

THE DYNAMIC BEHAVIOR OF INTEGRATED PLANTS

JOHN MORUD and SIGURD SKOGESTAD *

Chemical Engineering Dept., University of Trondheim, NTH
N-7034 Trondheim, Norway

March 15, 1994

KEYWORDS

Process dynamics; nonlinear systems; positive feedback; chemical reactor.

Abstract

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 of the linearized plant. This implies that recycle of mass and energy, which are feedback mechanisms, affect the poles and thus the plant stability, while parallel interconnections in a plant affect the zeros and thus the achievable performance of the plant control system.

1 Introduction

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 (Gilliland *et al.*, 1964, Denn and Lavie, 1982). Recycle and heat integration may dramatically alter the time constants of the plant, and may give rise to instability or oscillatory behavior (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 behavior of the system is very difficult. Although there exist mathematical tools such as bifurcation analysis, which in principle could be used to analyze 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 "rule of thumbs", or indicators, which could be used to warn us when complex behavior is plausible.

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. Jacobsen and Skogestad (1991) also studied distillation and found that positive feedback caused by the reflux may lead to instability and multiple steady states. Other related work that may be mentioned is Verykios and Luyben (1978), Luyben (1992), Papadourakis *et al.* (1987, 1989), and Uppal and Ray (1974).

Finally, in this introduction, we state the objective of the paper and define more clearly some of the terms, such as interconnections, feedback, loops and recycle.

The objective of this paper is to discuss the effect of the structure of the plant interconnections on plant dynamics. This means that we consider the processing units to be given, and ask how the dynamics of the plant is affected by the way the processing units are put together.

One very important interconnection of units is a *recycle loop* because this alters the response time

*Correspondence should be addressed to Sigurd Skogestad, E-mail: skoge@kjemi.unit.no, phone: +47-7359-4154, fax: +47-7359-4080

(eigenvalues) of the system. A recycle loop may be caused by mass recycle, but may also more generally be caused by heat recycle, for example, when the reactor feed is preheated by the effluent. A recycle loop is a special case of feedback, but the term “feedback” is 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 many cases a dynamic model of a unit may be formulated as

$$\frac{dx}{dt} = g(u) + f_1(x) + f_2(x) + \dots \quad (1)$$

where $g(u)$ yields the direct effect on the states x of changing an independent variable u , whereas $f_1(x), f_2(x), \dots$ represent secondary “feedback” effects which modify the dynamic behavior. If $a_i = \partial f_i / \partial x$ is positive (negative), then the feedback for effect i is positive (negative). As already stated, recycle usually yields positive feedback (although a couple of examples with negative feedback are presented below), but for stable systems the overall feedback effect must of course be negative, i.e., $\sum_i a_i < 0$.

In a previous paper (Morud and Skogestad, 1994) we studied in more detail various “internal” feedback effects $f_i(x)$ (in spite of the somewhat misleading title of the paper), such as the effect of reaction, heat transfer, flashing, evaporation etc. The idea of that paper was to understand the various effects, and in particular those resulting in positive feedback since this may result in instability. In summary, in the previous paper we also studied feedback effects that occur inside a unit, whereas the objective of the present paper is to study exclusively the effect of external interconnections of units in an integrated plant.

2 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. The main idea is to draw an analogy between interactions in a plant (e.g. caused by heat integration or mass recycle) and linear feedback control systems.

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 stabilized 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, which in a processing plant may correspond to e.g. having units in parallel or to having multiple downstream paths in a heat exchanger network.

In the paper we mainly discuss the effect of positive and negative feedback mechanisms. We therefore elaborate these concepts for scalar systems to illustrate their effect. 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 $u = k(s)y$. The poles of the system are then the roots of $1 - g(s)k(s)$. The steady-state behavior is found by setting $s = 0$. We distinguish between the following two cases:

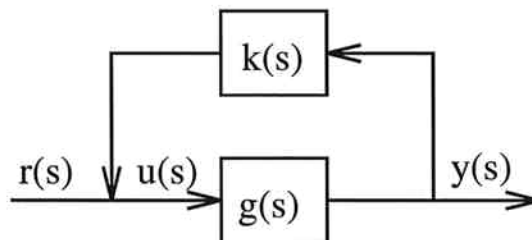


Figure 1: Feedback system

Case 1. $g(0)k(0) < 0$ means negative feedback. This is the most common case in feedback control, but it is less likely for a recycle loop. If the magnitude of the gain, $k(0)$, is increased, this will normally make a pair of complex conjugate poles cross the imaginary axis when $k(0)$ becomes sufficiently large (as long as there is at least 180° phase lag in $g(j\omega)$ at high frequencies, ω).

