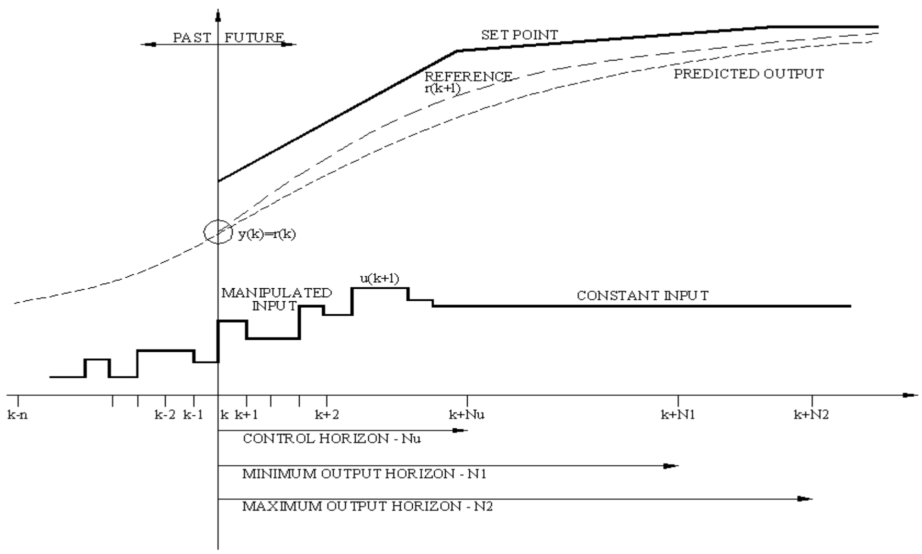

Fig. 2: The MBPC Prediction Strategy

In this paper, we deal with a simplified version of the MBPC 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:

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

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:

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

where:

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

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). It is obvious from the above definitions that if a designer is not looking beyond the dead time of the system β_* is zero. One must choose N_2 such that β is of the same sign as the process static gain and of sufficiently large amplitude. A possible criterion to be satisfied when choosing the horizon N_2 is:

$$\beta \operatorname{sign}(C_k^T(I - A)^{-1}\underline{b}) \geq \varepsilon |C_K^T(I - A)^{-1}b| \tag{6}$$

with $\varepsilon = 0.5$. Note that in the simple case of a minimum variance controller the matrix $(I - A)^{-1}b$ can be computed off-line as it depends only on the Laguerre filters. Additional computation has to be carried out on-line since the identified models (i.e., their Laguerre coefficients: C_k, C_{ff}, and C_d) are changing.

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 ($y_r(k + N_2)$):

$$y_r(k + N_2) = \propto^{N_2} y(k) + (1 - \propto^{N_2} y_{sp}) \tag{7}$$

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

$$\begin{aligned} u(k) = \beta^{-1}(y_r(k + N_2) - (y(k) + k^T l(k) + \\ k_d^T l_d(k) + k_{ff} l_{ff}(k) + \beta_d u_d(k) + \\ \beta_{ff} u_{ff}(k))) \end{aligned} \tag{8}$$

Indirect Adaptive Control Scheme

The indirect adaptive control scheme suggested uses a modified recursive least square algorithm [10] 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 [5] these issues are partially addressed. The adaptive control identification algorithm has a number of free parameters. A designer has to minimize this number since the scheme is implemented in real time. For instance, the choice of the Laguerre filter pole p can be restricted to a fixed value providing a good choice for the system sampling rate. For a given plant there is an optimal pole that will minimize the number of filters required to obtain a required accuracy for the model.

In a similar fashion, as in the case of a Pade approximation, the dead time of the process is well modeled by a Laguerre network, depending on its number of filters. A tradeoff has been observed between the dead-time modeling and the model settling time. Too many filters will result in a long process model settling time.

