

EFFECTS OF RECYCLE ON DYNAMICS AND CONTROL OF CHEMICAL PROCESSING PLANTS

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ABSTRACT

The effect of recycle of mass and energy on the dynamic characteristics of a processing plant is examined. The introduction of recycle of mass and energy may sometimes be considered analogous to feedback, and may change the plant eigenvalues and cause large time constants, instability or complex nonlinear behavior. The effects are greatly influenced by the choice of independent variables. Some simple effects are listed which may give rise to complex behavior in a plant.

INTRODUCTION

It is known that the overall dynamics of chemical processing plants with recycle can be very different from the dynamics of the individual processing units (Gilliland *et al.*, 1964, Denn and Lavie, 1982). Recycle may dramatically alter the time constants of the plant, and may give rise to instability or oscillatory behavior (limit cycles). The knowledge of these phenomena are important for controller design, and their effects may even pose a threat to plant safety if not foreseen. Unfortunately, even with a model of the system in terms of its nonlinear differential equations, the analysis of the possible behavior of the system is very difficult. For example, the behavior of a set of equations depends entirely on the parameter values as well as on the specification (choice of independent variables), and even for very simple sets of equations one may get complex behavior such as instability, multiple steady states, limit cycles and even chaotic behavior. The objective of this paper is not to analyze such systems in detail, but rather to examine what simple mechanisms that may give rise to complex behavior in chemical engineering systems, and in particular for cases with recycle of mass or energy.

General work in the area seems rather scarce even though issues like the effect of energy integration on reactor stability were discussed as early as 1953 by van Heerden (1953). Aris and Amundson (1957) analyzed the effect of feedback (control) on the dynamic characteristics of the continuous stirred tank reactor. Gilliland *et al.* (1964) studied the classical example with a reactor connected to a distillation column and total recycle of the column bottom product. They reported an increased sensitivity of the plant to feed disturbances compared to the reactor without recycle, and that the plant may become unstable even though the reactor itself is stable. Denn and Lavie (1982) argued that a recycle system may be considered analogous to a closed loop feedback control system with positive feedback. Hence, recycle may increase the overall response time of the plant and make the steady state gain large. They also considered the effect of time delays in the recycle path on plant dynamics. Kapoor *et al.* (1986) studied the effect of recycle structure on the time constants of distillation columns, and argued that the reflux may be viewed as a positive feedback effect which may result in very large time constants for high-purity separations. Other related work that may be mentioned is Verekios and Luyben (1978), Luyben (1992), Papadourakis *et al.* (1987, 1989) and Uppal and Ray (1974).

LINEAR SYSTEMS

For small deviations from the steady state, a processing unit may be well described by a linear transfer function. Before attacking the nonlinear complexities of a plant, it is therefore reasonable to review some basic results from linear systems theory. Our main reason for studying linear systems theory is that the introduction of recycle in a plant often can be thought of as a sort of feedback mechanism.

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Consider a system (or plant) with linear transfer function model $G(s)$. The response is mainly determined by the location (and possible direction) of the poles and zeros. For a scalar system the zeros z correspond to $g(z) = 0$, and the poles λ correspond to $|g(\lambda)| = \infty$. The poles are equal to the eigenvalues of Jacobi matrix for the states and are often referred to simply as "eigenvalues". The poles determine the speed (and possible oscillations) of the response whereas the zeros determine the shape of the response (e.g., overshoot for left half plane (LHP) zeros, and inverse response for RHP zeros). Plants with poles in the right half plane are unstable. If the plant has a pole near the origin, the response time will be large.

Assume that the original plant (e.g., without recycle) has transfer function $G(s)$, and that one somehow (e.g., by a recycle) introduces a modification $C(s)$. We now want to consider the effect of such modifications.

1. **Series interconnection, GC .** (Fig. 1a). In this case the poles and zeros of the combined system GC are given by the poles and zeros of the individual elements, G and C . Thus, in this case the overall response may be predicted directly from the individual elements.

2. **Parallel interconnection, $G + C$.** (Fig. 1b). The combination has the same poles as the individual elements, but the zeros are different. Thus, it may be difficult to predict in detail the overall response from knowledge of the elements. However, the overall response will usually not differ drastically from that of the individual responses, since it is simply their sum.

