Advances in pH Modeling and Control

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Abstract

Many chemical and biological processes have pH control loops. Good pH control can be important for product quality as well as environmental compliance. The extraordinary rangeability and sensitivity of pH as a concentration measurement poses exceptional challenges in many aspects of pH design and implementation. Advances in dynamic modeling, basic control, and advanced control embedded in a Distributed Control System are introduced and illustrated with field test results for a plant waste treatment pH system. Examples are also presented on how these advances can be potentially used to reduce the project and operating costs for multi-stage pH systems.

This paper details how models and control strategies are integrated in a DCS and used for an extensive variety of purposes. The model is used initially offline in a virtual plant to explore and prototype process control improvements running 10 to 100 times faster than real time. The improvements can be equipment, piping, and control system changes that reduce the capital and maintenance cost and reagent consumption that meet process objectives. An innovative configuration of a standard model predictive control is then developed to adapt model parameters to match up key process variables between the model and the plant. Test results and examples show how running and adapting the model online can provide increased monitoring and diagnostic besides control capability.

Meeting Expectations with Practical Limitations

The pH electrode offers by far the greatest sensitivity and rangeability of any industrial process measurement in terms of the measurement of concentration (hydrogen ions). To realize the full potential of this opportunity requires extraordinary performance of mixing equipment, control valves, reagent delivery systems, flow meters, control system design, and controller tuning. For pH control systems, not addressing any one of the automation and mechanical design requirements can cause the system not only to fail but to fail miserably (ref 1,2,3). Besides the opportunity for keeping the pH deviations within allowable limits, there are considerable often unknown opportunities to reduce operating costs. Based on the authors' experience, maintenance and reagent costs are often not correlated to production or waste treatment system design and operation.

Building a Virtual Plant

A virtual plant can be used to sort out fact from fiction important for insuring performance and reducing capital and operating costs. The virtual plant consists of a download of the actual control system configurations and displays, embedded advanced control tools, and a dynamic process model running on personal computer as shown in Figure 1. There is no emulation or translation of the control system (ref 3,4,5). Parts of the process or the whole virtual plant can be run much faster than real time (ref 6). The process model uses component, charge, and energy balances set up as modular blocks to provide a dynamic simulation based on first principles (ref 4,5,6,7). Since, only volumes flows, densities, heat capacities, and the dissociation constants of the acids and bases are essential for the simulation of pH systems, the complexity and interaction of physical properties and liquid and vapor equilibrium are avoided and the process aspects of the simulation are simplified (ref 5). Some would argue that activity coefficients should be modeled. Normally, waste treatment systems are dilute enough where these coefficients are unity. However, for those applications where a pH measured stream has exceptionally high acid or base concentrations, the dissociation constants can be adapted to compensate for the change in activity coefficients (ref 1). More important is the modeling of mixing and reagent injection delays. The dynamic response of different process, equipment, and control system scenarios can be explored with an embedded process model (ref 5). There are ten top reasons to use a virtual rather than a real plant for control improvement (ref 7).

Top Ten Reasons We Use a Virtual Plant Rather Than a Real Plant

(10) You can’t freeze, restore, and replay actual plant operation
(9) No separate programs to buy, learn, install, interface, and support
(8) No waiting on lab analysis
(7) No raw materials
(6) No environmental waste
(5) Virtual instead of actual problems
(4) Vessels line out within minutes rather than hours
(3) Plants can be operated on a tropical beach
(2) Last time we checked our wallet we didn’t have $100,000,000 for a real plant
(1) An actual plant doesn’t fit in our suitcase

