A Holistic Approach to the Application of Model Predictive Control to Batch Reactors

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Abstract: An advanced process control (APC) system using G2 and AspenTech's DMCplus controller was implemented on Anglo Platinum's Precious metals refinery. The APC was implemented on a batch reactor where an exothermic reaction occurred. The APC controller was able to counter the effects of an integrating process model and long time delay to improve overall stability of the reactor. The APC controller resulted in improved temperature stability, reduction in total batch time and reduction in a regent consumption.

Keywords: APC, refinery, batch reactor, time delay, stability

1. INTRODUCTION

Batch reactors are conventionally controlled using PID (Proportional, Integral and Derivative) control. Due to various factors, control of these reactors using PID control is difficult. Most of the literature covers process control of continuous reactors with individual heating and cooling jackets. While there have been numerous applications of advanced process control techniques applied to reactors in the petrochemical industry, few industrial applications have been cited on batch reactors or in the minerals industry. The application of advanced process control techniques, such as model predictive control, in the minerals industry applied to batch reactors can therefore be considered as novel.

Anglo Platinum's precious metals refinery (PMR) has an abundance of reactors employed in the separation and extraction of PGM's (platinum group metals). These reactors are integral to the refining process, and effective control of these is essential to ensure safe and efficient refinery operation. The separation processes rely on differences in the respective chemical properties of components in the process streams, and, as a result most separation steps typically include a reactor which adds reagents, and energy, in the form steam, and/or cooling water. The reactions occurring are either exothermic or endothermic.

1.1 Process Model and Control

In batch reactors various process phases are encountered. These could include heating, reaction, cooling and filtration phases. For each phase, the process needs to be controlled in order to achieve the objectives for that phase. A phase can also use one or all available control actions. This makes the control more difficult as different models are applicable for different phases of the process. Typically, the first phase in a reactor involves heating, which is accomplished by adding heat to achieve a desired temperature setpoint. When the heating phase is complete, the reaction phase starts, where reagents are added which result in either an exothermic or endothermic reaction. The process is then cooled and the reactor contents filtered. Temperature control, particularly, during the heating and reaction phases is very important to prevent the undesirable effects resulting from temperature runaways. Pressure control is also important as excursions can pose a safety hazard and can damage the reactor.

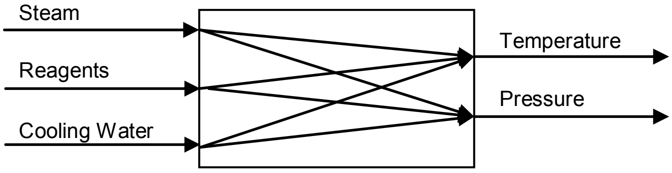

***Figure 1**:* Model for Batch Reactor

A simple process model for batch reactors at Anglo Platinum's precious metals refinery can be described by Figure 1. Figure 1 shows that for a change in any input (steam, reagents or cooling water) both pressure and temperature are affected. Hence individually acting PID controllers for temperature and pressure will not deliver accurate control due to the multivariate nature of the process. Also the model responses between inputs and temperature have an integrating model response with significant deadtime. Due to differing batch sizes, the gain of the integrator also changes from batch to batch. To overcome these limitations, it was decided to test a model predictive controller for temperature and pressure control on a reactor where an exothermic reaction occurred. A joint Anglo Platinum/BluESP control engineering team implemented an AspenTech DMCplus controller governed by G2 knowledge based system, herein referred to as APC.

2. APPLICATION OF DMCplus TO A BATCH REACTOR

The key performance indicators for the batch reactor where an exothermic reaction occurred were:

- Reactor Temperature Stability ± 3ºC of the required set point
- Achieve total batch duration of 8 hours or less
- Minimize Reagent consumption

2.1. Process Description

The batch reactor is filled with a measured quantity of liquor and heated (using steam) to a desired setpoint after which reagents are added. The start of reagent addition marks the start of the reaction phase. There is a period at the beginning of the reaction phase when no reaction occurs. This is referred to as the induction period. After the induction period, the exothermic reaction slowly starts building momentum. Initially the rate of reaction is too slow to maintain the reactor temperature but it then suddenly increases, often causing severe temperature overshoot. The control system must then counter this using cooling water passing through the same jacket that was initially used to heat the reactor using steam. The reaction kinetics are highly dependent on the reactor temperature. If the reactants are cooled too much, the reaction slows dramatically, while the higher the temperature goes, the rate of reaction increases, releasing energy and, causing a temperature runaway. It is very important to maintain the reactor temperature at setpoint for the duration of the reaction phase. After the reaction is complete, the batch is cooled down for filtering.

