

GENERAL PURPOSE ANALOG COMPUTATION

CHEMICAL/PETRO-CHEMICAL

APPLICATION STUDY: 6.2.19a

COMBINED FEEDFORWARD FEEDBACK CONTROL OF A CHEMICAL REACTOR

ABSTRACT: Control of product composition and stirred reactor temperature is difficult when composition is determined by a stream analyzer. The analyzer introduces a delay into the feedback path and the controller must be detuned considerably if stable operation is to be achieved. Combination of feedforward control with the conventional feedback action allows much tighter control since the sampling/analysis delay can be made less critical.

These notes describe the design of a combination feedforward feedback control system for a continuous flow stirred-tank reactor. The reactor, sampling system, and various conventional two-mode controllers were simulated using a PACE[®] TR-48 Analog Computer. The more sophisticated control action was implemented with Multipurpose PC-12 computing components tied directly to the simulated reactor system.

INTRODUCTION

The problem discussed here is suggested by the paper of Min and Williams (1). Those authors showed the dramatic loss of control associated with stream analyzer delays by study of a wellunderstood reactor system, the simulation of which had been previously compared to experimental data. Although the reactor is small, the percentage changes in pertinent quantities are thought to be indicative of performance for larger systems.

The reactor system is fed by two pure streams of reactants X and Y which form the product Z according to the equation

$$X + Y \longrightarrow 2Z$$
 (1)

The reaction is exothermic, so temperature control is effected by varying the flow of cooling water to both a surrounding jacket and an immersed coil. Reactor holdup is maintained constant by level control.

Min and Williams (1) studied a composition control loop which manipulated the flow of the X-reactant. In the present work, where more severe disturbances are postulated and tested, it is suggested that residence-time control accomplished by varying the reactor holdup leads to the best system performance, and it is this improved system which is to be described.

REACTOR SYSTEM

The system of equations presented by Min and Williams (1) have been simplified in some respects for purposes of the present demonstration. On the other hand, a varying hold-up volume must be considered here, so the equations are somewhat more nonlinear.

Material Balances

$$\rho_{o} \frac{d}{dt} [V_{o}X_{o}] = F_{2} - F_{o}X_{o} - \rho_{o}^{2} V_{o}kX_{o}Y_{o} \qquad (2)$$

$$\rho_{0} \frac{d}{dt} [V_{0}Z_{0}] = 2 \frac{M_{Z}}{M_{X}} \rho_{0}^{2} V_{0}kX_{0}Y_{0} - F_{0}Z_{0}$$
 (3)

$$X_{0} + Y_{0} + Z_{0} = 1$$
 (4)

Reactor Heat Balance

$$\rho_{o}C_{o}\frac{d}{dt}[V_{o}T_{o}] = F_{1}C_{1}T_{1} + F_{2}C_{2}T_{2} - F_{o}C_{0}T_{o} + Q\rho_{o}^{2}V_{o}kX_{o}Y_{o} + H_{a} + A^{*}h^{*}(T_{3} - T_{o})$$
(5)

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The coil and jacket of the original system (1) have been lumped together as an effective heat transfer area A^* . The term h^* represents the overall waterside plus process-side heat transfer coefficient.

Coolant Heat Balance

$$m^{*}C^{*}\frac{dT_{3}}{dt} = A^{*}h^{*}(T_{0} - T_{3}) + F_{3}C_{3}(T_{3i} - T_{3})$$
 (6)

Here m^*C^* represents the water-plus-metaloverall heat capacity. The flow F_3 is the sum of two rates, coil plus jacket, for cooling water. The heat sink term previously proposed (1) has been neglected.

Control Equations

$$\Delta F_{6} = \begin{pmatrix} K_{1} + \frac{K_{2}}{S} \end{pmatrix} \epsilon (T_{0})$$
(7)

(8)

$$\Delta V_{o} = \begin{pmatrix} K_{4} \\ K_{3} + \frac{K_{4}}{S} \end{pmatrix} \epsilon (Z_{o})$$
(9)

$$\Delta F_{o} = \begin{pmatrix} K_{6} \\ K_{5} + \frac{K_{6}}{S} \end{pmatrix} \epsilon (V_{o})$$
(10)

A cascade control is implied here, with the composition controller resetting level; feed flows are maintained in a fixed ratio. The combination feedforward feedback equations will be presented later. The dynamics of sensors and valves are neglected in any case.