3. **Feedback C around G .** (Fig 1c). The overall transfer function becomes $H(s) = G(s)[I - C(s)G(s)]^{-1}$. In this case the zeros of $H(s)$ are equal to the zeros of $G(s)$, but the poles are moved by the feedback, and the resulting response may of course be drastically different from that of the individual elements $G(s)$ and $C(s)$. For example, the individual elements may be stable and the overall response unstable and *vice versa*. Even the location of the poles may be difficult to predict. For example, consider the scalar case with static feedback, $c(s) = k$ ($k > 0$ corresponds to positive feedback). Then we know that for $k = 0$ the poles of the overall system $h(s)$ are equal to the poles of $g(s)$, and as $|k| \rightarrow \infty$ the poles of $h(s)$ approach the zeros of $g(s)$. However, as anyone with familiarity with a root locus plot knows, for intermediate values of k the poles may move widely about in the complex plane, and a detailed calculation is needed to obtain the location of the poles.

Of course, there are exceptions. For example, in this paper we mainly study simple first-order models such as $g(s) = 1/(s + a)$, and we get with constant gain feedback $h(s) = 1/(s + a - k)$. In this case the pole $\lambda = -a + k$ moves monotonically to the right along the real axis as k increases. Eventually, for $k > a$, we get instability, but before this occurs we will observe that "the response becomes slower" (since the time constant of $h(s)$ is $\tau = -1/\lambda = 1/(a - k)$) and "the gain gets larger" (since the gain of $h(s)$ is $1/(a - k)$). However, in the general case the behavior is much more complex, and statements such as "positive feedback makes the system slower and the gain larger" may not hold.

The conclusion from the above review of linear system theory is that the effect of feedback, and thus of recycle, is generally very difficult to predict just from considering the individual elements $G(s)$ and $C(s)$. This is discouraging, and the situation of course gets much more complicated for nonlinear systems.

CLASSIFICATION OF SIMPLE EFFECTS

Chemical engineering systems are usually quite accurately described by of a large number of coupled nonlinear differential equations which include a large number of feedback/recycle effects. From the above discussion of linear systems it seems almost hopeless to analyze such a system in its general case (taking into account various parameter values, specifications, etc.). Fortunately, it seems that most real chemical engineering processes behave in a relatively simple matter. In fact, most chemical engineers seem to believe that essentially all "natural" chemical engineering systems respond in a rather simple and sluggish way (of the form first order response plus delay), and that any oscillations or instability are due to poorly tuned controllers.

In this section we will make an attempt to classify some individual effects which by themselves may cause complex behavior in chemical engineering systems, and thus demonstrate that the above belief is to some extent false.

We define a "simple" or "individual effect" as an effect involving only one differential equation (balance equation), and study below in particular the location of the pole (eigenvalue) and the possibility for instability. An ideal mixing tank is used as the basic element in this analysis. Some of these involve recycle, most of them have some sort of "positive feedback" effect.

Notation. In all cases we consider a simple mixing tank with feed F [kmol/s] and constant holdup M [kmol]. Let z_A , x_A and y_A denote mole fractions of component A in the feed, liquid and vapor, respectively. We consider a

binary mixture of components A and B, and then we have $x_B = 1 - x_A$. For cases with reaction we consider the reaction $A \rightarrow B$ with rate $r(x_A, x_B, T)M$ (kmol A reacted / s) where for a 0th order reaction $r = k(T)$ and for a 1st order reaction $r = kx_A$.

Base case: Simple mixing tank. The base case has only one phase, one product stream and no reaction. In this case a material balance for component A yields

$$M \frac{dx_A}{dt} = F(z_A - x_A); \quad \lambda = -\frac{1}{\tau_0} \quad (1)$$

where $\tau_0 = M/F$ is the residence time in the tank. λ represents the eigenvalue of the linearized system and we note that the system is always stable and that the eigenvalue moves to the right and the response becomes slower as the residence time τ_0 increases. Clearly, at steady-state we get $x_A = z_A$.

We will below consider the effect of introducing a reaction, adding recycle, adding preheater, considering temperature effects and evaporation, etc.

