

## Appendix: First Principle Process Relationships

*Gregory K. McMillan, Emerson*

### GENERAL IMPLICATIONS

First principle relationships can define process cause and effects that can lead to improved controller tuning and performance by the selection of better tuning rules and process variables for scheduling of tuning settings. It also affects the choice of control valve trim and the feedforward and ratio control design. The understanding of these relationships does not require a degree in chemical engineering but presumes just some understanding of common terms (e.g., heat transfer coefficient and area), relationships (e.g., ideal gas law), and physical concepts (e.g., conservation of mass and energy).

Equations have been developed from first principle relationships for the process gains, deadtimes, and time constants of volumes with various degrees of mixing. The results show that for well-mixed volumes with negligible injection delays, the effect of flow cancels out for the controller gain if one of the following methods is used: Lambda self-regulating rule where Lambda is set equal to the deadtime, or the reaction curve method. The effect of flow also cancels out for the reset time besides the controller gain if the process is treated as a “near integrator” and the Lambda integrating tuning rule is used. This is because the flow rate cancels out in the computation of the ratio of process gain to time constant that is the “near integrator” gain. This ratio and “near integrator gain” are inversely proportional to the process holdup mass (e.g., liquid mass). However, for temperature control the effect of changes in liquid mass cancels out because a change in level increases the heat transfer surface area covered. Several authors have mistakenly tried to schedule controller tuning based on liquid level for reactor temperature control. One author has reported being bewildered by its failure. This is not the case for gas pressure control. The equations show that liquid level has a profound effect on the process integrating gain for vessel pressure control because it changes the vapor space volume without any competing effect. To summarize, the integrator gain for composition and gas pressure is inversely proportional to liquid level (liquid mass). For temperature, the effect of level cancels out unless the level is above or below the heat transfer surface area, which is unusual but can occur at the beginning or end of a batch when coils instead of a jacket is used for heat transfer. For temperature, the integrator gain is nearly always proportional to the overall heat transfer coefficient that is a function of mixing, process composition, and fouling or frosting.

The equations also show that if the transport delay for flow injection is large compared to the time constant, which does occur for reagent injection in dip tubes for pH control), then the controller gain will be proportional to flow. Note that pH control is a class of concentration control.

For the control of temperature and concentration in a pipe, the process deadtime and process gain are both inversely proportional to flow and the process time constant is essentially zero, which makes the actuator, sensor, transmitter or signal filter time lag the largest time constant in the loop. Thus, the largest automation system lag determines the deadtime to time constant ratio. For a static mixer, there is some mixing and the process time constant is inversely proportional to flow but is usually quite small compared to other lags in the loop. The controller gain is generally proportional to flow for both cases.

Finally, the above has implications so far as whether a flow feedforward multiplier or summer and whether a linear or equal percentage trim should be used. A flow feedforward multiplier and equal percentage trim, which both have a gain proportional to flow, can help compensate for a process gain that is inversely proportional to flow provided the process time constant is not also inversely proportional to flow. This is generally the case for temperature and concentration control of plug-flow volumes (pipelines, static mixers, and heat exchangers). For well-mixed volumes, feedforward summers and an installed linear characteristic for valves is generally best. For control valves this corresponds to a linear trim when the available pressure drop that is much larger than the system pressure drop or critical pressure drop so the installed is close to the inherent flow characteristic. For flow ratio control, the correction of the ratio bias and setpoint by the process controller corresponds to a feedforward summer and multiplier, respectively.

The results are also useful for determining the deadtime to time constant ratio, which has a profound effect on the tuning factors used and the performance of deadtime compensation, which has been discussed in “Control Talk Blogs — Missed Opportunities in Process Control, Parts 1–6,” [www.controlglobal.com/blogs/controltalkblog/](http://www.controlglobal.com/blogs/controltalkblog/), *Control* (2019).

## **BATCH IMPLICATIONS**

Plug-flow volumes can always be considered as continuous because the volume is completely full and anything entering will be discharged after a transportation delay.

A back-mixed volume is partially full. If the liquid discharge flow is zero, this volume can be considered to be in the batch mode rather than the continuous mode. If the flows are all sequenced and charged based on time and/or totals, the vessel operation can be considered to be pure batch. If reactor flows are ratioed and manipulated by a control loop, the vessel operation can be classified as fed-batch.

Level has an integrating response whether in the batch or continuous mode. In the batch mode, it is a zero load integrator in that all the feed flows must be zero for the level to stop rising. Level has a one-sided integrating response in the batch mode since the level can only rise and not drop assuming no appreciable vaporization. This type of response causes overshoot for any controller with reset action. Proportional plus derivative (PD) controllers with a zero or negative bias can be tuned for zero overshoot.