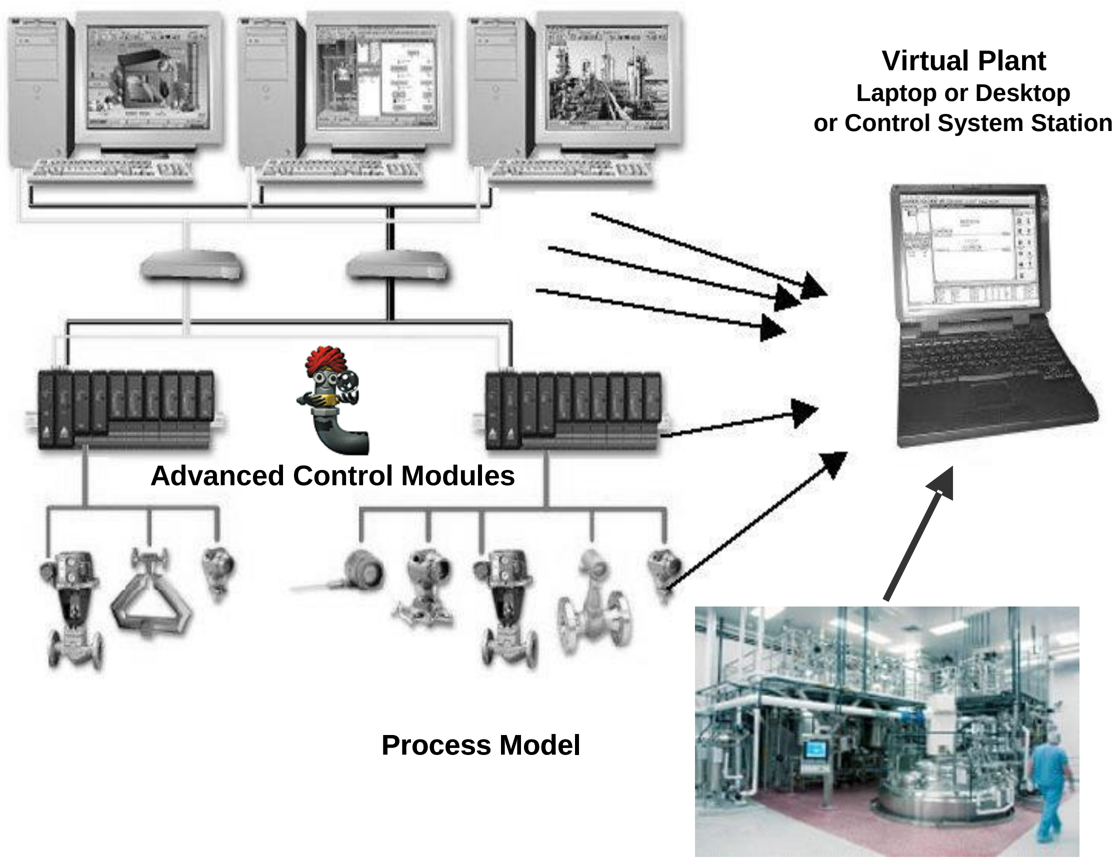

Figure 1 - Virtual Plant

Reducing Capital and Operating Costs

The capital cost of pH systems can be reduced by the use of static mixers instead of agitated vessels and by the use of high resolution control valves to eliminate a stage of neutralization (ref 1,2).

Static mixers are a section of baffled pipe that provides axial but little to no back mixing. Most of the residence time (typically 1-6 seconds) is a process dead time (transportation delay) rather than a process time constant.

The incredibly small almost negligible process time of a static mixer means that a feedback controller on a static mixer has difficulty in catching up with a fast disturbance. In fact, the peak error from a step disturbance to a static mixer is probably the same as if there was no control loop. Also, the pH at the mixer outlet tends to exhibit noise and fast oscillations from reagent injection because of the lack of back mixing. Various loop enhancements, such as signal filters, signal characterization, feedforward control, and a

“Kicker”, are used to help a pH control system on a static mixer deal with fast upsets, noise, and oscillations (ref 1,2,3). The same type of loop improvements can reduce the number of stages of neutralization required when combined with high resolution valves.

High resolution valves can respond to a change in signal less than 0.2%, which implies these valves have a half stick-slip and half dead band less than 0.2% (ref 8,9,10,11). The resolution of control valves can be tested per the ISA standard. It is important to realize that just the application of these mixers and valves does not insure a project or system will meet its objective. Successful capital and operating cost reduction by these mixers and valves require enhancements to the basic control system. The virtual plant provides a tool to develop, prototype, and test these improvements for typical plant disturbances and operating scenarios.