2.2. APET

The implementation and design of the APC controller was centred on APET[1] (Anglo Platinum's Expert toolkit). APET is an integrated product suite that has been developed by Anglo Platinum to provide tools for the design, deployment and support of advanced process control systems[1]. APET is based on G2's Expert system. Using APET the integration of ASPEN's DMCplus controller, sequence engine and plant PLC/DCS system was easily incorporated into the control philosophy. The control architecture is shown by Figure 2.

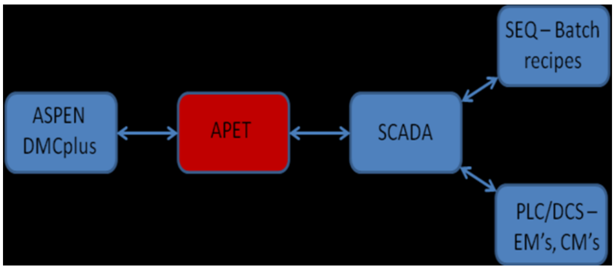

***Figure 2**:* Control architecture

As shown in Figure 2, APET communicates to the PLC/DCS and SEQ (sequence engine) via the SCADA using an OPC connection. DMCplus also communicates via APET. Any mode change, control actions and data transfer occurs via APET to the plant. This ensures that the control system fits into the plant control architecture seamlessly and allows for ease of implementation, support and troubleshooting.

An important aspect of this controller was the incorporation of the PLC EM (Equipment modules) and CM (control modules) and sequence engine into the control philosophy. It was a requirement that this was taken into the account for the design of the controller to ensure that the plant operators could interact with the control system as they currently were. This was accomplished using APET's sequence monitoring toolkit. APET monitored the phases of the batch process and hence the EM's and CM's that were being used in the different phases. An example of the phase monitoring is shown in Figure 3.

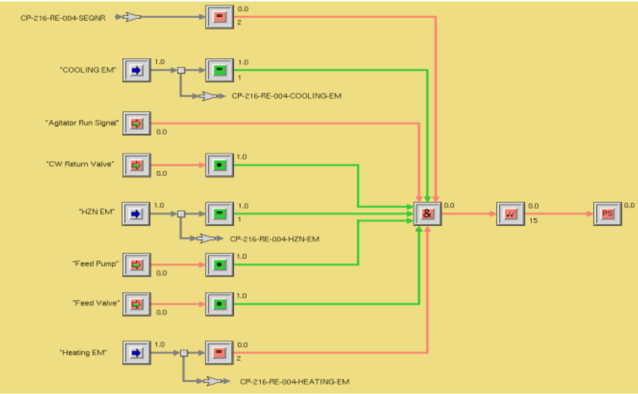

***Figure 3**:* APET Sequence Monitoring

Using the APET sequence monitor, it was decided which MV's and CV's should be used in the different phases. This was then transferred to DMCplus to activate and deactivate MV's and CV's. Limits of CM's as well as setpoints were also obtained by APET from the SCADA, sequence and EM's. This was also passed to DMCplus for the control during the various phases. Interlocks associated with CM's were retrieved by APET and used to manipulate the APC mode depending on the status of the interlocks. This philosophy implies that any APC controller is able to easily fit into the control architecture as a CM. This is a benefit when rolling out APC controllers as well as ease of interaction with the APC controller by operators.