Case 2. $g(0)k(0) > 0$ means 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 disturbances is high. It should be noted, however, that 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 (1993). As k is increased, the zeros of $1 - gk$ which remain finite approach the zeros of gk as $|k|$ is increased. For the ammonia synthesis case, complex conjugate poles approaching right half plane zeros of g 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 behavior.

While the feedback, $k(s)$, moves the plant poles, it does not move the zeros of $g(s)$, and may only introduce zeros in the left half plane. To see this, assume g and k to be rational, i.e. that they may be written as $g(s) = \frac{n_g(s)}{d_g(s)}$ and $k(s) = \frac{n_k(s)}{d_k(s)}$ 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 (Fig. 1):

$$y = \frac{g}{1 - gk} r = \frac{d_k n_g}{d_k d_g - n_k n_g} r \quad (2)$$

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 $g(s)$.

We will discuss separately the effects of feedback and parallel paths in integrated plants.

3 Feedback mechanisms in integrated plants

Two important sources of feedback in plants are material recycle and heat integration. Material recycle is used to reprocess unconverted material from a reactor, or to re-separate material as for the reflux in a distillation column. Heat integration is normally associated with energy conservation. Most sources of feedback in chemical plants yield a *positive feedback effect*: 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. Positive feedback due to mass recycle or heat integration will usually increase the plant time constant, and increase the sensitivity to slow disturbances, which corresponds to a pole being moved closer to the origin (approaching a pure integrator). 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 constants have been observed (e.g., Kapoor *et al*, -86).

Although this is usually the effect of mass or energy recycle, some care should be exercised. First,

positive feedback may in general just as well lead to e.g. limit cycle behavior than to slow responses, as explained in the previous section. Second, there are some examples of feedback in processing plants which correspond to negative feedback, and we shall give a few examples later. In these examples we have the somewhat unusual effect that a temperature increase in some location results in a temperature decrease at some other location.

4 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.

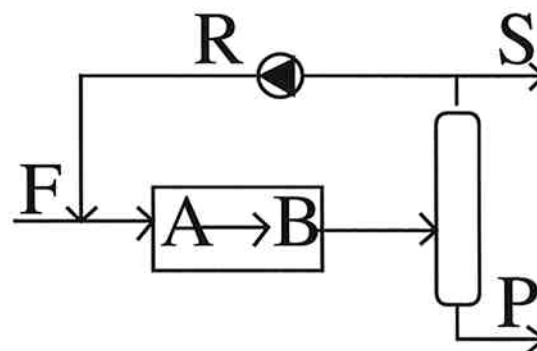


Figure 2: Reactor with mass recycle (positive feedback)

Material recycle. Consider the somewhat idealized system shown in Figure 2, where a reactant, A, forms a product B in a chemical reactor. The reactor outlet is separated in a separation unit, and a fraction α of the unreacted reactant, A, is recycled back to the reactor. Now, imagine that we increase the feed flow rate. This will normally increase the amount of unreacted component A from the separation unit, and hence the amount of A recycled. This is then an example of a *positive feedback mechanism*, and one would normally expect that one of the plant poles will be shifted towards the origin as the fraction A recycled is increased. With total recycle of A, and a feed flow rate slightly higher than the maximum capacity of the reactor, component A will accumulate in the system, which is equivalent to the system having a pole close to the origin. However, other dynamic behavior than slow responses are possible, such systems may be unstable or exhibit limit cycle behavior (see e.g. Eigenberger, 1985).

Feedback from heat integration. For the heat exchanger network shown in Fig 3 (Mathiesen and

Skogestad, -92), consider the effect of temperature disturbances in the hot stream (H1) on the outlet temperature y_1 . As can be seen, heat exchangers 1a and 1b form a positive feedback loop. This will therefore lead to a higher sensitivity and a slower response than if the heat exchangers were independent coolers working at the same steady state.

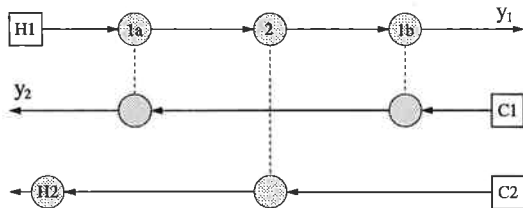


Figure 3: Heat exchanger network with energy recycle (positive feedback)

5 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 a heat exchanger or a reactor normally leads to an increase in outlet temperatures. For example, as shown by Mathiesen (1994) 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 instant 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.