Middle signal selection of 3 measurements can improve onstream time and reduce the amount of calibration and troubleshooting. With 2 measurements, which electrode is correct is a matter of personal opinion, whereas for 3 measurements, the measurement furthest from the middle signal is the real suspect.

The cost of reagent can be decreased by online performance metrics, reduced reagent cycling, and pH set points closer to the constraints (pH limits). Trends of online metrics of reagent usage that are relatively noise free and representative of shift and daily performance can be a powerful motivation and troubleshooting tool. ‘Kickers” can be made more intelligent to reduce the overdose of reagent when activated to prevent a constraint violation. Model predictive control combined with high resolution valves can eliminate limit cycles associated with split range points (ref 12). Model predictive control can also replace heuristic and rule based systems to optimize pH set points (ref 1).

Detailing the Existing Plant Control System

We applied a virtual plant to the waste treatment pH control system illustrated in Figure 2 and examined many of the issues associated with the use of static mixers and model predictive control to reduce capital and reagent cost. The neutralization system had an inline pH loop on each of the static mixers used for the two stages of reagent addition. The discharge from 2nd stage fed into an attenuation tank to smooth out the oscillations from the inline systems. In Figure 2, the waste from many production units are consolidated and depicted as a single waste stream entering at each stage. Any excursion of the tank discharge stream below the low environmental pH limit no matter how brief could be considered a recordable violation.

The control system employed several methods to always keep the effluent pH above the environmental limit despite large unknown changes in the strong acid concentration of the influent from various production units. Middle signal selection of 3 pH measurements for the inline loops and the tank was implemented to automatically prevent an excursion from an electrode failure of any type. Each stage of reagent addition employed multiple reagent valves to prevent the plugging or failure of a valve from disabling the pH loop. A kicker strategy was used to step open the 2nd stage reagent valves if the 2nd stage pH got too low. Finally, the effluent would be diverted if the tank pH got too low.

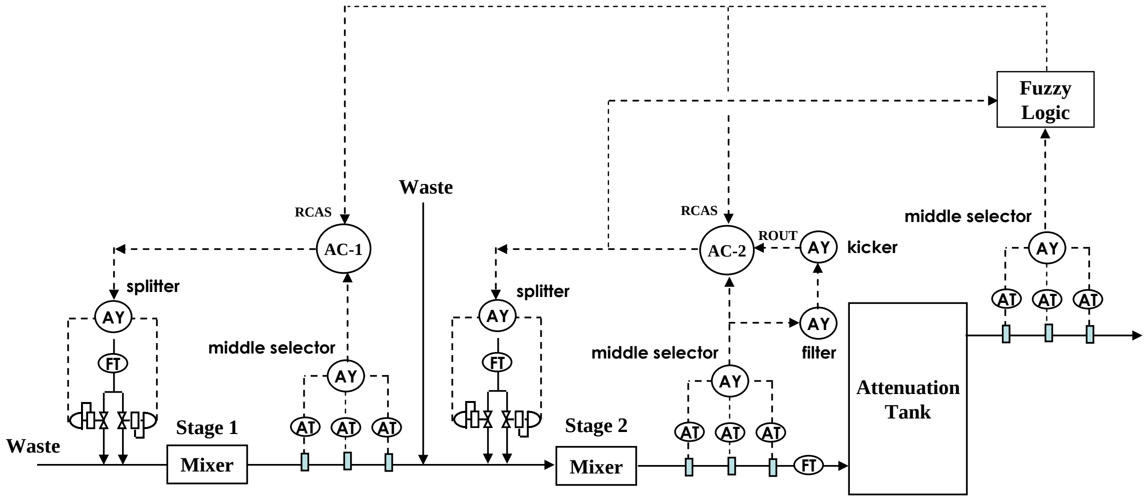

Figure 2 - Existing Plant Control System

The existing control system used fuzzy logic control (FLC) based on a heuristic rule set to automatically optimize the set points of the pH loops on the static mixers. If the pH in the tank was comfortably above the low pH constraint, the FLC would reduce the 2nd stage set point. The FLC would also decrease the 1st stage set point if the 2nd stage reagent valve was above some minimum throttle position. Operating the reagent valves too close to the seat increased stick-slip and the plugging and erosion of the trim.

