STABILITY AND DYNAMIC OPERABILITY ANALYSIS OF CHEMICAL PROCESSES

A thesis submitted for the degree of

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by

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Dedicated to my parents

CONTENTS

ABSTRACT

A number of well known techniques have been studied to investigate their use as simple tools for assesing the operability characteristics of nonlinear system.

Stability criteria for nonlinear systems are discussed and the second method of Lyapunov is applied to a CSTR and a Heat Exchanger system. Distributed systems, such as heat exchangers are dealt with by the application of discontinuous physical models. It has been shown that it is possible to obtain the stability regions for a CSTR and a heat exchanger provided a suitable Lyapunov function is constructed.

The operability analysis of a CSTR and a heat exchanger is carried out by making use of singular value analysis techniques. The dynamic characteristics of the system are investigated for the model linearised at several steady states over a range of frequencies for different operating conditions. The condition numbers of both unscaled and optimally scaled transfer function matrices of a CSTR and a heat exchanger have also been evaluated and applied in the analysis.

The condition numbers evaluated in a CSTR case show that high temperature and conversion are the optimum operating regions but it may not be feasible to operate the reactor in those regions because the system is much more difficult to control. In heat

exchanger analysis, the optimal scaling method reduces the condition numbers to very small values even in the case of high fouling, suggesting that fouling in heat exchangers does not seem to affect controllability significantly.

The condition numbers of unscaled state space matrices of both the systems are also obtained and it has been shown that the condition number of the scaled state space matrix is not a reliable measure of controllability. It masks potential problems with nonlinearities, and although it is scale dependent, scaling policies can remove important information from the analysis.

Dynamic simulation of both the systems is carried out by making use of the SpeedUp simulation package to verify the results obtained in dynamic operability analysis. It is hoped that the results of the present work may be of some value to practical situations in industry, particularly in the case of the systems having nonlinear behaviour.

DECLARATION

To the best of my knowledge, all the material presented in this thesis is original except where stated otherwise.

None of this material presented here has been previously accepted for the award of any other degree or diploma in any other University.

The author does not have any objection to the thesis being made available for photocopying and loan.

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CHAPTER 1

INTRODUCTION

"I keep six honest serving men
(They taught me all I know);
Their names are What and Why and When
And How and Where and Who."

Kipling, The Elephants' Child

Chemical processes are nonlinear in their behaviour at least over portions of their operational range so that linear methods of analysis are somewhat restrictive. Therefore the consideration of nonlinearities in the process is essential to understand its performance. A number of approaches have been proposed for assuring process operability but none consider nonlinearities explicitly. This thesis looks at how some of these methods may be extended to cover nonlinear systems.

Systems with nonlinear behaviour can exhibit stability problems and the stability analysis of these systems can be carried out by the help of Lyapunov's second method. This method can be utilized for certain naturally occurring systems of nonlinear simultaneous differential equations. The equations arise when there is a flow of some physical quantity such as heat, liquid flow, diffusion and chemical reaction. When these equations obey nonlinear conditions, their stability may not always be self evident, and it can be investigated by the use of Lyapunov method. This method provides information on the stability of a system by transforming the differential equations to a form from which one can see directly, that is without integrating the system equations, whether its trajectory approaches the state of rest or not. However, construction of Lyapunov function for a particular process system still remains a difficult task. The lack of a generally applicable guide to the construction of Lyapunov functions is the biggest drawback to the method's use. There have been attempts to generate successively general forms of Lyapunov functions by *Warden et al. (1964), Gurel and Lapidus (1965), Chen and Kinnen (1970), and Davison and Kurak (1970).* These approaches have not received a great deal of use. Numerous methods have been proposed in the literature to derive suitable Lyapunov functions to study the stability of nonlinear systems.