The temperature response of a back-mixed volume remains self-regulating even for zero liquid discharge flow unless the liquid level is above or below the heat transfer surfaces. However, the temperature response does lose some self-regulation and behaves more like a “near integrator.”

The concentration response of a back-mixed volume becomes integrating for a zero discharge flow. This is not obvious because the discharge flow cancels out of the differential equation from the application of the multiplicative rule of integration in the transition of the derivative from the rate of accumulation of component mass to the rate of accumulation of component concentration. The effect of zero discharge flow is more recognizable if we consider the case of a zero reaction rate so that the process time constant is simply the residence time (liquid mass divided by the liquid feed flow rate). The increase in mass for a fixed feed rate over the residence time is simply the feed rate multiplied by the residence time. The result is an increase in mass equal to the existing mass. This doubling of mass doubles the residence time and hence the process time constant. Consequently, the process never reaches a steady state because the process time constant is constantly increasing as the level is rising for a zero

discharge flow. For the case of zero reaction, the integrator is a zero load integrator because the feed of the component must be zero for the concentration of the component to stop rising. The concentration here has a one-sided integrating response in that the concentration can only increase and not decrease. This would also be the case for reaction products where there is only a forward reaction (no reverse or side reactions). As with level, overshoot is a problem unless Proportional-Derivative (PD) controllers are used. Alternatively, the controlled variable can be translated to a rate of change of concentration as noted in application of model predictive control for bioreactor biomass and product concentration.

Gas pressure is an integrator regardless of liquid discharge flow as long as the pressure in the vessel has a negligible effect on vent flow, which is the case for large or critical pressure drops. If this is not the case, the gas pressure response becomes self-regulating but for large volumes and small vent flows it behaves like a “near integrator.”

## RESULTS

The integrating process gain ( $K_{ip}$ ) for the control of liquid level by the manipulation of a flow:

$$K_{ip} = 1/(\rho_o * A_o) \quad (1)$$

The integrating process gain ( $K_{ip}$ ) for the control of pressure per gas law by the manipulation of a flow:

$$K_{ip} = [(R_g * T_g) / V_g] \quad (2)$$

For the manipulation of jacket temperature to control outlet temperature, the main process time constant ( $\tau_p$ ) is (positive feedback if heat of feed and reaction exceeds product of heat transfer coefficient and area):

$$\tau_p = (C_p * M_o) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (3)$$

For the manipulation of jacket temperature to control outlet temperature, the integrating process gain ( $K_p$ ) is:

$$K_p = (U * A) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (4)$$

For the manipulation of jacket temperature to control outlet temperature, the near-integrating process gain ( $K_{nip}$ ) is:

$$K_{nip} = (U * A) / (C_p * M_o) \quad (5)$$

For the manipulation of feed temperature to control outlet temperature, the process gain ( $K_p$ ) is:

$$K_p = (C_p * F_f) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (6)$$

For the manipulation of feed flow to control outlet temperature, the process gain ( $K_p$ ) is:

$$K_p = (C_p * T_f) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (7)$$

For manipulation of jacket temperature, the additional small secondary process time constant associated with the heat capacity and mass of the jacket wall is:

$$\tau_{p2} = (C_w * M_w) / [U * A] \quad (8)$$

The process deadtime ( $\theta_p$ ) from the turnover time for temperature and concentration control in a well-mixed volume is:

$$\theta_p = (M_o / \rho_o) / [(F_f + F_a + F_r) / \rho_o + F_v / \rho_v] \quad (9)$$

The process deadtime ( $\theta_p$ ) from injection delay for concentration control is:

$$\theta_p = V_1 / (F_1 / \rho_1) \quad (10)$$

For the manipulation of feed flow to control reactant concentration ( $X_{Ao}$ ), the main process time constant ( $\tau_p$ ) is:

$$\tau_p = M_o / (R_x + F_f) \quad (11)$$

For the manipulation of feed flow to control reactant concentration ( $X_{Ao}$ ), the process gain ( $K_p$ ) is:

$$K_p = X_{Af} / (R_x + F_f) \quad (12)$$

For the manipulation of feed flow to control reactant concentration, the near-integrating process gain ( $K_{nip}$ ) is:

$$K_{nip} = X_{Af} / M_o \quad (13)$$

For the manipulation of feed concentration to control reactant concentration, the process gain ( $K_p$ ) is:

$$K_p = F_f / (R_x + F_f) \quad (14)$$

For plug-flow volumes where different streams are being combined, the process gain ( $K_p$ ) for controlling the temperature of the mixture ( $T_f$ ) by the manipulation of flow is:

$$K_p = dT_f / dF_1 = T_1 / \sum F_i \quad (15)$$

For plug-flow volumes where different streams are being combined, the process gain ( $K_p$ ) for controlling the composition of component A ( $X_{Af}$ ) in the mixture by the manipulation of flow is:

$$K_p = dX_{Af} / dF_1 = X_{A1} / \sum F_i \quad (16)$$

For plug-flow volumes where different streams are being combined, the process deadtime for controlling the temperature or composition of the mixture by the manipulation of flow is:

$$\theta_p = V_1 / (F_1 / \rho_1) + V_p / \sum (F_i / \rho_i) \quad (17)$$

The process time constant is essentially zero for true plug-flow. For a static mixer there is some back mixing, the residence time in Equation 17 is split between a deadtime and time constant per Equations 18 and 19 where  $x$  is the fraction of volume that is plug flow:

$$\theta_p = V_1 / (F_1 / \rho_1) + x * V_p / \sum (F_i / \rho_i) \quad (18)$$

$$\tau_p = (1 - x) * V_p / \sum (F_i / \rho_i) \quad (19)$$

## DERIVATIONS

There are three types of processes; self-regulating, integrating, and runaway as shown in Figures 1, 2 and 3, respectively. A self-regulating process will decelerate to a new steady state. An integrating process will continually ramp. A runaway process will accelerate until hitting a relief or interlock setting.

Over 90% of the processes are self-regulating. However, many of the continuous and fed-batch processes in the chemical industry with the greatest direct economic benefits behave and can be best treated as “near-integrating” processes. The classic integrating process is a pure batch or level process. Less than 1% of the processes are runaway. When these exist, understanding the

runaway response is critical in terms of safety and control because of the propensity to accelerate and reach a point of no return. Runaway responses are almost exclusively associated with highly exothermic reactors used in plastics and specialty chemical production.

This note develops the equations for process dynamics for back-mixed volumes and plug-flow volumes. The back-mixed volumes section applies to volumes whenever an agitator pumping rate, an eductor or recirculation liquid flow rate, or gas evolution or sparge rate produces enough turbulence and back mixing to make the mixture more uniform in the axial besides the radial direction of the volume. Gas volumes generally have enough turbulence and a fast enough gas dispersion rates to be treated as a back-mixed volume. The equations therefore hold relatively well for an evaporator and a single distillation stage due to turbulence from the vapor flow. The plug volume section applies to static mixers, pipelines, coil inlets, and jacket inlets where the turbulence from pipe fittings or internal mixing elements creates enough radial mixing to make the mixture uniform over the cross-section of the pipe or nozzle inlet but little axial mixing.

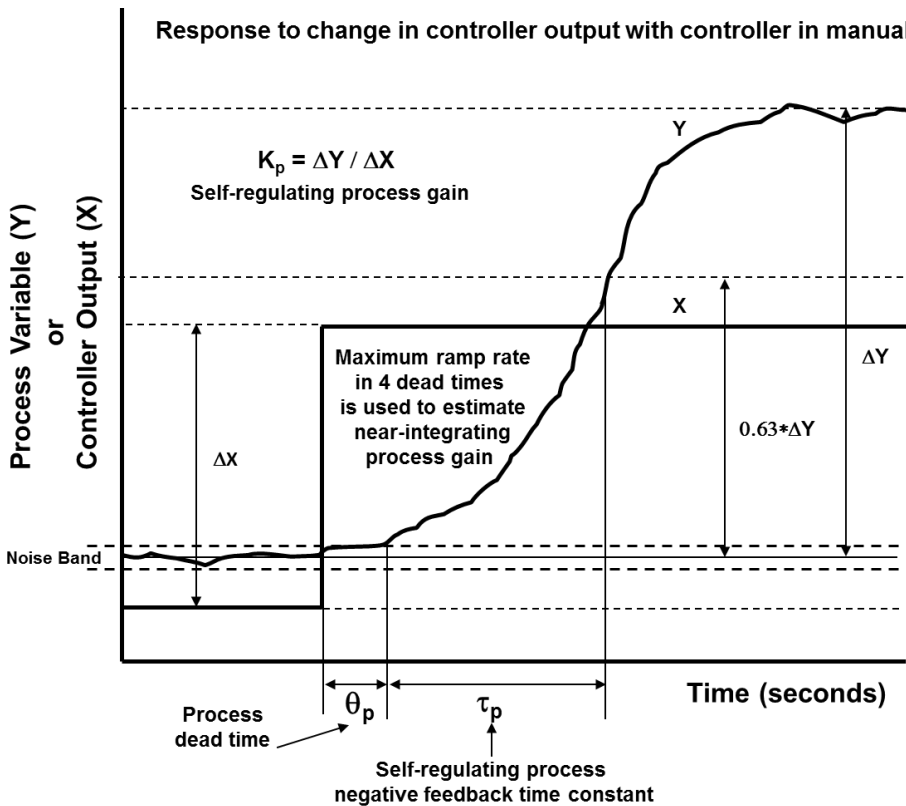


Figure 1 - **Self-Regulating** (Negative Feedback) Process.