Prototyping an Improved Control System

We developed and prototyped model predictive controllers (MPC) to replace the fuzzy logic control system. MPC-1 adjusted the 1st stage pH set point to keep the second stage reagent valve at a minimum position for good response and reliability. MPC-2 trimmed the 2nd stage set point to keep the pH in the tank at an optimum pH.

The strategy used by MPC-1 is an optimization technique commonly called “valve position control.” It has been used in many different applications such as optimization of compressor energy cost by reducing the compressor discharge pressure set point so the reactor feed valves are operating around a minimum effective throttle position. For our pH application, MPC-1 decreases reagent cost by reducing the 1st stage pH set point so the 2nd stage reagent valve is operating around a minimum effective throttle position. A conventional integral only feed back controller could be used for “valve position control” The proportional and derivative action of the PID controller are turned off to decrease the interaction between the “valve position control” loop and process control loops. The integral time setting is increased to make the optimization slower to further mitigate interaction problems. The tuning of this integral only controller is difficult (ref 13).

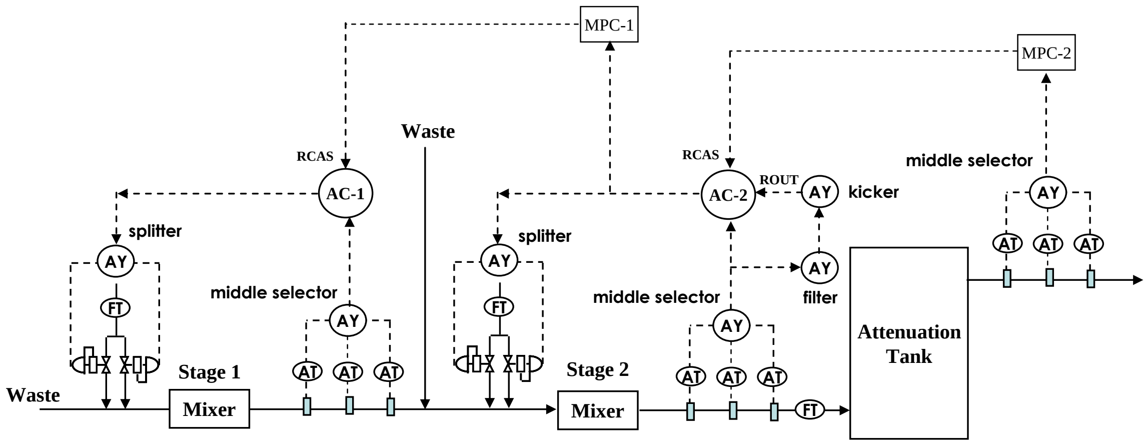

Figure 3 - Prototyped Plant Waste pH System with MPC Replacement of Fuzzy Logic

The use of model predictive control for the “valve position controller” has the advantage of built-in knowledge of the dynamic relationship between 1st stage pH and 2nd stage reagent valve position through its experimental model of the dynamic response. Thus, MPC-1 should be better able to sort out the interaction between valve position control and 1st stage pH control. Model predictive controllers also offer a tuning knob called “penalty on move” (PM) also known as “move suppression” that can slow down the manipulation of set points and final elements. For MPC-1, the PM was increased from the default setting computed automatically from the dynamic response (ref 14, 15).

A PID controller could be used to control tank pH by the manipulation of the 2nd stage pH set point. Since the tank is not agitated, there is considerable dead time and possibly non-uniform response from the lack of back mixing. In previous implementations on a poorly mixed tank, integral only controllers have been used to provide a slow and smooth trim of the set point for the inline pH system upstream.

