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Plantwide Control Study of a Vinyl Acetate Monomer Process Design

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A simulation of a vinyl acetate monomer (VAM) process design was developed and compared with the work of Luyben and Tyreus (1998). Two incremental changes were made to the two main control substructures. Specifically, the two schemes focus on improving the liquid inventory system control and controllability of the azeotropic distillation column. The level control strategy was tested and found to produce a faster response with less oscillatory behavior. Two alternative control techniques for the azeotropic distillation column were tested, a feed-forward model predictive controller and a static feed-forward ratio controller. The model predictive controller results illustrated the large difference between the water composition analyzer sample time and the controller step size. The static feed-forward ratio controller showed excellent disturbance rejection of large feed flow variations to the azeotropic distillation column. Simulation results are presented to illustrate the effectiveness of the new control strategies.

Keywords Vinyl acetate monomer; Simulation; Model predictive control; Ratio control

Introduction

Plantwide control system design and optimization has for many years been a recognized challenge in the research community (Mellichamp, 1993), and it continues to be a major topic of interest, with the focus on new methods for creating the most effective control structures. However, the task is a challenge due to the large number of variables involved and the resulting number of alternatives in plantwide control synthesis. Present-day techniques to overcome this difficulty range from the designer’s experience to formal sets of heuristics (Zheng et al., 1999, Luyben et al., 1997), to optimization with both steady-state and dynamic simulation (McAvoy, 1999).

Today it is recognized that one key tool to be used in designing more effective control structures is dynamic simulation. With the aid of simulation, both research and industrial practitioners can test their ideas and gain insight into process behavior that would not normally be intuitive given the complexity of an entire process design. Unfortunately for the research world, much plantwide information is proprietary and not available in open literature (Mellichamp, 1993). However, in recent years
several good case studies have been published that allow testing of new control ideas on the level of complexity seen in a typical industrial chemical manufacturing plant. One such study that has been presented by Luyben and Tyreus (1998) provides detailed process and rating information for the manufacture of vinyl acetate monomer (VAM). In addition, the authors propose and test an entire control structure using their nine-step approach to plantwide control design (Luyben et al., 1999). This study uses their work as a base case for testing several proposed changes to their decentralized control strategy. A simple incremental approach has been applied that looks for ways of improving the dynamic controllability of the base design. The results and conclusions of a new reboiler level strategy, use of a feed-forward model predictive control (MPC), and a simple static ratio controller are presented.

**Background Information**

**Process Description and Simulation**

In the process to be studied, the production of VAM is based upon the common gas phase catalyzed reaction of ethylene, acetic acid, and oxygen. In addition, a dominant CO₂ producing side reaction also occurs, consuming the key ethylene feedstock. It is assumed for this study that these two chemical reactions are the only ones that occur and are shown as follows:

\[
\begin{align*}
C_2H_4 + CH_3COOH + 0.5O_2 & \Leftrightarrow CH_2=CHOCOCH_3 + H_2O \\
C_2H_4 + 3O_2 & \Leftrightarrow 2CO_2 + 2H_2O
\end{align*}
\]

Figure 1 shows a schematic of the process. Only the central production units are included; the feed storage and product purification stages are not included as they are not germane to this study. The major unit operations include: a vaporizer,
a gas phase plug flow reactor, a heat exchanger, a vapor/liquid separator, an absorber column, and an azeotopic distillation column. There are two major recycle loops, one for gas reactant recovery and the other for liquid reactant recovery. In addition, there is a secondary liquid recycle stream to the absorber for the recovery of liquid carryover in the gas stream. Both liquid recycle loops are of particular interest as they introduce a dynamic that is dominated by the effects of lag.

The process simulation has been based on the design data given in Luyben and Tyreus (1998) and accomplished using the commercial process simulator HYSYS™. Standard unit operations were used for the entire flow sheet simulation. However, ActiveXTM extensions were written to model the complex structures of the reaction rate expressions defined in Luyben et al. (1999), representing the kinetic behavior of reactions (1) and (2). The HYSYS models developed in this article were provided to Hyprotech Ltd.