REACTOR PERFORMANCE

It is postulated that a major source of disturbance to the reactor is rapid variation (step changes) in the feed flow F₁. Hence, if level and temperature are held constant (1), the result is a step change in residence time and a resulting (say) increase in Z_0 . Then, with composition control manipulating F₂, this loop calls for an F₂ increase to offset the Z_0 error. Two factors are to be noted:

 System response is bound to be slow since the changing F₂ must act through the reactor time constant (residence time); and, (2) Severe loads on the system may make it impossible for the feedback loop to achieve the concentrations necessary for the specified conversion. $(X_0Y_0$ has a maximum value when $X_0 = Y_0$; unequal concentrations, sought by the controller action, would give low reaction rates).

These considerations suggest the proposed alternate of controlling the reactor residence time or level and maintaining a fixed ratio between the feed flows F_1 and F_2 . In this system, the X_0Y_0 product never gets out of hand and the required changes in level can be made quickly.

COMPARISON OF CONTROL SYSTEMS

Even though residence-time control is fast moving and more effective than flow/composition control, the behavior of the reactor system remains limited by the delay associated with the stream analyzer. A step change in feed flow is still felt initially as a step change in residence time, and it is only after a few sampling periods that the analyzer senses the load change, residence time is brought to a nearly correct value, and the composition Z_0 is brought back to set point. The initial excursion in Z_0 is nearly as large as would be experienced without any composition control.

This behavior is illustrated in Figure 1. A step change in $F_1 = F_2$ from 400 to 300 grams/minute was imposed on the system initially at steady state (i.e., $Z_0 = 39\%$, $T_0 = 75^{\circ}$ C, $V_0 = 1000$ cc.). Without control of composition or volume, Z_0 would change to 43%. As illustrated, the controlled system brings Z_0 back to set point after an excursion to 42%, during which time the volume makes most of the change to its final steady state value of 780 cc. The sampled-data character of Z_0 shows up clearly in the volume trace; level is tightly controlled and reset by the composition controller.

It is then clear that system behavior would be improved by sensing the need for a change in residence time before the analyzer puts out an error signal on a delayed basis. The required change in V_0 is easily deduced from the steady-state material balance for Z_0 , namely

$$\left(Z_{oss} = \frac{2M_Z \rho_o^2 V_o kX_o Y_o}{M_X F_o}\right)$$
(11)



Figure 1. Reactor Behavior with Conventional Control 25% Decrease in F1 Since steady state is implied, $F_0 = F_1 + F_2$. Thus, the volume required to accommodate a change in $F_1 + F_2$ so that Z_0 remains constant is

$$\left(V_{o} = \frac{M_{X} (F_{1} + F_{2}) Z_{oss}}{2M_{Z} \rho_{o}^{2} kX_{o} Y_{o}} \right)$$
(12)

Resetting of the level controller according to this equation would minimize variations in Z_0 .

ROLE OF THE ANALOG CONTROL COMPUTER

Equation (12) represents the statement of a design procedure for combination feedforward feedback control systems. The right-hand-side of the equation, it is to be noted, contains two distinctly different types of forcing functions:

- (1) A high-frequency term $(F_1 + F_2)$ which can change rapidly and which should be dealt with by feedforward action; and,
- (2) A low-frequency term (X_0Y_0) , a slowly changing variable which can be successfully associated with feedback control action.

To explain the nature of the design method being pursued, it is to be noted that any feedback controller (e.g., the reactor temperature controller in the present system) may be described as a device which computes the magnitude of some variable to offset the measured variation in some other variable. This computation is done by trial-and-error, using some part of the process for trial experiments until balance is achieved. Thus, the reactor temperature controller of the present system <u>computes</u> various values of cooling water flow until the variation in reactor temperature is made zero.

In these terms, one can think of a feedback controller acting on the error in Z_0 and computing a value for X_0Y_0 in Equation (12) such that Z_0 is made equal to Z_{OSS} . Looking to the remainder of Equation (12), F_1 or $(F_1 + F_2)$ are easily sensed and brought to the control computer; furthermore, in the case that temperature control is difficult, reactor temperature could be sensed and used to compute the reaction rate constant k as required in establishing the desired value of the volume V_0 .

The computer circuit so defined (Figure 2) represents an adaptive controller for reactor volume. The feedback control based on Z_O provides a "latest

estimate" of $(X_O Y_O)$ so that estimates of V_O may be made instantly as $(F_1 + F_2)$ make abrupt changes. In another light, the $(F_1 + F_2)$ term provides variable gain to the feedback signal so that at high flow rates and correspondingly high volume, when an error in Z_O means a big accumulation in terms of $(V_O Z_O)$, the feedback signal is applied at higher gain.

The reactor system under study here allows some simplification of the generalized controller given in Figure 2. Firstly, it was evident even before going to the TR-48 computer that temperature control would present no problem: the scaled form of Equations (5) and (6) points up the overdesign of the cooling system. As a result, the temperature control loop for the system could be tuned up tight with assurance that good performance would result. The benefit is further realized in implementing Equation (12) as a control law since the rate constant k may be assumed constant if reactor temperature is held within narrow limits.