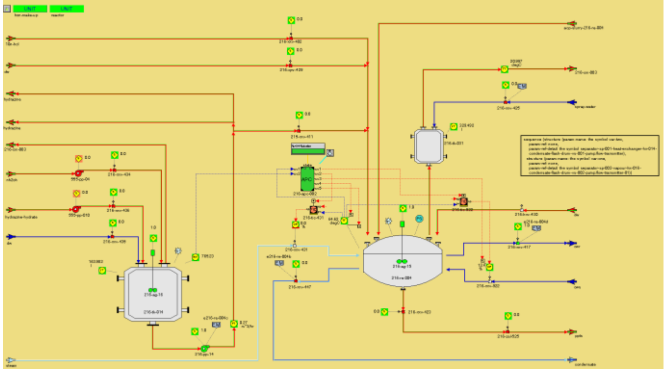

***Figure 4**:* APET APC Configuration

The configuration of APC from APET is given in Figure 4. The setup of the controller and the plant mimics follows object orientated programming. The various EM's, CM's, and sequences that are utilised for APC in this batch process are shown in Figure 3. Also shown is the MV's and CV's utilised by this APC controller.

The APC controller for this batch controller utilised rules and a model predictive controller (DMCplus). Rules were used for end point detection, adjusting limits, manipulating model process gains for different phases and determining end of a phase and pseudo phases within a phase. An example of end point detection is given in Figure 5.

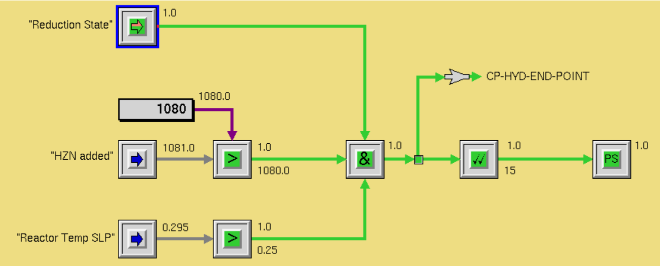

***Figure 5**:* APET End-Point Detection

2.3. DMCplus

DMCplus is a DMC type multivariable controller from AspenTech. DMC controllers are also called model predictive controllers. The technology is based on linear models that describe the process behaviour. At the heart of DMC lies the equation:

$$\delta CV = A * \Delta MV \qquad 1$$

Equation 1 is used to calculate how the controlled variables will change, based on controller input changes, or to calculate how to manipulate the manipulated variables in order to obtain the desired controlled variable response.

In calculating the dynamic move plan for the manipulated variables, δCV is the desired controlled variable response, ΔMV is the dynamic move plan to be calculated and A is the controller model.

The DMC controller executes periodically. Every execution cycle the controller will:

- Calculate the open loop prediction for each controlled variable.
- Decide on steady state values for all manipulated variables and controlled variables.
- Calculate a move plan for each manipulated variable.
- Implement the first move of the move plan

2.3.1 Open loop prediction

During the open loop prediction, the controller will update a vector holding the future open loop prediction for each controlled variable by considering the changes in all controller inputs (manipulated variables and feedforward variables). The controller model will be used as in equation 1, multiplied by the most recent changes in inputs, and added to the previous prediction from each controlled variable. Feedback will be applied by comparing the current value of each controlled variable with the predicted value from the previous execution cycle, and the new prediction will be shifted to start from the current controlled variable value.

2.3.2. Steady state values

Knowing what the open loop behaviour of the controlled variables will be, the controller must now calculate what to do with the manipulated variables to get the controlled variables to their desired values. The next step is therefore to use the:

- steady state gain information from the controller matrix
- the controlled variable setpoints or limits
- manipulated variable limits
- economic cost factors on manipulated variables and/or controlled variables

Using the above information the desired end values for all manipulated variables and controlled variables are determined.

2.3.4 Move plan calculation

Next the controller must determine how to move the manipulated variables from their current positions to the end positions. This path that the manipulated variables will follow is called the move plan of the controller. This move plan will be determined by calculating a number of future moves for each manipulated variable.

The response of the manipulated variables will be influenced by the magnitude of the controlled variable error, the controller models and the tuning of the controller.

2.4. Controller Design

An APET/DMCplus controller was designed, using steam during the heating phase and water and reagent volume during the reaction phases. A G2 APET knowledge base was developed that monitored the batch progress and the controller performance. APET then altered the behaviour of the DMCplus controller based on the current phase of the batch and the batch characteristics. APET also managed the use of manipulated variables, model gains and limits for manipulated and controlled variables. A very simple form of adaptive control was also implemented on the DMCplus controller from APET. APET used the rate of change on the initial heating phase to calculate the optimal gain that corresponds to the current batch size and heat capacity, which was then passed to DMCplus.

