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# Dynamic behaviour of integrated plants

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The effect of material recycle and heat integration on the dynamics and control of chemical processing plants is considered. In analogy to linear control theory, one may consider how plant interconnections affect the fundamental properties of the dynamics, such as the poles and zeros. This implies that recycle of mass and energy, which are feedback mechanisms, affects the poles and thus possibly the plant stability, whereas parallel interconnections in a plant affect the zeros and thus the achievable performance of the plant under feedback control.

**Keywords: process dynamics; nonlinear systems; positive feedback**

It is known that the overall dynamics of chemical processing plants with material recycle or heat integration can be very different from the dynamics of the individual processing units.[1,2] Material recycle and heat integration may dramatically alter the time constants of the plant, and may give rise to instability or oscillatory behaviour (limit cycles), even when the individual processing units are stable by themselves. Moreover, plant interconnections may introduce fundamental limitations in the achievable performance of any control system. The knowledge of such phenomena is 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 behaviour of the system is very difficult. Although there exist mathematical tools such as bifurcation analysis, which in principle could be used to analyse a plant, the systems describing whole plants are so large that a complete analysis by such tools is impractical if not impossible. Moreover, even if such an analysis were possible, there would still be a need for some 'rules of thumb', or indicators, which could be used to warn us when complex behaviour is plausible.

The main problem at hand is that even though we may have a thorough understanding of the dynamic behaviour of the individual units, it may be extremely difficult to predict the behaviour, even qualitatively, of an interconnected system. A well-known example is a distillation column which in most cases is well modelled as a number of interconnected flash tanks. Even though we may easily predict the response of the individual subsystems (the flash tanks), it is very difficult to predict the response of the overall system (the column). The main reason for the change in behaviour is the recycle of vapour and liquid (reflux). The strong effect recycle (feedback) may have on the dynamic response of a system is not appreciated by most engineers. In addition, for distillation columns the vapour–liquid relationship is nonlinear, and for persons familiar with nonlinear dynamics, it is well known that this combination of nonlinearity and feedback may lead to very complex dynamic behaviour. For example, a simple nonlinear function, $y = u \cdot (1 - u)$ may, when combined with dynamic feedback, for example, a simple gain and delay, $u(t) = k \cdot y(t - 1)$, yield a very complicated dynamic response, including chaos (try $k = 3.7$ with initial value $y(0) \in < 0,1 >$).[3] For linear systems the effects are not quite as drastic, although small changes in the feedback gain can also in this case drastically change the characteristics of the response.

In most cases recycle leads to positive feedback effects. For example, increasing the concentration of a chemical species in a process stream will normally increase the amount of this species in the recycle streams, and thus lead to a reinforcement of the original increase. In other words, there is a self-reinforcing mechanism associated with the recycle. This positive feedback will usually increase the plant time constant, and also increase the sensitivity to slow disturbances. This is because recycle will tend to 'store' material or energy within some part of the plant. An example is high purity distillation columns, where extremely long time constraints have been observed.[4]

From a linear systems point of view, the increased time constant corresponds to a pole (system eigenvalue) being moved closer to the origin in the complex

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plane (approaching a pure integrator). In some cases the positive feedback may move the pole past the origin and yield instability. One example is for distillation columns, where the use of mass reflux may lead to instability in some cases.[5,6] In other cases positive feedback may result in limit cycle behaviour. One example is the ammonia synthesis reactor with energy recycle studied by Morud and Skogestad.[7] Finally, it should be noted that there are a few cases where recycle may yield negative feedback. All of these issues are discussed in more detail in the paper.

General work in the area of the dynamics of integrated plants is rather scarce even though issues like the effect of energy integration on reaction stability were discussed as early as 1953 by van Heerden.[8] Aris and Amundson[9] analysed the effect of feedback (control) on the dynamic characteristics of the continuous stirred tank reactor. Gilliland *et al.*[1] studied the now classic example of a reactor connected to a distillation column with total recycle of the column bottom product. They reported an increased sensitivity of the plant to feed disturbances compared to the case without recycle, and that the plant may become unstable even though the reactor itself is stable. Denn and Lavie[2] 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. Other related work that may be mentioned is Verykios and Luyben;[10] Luyben;[11] Papadourakis *et al.*;[12,13] and Uppal *et al.*[14]

The main objective of this paper is to obtain qualitative insight into what dynamic behaviour can be expected for processing systems, and in particular to gain insight into the effect of various plant interconnections. For a given plant such insight can then provide a starting point for a more detailed analysis. Most of our analysis is based on linear systems theory, as this theory is well developed, and because it is difficult to obtain general results for nonlinear systems.

## Classification of interconnections

An interconnection refers to the way the subsystems are interconnected to form the overall system. We shall classify interconnections into external or internal interconnections, and into feedback, parallel or series interconnections.

*External interconnections.* In this case the subsystems are the individual processing units, and the term external interconnections refers to how these subsystems are connected together, that is, it refers to the structure of process flowsheet. One very important interconnection of units is recycle. A recycle loop may be due to mass recycling, but may also in a more general sense be due to heat recycling, for example when a reactor feed is preheated by the reactor effluent. Other common ways to arrange units, are in series and in parallel.

*Internal interconnections.* This is a somewhat more loosely defined concept. The 'subsystems' in this case usually refer to the dynamics of important state variables, such as the temperature dynamics (energy balance), the component dynamics (mass balance) and the pressure dynamics (momentum balance). The interconnection then refers to the coupling between these variables (balances). The term 'internal' is used because these couplings occur inside the individual processing units. The study of internal interconnections was the main focus of our earlier paper.[15]

A given interconnection, be it external or internal, may be subdivided into the following three broad classes:

1. *Feedback.* A recycle loop is a special case of feedback, but the term 'feedback' is often used for dynamical systems in a more general sense to include any secondary effect that modifies the original dynamic change, and includes also 'internal' feedbacks within the units. For example in some cases a dynamic model of a unit may be formulated as:

$$\frac{dy_1}{dt} = g(y,u) + f_1(y) + f_2(y) + \ldots \qquad (1)$$

   Here, $f_1(y), f_2(y), \ldots$ may be thought of as feedback effects modifying the 'original' behaviour given by $dy/dt = g(y, u)$. If $a_i = \partial f_i/\partial y$ is positive (negative), then the feedback for effect $i$ is positive (negative).
2. *Parallel paths (feedforward).* Two processing units in parallel is a special case of a parallel interconnection. However, here the term 'parallel path' is used in a general sense to include any system where an input affects an output through several independent subsystems or mechanisms. One specific example is the following system:

$$\frac{dy_1}{dt} = g_1(y_1, u) \qquad (2)$$

$$\frac{dy_2}{dt} = g_2(y_2, u) \qquad (3)$$

$$y = f(y_1, y_2) \qquad (4)$$

   Often the effects of the various subsystems ($g_1$, $g_2$, ...) on the output, $y$, have different signs, in which case they are denoted 'competing effects'. This is important as it may yield unstable zero dynamics, corresponding to inverse responses for linear systems.
3. *Series interconnections.* By a series interconnection of subsystems we mean that the output of one subsystem is the input to the next, that is, there is a one-way flow without feedback between subsystems. One example is the following system:

$$\frac{dy_1}{dt} = g_1(y_1, u) \quad (5)$$

$$\frac{dy}{dt} = g_2(y, y_1) \quad (6)$$

An example could be processing units in series, but in general we would allow series connections of any concrete or abstract systems, not only processing units.