To provide a more realistic basis for testing, the effects of sensor noise, dead time, and sample time have also been included. Specifically, process noise of 1% of each process variable range has been added to process and measured variables. In addition, a filter was applied to each measured variable. Finally, the effects of sample time and dead time resulting from the use of a water analyzer at the bottom of the distillation column have been assumed. A value of five minutes has been selected for this sample time.

The UNIQUAC (Abrams and Prausnitz, 1975) thermodynamic model was selected to model the VAM/water/acetic acid ternary mixture. The thermodynamic model interaction parameters were taken from low-pressure vapor-liquid equilibrium data given in the DEHEMA data series (Gmehling and Onken, 1977). The UNIFAC local linear estimator (LLE) estimation procedure (Frendenslund et al., 1975) was used to derive the VAM/water binary interaction parameters due to the lack of quantitative experimental LLE data for this binary. The liquid phase fugacities of the noncondensable components were derived using Henry’s Law coefficients. However, the ethane parameters used were the same as water in order to better match material balance information given in Luyben and Tyreus (1998). The vapor phase fugacities were calculated using the ideal gas law.

**Control Objectives**

In order to establish an understanding for the plantwide control system, a clear statement of the control objectives must be stated. For this VAM process design the control objectives, as outlined in Luyben et al. (1999), are:

1) Set the production of VAM while minimizing yield losses to carbon dioxide production.
2) Absorber must recover as much of the VAM, water, and acetic acid from the gas recycle loop to prevent losses to the CO₂ removal system.
3) Provide control during production turndown.
4) Oxygen concentration in the gas recycle loop must remain outside the explosivity range for ethylene.
5) Minimize losses of acetic acid to the overhead of the azeotropic distillation column.
6) Minimize VAM concentration in the bottoms stream of the azeotropic distillation column to below 100 ppm.
For this study, focus has been on objectives 5 and 6 above. The remaining objectives are handled by the base case plantwide control scheme discussed in the next section. For proper operation of the process several specific control requirements become apparent from these objectives. These specific control requirements are listed below and have been adapted from Luyben et al. (1999).

1) Provide set point tracking of key process variables (reactor outlet temperature, azeotropic distillation column bottoms waster composition, carbon dioxide and ethane concentration in the gas recycle stream).
2) Provide control with a water composition analyzer sample time of five minutes and demonstrate controllability under the influence of process noise.
3) Provide disturbance rejection due to a five-minute feed flow shutoff of the azeotropic distillation column feed pump.
4) Provide stable inventory control.

The focus of test work in this study has been on meeting these control requirements and searching for methods to improve their performance.

**Base Case Plantwide Control**

The derivation and the performance of the base plantwide control has been well documented in Luyben et al. (1999). The simulation used in this study has been compared against the results of this reference and found to agree well with the documented behavior. Figure 2 shows the base case control structure.

Of particular interest are the reboiler and the water composition control schemes of the azeotropic distillation column. In the base scheme, both the wash acid recycle stream and the total acetic acid feed flow to the vaporizer are on flow control. Therefore, changes in the reboiler level are controlled via the change in fresh feed flow rate of acetic acid. This pairing is justified for several reasons: the first is the need to prevent instability or “snowballing” of the liquid recycle loop by having the recycle
stream on flow control; second, putting the total acetic acid flow to the vaporizer on flow control ensures proper acetic acid concentration to the reactor; third, given that the reboiler level can be considered to be an indication of the plant acetic acid inventory, it is best to pair fresh feed flow with it. With this approach, the vaporizer level is free to be paired directly to the heat input to the vaporizer.

The azeotropic distillation column composition control is managed using two control loops: a bottoms water-reflux loop and a stage 14 temperature-reboiler duty loop. Interestingly, the water middle boiler and not the overhead acetic acid concentration is controlled. This approach ensures the overall plant water component inventory is regulated. The stage 14 tray temperature loop is key to maintaining the temperature profile of the column, thus ensuring the VAM concentration is less than 100 ppm in the bottoms stream.