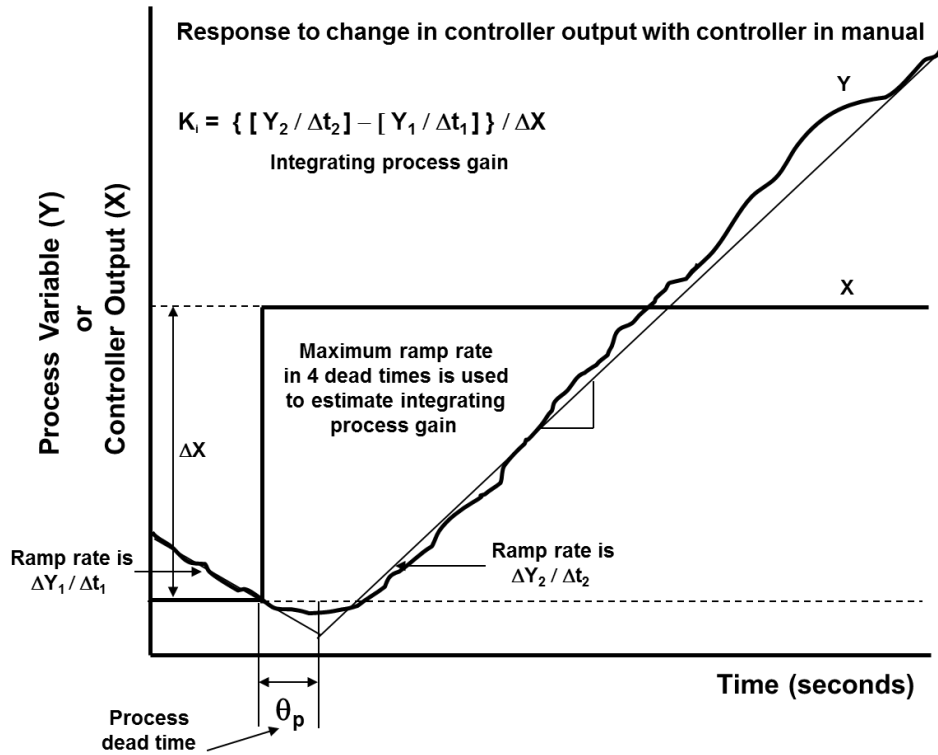


Figure 2 - Integrating (Zero Feedback) Process.

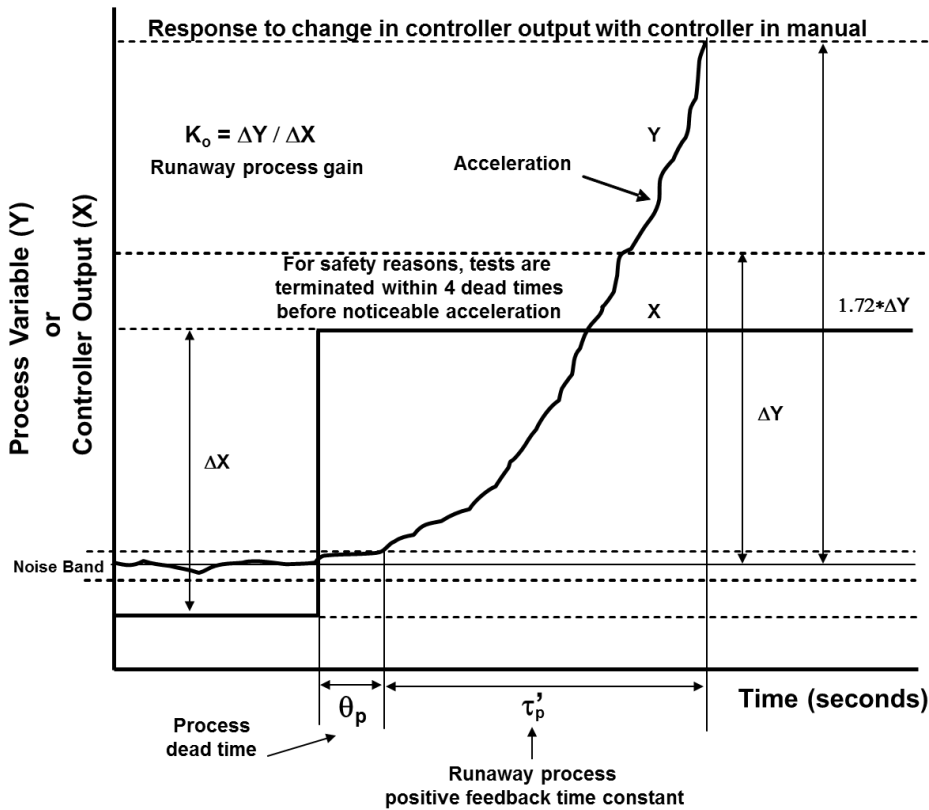


Figure 3 - Runaway (Positive Feedback) Process.