*Remarks*

1. As already mentioned, feedback may drastically change the dynamics of the system as compared to that of the subsystems. This is because feedback moves the poles of the system, and may, for example, yield instability.
2. Parallel interconnections do not generally yield responses which in themselves are drastically different from those of the subsystems. However, the presence of computing effects may lead to inverse responses and unstable zero dynamics (RHP-zeros in the linear case), which may lead to instability when feedback is applied to the system (for example, feedback control).
3. Series interconnections often yield responses that may be well predicted from those of the subsystems. It is therefore usually the simplest interconnection from a system point of view.
4. In many cases the responses within a unit may be described well by considering several 'internal' parallel paths. For example, changing a valve position may at the same time change the pressure (and thus flowrate), temperature and concentration at that location. The effect of the change in these three variables will propagate downstream with different speeds in a parallel manner (often pressure effects are the fastest and temperature effects the slowest). In this sense, we may also get parallel paths through processing units in series. In some cases these effects may be competing and very complex dynamic behaviour may be observed when feedback is applied to the unit.

These issues are discussed in detail for linear systems below, and are illustrated with process examples in subsequent sections.

## Linear systems

For small deviations from the steady state, a processing unit may be well described by a linear transfer function. It is therefore reasonable to review some basic results from linear systems theory.

The dynamic behaviour of a linear system is determined by its poles and zeros. For an uncontrolled system, the poles are the main issue, as they determine the stability of the plant. (The plant is stable if and only if all the poles are in the complex left half plane.)

However, plant instability may not necessarily be a problem, since an unstable process may be stabilised by feedback control. Essentially, control involves finding a way of inverting the process: one specifies the plant output, $y$, and the controller computes the necessary input, $u$, which (approximately) achieves this. With feedback control, as the bandwidth increases, the transfer function from the reference to the plant input approaches the inverse of the plant. This means that right half plane zeros in a plant would eventually end up as unstable poles in the closed loop system if the bandwidth were too high. Right half plane zeros in a plant therefore pose an upper limit to the achievable performance of any control system.

An important issue is therefore to understand how the poles and zeros of a plant are affected by plant integration. Here our insight from linear systems proves useful: Poles are changed by feedback, which in a processing plant will correspond to mechanisms that recycle mass or energy. On the other hand, zeros are changed or added by parallel interconnections.

We elaborate the effect of feedback, parallel and series interconnections for scalar linear systems to illustrate their effect.

*Feedback interconnection*

Consider a plant described by $y = g(s)u$ where $u$ and $y$ are the plant input and output respectively. Assume there is a feedback mechanism $k(s)$ as illustrated in *Figure 1*, such that $u = k(s)y + r$. The poles of the system are then the roots of $1 - g(s)k(s)$. The steady-state behaviour is found by setting $s = 0$. We distinguish between the following two cases:

*Case 1.* $g(0)k(0) < 0$ (negative feedback). This is the most common case in feedback control, but it is less likely to occur for a recycle loop. If the magnitude of the loop gain, $g(0)k(0)$, is increased, this will eventually yield instability where a pair of complex conjugate poles cross the imaginary axis (as long as there is at least 180° phase lag in $g(j\omega)k(j\omega)$ at high frequencies, $\omega$).

*Case 2.* $g(0)k(0) > 0$ (positive feedback). If $k(0)$ is varied from zero towards $1/g(0)$, $1 - g(0)k(0)$ approaches zero. This means that a pole goes through the origin as $k(0)$ passes $1/g(0)$. A pole near the origin means that the response of the plant is slow and that the sensitivity to slow disturbance is high.

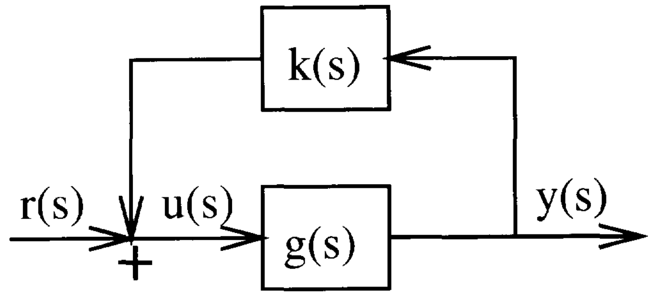


**Figure 1** Feedback interconnection

As the gain, $k(0)$ is increased, the system poles approach the zeros of the loop transfer function, $g(s)k(s)$. It should be noted that because of this, complex conjugate poles may cross the imaginary axis for values of $k(0)$ less than $1/g(0)$. One specific example is an industrial fixed bed ammonia synthesis reactor studied by Morud and Skogestad.[7] In the ammonia synthesis case, complex conjugate poles approaching right half plane zeros of the reactor transfer function crossed the imaginary axis for a loop gain $g(0)k(0)$ less than one (Hopf bifurcation). This made the reactor enter a stable limit cycle. Thus, it is not always true that positive feedback leads to slow responses and high sensitivity to disturbances, it may just as well lead to e.g. limit cycle behaviour. For this to happen, two conditions must be met. First, there must be at least 360° phase lag in $g(j\omega)k(j\omega)$ at high frequencies. Second, the magnitude of the loop gain $|g(j\omega_{360})k(j\omega_{360})|$ at the critical frequency $\omega_{360}$ where this happens must be larger than the loop gain at steady state $g(0)k(0)$.

While the feedback, $k(s)$ moves the plant poles, it does not affect the zeros of $g(s)$, and may only introduce new zeros at the locations of the poles of $k(s)$. To see this, assume $g$ and $k$ to be rational, i.e. that they may be written as $g(s) = n_g(s)/d_g(s)$ and $k(s) = n_k(s)/d_k(s)$ where $n_g$, $n_k$, $d_g$ and $d_k$ are polynomials in $s$. This gives an expression for the transfer function from $r$ to $y$ (*Figure 1*):

$$y = \frac{g}{1-gk} r = \frac{d_k n_g}{d_k d_g - n_k n_g} r \tag{7}$$

The zeros of the closed loop system thus consist of the poles of $k(s)$ and the zeros of $g(s)$. As long as $k(s)$ is stable, i.e. $d_k$ does not have roots in the right half plane), the closed loop system has the same right half plane zeros as $g(s)$.

*Parallel interconnection*

Now consider parallel interconnection of two transfer functions, as shown in *Figure 2*. For rational transfer functions, the overall transfer function from $r$ to $y$ becomes:

$$y = (g+k) = \left(\frac{n_g}{d_g} + \frac{n_k}{d_k}\right) r = \frac{n_g d_k + n_k d_g}{d_g d_k} r \tag{8}$$

As can be seen, the poles are the poles of $g$ and $k$, while the zeros are changed.

Right half plane zeros (often denoted 'unstable zeros', since the inverse is unstable) are often associated with competing effects, i.e. when $g(s)$ and $k(s)$ have opposite effects on the output $y$. In terms of time responses, right half plane zeros cause an inverse response (undershoot) in the step response. Left half plane zeroes close to the origin yield large overshoots in the step response.