The control loops were tuned using an auto tuning variation relay technique (Åström and Hagglund, 1984). All pressure and level loops were set on proportional control only with a high gain for tight pressure regulation and averaging control for the levels.

In this work, incremental changes were made to the base design by evaluating two main control substructures. A new reboiler level control strategy was implemented along with two alternative control arrangements for the azeotropic distillation column. The first is the implementation of an MPC centralized controller and the second is a static feed-forward ratio controller. The results of each are compared to the base case performance in the following sections.

**Base Case Control Performance**

Two tests were selected for study based on the specific control requirements mentioned above. There was a step change from 0.09 to 0.18 mole fraction water composition in the distillation column bottoms and an interruption in distillation column feed flow for five minutes. Figure 3 shows the results for the first test. The response proved to be underdamped, resulting in an overshoot of the set point and oscillatory behavior in liquid inventory levels and flows. The cause of this oscillatory behavior is attributed primarily to the structure of the base case reboiler level control strategy. With the fresh acetic acid feed introduced immediately upstream of the vaporizer, a considerable amount of dead time is introduced into the system. As a result, the interaction lag between the reboiler level and the fresh acetic acid feed adversely affects all other flow rate and composition controls. However, excellent set point tracking was attained for the stage 14 temperature controller. Through the tight temperature control, the VAM composition in the column bottoms stream remained below the specified 100 ppm constraint, reaching a maximum of only 10 ppm.

Figure 4 illustrates the ability of the base case to reject the five minute feed flow interruption disturbance. Due to the short time duration, the capacity controls were not significantly affected. However, composition and temperature effects were significant. Despite the initial large variations in these variables, the process was brought under control and stabilized at the appropriate set points after the pump was restarted. The water composition response took approximately seven hours to reach steady state whereas the stage 14 temperature took only one hour. Finally, the VAM concentration in the bottoms reached a maximum of 40 ppm, remaining
Figure 3. Step test of WATER composition in azeotropic distillation column bottoms from 0.09 to 0.18 mole fraction – base case.

Figure 4. 5-minute shut-off of azeotropic distillation column feed pump – base case.
below the 100 ppm limit. Again this result is attributed to the fast temperature control loop dynamics.

**Plant Inventory Control Structure**

*Design*

The design of the new reboiler level control structure is shown in Figure 5. In this arrangement the acetic acid feed flow is paired with the vaporizer level and the distillation column reboiler level is paired with the bottoms flow. The decision to use this control structure was for two reasons: to minimize the dead time introduced into the process by the base case design as discussed above and to maintain a constant temperature of the vaporizer overhead gas stream. It is concluded that any undesirable propagation of disturbances in the liquid recycle loop would be held in check. That is, the acetic acid feed flow is being used to directly control the level of the vaporizer, minimizing dead time in the system. Second, the vaporization rate remains fixed by using a temperature controller on the vaporizer outlet. Therefore, the liquid recycle is essentially under flow control preventing any “snowball” effects due to disturbances in the liquid inventory system. Pairing of reboiler level with bottoms flow results in rapid rejection of any fluctuations in level and passes the flow rate changes onto the vaporizer level control.

However, two implementation issues should be noted. First, extra precaution would have to be taken to ensure that the temperature sensor is accurate, as a faulty sensor can result in little or no vaporization. Therefore, operations would be responsible for ensuring the integrity of this temperature sensor. In addition, acetic acid inventory is now regulated within the vaporizer given the pairing of acetic acid fresh feed with vaporizer level. Therefore, depending on the dynamics, the process design

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**Figure 5.** New reboiler level control structure.
may need to be changed to incorporate more capacity in the vaporizer or utilize an intermediate tank in the acetic acid recycle loop.

**Results**

To test the new configuration, the same step test of WATER bottoms composition from 0.09 to 0.18 mole fraction was performed. The results shown in Figure 6 verify stable capacity and composition control of the key process variable. In comparison to Figure 3, better performance was achieved, as less time was required to stabilize the variables at their set points. The conclusion is that given the elimination of additional dead time in the reboiler level control strategy, less oscillatory behavior occurred in the process, resulting in better performance.