## BACK-MIXED VOLUMES

For a back-mixed volume, the process gains and time constants can be readily identified if the ordinary differential equations for the rate of accumulation of energy or material in the volume are set up so that the process output of interest ( $Y$ ) is on right side with a unity coefficient. From this simple generic form we can identify the process time constant ( $\tau_p$ ) as the coefficient of derivative of the process output ( $dY/dt$ ) and the process gain ( $K_p$ ) as the coefficient of the process input ( $X$ ). The process output ( $Y$ ) and input ( $X$ ) can be viewed as the controlled and manipulated variables, respectively. Many other terms can exist but these are not shown in the following equations. These missing terms can be categorized as disturbances.

If the sign of the unity coefficient of the process output on the right side is negative (Equation 20), the process has negative feedback. As the process output changes, the negative feedback slows down and eventually halts the excursion of the process output at its new steady state when it balances out the effect of the process input and the disturbances.

$$\tau_p * dY / dt = K_p * X - Y \quad (20)$$

The integration of this equation provides the time response of a change in the process output ( $\Delta Y$ ) for a step change in the process input ( $\Delta X$ ). The step occurs at  $t = 0$ .

$$\Delta Y = K_p * (1 - e^{-t/\tau_p}) * \Delta X \quad (21)$$

If the process output does not appear on the right side (Equation 22), there is no process feedback. As the process output changes, there is no feedback to slow it down or speed it up so it continues to ramp. There is no steady state. The ramping will only stop when  $X$  is zero or balances out the disturbances.

$$dY / dt = K_i * X \quad (22)$$

$$\Delta Y = K_i * t * \Delta X \quad (23)$$

Often in the more important loops for concentration, pressure, and temperature control of large volumes, the time constant in Equation 20 is so large that the time to reach steady state is beyond the time frame of interest. Since these loops with small deadtime to time constant ratios should be tuned with high controller gains for maximum disturbance rejection, the controller only sees the first part of the excursion before the inflection point and deceleration by negative process feedback. In this case, the response is best characterized by a near-integrating process gain calculated per Equation 24.

$$K_{nip} = K_p / \tau_p \quad (24)$$

If the sign of the unity coefficient of the process output on the right side is positive (Equation 25), the process has positive feedback. As the process output changes, the positive feedback speeds up the excursion unless disturbances counteract the effect of the process input and output.

$$\tau_p' * dY / dt = K_p * X + Y \quad (25)$$

$$\Delta Y = K_p * (e^{t/\tau_p'} - 1) * \Delta X \quad (26)$$

Consider a mixed volume with a jacket and vapor space. There are liquid reactant feeds, gas feeds (sparged through the liquid and added directly to the vapor space), an outlet liquid flow, a vent gas flow, and a jacket coolant flow. There is normally multiple components interest. For example, consider liquid or gas acid and base reagent or reactant components (a, b) to

produce primary and secondary liquid or gas products (c, d, e). Consider also there are typically water and nitrogen gas components (w, n).

The ordinary differential equation for the accumulation of liquid mass as shown in Equation 27 includes inlet flows added directly to the liquid volume ( $\sum F_i$ ), vapor flow rates from evaporation and vaporization ( $\sum F_v$ ), and an outlet liquid flow rate ( $F_o$ ). The liquid level depends upon density and cross section area of the liquid. Equation 27 can then be reformulated to Equation 28 to include the process variable of interest, liquid level ( $L_l$ ), in the derivative.

$$dM_o / dt = \sum F_i - \sum F_v - F_o \quad (27)$$

$$d(\rho_o * A_o * L_o) / dt = \sum F_i - \sum F_v - F_o \quad (28)$$

If we consider the density ( $\rho_o$ ) to be a weak function of composition and therefore constant like the cross-sectional area ( $A_o$ ) we can take these terms outside the derivative and divide through to get an equation for level ( $L_o$ ) in the form of Equation 27. Now it is clearly evident that the integrating process gain ( $K_{ip}$ ) for manipulation of flows in or flow out is simply the inverse of the product of the liquid density and cross section area (Equation 30).

$$dL_o / dt = [1/(\rho_o * A_o)] * [\sum F_i - \sum F_v - F_o] \quad (29)$$

$$K_{ip} = 1/(\rho_o * A_o) \quad (30)$$

The ordinary differential equation for the accumulation of gas mass as shown in Equation 31 includes inlet flows added directly to the gas volume ( $\sum F_i$ ), vapor flow rates from gas sparging, evolution, and vaporization ( $\sum F_v$ ), and an exit gas flow rate ( $F_g$ ). Equations of state such as the ideal gas law can be used to express this relationship for a given composition. Equation 31 can then be reformulated to Equation 32 to include the process variable of interest, gas pressure ( $P_g$ ), in the derivative.