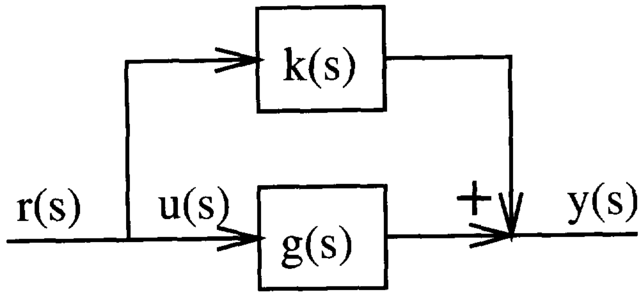


**Figure 2** Parallel interconnection

*Series interconnection*

The series interconnection is shown in Figure 3. The overall transfer function becomes:

$$y = g(s)k(s)u \tag{9}$$

The poles and zeros of the combined transfer function, $g(s)k(s)$, are the poles and zeros of the individual transfer functions, $g(s)$ and $k(s)$. Thus there are really no surprises. Note, however, that right half plane zeros may yield a peak in the frequency response and at the same time yield a large phase lag. In a series connection of a large number of transfer functions with right half plane zeros (think of a distributed parameter system), there may therefore be peaks at very large phase lags.

In summary, feedback effects move poles, which affect the plant time constants and determine its stability, while parallel paths change or add zeros, which affect the plant behaviour under feedback, whether it be a controller or feedback due a recycle loop.

With the linear theory in mind, we now turn to the plant, and give some examples to illustrate the effect of interconnections on the dynamic behaviour of plants. We will discuss separately the effects of feedback and parallel paths in integrated plants.

## Models used for the examples

In the examples we make use of some very simple models to illustrate the dynamics. Since they are used repeatedly, we have given the models a unified treatment in the Appendix. Here, we only present their essential features. For numerical calculations we have used standard MATLAB functions (ode45, rlocus) with numerical values as listed in the Appendix.

*The CSTR.* The CSTR model used has constant molar holdup and at most three chemical species, A, B, C. The reaction is a simple reaction A → B (or B → C) of the

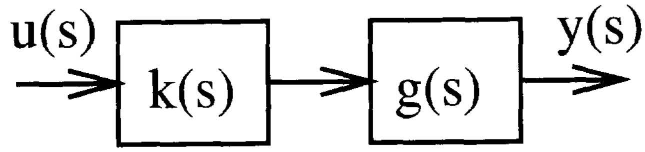


**Figure 3** Series interconnection

Arrhenius type. We allow the presence of a catalyst in the reactor, yielding a larger time constant for the energy balance than for the mass balance. For simplicity we have assumed constant heat capacities of the fluid and the catalyst.

*Heat exchanger without dynamics.* The model used is a standard $\varepsilon$-NTU model with no dynamics. For constant flow rates this reduces to a linear relation between inlet and outlet temperatures when the fluid heat capacity is assumed to be a constant.

Cases involving dynamic heat exchanger models are taken from the thesis by Mathiesen.[16]

*The perfect separation unit.* The perfect separation unit with no dynamics splits a mixture of components A, B, C into pure B at the bottom and a mixture of A and C at the top.

## Examples of recycle causing positive feedback

Material recycle and heat integration in plants usually lead to positive feedback. We therefore present some examples to illustrate their effects on plant dynamics.

*Example 1: Material recycle*

Consider the somewhat simplified system shown in *Figure 4a*, consisting of an isothermal continuous stirred tank reactor (CSTR) followed by a separation unit. The feed to the reactor consists of two streams, F and R, consisting of a reactant, A, and an inert, C. The reaction taking place in the reactor is a first order reaction A → B. The separation unit separates the reactor effluent into pure product, B, at the bottom and a mixture of reactant, A, and inert, C, at the top.

Now, in order to reprocess unreacted A, one might consider material recycling, as shown in *Figure 4b*. Assuming that the two systems operate at the same steady state, we ask how the material recycle affects the dynamic behaviour of this system.

For the sake of example, assume that the separator is perfect, with no dynamics. The model and the numerical values used are listed in the Appendix.

*Figure 5* shows the time responses to a very small step disturbance in $z_F$, the mole fraction of the reactant in the feed stream. As can be seen, the positive feedback due to the recycle has in this case made the response slower, and the steady state sensitivity higher.

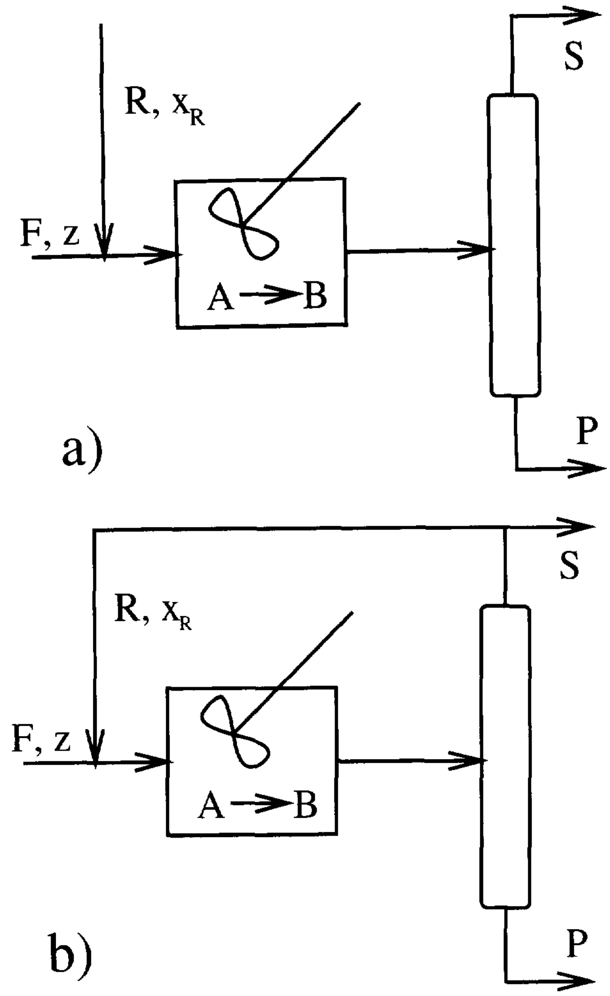


**Figure 4** Reactor with material recycle (positive feeback)

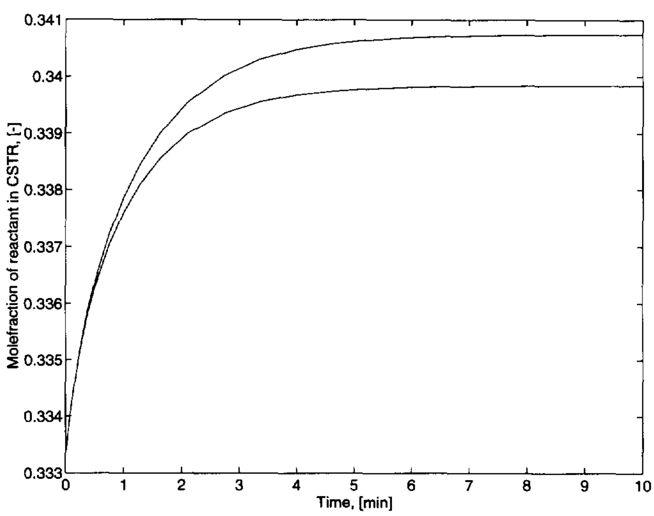


**Figure 5** Step response of recycle system (upper curve: with recycle, lower curve; without recycle

*Example 2: Feedback from heat integration*

Consider the system shown in *Figure 6a* showing a CSTR where a simple first order reaction A → B is taking place. The feed, F, is preheated in a preheater before entering the reactor.

