CATALYST CONTROL USING A REAL-TIME PROCESS MODEL

P L Hastings

Dupont Sabanci Polyester, PO Box 1923, Redcar, Cleveland, UK

Philip.l.hastings@dupontsa.com

Keywords

Control, Process model, Robust, Catalyst, Reliable

Abstract

Controlling the reaction and the product quality in a large Polyester Intermediates plant has been an intractable problem for many years. Handling difficulties and the hazardous nature of the process has made it impossible to get real time measures of the product or of the dissolved catalyst. Model Predictive Control was implemented, but failed to give reliable control. Now a simplified Process Model is used with just the right level of detail to estimate the catalyst concentrations around the plant in continuous real-time. Data quality handling logic keeps the model sufficiently robust. The model is described and how it is implemented in the closed loop control schemes. The whole process has highlighted major lessons in the pragmatic approach to implementing Advanced Process Control in the process industry.

Process Description

There are two sister plants on site producing Terephthalic Acid from Paraxylene, each with several reactors. The process is shown simplified in figure 1. The reaction between paraxylene and air occurs in two stages, with the secondary reaction only finishing the last 2% of the conversion, but key to producing the right specification at a competitive cost. The processing and separation section constitutes a large inventory, in some 7 major vessels with residence times totalling 4 hours. Controlling the reaction and the catalyst is only one of the complex tasks in operating the plant – several factors complicate all tasks and the smooth operation of all plant equipment:

- the reaction is between a flammable liquid and air at high temperatures, pressures and volumes, posing a major explosion hazard
- the main solvent, Acetic Acid, is a highly corrosive strong acid
- all stages of the plant operate across the solid, liquid and vapour phases. This inevitably leads to process handling problems giving rise to process disturbances.

Control objectives

The reaction proceeds via several intermediates, the last of which, 4CBA, is never fully converted and remains as a product impurity. The first control objective for the reaction is to keep the 4CBA in the product at the optimum concentration. If the impurity exceeds an upper target, the cost penalty on the downstream processing plant rises very steeply. When the impurity is below a lower target, the material usage on this plant increases. Due to the asymmetry of these costs, when the reaction conditions are controlled manually, the impurity typically runs slightly below the lower target, costing around £¼ million per annum.