The use of model predictive control for tank pH control has the advantage of built-in knowledge of the large dead time through its experimental model of the dynamic response (ref 14,15). Thus, MPC-2 should exhibit more patience and provide a smoother response than a PID controller and a faster response than an I-only controller.

We conducted automated pseudo random binary step (PRBS) tests in an offline virtual plant. Before the PRBS tests were initiated, the 1st and 2nd stage loops were tuned since their tuning affects the dynamic response seen by MPC-1. Also, the tank model was speeded up to reduce the test time. When the virtual plant was operated real time, the time constant for MPC-2 was increased accordingly. The experimental models were automatically identified from the PRBS tests and the controllers were downloaded. Runs of the offline virtual plant indicated MPC-1 and MPC-2 did well for set point changes.

Putting the Virtual Plant Online

In order to study and improve performance of the control system and the fidelity of the process model for actual process conditions, we put the virtual plant in a read-only mode online running real time. A simple interface module was configured that used object link embedding for process control (OPC) to read indicated waste flows, controller set points, and controller modes from the actual plant. An important concept to realize here is that the signals written into a virtual plant (VP) to keep it in sync with the actual plant are the set points of the highest level of active controllers plus the process variables that are not controlled in the virtual plant. Consider a VP cascade loop whose primary controller can get a set point from an even higher level of VP MPC control. When the secondary loop is in the "auto" and "RCAS" modes, the secondary loop set point comes from the actual plant and the primary loop in the VP, respectively. Similarly, when the primary loop is in the "auto" and "RCAS" modes, the primary loop set point comes from the actual plant and the model predictive control in the VP, respectively. Thus, the flows that result from manipulation of final elements in the VP are determined by the loops in the VP. Only, wild flows or flows whose controllers are outside of the scope of the VP are read and set in the VP to match the actual plant. How well the manipulated flows in the VP match up with the actual plant are a good indication of the process model fidelity. How well the valve positions match up depends upon the fidelity of pressures and valve characteristics.

Adapting the Process Model

We developed a third model predictive controller (MPC-3) to adapt the concentration of the strong acid in the waste going to the 1st stage of the VP to match the actual plant. An innovative configuration of a standard model predictive controller was used to match up a key process variable in the VP with the actual plant by the automatic manipulation of the associated model parameter (ref 15,16). The key process variable and set point for the controlled variable was the ratio of reagent to influent flow from the virtual and actual plant, respectively as shown in Figure 4. The ratio of reagent to influent flow rather than just reagent flow was used as the key performance variable to match up in order to build in knowledge of the plant production rate. The experimental model for MPC-3 was automatically identified from an automated PRBS test of the offline VP. An important point here is that the dynamics of this experimental model depends upon the tuning of the control system and changes in other model parameters. Consequently, if the tuning of the control system is significantly changed, the model should be retested and identified. Also, if other model parameters need to be adjusted, the adaptation of these parameters should be done as much as possible in the same model predictive controller so the interaction between model parameters and key process variables are automatically addressed (the forte of MPC). We envision two additional adaptations for future testing. We would adapt the effective pressure drop in the model across the flashing reagent valves in the

VP by matching up the valve positions in the VP with the actual plant. Also, we would adapt the acid dissociation constant in the VP by matching up the change in the 2nd stage pH of the VP with the actual plant when the kicker as activated.