Since the model of the plant at crossover frequency is very important from the perspective of the transient response of the closed loop system, a good choice for the Laguerre pole will be in that area. If, for other reasons, a fixed choice for the pole is required, then choosing an appropriate sampling time can change the time scale of the system. 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. This path is motivated by the choice of the cost function used in computing the optimal control movement *(u(k))*. Another version, under development, includes a full MBPC cost function. This approach, as described [11], augments the plant model (including the known marginally stable or unstable part) with the disturbance model and computes the control movement based on the prediction of the augmented model. The closed loop system is depicted in Fig. 3. The advanced controller was implemented in C++ and runs on the Windows-NT™ operating system. An OLE for process control (OPC) data server is used to communicate to the Distributed Control System (DCS). Logic was programmed in the DCS device to allow operation from the existing operator console. The operator can select between manual, PID (DCS) or advanced control modes.

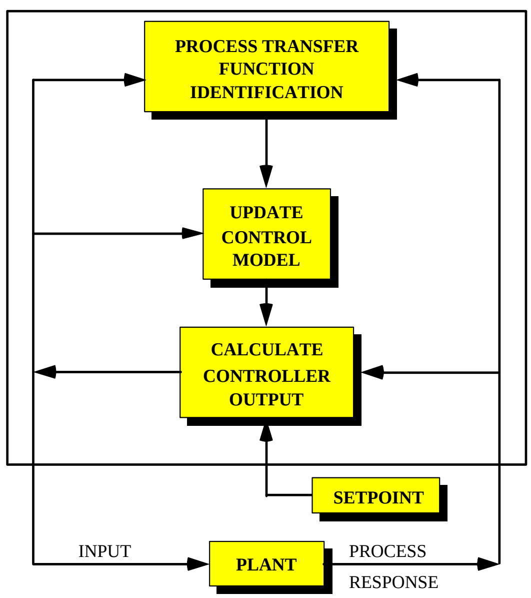

Fig. 3: The Closed Loop Advanced Control System

3. PVC BATCH REACTOR APPLICATION

Poly Vinyl Chloride (PVC) is produced by a suspension polymerization process. The process reaction is highly exothermic. Product quality is based on molecular weight, which in turn is effected by the reaction temperature. In addition, poor temperature control results in the production of undesired copolymers that build up on the walls of the reactor vessel and require cleaning about every ten batches. The copolymer deposits also affect the cooling capacity of the reactor and thus the process dynamics of the rector temperature control system.

The existing PID based control scheme adjusted both the flow of cooling water to the reactor jacket and catalyst feed rate to control reactor temperature as shown in Fig. 4. The temperature variability was typically about ± 5°C. Production capacity is reduced whenever the cooling system is not providing maximum cooling, as the exothermic reaction would cause the reactor temperature to rise too high if the catalyst feed rate was not reduced. It is therefore desirable that the cooling rate be maintained at the maximum level that the system can provide and then regulate catalyst feed rate as high as possible provided that the reactor temperature target is not exceeded. The plant had attempted to control the reactor temperature by manipulating catalyst feed rate only using PID control but found that the temperature excursions were unacceptably high.