**Distillation Column Composition Control**

**Feed-Forward MPC**

The first modification to the composition control substructure in the azeotropic distillation column was to implement a model predictive controller (MPC). The reason that MPC was chosen is that it has become arguably the most widely implemented advanced process control strategy in industry (Seborg, 1994). The controller was applied to the $2 \times 2$ composition control loop consisting of the water composition in the bottoms stream and the tray 14 stage temperature. Due to the nature of the investigation in implementing an MPC, we decided to minimize the number of variables at two. We selected the composition control loops in light of their importance for product purity and overall operation stability, these loops being key to quality

![Graphs](image)

*Figure 6.* Step test of WATER composition in azeotropic distillation column bottoms from 0.09 to 0.18 mole fraction – new reboiler level control.
control for this distillation column (Olsen et al., 2002) and assuming the work of Luyben et al. (McAvoy, 1999; Luyben et al., 1999) in developing the regulatory control structure was optimal in some sense. Note that is also important to consider the restrictions of the manipulated variables in the development of an MPC. However, no data related to restrictions on manipulated variables were given in the original reference. As a result this was considered in the following manner. All valves were simply sized using standard control valve Cv sizing algorithms. The values were checked to ensure saturation did not occur. The details of the controller and the results are presented in the following sections.

**Design Details**

The MPC algorithm used in this study is the well-known dynamic matrix controller (DMC) formulation (Cutler and Ramaker, 1979). For this study, a feed-forward component was included in the overall calculation to account for feed flow disturbances. Therefore, the full prediction horizon can be calculated as:

\[
Y = Y_{past} + Y_{FF} + A \times \text{delU} + b
\]

where \( Y_{past} \) accounts for the effects of past moves in the manipulated variable, \( A \) is the dynamic matrix of step coefficients, \( \text{delU} \) is the future moves of manipulated variables, and \( b \) accounts for model error. To account for measured disturbance variables, a feed-forward component \( Y_{FF} \) is applied to the truncated step response model based on the approximation of constant future disturbances (Hokanson and Gerstle, 1992). The step response models were easily obtained by introducing positive changes in the manipulated variables. Given all this information, future \( \text{delU} \) moves are calculated using standard least squares to find the minimum error from set point with only the first move actually being implemented.

To avoid the complexity of the open-loop behavior as discussed in Olsen et al., (2002), a partial closed-loop strategy has been used. As a result, the temperature controller set point is controlled directly as shown in Figure 7. The MPC controller

![Figure 7. High-level MPC design showing relation between manipulated and controlled variables.](image-url)
calculations were implemented in a custom computer program linked together with HYSYS™ and Matlab™ (van der Lee et al., 2001).

Due to the aggressive settings of the stage 14 temperature control loop, they were detuned to provide a more critically damped response. This action was necessary in order to obtain an adequate step response model to allow stable performance of the controller. Using the detuned control loop proved beneficial in two aspects: the oscillatory behavior of the underdamped response was removed and the difference between the two composition controller time constants was reduced to an adequate level. A 30-second step size was selected based on the time constant of the detuned temperature control loop. Also, the step response model horizon was selected to be 200 step coefficients. Tuning of the MPC controller used the method in Maurth et al. (1988) whereby a control horizon of 1 was set and the prediction horizon adjusted as a tuning parameter. Finally, the weighting and move suppression matrix were set to the identity matrix to provide equal weighting to each control variable and maintain conservative movements in the controller actions.

Results
Performance of the MPC controller is shown in Figures 8 and 9. Performance proved unacceptable for a set point change in water composition and acceptable for a five-minute feed flow interruption. The VAM concentration in the bottoms stream violated the constraint of 100 ppm, as shown in Figure 8. In the case of feed flow disturbance the control scheme was able to meet the control objectives. However, the temperature on stage 14 was poorly regulated, resulting in a large drop in temperature. Due to this poor temperature regulation, it may have been possible for the VAM concentration to rise above the 100 ppm constraint. Even though in this case it

Figure 8. Step test of WATER composition in azeotropic distillation column bottoms from 0.09 to 0.18 mole fraction – feed-forward MPC.
did not, there is potential for the VAM to rise to unacceptable levels given the low temperatures on stage 14 required by the controller.