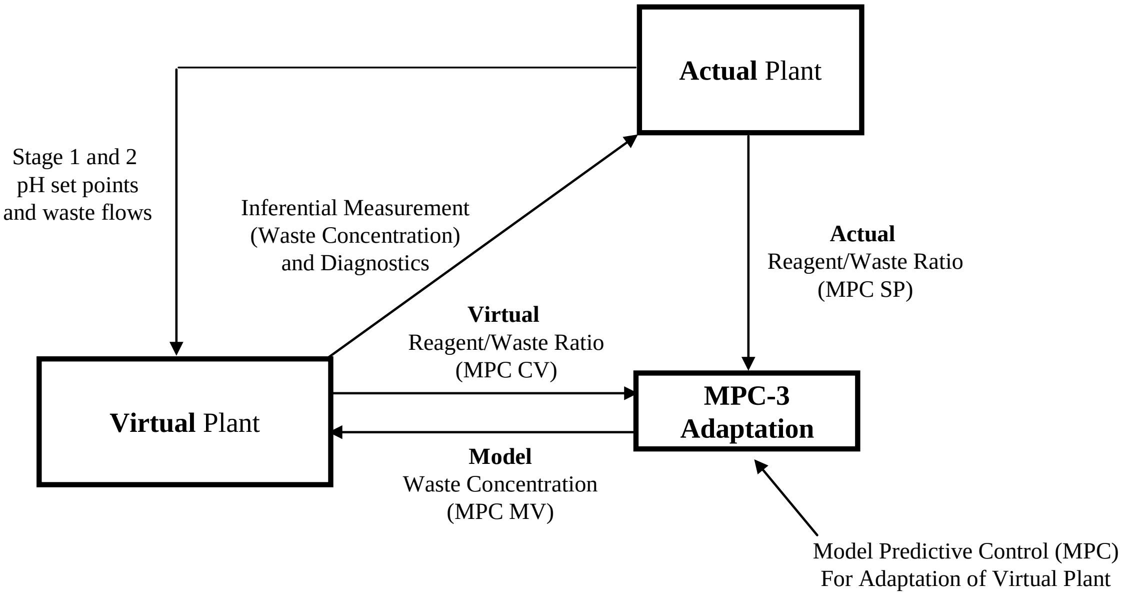

Figure 4 - Setup of Virtual Plant with MPC Adaptation of Acid Concentration

Rocking-N-Reeling

When we did initial tests with the virtual plant running online, everything was smooth and the application looked rather straight forward. While at lunch the calm turned to storm and the loops were all rocking and reeling. We looked at MPC-3 and it was doing a much better than expected job of chasing big changes in reagent to influent flow by adjusting the waste concentration coming into the VP as shown in Figure 5. We realized that the action of the MPC-3 could be used to troubleshoot operating problems originating in the production units. MPC-2 was doing a great job as well keeping the tank pH on target. However, MPC-1 was having a heck of time trying to keep the 2nd stage reagent valves at an effective throttle position particularly during the periodic activations of the "kicker." The fact that MPC-1 had taken a back seat and that MPC-1 and MPC-2 was driving the show was consistent with the relative importance of the controllers. However, it was surmised that the performance of MPC-1 could be improved if it was included with MPC-2 into a single larger MPC so the valve position controller knew about the actions of the tank pH controller. Also, it was obvious that the kicker was over active and over dosing reagent. This was corrected by significantly increasing the filter on the pH used to trigger the "kicker." In principle, the filter time could be increased to the effective process time constant of the tank seen by MPC-2.