The most useful thing would be to have an on-line measure of

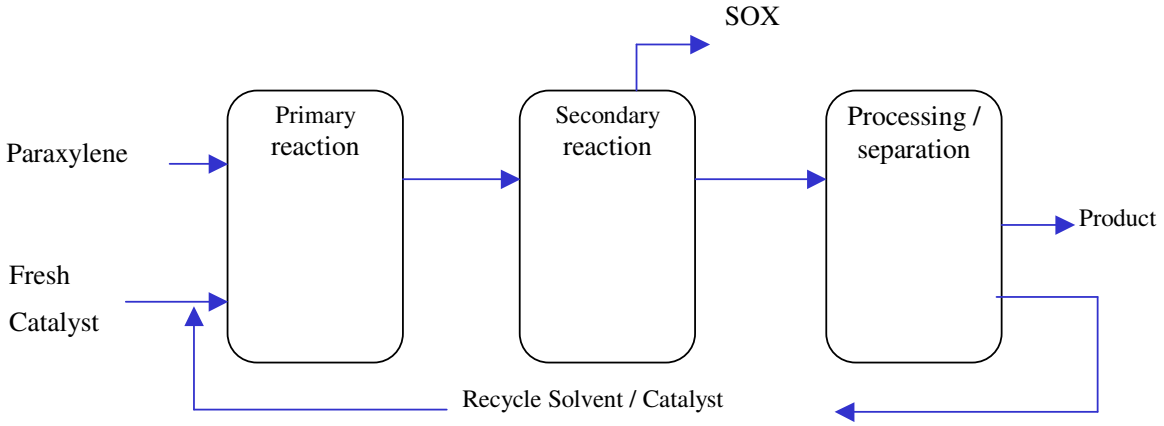

Figure 1 – Simplified Process Block Diagram

the 4CBA concentration in the secondary reaction. This has proved impossible, so the only indication we have is a laboratory analysis of a product sample taken after the processing and separation stage of the plant. The lag time from reaction to sample point is 4 hours, the analysis processing time is 35 minutes and, due to the complexity of the analysis, it is only practical to perform this every 4 hours. By setting up the reaction in a particular way, however, we can measure a parameter called SOX on the secondary reaction which provides a good inference of the 4CBA. Data analysis (prior to the implementation of the reaction control scheme) showed a correlation of 70% and an offset of 4 hours between the SOX and the laboratory measurement of impurity. (Interestingly - a neural network model was also built using 8 plant instrument signals, but this did not give a significantly better inference of 4CBA.) This parameter is used as an inferential measurement and is the controlled value or Process Variable (PV) input to the main controller for reaction. Hence the control scheme is known as "SOX Control".

The primary objective, therefore, is to control the 4CBA to target in order to achieve the minimum operating costs. This is achieved by controlling the SOX to a target, which is adjusted manually based on laboratory results. The SOX controller works by manipulating a number of reaction conditions.

Manipulated variables

There are four key variables that affect the SOX and can be used to control the reaction onto the target. These all have to be used in balance and within certain constraint rules, because they each have other effects on the process affecting: costs of production, product quality, corrosion rates, safety limits, etc.. The variables are:

- reactor level
- reactor pressure
- water draw off rate
- and catalyst concentration.

The first attempt at a robust SOX control, was based on two Model Predictive Controllers (MPC) using a costly proprietary package. A single controller was built for SOX control with three inputs, six outputs and two feedforward inputs. It had full constraint handling capabilities and manipulated the level, pressure and water draw off on both of the two parallel reaction streams. In order to keep the reaction in the correct range it was linked to a separate MPC via a LP Optimiser, which controlled the catalyst concentration. An on-line XRF analyser was installed, specifically to measure the catalyst concentration in the reactor feed, which was a critical input to the catalyst concentration controller.

The Achilles heel of the MPC solution proved to be the poor availability of the on-line XRF analyser. The difficulty of the analysis and the sample handling could not be overcome consistently despite the best efforts of the plant maintenance team. The catalyst concentration was then neither measured nor controlled but was drifting up or down to a point where the SOX controller, with the variables it had available to manipulate, could not be kept within its target range. Its manipulated variables ended up on their constraint limits as far away from optimum as they were permitted.

Catalyst Concentration

It became evident that the fundamental problem for reaction control is the ability to control the catalyst concentration. The difficulty is compounded by:

- the high recycle ratio of mother liquor at around 85%, means that fresh catalyst injection rate, which is how catalyst concentration is controlled, only accounts for 15% of the concentration. It therefore requires bold changes to catalyst injection to make significant corrections for recycle rate.
- The inventory and residence time in the processing/separation stage means that the overall response of catalyst concentration to changes in fresh catalyst flow is around 30 hours (or more than 3 shifts). The step response to changes in catalyst flow, modelled using VisSim in figure 2, shows that there is an immediate response followed by a large slow tail that hits later as it comes round in recycle.
- The catalyst is comprised of three components working together (Cobalt, Manganese and Bromine) in solution. Each of these travels through the plant and back in recycle differently. Bromine has a tendency to convert to a volatile form that vents off and is lost from recycle, Manganese can complex with one of the impurities and come out with the product and Cobalt is more stable in solution.