A reactor example. An other example where a loop yields negative feedback is the system shown in figure 4. Feed is preheated with the product, further heated in a second heater, and sent through two reactors. In the first reactor, a reaction with negligible heat of reaction $A \rightarrow B$ takes place (i.e. $T_3 = T_2$). The reaction rate, r , is assumed to be $r = k_0 e^{-\frac{E}{R}(\frac{1}{T_2} - \frac{1}{T_0})}$. Here k_0 , E and R are the rate constant, activation energy and the gas constant respectively. 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):

$$T_4 - T_2 = -\Delta T_0 e^{-\frac{E}{R}(\frac{1}{T_2} - \frac{1}{T_0})} \quad (3)$$

with some proportionality constant, $-\Delta T_0$, which is seen to be equal to the temperature drop when $T_2 = T_0$, the reference temperature. Consider an increase in T_2 , the inlet temperature of the first reactor. With a proper choice of numerical values, the outlet temperature of the second reactor, T_4 , will decrease, that is

$$\frac{dT_4}{dT_2} = 1 - \frac{E\Delta T_0}{RT_2^2} e^{-\frac{E}{R}(\frac{1}{T_2} - \frac{1}{T_0})} < 0 \quad (4)$$

A specific numerical example is $E=60$ kJ/mol, $R=8.31$ J/mol.K, $T_0=T_2=782$ K, $T_4=626$ K, $\Delta T_0=156$ K). This is then an example of a *negative feedback effect*. Negative feedback will usually have a stabilizing effect on the system, but may cause instability if the loop gain is large enough.

6 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 temperatures and flows, and destabilize a plant. Take for example the reactor example analyzed in the previous section (Fig 4), and assume that the feed is liquid which is partially evaporized 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. 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 (1985).

7 Parallel paths in plants

While the effect of feedback is to shift the plant poles, parallel paths in plants affect the plant zeros. Of most concern are zeros in the complex *right half plane*, as these make the phase of the plant transfer function drop, while increasing the gain. If parts of

the plant containing right half plane zeros are contained in a feedback loop, instability or oscillatory plant behavior becomes very likely, as discussed in section 1.

The most obvious examples of parallel paths occur when there are processing units in parallel, e.g. two reactors in parallel, or e.g. in heat exchanger networks when there are several downstream paths from one unit to another, as in the heat exchanger network shown in Fig 5. A disturbance in the hot stream H2 affect the outlet of cold stream 2 by two paths: through exchangers 3-1-2 and directly through exchanger 4 (Mathiesen and Skogestad, -92). There are also cases where one variable in the plant affect another through different effects through the same units. E.g., in an adiabatic fixed bed where an exothermic reaction is taken place, decreasing the inlet temperature to the bed will affect the temperature near the outlet by two mechanisms: through changes in the concentration of reactant in the bed, and through the migration of temperature waves in the bed. Typically, the concentration waves are travelling much faster than the temperature waves due to high heat capacity of the catalyst. Moreover, the two effects will typically have an opposite effect on the temperature at the bed outlet, such that when the inlet temperature decreases, the outlet temperature will initially increase, then decrease. Such *inverse response characteristics* are typical of *right half plane zeros*. If the heat from the reactor bed is recycled, e.g. if the reactor feed is preheated with the reactor effluent, limit cycle behavior or runaway become possible under certain operating conditions. References to several such examples are given by Eigenberger (1985).

8 Effects on plant control

Consider a system with recycle, as shown schematically in Fig 6, where a fraction α 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, α , may typically look something like the plot illustrated in Fig 5. For high values of the fraction recycled, α , 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,

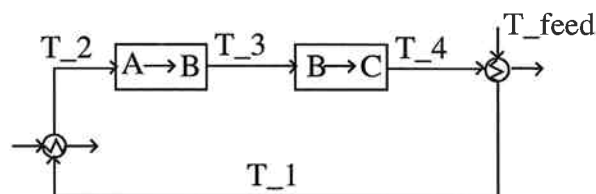


Figure 4: Endothermic reaction system with energy recycle (negative feedback)

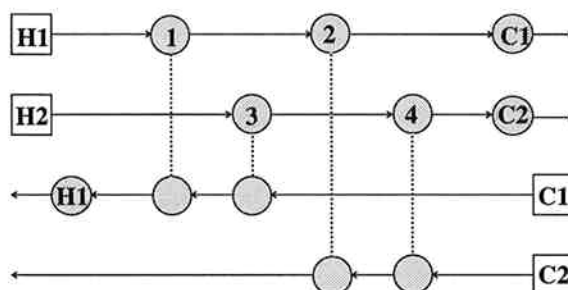


Figure 5: Heat exchanger network with parallel downstream paths (from inlet temperature of stream H2 to outlet temperature of stream C2)