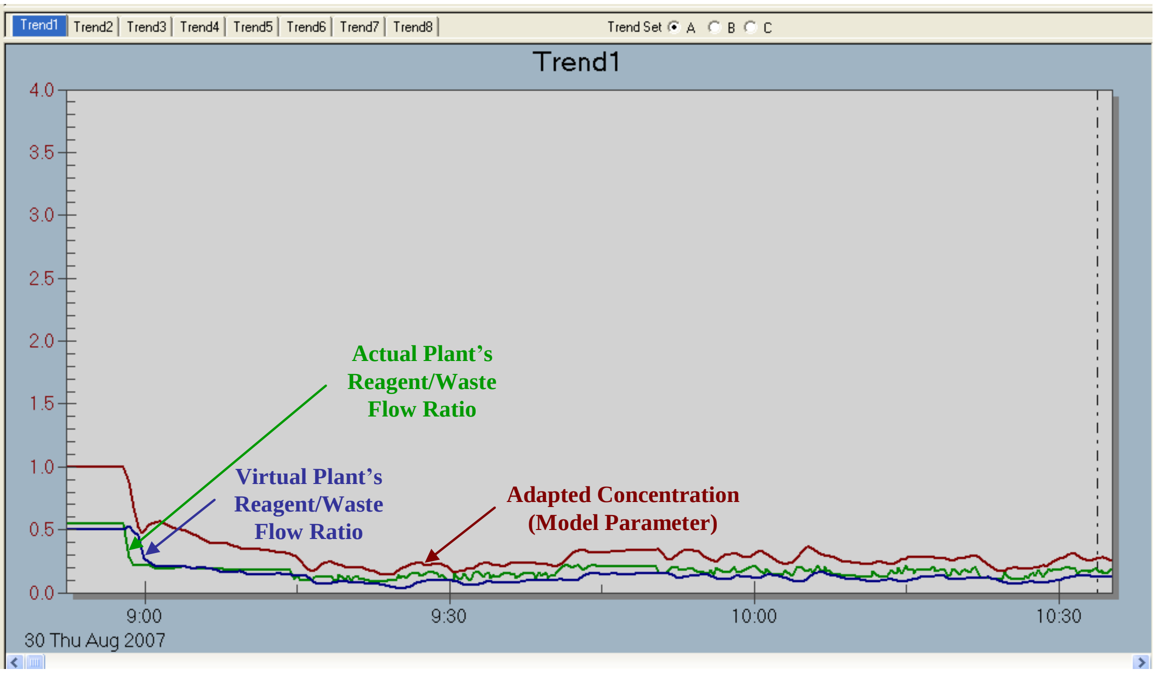

Figure 5 - Online Adaptation of Model's Acid Concentration

Finding Future Opportunities

We learned about several new opportunities while using the virtual plant that can be developed and prototyped in the future.

An increase in an online metric that is the ratio of reagent flow to influent flow indicates either a production unit or waste treatment performance problem. However, if adaptation of the VP shows a significant increase in waste concentration, the problem originates in the production unit. If the ratio is computed based on a running total of flow over the last x hours, the noise and confusion of short term fluctuations is reduced. Furthermore, if the last x hours correspond to a shift, the performance of different shifts can be compared. Both totals and ratios for each shift could be indicated. Shift metrics could be treated similar to batch metrics where each shift is like a different piece of equipment running the same batch process. The shift metrics could be plotted similar to batch metrics.

The VP can provide an inferential measurement of this concentration useful for feedforward control and diagnostics. The inferential concentration measurement with the actual waste flow measurement can be used to compute a component acid waste flow that can provide a more accurate feedforward signal for the pH loops and a more direct metric of a running total of the reagent to acid waste flow.

Online metrics improve performance by better operating and maintenance practices from increased awareness and provide the justification, motivation, and knowledge for process control improvements. The quality of these metrics depends upon the availability, rangeability, and repeatability of individual waste and reagent flow measurements.

Watching the kicker, we realized that the single step to pop open the 2nd stage reagent valves to 50% was an over reaction. The "kicker" should instead increment open the reagent valves by about 1% per second when the pH was below the trigger point. Even if the 2nd stage pH loop took almost a minute to get the reagent valves open to 50%, the tank was large enough to handle the pH deviation.

We also recognized the opportunities to use the virtual plant to teach operators, process engineers, automation engineers, and maintenance technicians how to troubleshoot and deal with disturbances, failures, startups, and shutdown.

Unrelated to this pH control system is a three vessel neutralization system in a production unit where pH is critical for product quality. We expect to use a virtual plant to study how the cost and performance of this system could be improved in a future project.

Summarizing the Big Picture

A virtual plant was used to provide knowledge of the operation of the process, equipment, and control system that lead to improving the control and performance of a waste treatment pH system. The insight into principles and relationships decreased the reagent costs and is expected to reduce the capital cost of plant projects for pH control.

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Biographies

Gregory K McMillan is a retired Senior Fellow from Solutia Inc who presently is a principal consultant at Emerson Process Management. Greg is an ISA Fellow and received the ISA “Kermit Fischer Environmental” Award for pH control in 1991.

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