The philosophy adopted for manual control had been to keep the catalyst flow as steady as possible (close to a standard rate for the prevailing plant conditions), hope that there are few disturbances, and only make small adjustments infrequently. This made sure that the concentration didn't ramp off a long way from the requirement and that the reaction could be

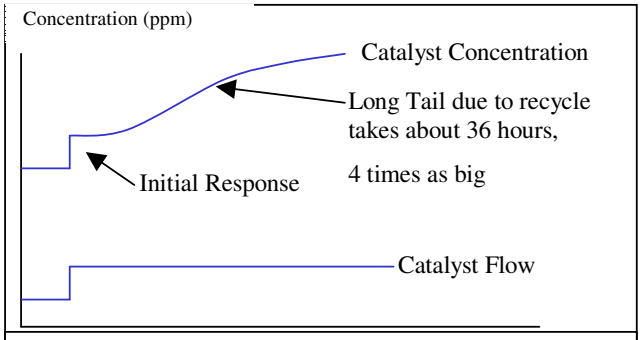

Figure 2 – Concentration response to change in catalyst injection

brought back to target in about 24 hours. This approach,

however is extremely slow to respond to changes in process conditions.

On-line Catalyst concentration model

The solution adopted is to maintain a real-time model tracking the catalyst concentration, based on flow and level readings, and use this to set the catalyst concentration as required for the reaction. The model was developed and trialled in a standard spreadsheet, using historical data downloaded from the process historian, to prove its stability, convergence and correlation with the (infrequent) off-line analysis.

The model tracks the concentration of the catalyst through the main stages of the plant and in the mother liquor recycle. The model uses as inputs the main flows round the plant, the fresh catalyst flow, and the purge of mother liquor. It also uses the main vessel level readings to calculate the inventories. The XRF analyser has been made redundant so we do not use an on-line measure of catalyst concentration. The model therefore, works in an iteration, calculating the change in catalyst at each point every minute and adding this to the previous value. It therefore starts, when reset from some typical values, and takes 5 to 10 hours to converge onto a realistic live value.

Much of the model has been based on the simple form:

Accumulation of catalyst in the vessel =

Total flow of catalyst in - Total flow of calayst out

Which in the simplest case is the equation:

$$\frac{d}{dt} M_i C_i = F_{i-1} C_{i-1} - F_i C_i$$

Where: Mi is Inventory of ith vessel

Ci is Concentration in ith vessel

Fi is Flow from ith vessel

Most of the vessels are maintained at a constant level setpoint and the catalyst concentration is incremented by:

$$C(t+\Delta t) = C(t) + \frac{F_{i-1} C_{i-1} - F_i C_i}{M_i} . \Delta t$$

For vessels that have deliberate changes in inventory the 'rate of change' of level has to be used, this gives rise to noisy signals that have to be handled carefully. For many of the process streams there is no reliable measure of flow and the design and simplification of the model has been built around these limitations. The model uses 6 flowmeter readings and 13 level readings.

T8 Catalyst Model 4.0 Equations

Constants		**Flow Rates**
Fresh catalyst conc	81000 ppm	Qa = FC104/1000
Frovac	0.98	Qb = FC120+FC108
Frecycle	0.95	Qc = 0.9*qb
		Qd = qc
Starting concentrations		Qe = qc
Feed mix drum	450	Qf - not used -
Reactors	450	Qg = qe-dM5/dt – dM6/dt
1st Xyst	450	Qh = FC403+FC406+dM7/dt
2nd Xyst	450	Qi = FC403
3rd Xyst	450	Qj = FC406
Filter Feed drum	500	Qk = FC102 + dM8/dt
Mother Liquor Drum	550	
Solvent Charge Drum	310	**Concentrations**
		db/dt = (qkck+qaca-qbcb)/(12*M1)
Mass Inventory		dc/dt = (qbcb-qccc)/(12*M2)
M1 = (68.9*LC239/100)+11.3		dd/dt = (qccc-qdcd)/(12*M3)
M2 = (36*(LC241+LC244)/100)+2		de/dt = (qdcd-qece)/(12*M4)
M3 = (63.1*LC245/100)+34.3		dg/dt = (qece-qecg)/(12*(M5+M6))
M4 = (67.8*LC246/100)+36.4		di/dt = (frovac*qgcg-qhci)/(12(M7+M9)
M5 = (70*LC248/100)+15.1		dk/dt = (frecycle*qici-qkck)/(12*M8)
M6 = (27.3*LC251/100)+3.81		
M7 = (54.8*LC456/100)+7.3		
M8 = (47.8*LC237/100)+7.5		
M9 = (10*(LC254+LC256)/100)+4		

Model Reliability

In order for the concentration model to be used to control the reaction, not only does it have to be representative, it also must be reliable to win and maintain the confidence of the operators. We set a target that it must be available for use for at least 95% of the time. Given that it takes 5 to 10 hours for the model to converge after a significant interruption, that is a challenging target. If a critical input to the model fails then the concentration controller is automatically disabled for 5 hours while it resets.