2.4.1 Control variables and manipulated variables

The DMCplus controller has two manipulated variables, no feedforward variables and three controlled variables. The manipulated variables are the steam valve to the reactor jacket and the cooling water to the same reactor jacket. As both manipulated variables use the same jacket, they can not be used at the same time, and switching between them is a time consuming process.

The reagent to the reactor was initially considered as a feedforward variable, but because the effect of adding reagent varies dramatically over the batch time, it was discarded.

The controlled variables are the reactor temperature, the first derivative of the temperature and the reactor pressure.

2.4.2 Heating Phase

During the heating phase, the steam valve is opened to the high limit. This will cause the reactor contents to heat up at a constant rate of change. This rate of change is indicative of the heat capacity of the reactor contents and therefore a calculation was developed that used the rate of change to adjust the controller models accordingly.

One substantial difference between continuous and batch processes is that most manipulated variables can only affect a change in one direction. In most continuous processes, if steam is added, the process will heat up. If steam is decreased, temperature will drop because fresh feed material is continuously fed to the process. In batch processes, this is not true. If the temperature on a batch reactor overshoots, taking all the steam out will only cause the temperature to remain at a value higher than the setpoint. Only temperature losses to the environment are available to slowly cool the reactor. In the same way, too much cooling water will only cool the reactor down, and reducing the cooling water to zero will never heat up the process.

For this reason, the desired temperature setpoint will be overshot by 2 degrees Celsius during the heating phase. This temperature offset will be used by the cold reagent that will be added until the exothermic reaction starts.

After completion of the heating phase, APET then activates the DMCplus controller for the reaction phase.

2.4.3 Reaction Phase

During the reaction phase APET disables steam and activates cooling water.

At the start of the reaction phase, APET will also prevent the DMCplus controller from using the cooling water to cool the batch down, even though the temperature is above the setpoint. At the start of the reaction phase, the cold reagent will cool the batch down. If a controller adds cooling water continuously to the process at this time to control the temperature to setpoint, the temperature will drop to a value where the exothermic reaction will not start. Once a minimum time has passed and a minimum volume of reagent added (the induction phase – pseudo phase with reaction phase), and the rate of change of the temperature becomes positive, APET will open the manipulated variable limits to enable DMCplus to manipulate the cooling water.

The temperature of a batch reactor is an integrator. The model exhibits significant deadtime because the metal reactor wall and a glass wall separate the reactor contents from the heating or cooling medium. Another challenge when using cooling water on a batch reactor is that if a large amount of cooling water is added to the jacket, it will keep cooling the reactor contents until the cooling water reaches the same temperature as the reactor.

If the exothermic reaction pushes the temperature up, DMCplus or PID will add cooling water to the jacket. Often at the time when the temperature is still high, there will already be too much cooling water and the temperature will drop much lower than setpoint. This will kill the exothermic reaction, and a significant time will go by before the temperature will increase again. For this reason, a rule is enforced from APET that even if the temperature is above setpoint, if the rate of change of the temperature is negative, the cooling water is closed.

2.4.4 Endpoint

At the end of the batch when the reaction is complete, secondary reaction occurs. This reaction is hugely exothermic, causing a severe temperature spike that the normal DMCplus tuning is not able to control. During this occurrence, APET will change the DMCplus models and tuning to make the controller much more aggressive. APET will also increase the high limit on the cooling water manipulated variable. When this state is detected, APET will notify the sequence the reaction is complete. The sequence will then stop the addition of reagent and move into the cooling phase. During the cooling phase APET will fully open the cooling until a minimum desired temperature is reached after which the contents of the reactor will be filtered.

3. RESULTS

The results achieved are presented in Figures 5, 6 and 7 below.