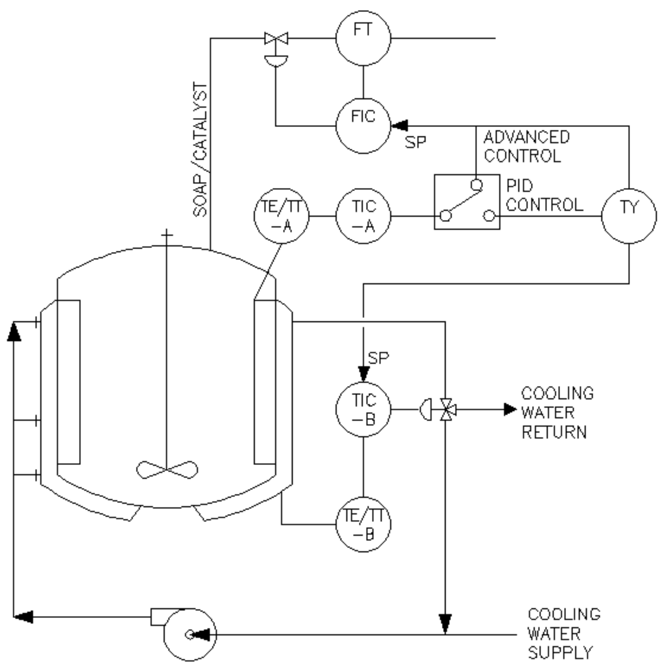

Fig. 4: PVC Batch Reactor Schematic

The adaptive controller was configured to control the reactor temperature by adjusting catalyst feed rate only. Logic in the DCS ensured that the reactor cooling system was maintained at maximum cooling capacity. The adaptive controller was able to maintain the reactor temperature to within about ± 2°C. The improved reactor temperature stability enables the reactor to produce PVC with a more consistent molecular weight with reduced production of undesired copolymers.

The batch cycle times for the PID controlled batches using the original control strategy would range from 12 to 18 hours, with a typical batch time of about 15 hours. The adaptive controller using the new control scheme was able to complete the same product batches with cycle times that ranged between 8.5 and 10.5 hours, with a typical batch time of about 9.5 hours as shown in Fig. 5. The adaptive controller increased the production capacity of the plant by about 35%. This was not possible with the PID controller as it was not capable of maintaining adequate control of the reactor temperature by adjusting catalyst flow alone.

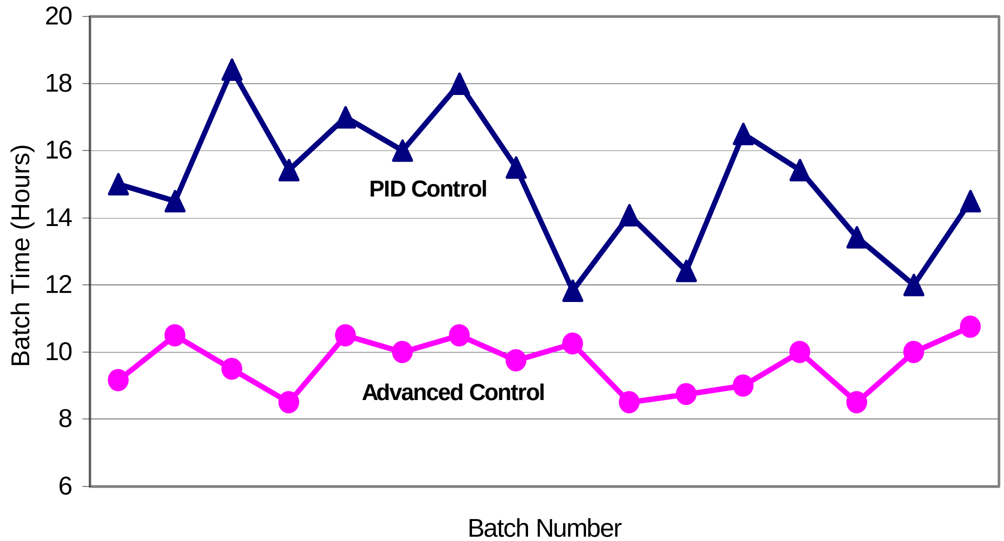

Fig. 5: PVC Batch Reactor Cycle Time Comparison

4. ETHOXYLATED FATTY ACID REACTOR APPLICATION

This process involves reacting fat (typically beef tallow) with ethylene oxide (E.O.) to produce a white, tasteless, edible product that is used as component in many common food products. The reaction is highly exothermic. Ethylene Oxide is charged into the E.O. tank at a pressure of about 60 psi and the E.O. feed control valve is opened such that the reactor pressure reaches about 40 psi. The contents of the reactor are circulated through a heat exchanger that can be heated with steam or cooled with water. Initially the reactor contents must be heated above about 140°C before the reaction with the ethylene oxide will start. As the reaction commences, the steam supply is switched out from the heat exchanger and cooling water in switched in. The cooling water flow is then regulated to maintain reactor temperature with a set point of about 155°C. As the reaction occurs, E.O. is consumed in the reactor and the pressure falls below 40 psi. A pressure controller automatically opens the E.O. feed supply valve to maintain reactor pressure at the pressure set point. The reaction continues until all of the E.O. is consumed.