Class 1. Reaction. Consider an isothermal continuous stirred tank reactor (CSTR) with a 1st order reaction taking place (the reaction is assumed isothermal such that r depends on x_A only). We get

$$\frac{dx_A}{dt} = \frac{1}{\tau_0}(z_A - x_A) - kx_A; \quad \lambda = -\frac{1}{\tau_0} - k \quad (2)$$

At steady-state we get $x_A = z_A/(k\tau_0 + 1)$. We note that the reaction introduces a negative feedback which "stabilizes" the system and makes the response faster. To get instability from the reaction alone we would need an autocatalytic reaction, e.g. $r = kx_B$. With autocatalytic reactions, the number of different possible dynamic behavior is virtually endless: multiple steady states, instabilities, limit cycle behavior or even chaotic behavior. An extensive analysis of autocatalytic reactions may be found in Gray and Scott (1990). However, in this paper we restrict ourselves to simple kinetics.

Class 2. Reaction with recycle. Consider the same example as above, but introduce recycle of unreacted A (Fig. 2) such that all the reactor outlet except $(1 - \alpha)F$, $\alpha \in [0, 1]$ is sent to the perfect separation unit. If the dynamics of the separation unit is neglected, a component balance around the total system yields:

$$\frac{dx_A}{dt} = \frac{1}{\tau_0}(z_A - (1 - \alpha)x_A) - kx_A; \quad \lambda = -\frac{1}{\tau_0} - k + \frac{\alpha}{\tau_0} \quad (3)$$

As can be seen the introduction of the recycle has introduced *positive feedback* and the eigenvalue of the system is moved to the right ("slower response") as the recycle α increases.

However, the system never becomes unstable since we get $\lambda = -k$ for the limiting case with $\alpha = 1$ (all unreacted A is recycled). In this case the eigenvalue is independent of the residence time, but of course the actual conversion will depend on τ_0 , as we have at steady-state $x_A = z_A/(k\tau_0)$ (this also puts a lower limit on τ_0 since we must have $x_A \leq 1$). We also note from this equation that the sensitivity ("gain") of x_A to changes in z_A has increased by introducing the recycle.

Class 3. Temperature dependent exothermic reaction. Consider an adiabatic CSTR with a 0th order exothermic reaction, i.e. $r = k(T)$ (the reason for assuming a 0th order reaction is to show that we are dealing with a pure temperature effect). An energy balance assuming constant c_P and $c_P = c_V$ yields:

$$\frac{dT}{dt} = \frac{1}{\tau_0}(T_{in} - T) + f(T); \quad \lambda = -\frac{1}{\tau_0} + T_{ad}k'(T) \quad (4)$$

where the "energy production term" is $f(T) = k(-H_{rx})/c_P = kT_{ad}$ where $T_{ad} = (-H_{rx})/c_P$ is the adiabatic temperature rise. For an Arrhenius type of rate expression we get $k'(T) = dk(T)/dT = kE/(RT^2)$ where E [J/kmol] is the activation energy. Hence, the temperature dependency of the reaction has introduced *positive feedback* which moves the eigenvalue to the right and makes the response slower or even unstable. The positive feedback may be explained as follows: increasing the temperature causes an increased reaction rate, which again increases the energy production due to the exothermic reaction.

Class 4. Recycle of energy by preheating. Consider a mixing tank where the feed is preheated with the product (Fig.3). To isolate the effect of the preheating we assume no reaction. Energy balances yield: Tank

by itself:

$$\frac{dT}{dt} = \frac{1}{\tau_0}(T_1 - T); \quad \lambda = -\frac{1}{\tau_0} \quad (5)$$

Heat exchanger:

$$T_1 = \alpha T + (1 - \alpha)T_{in}; \quad \alpha \in [0, 1) \quad (6)$$

where α is independent of temperature. The overall model then becomes:

$$\frac{dT}{dt} = \frac{1 - \alpha}{\tau_0}(T_{in} - T); \quad \lambda = -\frac{1}{\tau_0} + \frac{\alpha}{\tau_0} \quad (7)$$

The preheating introduces *positive feedback* which moves the eigenvalue towards the right, and thus makes the response slower. The system gets increasingly slower as the exchanger becomes more effective, but it never becomes unstable as $\alpha < 1$. Also note that (7) is identical to the recycle example in (3) with no reaction.