In order to save energy, one might consider preheating the feed by the effluent, as shown in *Figure 6b*. The two systems are supposed to operate at the same steady state. For the example, we neglect the dynamics of the heat exchanger. The models and numerical values are described in the Appendix.

*Figure 7* shows the time response of the two systems when they are given a one degree K step disturbance in the feed temperature, $T_F$. Like in the previous example,

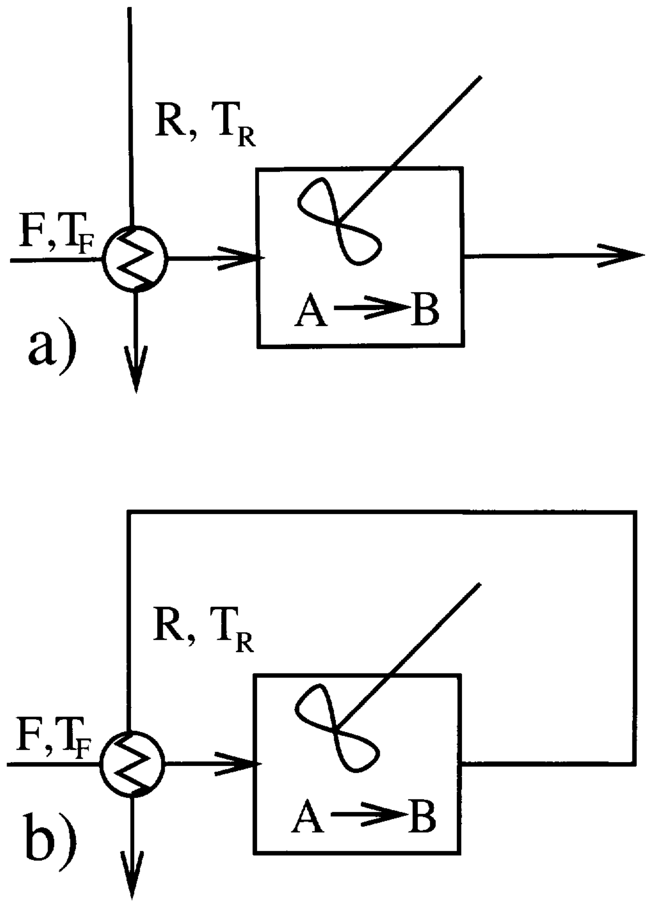


**Figure 6** Reactor with feed/effluent preheating (positive feedback)

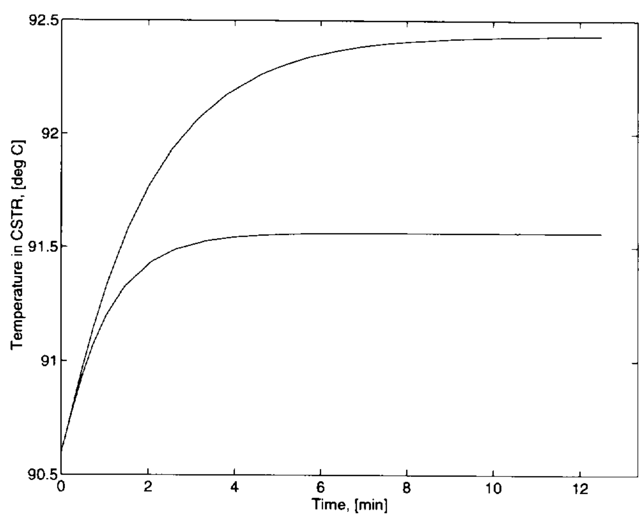


**Figure 7** Step response of preheating system (upper curve: with feed/effluent preheating, lower curve: independent preheater

the feedback due to heat integration has increased the time constant and the steady state gain.

*Example 3: Heat exchanger network example*

As another example of positive feedback from heat integration, take the heat exchanger network shown in *Figure 8*.[17] Consider the effect of temperature disturbance in the hot stream (H1) on the outlet temperature $y_1$. As can be seen, heat exchangers 1a and 1b form a positive

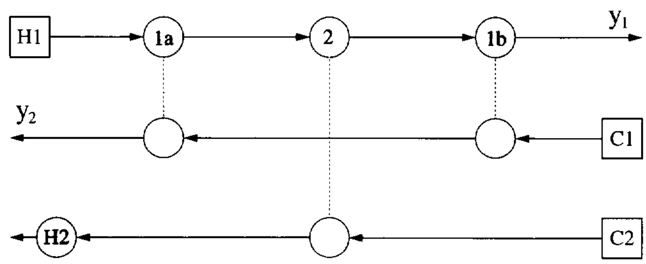


**Figure 8** Heat exchanger network with energy recycle (positive feedback)

feedback loop. In this case, this leads to a higher sensitivity and a slower response than if the heat exchangers were independent coolers working at the same steady state.

## Examples of recycle causing negative feedback

Material recycle and heat integration may also lead to negative feedback effects. This is less common but it is nevertheless important to be aware of the possibility. It is rare because units in a plant usually have a positive gain: increasing an inlet temperature of an heat exchanger or a reactor normally leads to an increase in outlet temperature. For example, as shown by Mathiesen,[16] this is always the case for heat exchanger networks. Similarly, increasing the inlet concentration of a chemical species to a system usually leads to an increase of outlet concentration of the species.

However, there are exceptions: take for instance a distillation column where the distillate flow and the boilup are the independent variables (DV configuration). Increasing the temperature of the boiler medium increases the boilup, which leads to higher purity, and hence a lower temperature, in the top of the column. The column is therefore a negative gain element from the boiler medium temperature to the top temperature. With heat integration, the column can therefore act as a negative gain element and lead to negative feedback if contained in a loop.

*Example 4: A reactor example*

Another example where a loop yields negative feedback is the system shown in *Figure 9*. Feed is preheated with the product, further heated in a second heater, and sent through two reactors. In the first reactor, a reaction A → B with negligible heat of reaction takes place

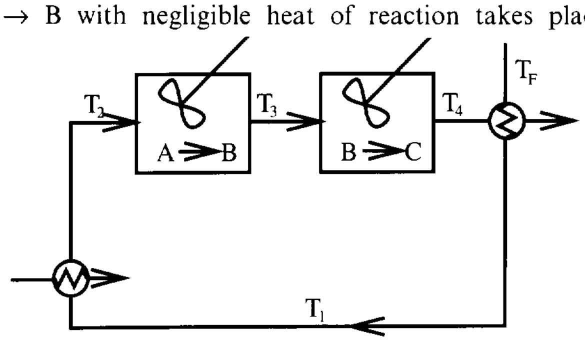


**Figure 9** Endothermic reactor system with energy recycle (negative feedback)

(i.e. $T_3 = T_2$). In the second reactor, an endothermic reaction takes place, with total conversion of component B to component C. The temperature drop over the two reactors taken together is therefore proportional to the reaction rate, $r$, of the first reactor (assuming constant heat capacity). Details in the mathematics are given in the Appendix. Consider an increase in $T_2$, the inlet temperature of the first reactor. With a proper choice of numerical values (Appendix), the outlet temperature of the second reactor, $T_4$, will decrease, that is $dT_4/dT_2 < 0$. This is then an example of a negative feedback effect. Negative feedback will usually have a stabilizing effect on the system and make it faster, but may cause instability if the loop gain is large enough.