Each of the plant readings used as inputs to the model are analysed to define: the level of criticality; what ranges indicate a believable result; and what response the model should take in the event of a suspect reading.

Non-critical inputs	Flag reading as bad value. Continue with catalyst model and control
Short term non-critical inputs	For up to 20 minutes, freeze model concentrations. Continue with automatic control After 20 minutes trip out automatic control and reset model
Critical inputs	Trip out automatic control Reset model and re-initialise when input is good again.

Control Structure

Once we had achieved a model that representatively tracks the changes in catalyst concentration, this was programmed into the plant Distributed Control System using conventional control building blocks. This is set up as a controller that adjusts the catalyst injection rate to maintain the calculated (modelled) concentration onto whatever target value is required.

As there was no effort initially to re-model or rebuild the MPC controller for SOX. The two controllers are tied together using a simple constraint controller. The constraint controller is a conventional P+I control block. As an input it has a value showing where the Manipulated Variables of the MPC are relative to their constraints. The output then sets the target concentration for the catalyst concentration controller. Thus if the SOX controller is winding its manipulated variables above the optimum settings and towards the upper limits in order to keep the SOX on control, then the constraint controller will recognise this and adjust the setpoint of the catalyst concentration controller to allow the SOX to remain in control around the optimum reaction conditions.

This structure illustrated in figure is not the preferred way to build in catalyst concentration control, but it was a pragmatic option to avoid modifying the MPC at the time.

Concentration Control Performance

We have not managed to make any absolute measures of the performance of the catalyst concentration control. The laboratory measurements of concentration are too infrequent to verify the dynamic performance of the model. Since the model was installed there has only been one 36-hour run in which the on-line XRF analyser was working, and that was before final improvements were made to the model. This did however provide sufficient support for the model to proceed with commissioning the control scheme.

The performance of the controller is show in figure 4. These trends are the raw data from the very first time it was switched on. The left hand side is with manual adjustments to the fresh catalyst injection and the SOX controller is switched on. Here you can see the operator's practice of making small infrequent adjustments to the catalyst on the top line. With this practice the manipulated outputs of the SOX controller are seen averaged on the bottom line to be all over the place and riding on their limits for part of the time. On the right hand side the constraint controller and the concentration controller have been switched on. Large adjustments are required to the fresh catalyst flow as this only accounts for about 15% of the concentration. The MPC manipulated variables are now kept close to the optimum.

There is no requirement for absolute accuracy in the catalyst model. Because it is incorporated as part of a feedback control scheme, any long-term drifts are compensated for.

Simplification of SOX Controller

Since the Catalyst concentration control scheme has been proven to be robust, it has been possible also to simplify the SOX controller. The MPC controller for SOX had become rather oscillatory and was not keeping the SOX close to target, but in the plant team we have not got resource or expertise to re-model the controller. Now that it was possible for the first time to control catalyst concentration as required, a trial was arranged, replacing the SOX controller with a version based on standard control blocks. The new version uses a P+I controller with two outputs and a feed-forward from plant throughput. This simplified version has actually proved much better than the MPC controller with its out-of-date model and has now been adopted as the standard control. This means that we now have no reliance on outside experts to maintain MPC technology and the corresponding charges.