Class 5. Heating or cooling. Consider a mixing tank with heating or cooling and no reaction. An energy balance yields:

$$\frac{dT}{dt} = \frac{1}{\tau_0}(T_{in} - T) - \beta(T - T_{cool}); \quad \lambda = -\frac{1}{\tau_0} - \beta \quad (8)$$

where $\beta = UA/Mc_p$ is the number of heat transfer units, T_{in} the feed temperature, and T_{cool} the cooling (or heating) water temperature. The heating or cooling thus introduces negative feedback which makes the response faster, which is the opposite of the preheating considered above.

Class 6. Flash tank with heating. Consider a flash tank where products are withdrawn both as vapor V and liquid L . The material balance for component A yields

$$M \frac{dx_A}{dt} = Fz_A - Lx_A - Vy_A \quad (9)$$

If we assume that V (or $L = F - V$) is an independent variable (and specifically does not depend on composition) then the pole (eigenvalue) becomes

$$\lambda = -\frac{1}{\tau_0} \left(K \frac{V}{F} + \frac{L}{F} \right) \quad (10)$$

where $K = dy_A/dx_A$ is the local slope of the equilibrium line. In most cases K is reasonably close to 1 and we find that λ is close to $-1/\tau_0$, but in theory it may take on any negative real value.

Now consider the case where *the heat input Q is the independent variable*, and where V indirectly depends on composition because H_{vap} depends on composition. In this case rather surprising effects may occur. By neglecting heat capacity terms in the energy balance we get

$$V = Q/H_{vap}; \quad H_{vap} = x_A H_{vap,A} + x_B H_{vap,B} \quad (11)$$

Here we have assumed that the heat of vaporization depends linearly on composition. Introducing this into (9) and using $L = F - V$ results in the eigenvalue

$$\lambda = -\frac{1}{\tau_0} \left(K \frac{V}{F} + \frac{L}{F} \right) + \frac{1}{\tau_0} \frac{V}{F} \frac{H_{vap,B} - H_{vap,A}}{H_{vap}} (x_A - y_A) \quad (12)$$

Assume that component A is the least volatile component such that $x_A > y_A$ and at the same time has the smallest heat of vaporization such that $H_{vap,B} > H_{vap,A}$ (this is not very common but does happen). In this case we find that the composition dependency of V has introduced *positive feedback* in the system, and the response may even become unstable.

Class 7. Exothermic reaction with evaporation. Next consider an example which is quite similar to the one above in that V depends on composition.

First consider the material balance for a flash tank with a 1st order reaction $A \rightarrow B$. The temperature is assumed constant (e.g., by adjusting the pressure). The material balance for component A yields

$$M \frac{dx_A}{dt} = Fz_A - Lx_A - Vy_A - kx_A M \quad (13)$$

If we assume that V (or alternatively $L = V - F$) is an independent variable then the eigenvalue becomes

$$\lambda = -\frac{1}{\tau_0} \left(K \frac{V}{F} + \frac{L}{F} \right) - k \quad (14)$$

and we note as found before that the reaction as introduces additional negative feedback.

Now consider the case where an exothermic adiabatic reactor is cooled by evaporation, that is, the vapor flow V is caused by the heat released by the reaction and thus V depends on composition. This may change the dynamics drastically as is shown next. By neglecting heat capacity terms in the energy balance we get

$$V = M x_A (-H_{rx}) / H_{vap} \quad (15)$$

where $\tau M = k x_A M$ [kmol/s] is the reaction rate. Introducing this into (13) and using $L = F - V$ results in the eigenvalue

$$\lambda = -\frac{1}{\tau_0} \left(K \frac{V}{F} + \frac{L}{F} \right) - k + \frac{(-H_{rx})}{H_{vap}} (x_A - y_A) \quad (16)$$

Assume that A is the heavy component such that $x_A > y_A$. Then we find that the composition dependency of V has introduced *positive feedback* in the system, and the response becomes slow, and even unstable if the heat of reaction, $(-H_{rx})$ [J/kmol] is sufficiently large. The positive feedback can be explained as follows: An increase in x_A yields an increased reaction rate, which increases V , which removes relatively more of light component B from the liquid, which increases x_A even more, etc.