$$dM_g / dt = \sum F_i + \sum F_v - F_g \quad (31)$$

$$d[(P_g * V_g)/(R_g * T_g)] / dt = \sum F_i + \sum F_v - F_g \quad (32)$$

If we consider changes in the gas volume ( $V_g$ ) and gas temperature ( $T_g$ ) to be much slower than changes in the gas pressure ( $P_g$ ) and therefore relatively constant during the integration step we can take these terms outside the derivative and divide through to get an equation for pressure in the form of Equation 22. Now it is clearly evident that the integrating process gain ( $K_{ip}$ ) for manipulation of flows in or flow out is simply the product of the universal gas coefficient ( $R_g$ ) and the absolute gas temperature divided by the gas volume (Equation 34).

This assumes a change in pressure does not significantly change the gas glow out of the volume, which is normally the case for a pressure drop across the vent valve that is large or critical.

$$dP_g / dt = [(R_g * T_g)/V_g] * [\sum F_i + \sum F_v - F_g] \quad (33)$$

$$K_{ip} = [(R_g * T_g)/V_g] \quad (34)$$

The ordinary differential equation (ODE) for the accumulation of energy as shown in Equation 35 includes the effects of feed temperature, heat of reaction as a function of temperature, heat of vaporization, and heat transfer to the jacket. If we consider the specific heat capacity relatively constant and use the multiplicative rule of integration, we can express the differential equation in the generic form of Equation 20 in terms of temperature to show the



process feedback in Equation 40, the final form of the ODE. The relative magnitude of the terms in the denominator of Equation 41 determines the feedback sign.

$$dQ_o / dt = C_p * \sum(F_i * T_i) - C_p * F_o * T_o + (\Delta Q_r / \Delta T_o) * T_o + H_x * R_x - H_v * F_v - U * A * (T_o - T_j) \quad (35)$$

$$dQ_o / dt = d(C_p * M_o * T_o) / dt = C_p * (dM_o / dt) * T_o + C_p * M_o * (dT_o / dt) \quad (36)$$

$$F_f = \sum F_i \quad (37)$$

$$T_f = \sum(F_i * T_i) / \sum F_i \quad (38)$$

$$C_p * (dM_o / dt) * T_o = C_p * (F_f - F_o) * T_o \quad (39)$$

$$C_p * M_o * (dT_o / dt) = C_p * F_f * T_f + H_x * R_x - H_v * F_v + U * A * T_j - [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] * T_o$$

(40)

For the manipulation of jacket temperature to control outlet temperature, the main process time constant ( $\tau_p$ ) is (positive feedback if heat of feed and reaction exceeds product of heat transfer coefficient and area):

$$\tau_p = (C_p * M_o) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (41)$$

For the manipulation of jacket temperature to control outlet temperature, the process gain ( $K_p$ ) is:

$$K_p = (U * A) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (42)$$

For the manipulation of jacket temperature to control outlet temperature, the near-integrating process gain ( $K_{nip}$ ) is:

$$K_{nip} = (U * A) / (C_p * M_o) \quad (43)$$

For the manipulation of feed temperature to control outlet temperature, the process gain ( $K_p$ ) is:

$$K_p = (C_p * F_f) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (44)$$

For the manipulation of feed flow to control outlet temperature, the process gain ( $K_p$ ) is:

$$K_p = (C_p * T_f) / [C_p * F_f - \Delta Q_r / \Delta T_o + U * A] \quad (45)$$

For manipulation of jacket temperature, the additional small secondary process time constant associated with the heat capacity and mass of the jacket wall is:

$$\tau_p = (C_w * M_w) / [U * A] \quad (46)$$

Any change in the temperature at the heat transfer surfaces or the feed inlet must be dispersed and back-mixed into the volume. This process deadtime ( $\theta_p$ ) is the turnover time that can be approximated as the liquid inventory divided by the summation of the feed flow rate ( $F_f$ ), agitator pumping rate ( $F_a$ ), recirculation flow rate ( $F_r$ ), and vapor evolution rate or vapor bubble rate ( $F_v$ ). Since this turnover time is computed in terms of volumetric flow rates, the liquid mass and the mass flow rates are divided by their respective densities as shown in Equation 47.

$$\theta_p = (M_o / \rho_o) / [(F_f + F_a + F_r) / \rho_o + F_v / \rho_v] \quad (47)$$

If there is an injector (dip tube or sparger ring) volume, a change in composition at the nozzle must propagate by plug flow to the discharge points of the dip tube or sparger ring. The

deadtime for a feed flow ( $F_1$ ) is the injector volume ( $V_1$ ) divided by the injection mass flow ( $F_1$ ) divided by its respective density ( $\rho_1$ ).