The existing PID based temperature control was supplemented with override logic in the DCS to prevent high or low temperature excursions. The plant found tuning the PID controller to be difficult, and the best temperature control they could achieve relied upon the override logic extensively. The temperature of the reactor essentially oscillated between the temperature limits set in the override logic. The plant also considered the E.O. feed rate to be operating at high as possible due to the fact that the cooling water supply was spending long periods of time at 100% cooling. A chart of the existing reactor temperature control is shown in Fig. 6.

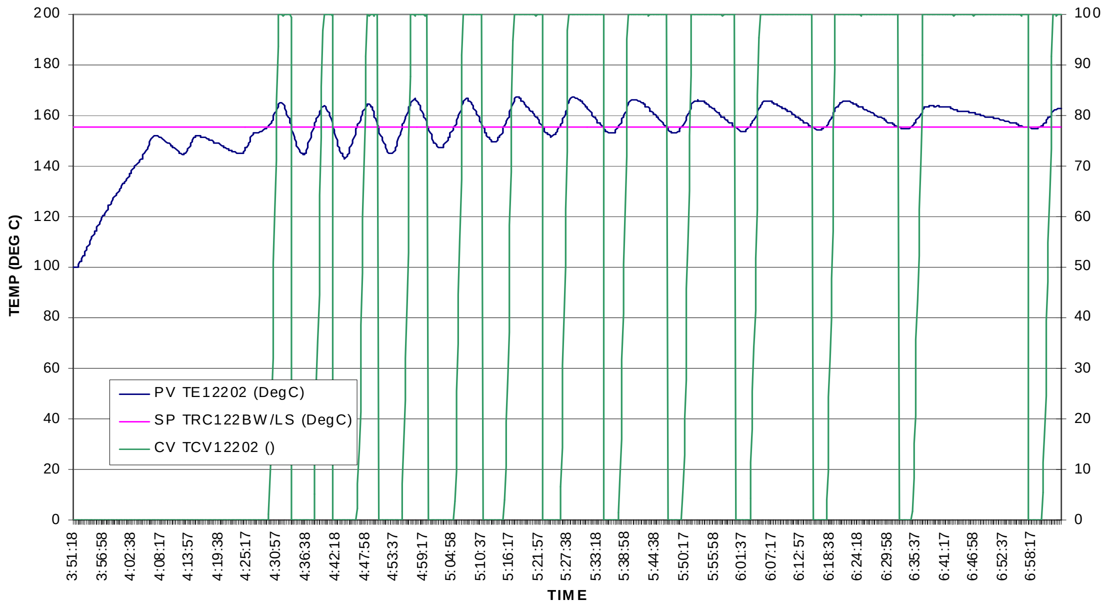

Fig. 6: Existing PID Temperature Control Performance

The reaction rate increases significantly as the reactor temperature rises from 155°C to 170°C. Above 170°C, the product will begin to discolor, so this becomes a constraint for increased production in addition to the amount of available cooling. The temperature excursions with the existing control scheme were about 20°C.

The adaptive controller was installed to replace the existing PID temperature controller on the cooling water circuit. The existing DCS temperature control override logic was retained as a safety precaution. Examination of the cooling system utilization under PID control indicated that there was unused cooling capacity available. This was deduced from the duty cycle of the cooling water valve averaging a maximum of about 80% open.