Class 8. Composition dependent recycle: Mass reflux in distillation. It was recently recognized by Jacobsen and Skogestad (1991) that one may get instability and multiple steady states in ideal two-product distillation if the liquid reflux is specified on a mass (or volume) basis, L_w [kg/s], instead of on a molar basis, L [kmol/s]. This may even happen for cases with a single equilibrium stage, and a closer analysis shows that the cause for the instability is that the reflux $L = L_w / M_w$ becomes dependent on composition since the mole weight of the reflux is $M_w = M_{wA} x_A + M_{wB} x_B$ [kg/kmol]. This is very similar to what caused the possible positive feedback in Classes 6 and 7.

DISCUSSION

By combining a few simple effects like the ones above one may easily get very complex behavior. Consider for example the CSTR with a 1. order reaction and an Arrhenius type rate expression. For the adiabatic case (combined class 1 and 3) there may be several steady states (van Heerden, 1953), and if heating or cooling is introduced, the system may behave in a number of qualitatively different ways, including limit cycle behavior (Uppal *et al.*, 1974).

The analysis of a system is further complicated by the fact that there are a number of ways of choosing the controlled (specified) variables of a plant, and because this choice may have a large impact on the dynamic characteristics. Even the choice of specification of a flow on mass or volume basis instead of on molar basis, as in class 8 above, may change a system from having a unique stable steady state to having multiple steady states or instability. In addition, there are normally many different ways of choosing which variables should be the independent ones.

CONCLUSION/PROPOSITION FOR FURTHER WORK

A plant with recycle of mass or energy may sometimes be considered analogous to a closed loop feedback control system with positive feedback. Hence, the plant eigenvalues may be shifted closer to the right half plane, and give the plant longer response times and greater sensitivity to disturbances. The positive feedback effect may also cause instability or nonlinear behavior such as limit cycles or even chaotic behavior. In the general case the positive feedback analogy may not hold. The feedback effect caused by e.g. recycle may in general move the poles of the plant to almost any point in the complex plane, complicating any unified approach to analyzing recycle systems.

A further complication arise from the fact that the choice of specified (independent) variables has a large impact on the plant behavior. The number of possible set of specified variables for a given plant is usually very large.

There is a need for a systematic classification of effects which may introduce complex behavior in a plant. By labelling and analyzing different effects, it should be possible to increase the understanding of different phenomena, and to provide some indicators as to when they occur.

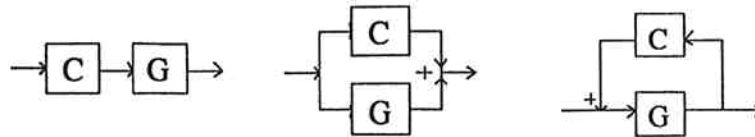


Figure 1: Interconnections of transfer functions

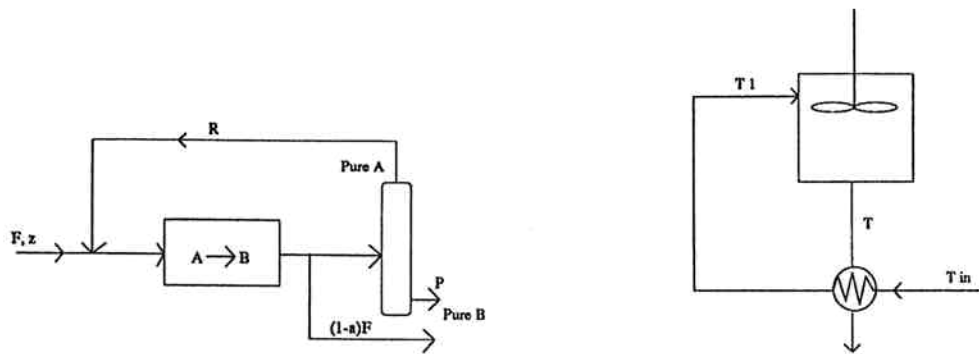


Figure 2: Reactor with recycle of unreacted feed Figure 3: Preheating the feed with the product

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