## More complex feedback effects caused by recycle

*Flow/heat transfer interactions.* The effects mentioned above are either pure temperature effects or pure recycle effects. Introduction of heat integration in plants may sometimes provide a coupling between temperature and flows, and destabilise a plant. Take for example the reactor example analysed in the previous section (*Figure 9*), and assume that the feed is liquid which is partially evaporated in the preheater, such that the flow between the preheater and the second heater is two-phase. The pressure drop of the system is now affected by the heat transfer in the preheater, which is influenced by the outlet temperature of the reactors. The outlet temperature of the reactors is affected by the flow rates, which are affected by the pressure drop. With the resulting coupling between temperature and flows, one should be concerned about the stability of the plant, as it could easily be unstable. Such instabilities are discussed thoroughly by Eigenberger.[18]

*Example 5: Industrial example*

An industrial example of a flow/heat transfer interaction was given by Anderson.[19] A reactor/preheater system in a new plant turned out to be unstable for large throughputs. *Figure 10* shows a simplified sketch of the system. The saturated liquid feed, $F_0$, was vaporised in an evaporator using the reactor effluent and superheated in a superheater before entering the reactor. The pressures and temperatures in the system were tightly controlled. To understand the instability, assume that the flow rate, $F_1$, through the reactor increases (due to some disturbance) while the feed flow rate, $F_0$ is kept constant. The resulting increase in the hot stream flow rate (inside the 'coil' in the figure) in the boiler has two effects on the evaporator. In the long run, the liquid holdup in the evaporator will decrease, reducing the heat transfer area and thus eventually reducing the flow rate $F_1$ (negative feedback effect). Initially, however, the liquid level in the evaporator will increase due to swelling of the boiling liquid and thus increase the heat transfer and thus tend to increase the vapour production, $F_1$, i.e. there is a positive feedback effect. In the industrial case, the loop gain due to this positive feedback was larger than one, resulting in instability of the steady state. As the flow, $F_1$, is constrained by the mass balance to be equal to $F_0$ on the average, the phenomenon manifests itself as limit cycles.

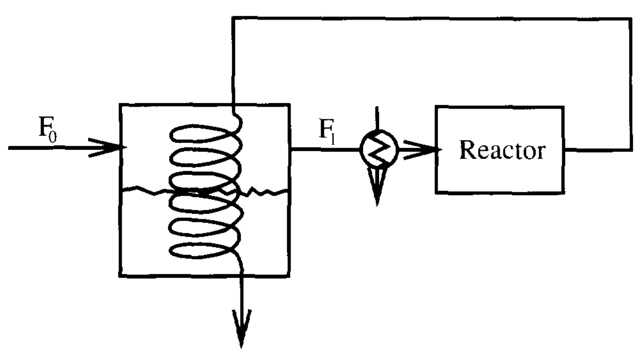


**Figure 10** Reactor with feed preheating

## Parallel paths in plants

Manipulating an actuator in an integrated plant often has more than one effect on the plant. First, different parts of the plant may be affected, several of which may influence a given measurement. This may correspond to e.g. having units in parallel or when there are several downstream paths in a heat exchanger network. Second, several different physical effects, such as pressure, flow rate, temperature and concentration may be affected. The influence of these effects on a measurement may vary in strength and speed, and the measurement will often be the sum of several such effects. In both cases there exist parallel paths between the actuator and the measurement. Often the parallel paths have an opposing influence on the measurement, i.e. they are competing effects. We present some examples of parallel paths in plants.

*Example 6: Units in parallel*

As an example of parallel units, consider the system shown in *Figure 11*, showing two CSTRs in parallel. The feed stream, F, consisting of pure reactant, A, is divided equally in a splitter (split fraction $\alpha = 0.5$), and fed to the reactors, where a simple reaction A $\rightarrow$ B takes place. The outlet streams from the reactors are mixed to form a product, P.

With a specific choice of numerical values of the parameters (Appendix) the response to a small step in the split fraction, $\alpha$, yields an inverse response, as shown in *Figure 12*. This reflects the existence of right half plane zeros for the particular choice of numerical values chosen.

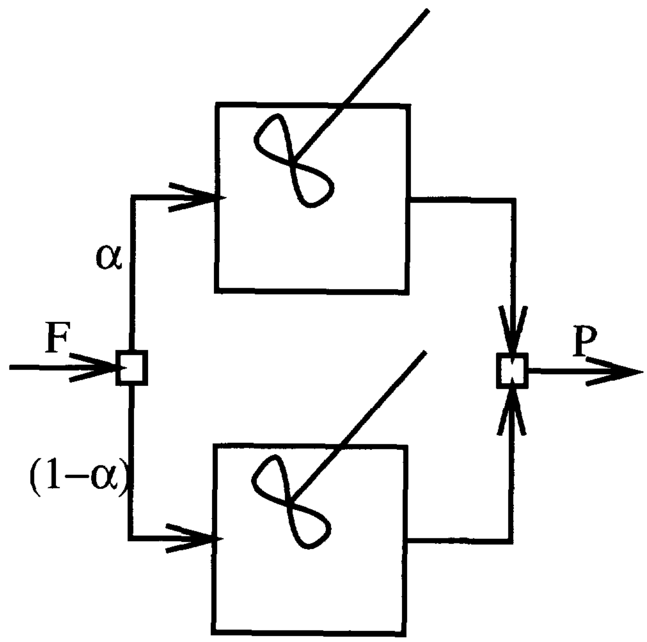


**Figure 11** Reactors in parallel (parallel path)

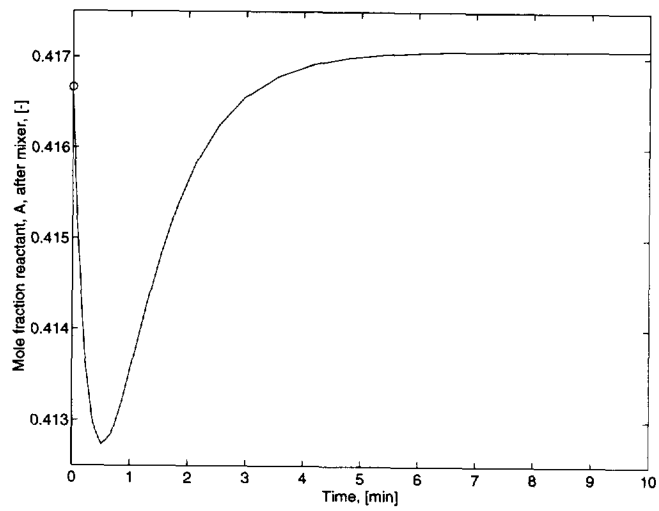


**Figure 12** Step responses of CSTRs in parallel

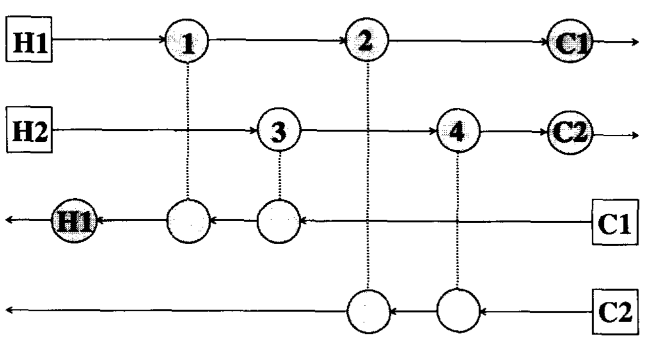


**Figure 13** Heat exchanger network with parallel downstream paths (from inlet temperature of stream H2 to outlet temperature of stream C2)