Based on this information, the E.O. feed rate pressure control scheme was reassessed. Fundamentally, there is no reason for the reactor pressure to be maintained at 40 psi as the reactor vessel is rated 150 psi, particularly considering that the maximum pressure that could be achieved is equal to the E.O. tank feed pressure of 60 psi. The E.O. feed rate control was thus changed from pressure control to reactor temperature control. A schematic of the new control scheme is shown in Fig. 7. The complete control strategy consisted of the cooling circuit that was attempting to maintain reactor temperature at 165°C (TIC-B), and the E.O. feed rate control that was simultaneously trying to maintain the reactor temperature at about 170°C (TIC-A). These competing objectives automatically maximize the E.O. feed rate, and thus the production rate of the reactor, as the E.O. feed valve will remain 100% open as long as the cooling system is able to maintain reactor temperature below the high limit of 170°C. If the cooling system is overloaded and the reactor temperature begins to exceed 170°C, the E.O. feed rate is automatically reduced by TIC-A. The adaptive controller was used for both TIC-A and TIC-B. The control loop dynamics exhibit an integrating response with a dead time of about 800 seconds and a time constant of about 1,600 seconds.

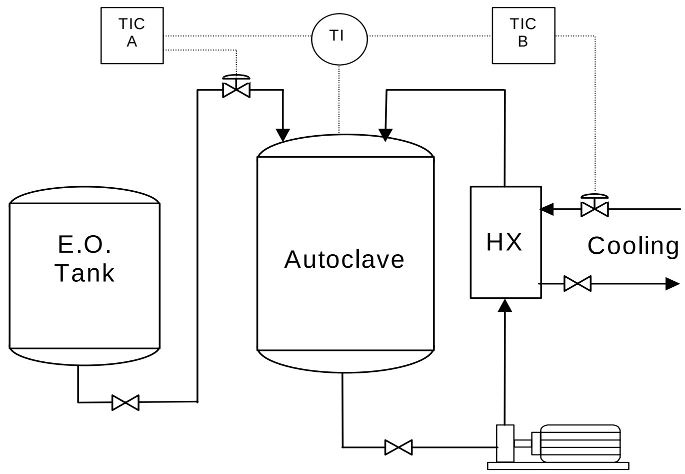

Fig. 7: Reactor Temperature Control Schematic

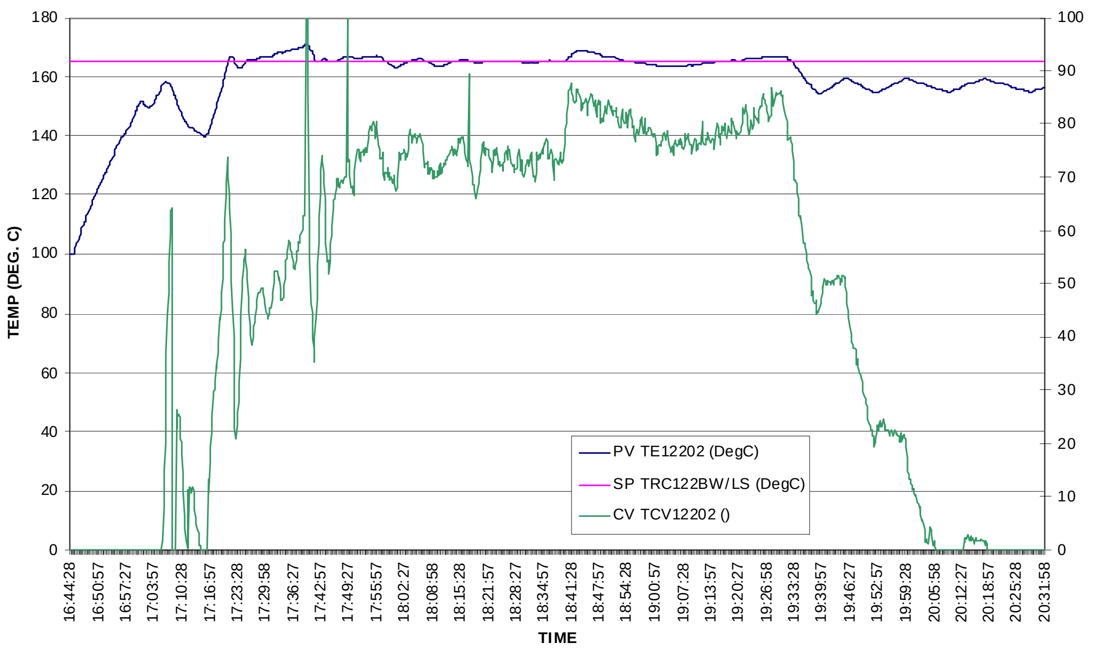

Fig.8: Advanced Temperature Control Performance

The adaptive controller reduced temperature variability by 75% and was able to maintain reactor temperature within about 5°C of set point without excessive operation of the temperature override logic. A chart of the temperature control with the adaptive controller is shown in Fig. 8. It is apparent that there is still some cooling capacity available as the cooling water valve experienced a maximum opening of 85%. The improved temperature control allowed the temperature set point to be raised from 155°C to 165°C without exceeding the high temperature constraint of 170°C.