$$\theta_p = V_1 / (F_1 / \rho_1) \quad (48)$$

The ordinary differential equation (ODE) for the accumulation of liquid reactant mass ( $M_A$ ) as shown in Equation 49 includes the effects of feeds ( $F_i$ ) with a reactant mass fraction ( $X_{Ai}$ ), reaction rate ( $R_x$ ), and outlet flow ( $F_o$ ). The feeds can be from raw material, intermediate products, recycle streams, or multi-stage reactors. If we use the multiplicative rule of integration, we can express the differential equation in the generic form of Equation 20 in terms of concentration to show the process feedback in Equation 54, the final form of the ODE.

$$dM_A / dt = \sum(F_i * X_{Ai}) - (R_x + F_o) * X_{Ao} \quad (49)$$

$$dM_A / dt = d(M_o * X_{Ao}) / dt = (dM_o / dt) * X_{Ao} + M_o * (dX_{Ao} / dt) \quad (50)$$

$$F_f = \sum F_i \quad (51)$$

$$X_{Af} = \sum(F_i * X_{Ai}) / \sum F_i \quad (52)$$

$$(dM_o / dt) * X_{Ao} = (F_f - F_o) * X_{Ao} \quad (53)$$

$$M_o * (dX_{Ao} / dt) = F_f * X_{Af} - (R_x + F_f) * X_{Ao} \quad (54)$$

For the manipulation of feed flow to control reactant concentration ( $X_{Ao}$ ), the main process time constant ( $\tau_p$ ) is:

$$\tau_p = M_o / (R_x + F_f) \quad (55)$$

For the manipulation of feed flow to control reactant concentration ( $X_{Ao}$ ), the process gain ( $K_p$ ) is:

$$K_p = X_{Af} / (R_x + F_f) \quad (56)$$

For the manipulation of feed flow to control reactant concentration, the near-integrator gain ( $K_i$ ) is:

$$K_i = X_{Af} / M_o \quad (57)$$

For the manipulation of feed concentration to control reactant concentration, the process gain ( $K_p$ ) is:

$$K_p = F_f / (R_x + F_f) \quad (58)$$

The process deadtimes from turnover time and from feed injection are the same as computed in the section for temperature control (Equations 47 and 48).

## PLUG-FLOW VOLUMES

For plug-flow volumes where different streams are being combined, the process gain for controlling the temperature ( $T_f$ ) or composition ( $X_{Af}$ ) of the mixture (often a feed to a downstream equipment) can be computed by taking the derivative of Equations 38 and 52 with respect to the manipulated flow stream 1 ( $F_1$ ) to give Equations 59 and 60, respectively. In both cases, the process gain is inversely proportional to total flow ( $\sum F_i$ ).

$$K_p = dT_f / dF_1 = T_1 / \sum F_i \quad (59)$$

$$K_p = dX_{Af} / dF_1 = X_{A1} / \sum F_i \quad (60)$$

The process deadtime for the manipulation of a flow for stream 1 ( $F_1$ ) is the summation of the injection delay for steam 1 and the piping delay from the point of injection to the point of temperature or composition measurement. For plug flow, the residence time, which is the second expression in Equation 61 completely becomes deadtime.

$$\theta_p = V_1 / (F_1 / \rho_1) + V_p / \sum (F_i / \rho_i) \quad (61)$$

The process time constant is essentially zero for true plug flow. For a static mixer, there is some back-mixing, the residence time in Equation 61 is split between a deadtime and time constant per equations 62 and 63.

$$\theta_p = V_1 / (F_1 / \rho_1) + x * V_p / \sum (F_i / \rho_i) \quad (62)$$

$$\tau_p = (1 - x) * V_p / \sum (F_i / \rho_i) \quad (63)$$

It is obvious from the above that both the process gain and deadtime are inversely proportional to total flow.

### CONTROLLER TUNING

The implication of the results can be best seen if Lambda is set equal to the total loop deadtime ( $\theta_o$ ) resulting in Equation 64 for the PID gain for a self-regulating process. If the open-loop time constant ( $\tau_o$ ) is large compared to the deadtime, the process response is termed near-integrating and the ratio of the open-loop self-regulating process gain ( $K_o$ ) to the time constant is used to approximate the open-loop integrating process gain ( $K_i$ ) in Equation 65. This PID gain is about 1/2 of the PID gain estimated by the Ziegler Nichols reaction curve method.

$$K_c = 0.5 * \frac{\tau_o}{K_o * \theta_o} \quad (64)$$

$$K_c = 0.5 * \frac{1}{K_i * \theta_o} \quad (65)$$

The open-loop time constant ( $\tau_o$ ) in the numerator of Equation 64 is the largest time constant in the loop wherever it occurs. Hopefully, the process is mixed well enough and the instrumentation is fast enough that the largest time constant is in the process ( $\tau_o = \tau_p$ ) and not the automation system. A large time constant in the process slows down the disturbance and is desirable. A large time constant in the measurement and final element is detrimental because it slows down the ability of the controller to see and react to disturbance, respectively.