The cause of the poor performance is attributed to the difference in sample time of the water composition controller relative to the controller sample time (five minutes versus 30 s). As a result, the temperature response is too aggressive given the delay in water composition measurement, resulting in too low a stage 14 temperature and as shown in Figure 8 too high a VAM concentration in the column bottoms stream. It is postulated that a continuous measurement via an inferred water composition such as a Kalman filter, neural network, or other soft sensors could allow adequate performance of the MPC controller in this situation (Quek et al., 2000).

**Static Ratio Control**

*Design Details*

The final test involved using a static ratio control scheme within the azeotropic distillation column composition control substructure (Ryskamp, 1980). Ratio control of this type is an example of a more advanced regulatory control strategy than the base regulatory control structure. However, we are assuming the work of Luyben et al. (McAvoy, 1999; Luyben et al., 1999) in developing the regulatory control structure was optimal, in some sense. We did not try to further improve their regulatory structure and instead focused on classical advanced control techniques. In this arrangement, a mass ratio of reflux flow to feed flow ($L/F$) is utilized to minimize the effects on bottoms water composition due to fluctuations in the feed flow rate variable. It is reasoned that effects of feed flow would be a frequent process disturbance, and therefore accounting for the effects in a feed forward manner would be a simple yet effective control method. The ratio of reboiler duty to feed-flow was not

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Figure 9. 5-minute shut-off of azeotropic distillation column feed pump – feed-forward MPC.
implemented, as it was concluded that the PI stage 14 temperature controller was aggressive enough to reject temperature disturbances and would not provide significant control benefits. Figure 10 shows the control scheme using $L = F$ as the new control variable.

Results

The results for the two test cases are shown in Figures 11 and 12. In the first test, the performance of the ratio scheme in changing the water composition proved to be the same as in the base case. The cause is attributed to the dominant effects of reboiler vaporization rate on water composition in comparison to the resulting small feed flow variation. Therefore, it is concluded there is no advantage to using the ratio scheme for water composition changes. However, the second test showed improved performance at minimizing the effects of a significant feed flow interruption. In particular, both the changes in water composition and stage 14 temperature variables deviated less from their set points and stabilized more quickly. The control scheme was able to immediately start to account for the drop in feed flow, providing the control action before the composition controller measured any changes. Through the use of the static $L/F$ ratio, the composition controller was required to make less aggressive reflux flow adjustments. It is concluded that a static $L/F$ ratio controller is a good column controller design option for feed flow disturbance rejection.
Conclusions

Dynamic modeling of a plantwide regulatory control system for a VAM process design has been completed and compared with the work of Luyben and Tyreus (1998).

Figure 11. Step test of WATER composition in azeotropic distillation column bottoms from 0.09 to 0.18 mole fraction – static feed-forward ratio control.

Figure 12. 5-minute shutoff of azeotropic distillation column feed pump – static feed-forward ratio control.

Conclusions

Dynamic modeling of a plantwide regulatory control system for a VAM process design has been completed and compared with the work of Luyben and Tyreus (1998).
Incremental changes were made to two main control substructures, the liquid inventory system and the $2 \times 2$ composition control of the azeotropic distillation column. A reboiler level control strategy was tested and found to produce a faster response with less oscillatory behavior. Two alternative control techniques for the azeotropic distillation column tested included a feed-forward model predictive controller and static feed-forward ratio controller. The model predictive controller results were poor due to the large difference between the WATER composition analyzer sample time and the controller step size. As a result, it was concluded that options for an inferred composition analyzer would be needed to effectively implement a model predictive controller for the VAM azeotropic distillation column. Finally, the static feed-forward ratio controller was implemented to maintain a constant reflux to feed flow ratio. The results showed excellent disturbance rejection of large feed flow variations to the azeotropic distillation column. This study represents a thorough simulation study and is valuable as a reference for future work.

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References