*Example 7: Different downstream paths*

Consider the heat exchanger network shown in *Figure 13*. A disturbance in the hot stream H2 affects the outlet of cold stream C2 by two paths: through exchangers 3–1–2 and directly through exchanger 4.[17] In this particular case there may be only left half plane zeros due to the parallel paths.[16]

*Different physical effects.* There are also cases where one variable in the plant affects another through different physical effects through the same units. For example, manipulating an actuator may typically change pressures, flow rates, concentrations and temperatures. These effects propagate with different velocity through the plant. Changes in flow rates and pressures often propagate quickly, while changes in concentrations and temperatures usually propagate somewhat slower. Slow propagation is often associated with large hold ups or storage capacities.

*Example 8: Heat exchanger network*

As an example, take the simple heat exchanger network shown in *Figure 14*. The temperature, $T_2$, is supposed to be lower than $T_1$. Manipulating the valve position, $u$, affects the outlet temperature, $T = y$, by two different effects: through the change in the flowrate of the stream H2, and by a change in the operation of the heat exchanger. The two effects are competing: the former tends to decrease $T$ in response to an increase in the flow rate H2, the latter to increase $T$. As shown in the thesis by Mathiesen[16] (*Figure 15*), this may cause inverse response behaviour, reflecting the existence of right half plane zeros.

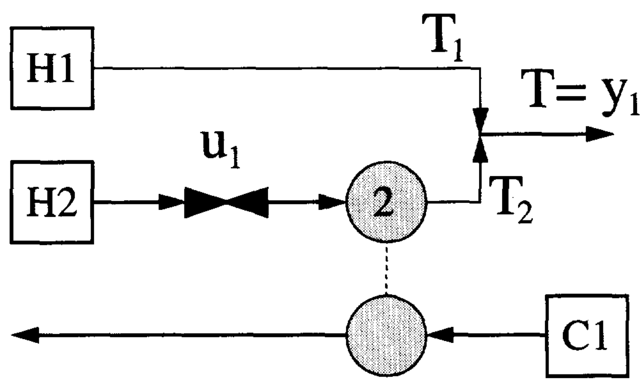


**Figure 14** Heat exchanger network with 'internal' parallel paths (flow rate and temperaure)

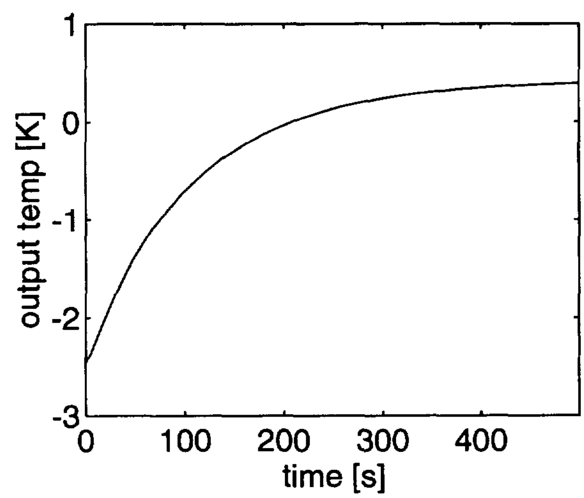


**Figure 15** Step response to change in flow rate, $u_1$

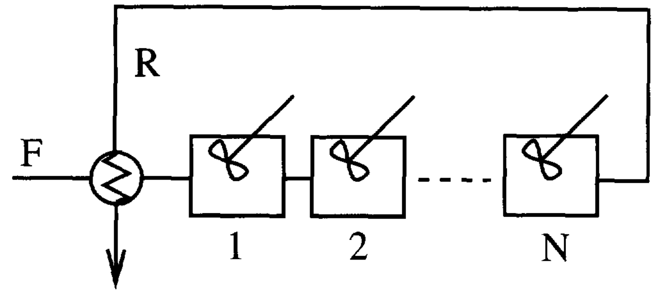


**Figure 16** Reactors in series with feedback of heat (positive feedback)

## Effects of combining recycle with parallel paths

In the heat recycle example above, the result of the feedback was to make the system slower. We now give a similar example where the positive feedback due to the heat recycle leads to oscillatory instability due to right half plane zeros introduced by 'internal' parallel paths.

*Example 9: CSTRs in series with heat integration*

Consider the system shown in *Figure 16*, which might represent a crude model of a fixed bed autothermal reactor. Feed gas, consisting of pure reactant, A, is preheated in a feed/effluent heat exchanger and fed into a train of CSTRs filled with catalyst before it leaves the system through the feed/effluent exchanger. The reaction is a simple A → B of the Arrhenius type.

As a specific numerical example, we take a system with 15 CSTRs in series. The numerical values used for the parameters are listed in the Appendix. The time constant for the energy balance is chosen an order of magnitude larger than the residence time, reflecting a large heat capacity of the catalyst. As a basis of comparison, we use a similar system with an independent preheater.

*Figure 17* shows the responses to a small step disturbance in the feed temperature, $T_F$. As can be seen, the system with preheating is unstable. Moreover, the instability manifests itself as oscillations of growing amplitude, indicating that the instability is due to a pair of complex conjugate poles, and not the pole approaching the origin. This is confirmed in *Figure 18*, showing a numerically computed pole/zero map of the linearised system. As can be seen, there are right half plane zeros in the system. These may be explained by the existence of 'internal' parallel paths in the reactor train, since there are changes in both reactant concentration and temperature. Consider for instance an increase in the inlet temperature of the first bed. This has two effects on the last reactor in the train. First, as the reaction rate in the first reactor increases, there is less reactant left to the last reactor, which tends to decrease its outlet temperature. This is the fast effect. Second, the heat produced in the first reactor will eventually reach the last reactor, tending to increase its outlet temperature. This is a slow effect due to the heat capacity of the catalyst. However, the second effect is the strongest, yielding right half plane zeros. Now, the feedback gain from the heat recycle makes these right half plane zeros attract a pair of complex conjugate poles, as may be seen from the figure. This makes a pair of complex conjugate poles cross the imaginary axis, yielding the instability.