The open-loop self-regulating process gain ( $K_o$ ) in the denominator is dimensionless.

The process gain is actually the product of the manipulated variable gain, the process gain ( $K_p$ ), the gain of nonlinear process variables, such as pH (slope of the titration curve), and the controlled variable gain. For a loop that throttles a control valve, the manipulated variable gain is the slope of the valve's installed characteristic. For the primary loop of a cascade control system, the manipulated variable gain is the secondary loop set point span divided by 100%. The controlled variable gain is 100% divided by the process variable span. Thus, changes in calibration span affect the computed controller gain, which provides robustness and a less oscillatory response.

Finally, the deadtime ( $\theta_o$ ) in the denominator is really the total loop deadtime, which is summation of the process deadtime ( $\theta_p$ ) plus all the small time lags and delays in the loop. While the names open-loop time constant ( $\tau_o$ ), open-loop self-regulating process gain ( $K_o$ ), and total loop deadtime ( $\theta_o$ ) for the parameters in Equation 64 are more definitive, nearly all of the control literature uses the terms process time constant, process gain, and process deadtime indiscriminately.

## NOMENCLATURE

### *Process Parameters:*

- $A_o$  = cross sectional area of liquid level (m<sup>2</sup>)
- $A$  = heat transfer surface area (m<sup>2</sup>)
- $C_p$  = heat capacity of process (kJ/kg\*°C)
- $C_w$  = heat capacity of wall of heat transfer surface (kJ/kg\*°C)
- $F_a$  = agitator pumping rate (kg/sec)
- $F_f$  = total feed flow (kg/sec)
- $F_g$  = gas flow (kg/sec)
- $F_i$  = feed stream i flow (kg/sec)
- $F_o$  = vessel outlet flow (kg/sec)
- $F_r$  = recirculation flow (kg/sec)
- $F_v$  = vaporization rate (kg/sec)
- $H_v$  = heat of vaporization (kJ/kg)
- $H_x$  = heat of reaction (kJ/kg)
- $L_o$  = liquid level (m)
- $M_A$  = component A mass (kg)
- $M_g$  = gas mass (kg)
- $M_o$  = liquid mass (kg)
- $M_w$  = mass of wall of heat transfer surface (kg)
- $P_g$  = gas pressure (kPa)
- $T_f$  = total feed temperature (°C)
- $T_g$  = gas temperature (°C)
- $T_i$  = feed stream i temperature (°C)
- $T_o$  = vessel outlet temperature (°C)
- $t$  = time (sec)
- $Q_o$  = total heat of liquid (kJ)

$Q_r$  = heat from reaction (kJ)  
 $R_x$  = reaction rate (kg/sec)  
 $R_g$  = universal constant for ideal gas law (kPa·m<sup>3</sup>·°C)  
 $\rho_g$  = gas density (kg/m<sup>3</sup>)  
 $\rho_i$  = stream i density (kg/m<sup>3</sup>)  
 $\rho_o$  = liquid density (kg/m<sup>3</sup>)  
 $\rho_v$  = density of vapor (kg/m<sup>3</sup>)  
 $U$  = overall heat transfer coefficient (kJ/m<sup>2</sup>·°C)  
 $V_g$  = gas volume (m<sup>3</sup>)  
 $V_i$  = injection (e.g., dip tube or sparger ring) volume (m<sup>3</sup>)  
 $V_p$  = piping volume (m<sup>3</sup>)  
 $x$  = fraction of volume that is plug-flow  
 $X_{Af}$  = total feed component A concentration (mass fraction)  
 $X_{Ai}$  = feed stream i component A concentration (mass fraction)  
 $X_{Ao}$  = vessel outlet component A concentration (mass fraction)

*Generic Terms:*

$X$  = process input (manipulated variable) (eu)  
 $Y$  = process output (controlled variable) (eu)

*Dynamic Parameters:*

$K_c$  = PID controller gain (dimensionless)  
 $K_i$  = open-loop integrating process gain (1/sec)  
 $K_{ip}$  = integrating process gain (eu/eu)  
 $K_o$  = open-loop self-regulating process gain (dimensionless)  
 $K_p$  = process gain (eu/eu)  
 $K_{nip}$  = near-integrating process gain (eu/eu/sec)  
 $\tau_p$  = negative feedback process time constant (sec)  
 $\tau_p'$  = positive feedback process time constant (sec)  
 $\tau_o$  = open-loop time constant (sec)  
 $\theta_p$  = process deadtime (sec)  
 $\theta_o$  = total loop deadtime (sec)