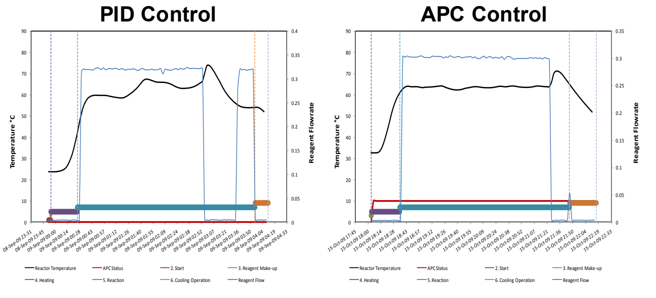

***Figure 5**:* Temperature control PID vs. APC

Figure 5 shows temperature control for a typical batch operation with PID and APC control. It is clear that the APC controller out-performs PID control. APC is able to control the reactor temperature using cooling water during the reaction phase even when an exothermic reaction is occurring. With PID control, temperature stability is very difficult especially when the exothermic reaction is occurring. This is clearly visible from Figure 5 for PID control, shown by the sudden rise in temperatures that is indicative of the exothermic reaction.

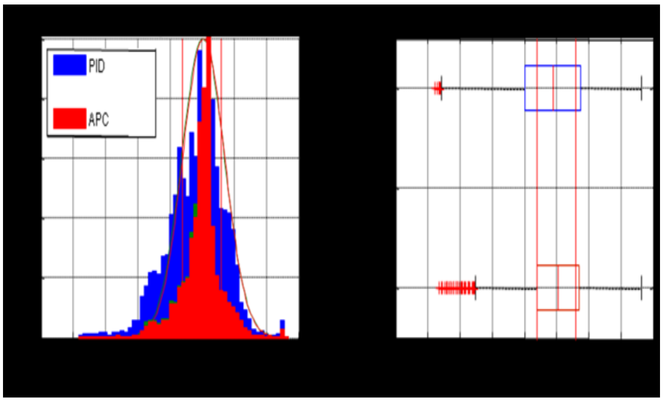

***Figure 7**:* Temperature Stability

The temperature stability during the reaction phase is shown in Figure 7. The standard deviation of temperature with PID control was 4.2°C and 3.2°C with APC. This reduction in standard deviation can also be seen by the distribution and box plots in Figure 7. Tighter temperature control allowed the reactor to be operated at higher which had a positive impact on the particle size distribution of the product, and hence filtration rate, ultimately reducing total batch time.

The individual phase times, total batch times and volume of reagent used per batch is presented in Figure 8. With PID control, the average batch duration was 8.8 hours which reduced to 7.5 hours with APC. This result is statistically significant at 95% confidence level. This batch time reduction corresponds to a potential throughput improvement of 10.5%.

The average reagent consumption reduced by 2.3% with APC. This result is statistically significant at the 95% confidence level.

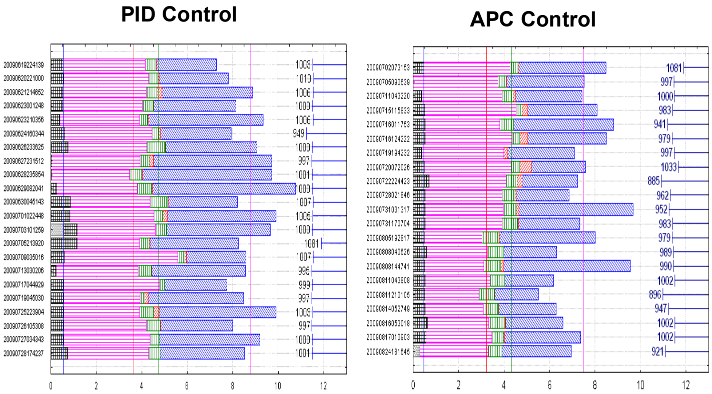

***Figure 8**:* Batch Duration and Reagent Consumption

5. CONCLUSIONS

APC has been successfully implemented on a batch reactor where an exothermic reaction occurs. It also demonstrated successful implementation of AspenTech’s DMCplus controller with Anglo Platinum’s Expert toolkit (APET). The advanced controller delivered a greater than 20% reduction in temperature standard deviation from the setpoint value, ultimately resulting in a 10.5% reduction in total batch duration, and 2.3 % saving in reagent consumption.

5. References

1. De clerk, D.J., de Villiers, P.G.R. and Humphries, G. *A Sustainable Approach to Process Optimization through Integrated Advanced Control Software Standards*, to be presented at IFAC MMM, 2010, Cape Town

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