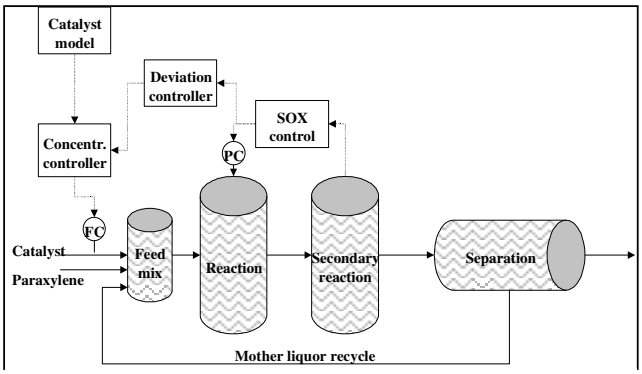

Figure 3 – Control structure

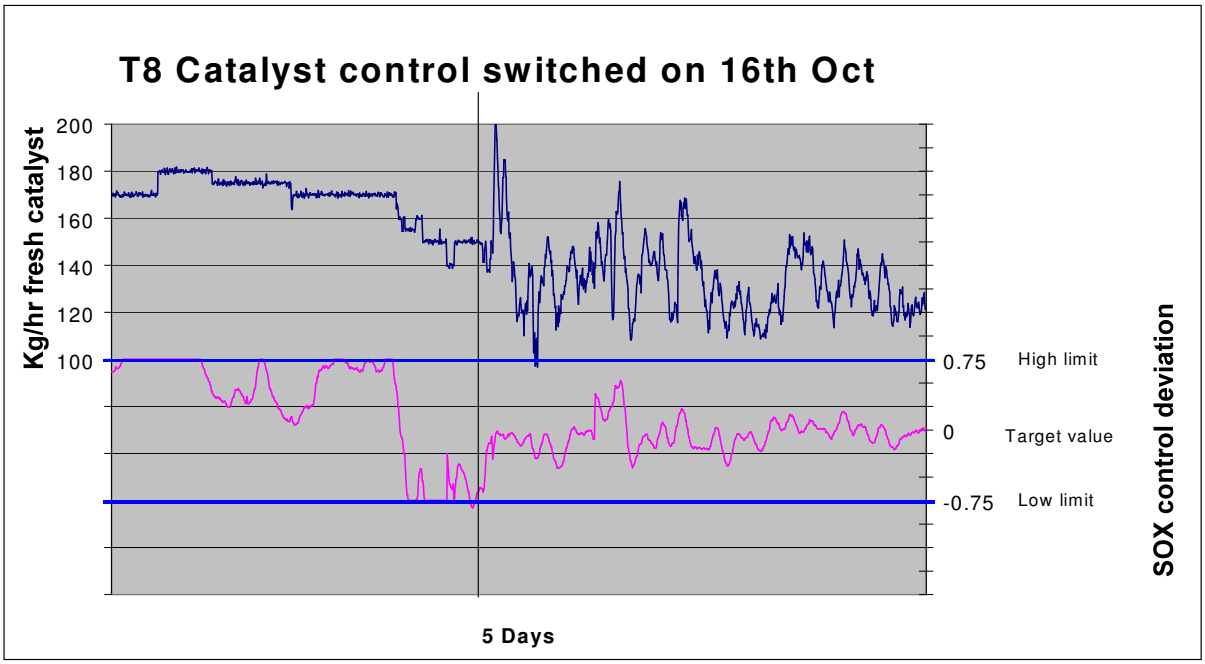

Figure 4 – Before and After switching on

Conclusion

The catalyst model, despite its dependence upon a wide range of plant instruments, has been reading, since commissioning, for greater than 98% of the time the plants have been running, even though it takes 5 hours to reset following a failure. This has allowed for very consistent and reliable use of the concentration controller. The variance of the reaction conditions from optimum had been reduced by a factor of three and the product 4CBA levels maintained in the target range for all normal operation of the plant. All this has contributed a significant saving on operating costs.

We have also learned a lot through the failures and successes about implementation of improved control on a Process Plant:

- Make sure we use the right level of technology for the application
- Which parts of the implementation should be done with reliance on expert consultants and which should be lead in-house
- It is preferable to aim at a clearly visible structure for the process control and avoid the “back box” approach.
- Keep it as simple as possible