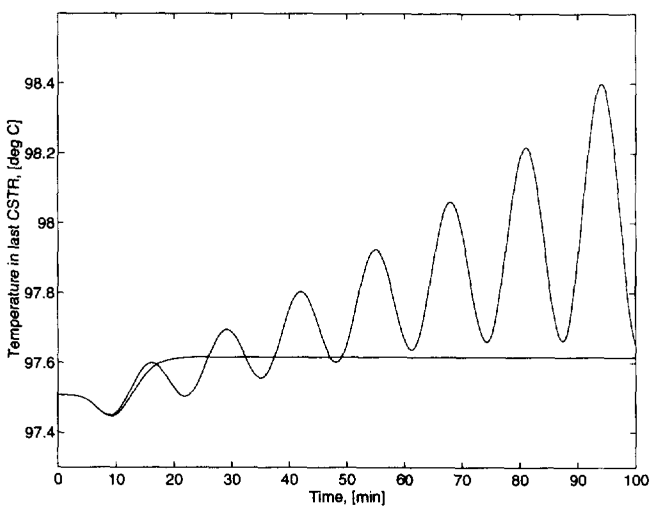


**Figure 17** Step response of CSTRs in series with preheating (wavy curve: with feed/effluent preheating; other curve: independent preheater)

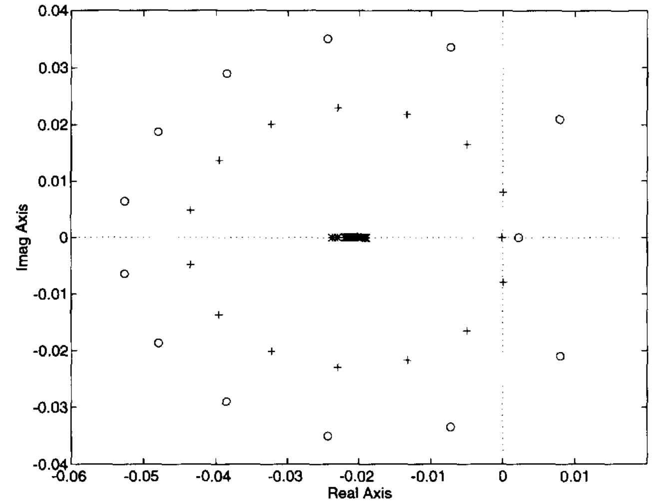


**Figure 18** Pole and zero locations of reactor systems ('0'-zeros, 'X'-poles when independent preheater, '+'-poles with heat recycle)

This kind of behaviour is more likely the larger the number of CSTRs in series. With right half plane zeros in the individual CSTR transfer functions there will typically be a peak in the frequency response and at the same time a phase lag. By compounding a large number of such units, the peak in the frequency response of the reactor train may easily extend to phase lags beyond 360°. As explained in the linear systems section this implies that a pair of complex conjugate poles cross the imaginary axis before the real pole passing the origin.

Limit cycle behaviour due to such effects has been observed in industrial fixed bed reactor systems. A particular industrial example was studied by Morud and Skogestad[7] based on an incident in an ammonia synthesis plant. References to several other examples are given by Eigenberger.[18]

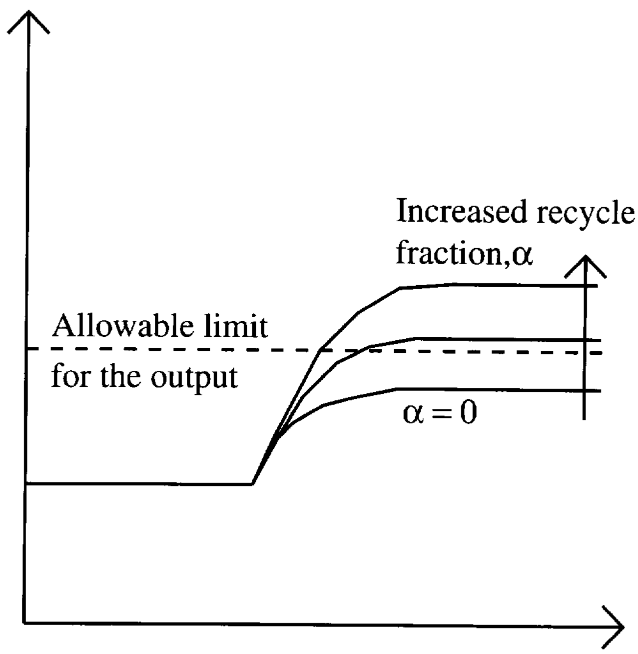


**Figure 19** Response in output to step disturbance

## Discussion

Plant integration has an impact on the control aspects of the plant. Feedback effects due to e.g. mass recycle may make the plant unstable or more sensitive to disturbances and increase the need for control, while parallel paths may introduce fundamental limitations in the performance of the plant under feedback control.

Consider a system with recycle, where a fraction $\alpha$ of the outlet is recycled. For a step disturbance in e.g. the feed concentration, the output, e.g. the outlet concentration of some chemical, has to stay within some acceptable limits. The response, for different values of the fraction recycled, $\alpha$, may typically look something like the plot illustrated in *Figure 19*. For high values of the fraction recycled, $\alpha$, the outlet concentration is sensitive to disturbances in the input stream, and will typically exceed its allowable limit. For low values of the amount recycled, there is in this case no need for control, as long as the output keeps within the specified limits. The recycle will typically make the sensitivity high for slow disturbances, such that the recycle does not necessarily introduce a need for fast control, but it introduces a need for control where it otherwise might not have been needed. With control, disturbances may be rejected, or the plant response may be speeded up if necessary, as long as the plant does not have inherent limitations in achievable control performance.

It is known that right half plane zeros in a plant limit the achievable control performance obtainable by any controller. Hence, if there are parallel paths between the manipulated variables and the controlled variables, this may lead to inherent limitations in what can be achieved by the control system. Hence, it is important to be aware of this when doing e.g. heat integration, as it may introduce many parallel paths in the plant, some of which may lead to poor control of the resulting plant.

In this paper we have only discussed linear systems. However, many of the concepts involved may be generalised to nonlinear systems. Instead of poles, one may study the internal dynamics of the plant, i.e. the evolution of the states of the plant when the input follows a given trajectory. Instead of zeros, one may study the zero dynamics of the plant, which is the evolution of the states of the plant when the output is forced to be zero by the input. Unstable zero dynamics means that there are right half plane zeros if the plant is linear, and may be through of as a generalisation of right half plane zeros for non-linear plants. Unfortunately, nonlinearities make the analysis of possible dynamic behaviour much more difficult. Nonlinear systems may exhibit other types of behaviour, such as chaos, which may never occur in a linear system.

## Conclusion/proposition for further work

The dynamics of plants with material recycle or heat integration may be very different from the dynamics of the individual processing units. The effect of material recycle or heat integration may be thought of as moving the plant poles and zeros. Feedback effects due to recycle of material or energy are typically positive, which often leads to slow responses and high steady state sensitivity, and in some cases to instability. This will lead to an increased need for control. Parallel paths caused by e.g. heat integration change the zero locations of the plant, and may introduce limitations to the achievable performance of the plant control system. In addition, combinations of these effects may lead to instability, reactor runaway, limit cycles, etc, in the plant if not foreseen.

There is a need for a systematic classification of the effects of integration on the plant dynamics, as tight integration may lead to plants which are almost impossible to control. Some simple indicators which could be used to tell us when problems are probable, would be of great help.