As mentioned earlier, the reaction rate is highly sensitive to temperature, so the increased average temperature allowed the reaction to be completed much sooner than before. Fig. 9 shows a comparison of E.O. feed rates for a batch using the old PID control scheme and the new adaptive control scheme. The E.O flow for the adaptive controller batch maintained consistent feed rates of over 5,000 pounds per hour for most of the batch. As a result, the batch was completed about 20% sooner than with the existing PID control scheme, representing a 20% increase in plant capacity.

During this batch, the temperature did not exceed the temperature set point of 170°C for TIC-A so the E.O. feed control valve remained 100% open for the entire batch. In fact, this indicates that the E.O. tank charge pressure should be raised above 60 psi or the E.O. flow control valve size should be increased to achieve even higher reaction rates to exploit the available cooling system capacity.

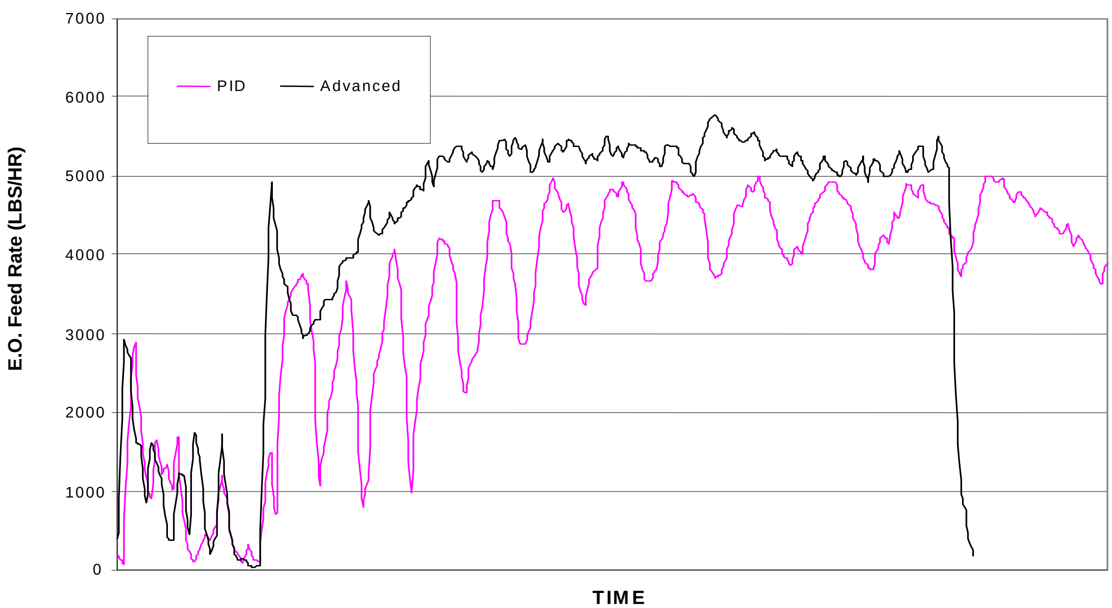

Fig. 9. Ethylene Oxide Feed Rate Comparison

5. 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. An advanced model-based predictive controller (MBPC) 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 of 60% or more and enabled the use of control strategies that optimize production capacity of the reactor. These improvements resulted in increases in plant production capacity of 20% for the Ethoxylated fatty acid reactor and 35% for the PVC reactor without modification to the process equipment.

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