A second simplification is allowable because of the ratio control chosen for the feed flow F₂. With $F_2/F_1 = K_0$, and considering just what residence time control will do, it is logical to assume that (X_0Y_0) will vary only slightly, and so a linearized form of Equation (12) is acceptable.



Figure 2. General Circuit for Solution of Equation (12)

$$V_{o} = \left[\frac{\frac{M_{X}(F_{1} + F_{2})Z_{oss}}{2M_{Z}\rho_{o}^{2}k(X_{o}Y_{o})_{ss}}\right]$$
$$\left[\frac{1 - (x_{o}y_{o})}{(X_{o}Y_{o})_{ss}}\right]$$

(13)

where $(x_O y_O)$ is the variation around $(X_O Y_O)_{SS}$. Here the automatic gain control feature mentioned previously is clear. If $(x_O y_O)$ is the output from an ordinary controller, the factor is multiplied by $(F_1 + F_2)$ in the calculation of V_O . The system performance with this type of control is illustrated in Figure 3.

The much sharper response of reactor volume is evident, as is the resulting smaller excursion in Z_0 . For the curves shown, it was assumed that the maximum allowable value for F_0 was about 2400 grams/minute, and, with the severe 25% step change in flows illustrated, this limit applies to the initial volume behavior. The large change in heat load on the system drives the cooling water flow rate to zero in the example, so the temperature behavior is somewhat less impressive than one would expect in the continuous, unlimited situation. Less severe (and more practical) steps in input flow would allow behavior within these limits, and Z_0 would exhibit excellent behavior.

CONCLUSIONS

Combination feedforward feedback control systems offer significant improvements in the performance of systems displaying large lag times, either because of large system time constants or by virtue of analyzer dead times. The controller equation is easily derived from the system equations, and recognition of high-frequency and low-frequency terms points logically to the proper division between feedforward and feedback computations.

While the suggested design technique may not be universally applicable, any failure of a design is apparent from a simulation of the process and the suggested control action. On-line analog computers can be used to implement any of the derived control functions, and they offer special advantages when these functions are nonlinear.

REFERENCES

 Min, H.S., and T.J. Williams, Chem. Engr. Prog. Symposium Series <u>57</u>, #36, page 100 (1961).



Figure 3. Reactor Behavior with Combination Feedforward Feedback Control 25% Decrease in F1

NOMENCLATURE

A - heat transfer area

 $C\,$ - specific heat

- F mass flow rate
- h heat transfer coefficient
- H_a agitation energy input rate

K - constants

- k reaction rate constant
- M molecular weight
- Q heat of reaction
- T temperature
- t time

- V volume
- $X\;$ weight fraction of material X
- Y weight fraction of material Y
- $\rm Z~$ weight fraction of material $\rm Z$
- ρ density
- ϵ error function

SUBSCRIPTS

- o output or reactor
- i input
- 1 in Y feed
- 2 in X feed

(1) Combined Operation of the TR-48 Analog Computer and Multi-Purpose PC-12 Components.

EAI's PC-12 systems are completely flexible with regard to input and output. Thermocouple or strain gage signals, for example, may be brought directly to the PC-12 terminal strip for introduction into a control law computation. Similarly, common outputs such as 4-20 ma. or 10-50 ma. are easily generated.

To preserve some of the plant atmosphere in using a PC-12 system to control the plant simulated on the PACE TR-48 computer, these two devices were not slaved together in the usual fashion of analog computing. Indeed, there was no control common to the two machines. Signals going from one device to another were treated in a differential manner so that common grounding was unnecessary.

(2) Simulation of Sampling/Analysis Delay with a PACE TR-48 General Purpose Analog Computer.

One of the many distinctive features of the TR-48 computer is the completely flexible sys-

tem of integrator mode control. Point storage and multi-speed computations are thus easily implemented.

The sampling and analysis system studied here was assumed to have a pure time delay characteristic; a sample drawn at time t was then analyzed and a result delivered at time t + T_s . Simultaneous with the completion of an analysis, the next sample was taken.

Simulation of these characteristics was accomplished here by the use of four integrators, two summing amplifiers, and a comparator. One integrator and the two summers were set up in a circuit which produces a square wave, a triangular wave, and the sum of these two periodic signals; this last function, displaying a narrow peak, was used to drive the comparator switching relay voltage on and off to the mode control (operate) relay of the remaining integrators. These sampled the continuous signal Z_0 , stored the value for a period T_S , and delivered a delayed reading just as the real analyzer would operate.

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