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## Nomenclature

| | |
|---|---|
| $C_{p,\text{fluid}}$ | fluid heat capacity (J/mol K) |
| $C_{p,\text{solid}}$ | catalyst heat capacity (J/kg K) |
| $E$ | activation energy (J/mol) |
| $F$ | flow rate (mol/s) |
| $k(T)$ | reaction rate constant ($s^{-1}$) |
| $k_0$ | Arrhenius constant ($s^{-1}$) |
| $M_{\text{fluid}}$ | fluid holdup in CSTR (mol) |
| $M_{\text{solid}}$ | amount of catalyst in CSTR (kg) |
| $r$ | reaction rate ($s^{-1}$) |
| $R$ | universal gas constant (8.31J/mol K) |
| $T$ | temperature (K) |
| $T_0$ | reference temperature (K) |
| $x$ | mole fraction of chemical species (–) |
| $z$ | mole fraction of chemical species in the feed (–) |

*Greek*

| | |
|---|---|
| $\alpha$ | flow split fraction in splitter $F_{\text{out}}/\Sigma_{\text{out}}F_{\text{out}}$ (–) |
| $-\Delta H_{\text{rx}}$ | heat of reaction (J/mol) |
| $\varepsilon$ | heat exchanger efficiency (–) |
| $\tau$ | fluid residence time in CSTR (s) |
| $\tau_T$ | time constant of energy equation (s) |

*Subscripts*

| | |
|---|---|
| A, B, C | chemical species |
| F | feed stream |
| $i$ | index taking the values A, B, C |
| in | index over all inlet streams |
| out | index over all outlet streams |
| R | recycle stream |

## Appendix

The models used for the examples are:

*The CSTR.* The CSTR model used has constant molar holdup, $M_{\text{fluid}}$, and at most three chemical species, A, B, C. The reaction is a simple reaction of the Arrhenius type A → B or (B → C). The reaction rates, $r_i$, $i$ - A, B, C are given by ($r_C = 0$ when C is an inert):

$$r_A = -r_B = k(T)\cdot x_A, \qquad k(T) = K_0 e^{-\frac{E}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)} \tag{10}$$

Mass balance for component $i$, $i$ = A, B, C:

$$\dot{x}_i = \frac{1}{\tau}(x_{\text{in},i} - x_i) - r_i \tag{11}$$

Energy balance (constant heat capacity):

$$\dot{T} = \frac{1}{\tau_T}(T_{\text{in}} - T) + \frac{-\Delta H_{\text{rx}}}{C_p}\cdot r_A \tag{12}$$

The time constants in these equations are given by:

$$\tau = M_{\text{fluid}}/F, \qquad \tau_T = \frac{C_{p,\text{fluid}}M_{\text{fluid}} + C_{p,\text{solid}}M_{\text{solid}}}{C_{p,\text{fluid}}F} \tag{13}$$

*Heat exchanger without dynamics.* The model used is a standard $\varepsilon$-NTU model (Two streams, 1 and 2):

$$T_{1,\text{out}} = \varepsilon_1 T_{2,\text{in}} + (1-\varepsilon_1)T_{1,\text{in}} \tag{14}$$

where the heat exchanger efficiency, $\varepsilon_1 \in [0\ 1]$, is a function of the flow rates only. In the examples where it is used, it is just a constant, as the flow rates are constant in these examples.

*The perfect separation unit.* The perfect separation unit with no dynamics splits a mixture of components A, B, C into pure B at the bottom (i.e. $x_{\text{bottom,B}} = 1$, $x_{\text{bottom,A}} = x_{\text{bottom,C}} = 0$) and a mixture of A and C at the top. The mass balance for component $i$, $i$ = A, B, C becomes:

$$Fx_{\text{in},i} = F_{\text{top}}x_{\text{top},i} + F_{\text{bottom}}x_{\text{bottom},i} \tag{15}$$

*Splitters and mixers.* The mass balances of splitters and mixers are taken as (component $i$, $i$ = A, B, C):

$$\sum_{\text{in}} F_{\text{in},i}x_{\text{in},i} = \sum_{\text{out}} F_{\text{out},i}x_{\text{out},i} \tag{16}$$

For the mixer, the inlet streams are fully specified. For the splitter, the mole fractions of all streams are the same. The outlet flowrates are $F_1 = \alpha F$, $F_2 = (1-\alpha)F$, where $F$ is the inlet flow rate.

## Numerical values for the examples

*Example 1*: $z_A = 0.95$. $z_C = 0.05$, $x_{R,A} = x_{R,C} = 0.33$, $F$ = 1 vol.units/min, $R$ = 1.7 vol. units/min, $k(T)$ = 2.7 $\text{min}^{-1}$ (isothermal), $\tau$ = 1 min, step size $\Delta z_A = 0.01$.

*Example 2*: $z_A = 1$, $z_C = 0$, $T_F = 25°C$, $T_0 = 60°C$, $T_R = 90.6°C$, $F$ = 1 vol.units/min, $R = F$, $k_0 = 1\ \text{min}^{-1}$, $\tau = M/F = 1$ min, $-\Delta H_{r,x}/C_P = 50K$, $-E/R = -7693K$, $\varepsilon_{\text{feed}} = 1/3$ (Feed is stream 1 in eq. 14), step size $\Delta T_F$ = 1K.

*Example 4*: $E$ = 60 kJ/mol, $R$ = 8.3 J/mol.K, $T_0 = T_2$ = 573.15K, $-\Delta H_{rx}/C_p = -1000K$, $k_0 = 5.76 \cdot 10^{-4}\ s^{-1}$, residence time of first reactor $\tau$ = 300 s, inlet to first reactor $z_A = 1$.

*Example 6*: Feed to system: $z_A = 1$, $\alpha = 0.5$, $F = 1$ vol.units/min, Bottom reactor: feed $(1 - \alpha)F$, $k(T) = 2\ \text{min}^{-1}$ (isothermal), $M = 0.5$ vol.units, Upper reactor: feed $\alpha F$, $k(T) = 1/2\ \text{min}^{-1}$ (isothermal), $M = 1$ vol.units, step size $\Delta\alpha = 0.05$.

*Example 9*: $T_0 = 60°C$, $T_F = 2°C$, $z_A = 1$, number of reactors 15, $\varepsilon_{feed} = 0.5$, $\tau = 1$ min, $\tau_T = 60$ min, $-\Delta H_{rx}/C_p = 5K$, $k = 1\ \text{min}^{-1}$ (isothermal), $-E/R = -7693K$, $T_R = 97.5°C$, step size $\Delta T_F = 1K$

## Details of example 4

See the example. Throughout the derivation, $\tau$, $z_A$ and $x_B$ are the residence time, the inlet mole fraction of reactant and the outlet mole fraction of the *first* reactor. The mole fraction at the outlet of the first reactor (isothermal) at steady state is found from the mass balance, eq. (11):

$$0 = \frac{1}{\tau}(z_A - x_A) - k(T_2) \cdot x_A \tag{17}$$

which yields:

$$x_B = 1 - x_A = 1 - \frac{z_A}{1 + k(T_2)\tau} \tag{18}$$

Total conversion of this in the second reactor yields the temperature difference (energy balance):

$$T_2 - T_4 = T_3 - T_4 = -\frac{-\Delta H_{rx}}{C_p} x_B \tag{19}$$

which yields (dropping argument of $k$, i.e. $k = k$(T2)):

$$\begin{aligned}\frac{dT_4}{dT_2} &= 1 + \frac{-\Delta H_{rx}}{C_p} \frac{z_A \tau}{(1 + k\tau)^2} \frac{dk}{dT_3} \\ &= 1 + \frac{-\Delta H_{rx}}{C_p} \frac{z_A \tau}{(1 + k\tau)^2} \frac{E}{RT_2^2} k\end{aligned} \tag{20}$$

With a proper choice of numerical values (listed above), this is a negative quantity.