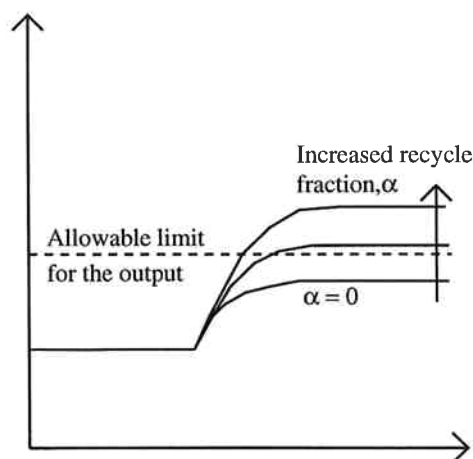


Figure 6: Response in output to step disturbance

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.

9 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. Typically, 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.

REFERENCES

- Aris, R. and Amundson, N.R. (1958). An analysis of chemical reactor stability and control. *Ch.Eng.Sci.*, vol 7, no 3, pp 121-155.
- Denn, M.M. and Lavie, R. (1982). Dynamics of Plants with Recycle. *The Chem. Eng. J.*, 24, pp 55-59.
- Eigenberger, G. (1985). Dynamics and stability of chemical engineering processes. *Int. Chem. Eng.*, vol 25, no. 4, pp 595-610
- Gilliland, E.R., Gould, L.A. and Boyle, T.J. (1964). Dynamic effects of material recycle. Preprints JACC, Stanford, California pp 140-146.

- Gray, P. and Scott, S.K. (1990). *Chemical Oscillations and Instabilities. Nonlinear Chemical Kinetics.* Clarendon Press, Oxford, ISBN 0198556462
- Jacobsen, E.W. and Skogestad, S. (1991). Multiple Steady States in Ideal Two Product Distillation. *AIChE Journal*, vol 37, No. 4., pp 499-511.
- Jacobsen, E.W. (1994). Dynamics of systems with input multiplicity with binary distillation as an example, Lecture at Chem. Eng. Dept, NTH, Trondheim, March 11, 1994.
- Kapoor, N., McAvoy, T.J, Marlin, T.E. (1986). Effect of Recycle Structure on Distillation Tower Time Constants. *AIChE J.* vol. 32, no. 3, pp 411-418
- Luyben, W.L. (1992) Dynamics and Control of Recycle Systems. Part 2 - Comparison of Alternative Process Designs. Paper submitted to IEC Research.
- Mathiesen, K. W., and Skogestad, S. Design, Operation and Control of Resilient Heat Exchanger Networks. *AIChE Annual Meeting*, Miami Beach, Nov 1-6, 1992, Session: Design and Control.
- Mathiesen, K. W. (1994). Integrated Design and Control of Heat Exchanger Networks. PhD thesis, University of Trondheim, NTH, Norway, 1994
- Morud, J.C. and Skogestad, S. (1993). The Dynamics of Chemical Reactors with Heat Integration. Paper 26e at *AIChE Annual meeting*, St. Louis, USA, Nov. 8-12, 1993.
- Morud, J.C. and Skogestad, S. (1994). Effects of Recycle on Dynamics and Control of Chemical Processing Plants. *Computers and Chemical Engng* 18, Suppl S529-S534
- Papadourakis, A., Doherty, M.F. and Douglas, J.M. (1989). Approximate Dynamic Models for Chemical Process Systems. *Ind. Eng. Chem. Res.* 28, No. 5, 546-552
- Papadourakis, A., Doherty, M.F. and Douglas, J.M. (1987). Relative Gain Array for Units in Plants with Recycle. *Ind. Eng. Chem. Res.*, Vol 26, 1259-1262.
- Pareja, G. and Reilly, M.J. (1969). Dynamic Effects of Recycle Elements in Tubular Reactor Systems. *IEC Fund.* 8, 442.
- Uppal, A., Ray, W.H. and Poore, A.B (1974). On the dynamic behavior of continuous stirred tank reactors. *Ch.Eng.Sci.* vol 29, pp 967-985
- Uppal, A., Ray, W.H. and Poore, A.B. (1976). The classification of the dynamic behavior of continuous stirred tank reactors-Influence of reactor residence time. *Ch.Eng.Sci.* vol 31, pp 205-214.
- van Heerden, C. (1953). Autothermic Processes. Properties and Reactor design. *Industr. Engng. Chem. (Industr.)*, 45, 1242
- Verykios, X.E. and Luyben, W.L. (1978). Steady-state Sensitivity and Dynamics of a Reactor/Distillation Column System with Recycle. *ISA Transactions*, vol 17, no. 2. pp 31-41.