Once the stability criteria of these systems are established, then they are subjected to dynamic operability analysis. Dynamic operability of a process refers to the ability of the plant to perform satisfactorily under conditions different from the nominal design conditions. The plant should be able to make the transition from operating conditions to stand-by or shutdown conditions without violating its environmental or safety constraints. Dynamic operability assessment can be made by making use of singular value analysis techniques. The singular values depend only on the process design and are independent of the particular controller used. They are easy to compute and utilize as a dynamic operability measure. By analysing the singular values of the system matrix or of the transfer function matrix, its condition number (the ratio of maximum to minimum singular values) can be evaluated which can be used as a measure of sensitivity of control performance to modelling error and as such is a measure of controllability *(Morari, 1983).*

Since the condition number is a measure of sensitivity of the system, therefore, it is desirable that this number should be small. The smaller the condition number, the more it will tolerate a larger uncertainty before going unstable.

Since the singular values depend on the scaling of the system, ie; the physical dimensions which are used in defining the variables and the equations, a method of optimum scaling is suggested by *Perkins and Wong (1985).* The method entails comparing transfer function matrices only on the basis of the optimal condition number in the maximum norm as defined by *Bauer (1963)* which is an upper bound on the optimal condition number in the 2-norm.

Operability analyses have been developed to avoid extensive use of dynamic simulation. A multipurpose simulation programme was developed *(Perkins, 1981)* which performs steady state and dynamic simulation with the same set of models. It is used in this thesis to evaluate results predicted by the operability analysis.

In Chapter 2, stability criteria for nonlinear systems are discussed and the second method of Lyapunov is described in detail. A standard form of Lyapunov function due to Krasovskii has been utilized and applied to a CSTR and a heat exchanger system and the stability regions of these systems are examined. Mathematical and geometrical interpretations of the method are also given. A literature survey is also provided including the recent developments in the construction of Lyapunov functions.

Chapter 3 deals with an overview of dynamic operability analysis. It provides an insight into the methodology developed for operability analysis. This chapter highlights the significance of the condition number which quantifies the sensitivity of the system with respect to uncertainties in the model. Mathematical interpretations of singular values and process control properties provided by them have also been described. Since singular values are scale dependent, a method of scaling the system matrix is also provided. The optimal scaling method suggested by *Perkins and Wong (1985)* has been utilised.

The dynamic operability concepts presented in Chapter 3 are applied to a CSTR system in Chapter 4. As the CSTR system is nonlinear, the dynamic characteristics of the system are investigated for the model linearised at several steady states over a range of frequencies for different operating conditions. The control potential of the system is established by analysing the singular values of the steady state system matrix and extending it to include the dynamics of the system. The condition numbers of both unscaled and optimally scaled transfer function matrices of the CSTR at different operating conditions were evaluated for the analysis. Also the condition numbers of unscaled state space system matrix were evaluated. All these numbers obtained were plotted on a log-log plot in function of frequency to assess the controllability of the system.

In Chapter 5, dynamic operability and sensitivity analyses are carried out on heat exchangers undergoing fouling. The analysis is performed at three different stages, when the exchanger is clean, with moderate fouling and with high fouling.

Chapter 6 deals with the dynamic simulation of a CSTR and heat exchangers undergoing fouling. Simulation work is carried out using the SpeedUp programme. The main idea of using the simulation was to see whether the results obtained during the simulations are in agreement with the dynamic operability analysis carried out in Chapters 4 and 5.

Finally, Chapter 7 gives general conclusions on the overall work in the thesis and some suggestions for future investigations.

CHAPTER 2

STABILITY OF NONLINEAR SYSTEMS

"All these tidal gatherings, growth and decay,
Shining and darkening, are forever
Renewed; and the whole cycle impenitently
Revolves, and and all the past is future:-
Makes it a difficult world... for practical people."
Robinson Jeffers, Practical People

In this Chapter, stability criteria for nonlinear systems are discussed and the well known second method of Lyapunov is described in detail. Geometrical interpretations of the Lyapunov function are also given. However, detailed analysis may be found in literature discussed by *Berger and Perlmutter (1964), Luecke and McGuire (1965) and Berger and Lapidus (1969).*

A literature survey is also provided and recent advancements in construction of Lyapunov functions have been highlighted.

The Lyapunov method is applied to a CSTR and a Heat Exchanger system and the stability regions of these systems are examined. Mathematical results are also obtained for these systems. Distributed systems, such as heat exchanger, give rise to partial differential equations; these systems are dealt with by the application of discretized physical models.

2.1 Introduction

In practical applications most control systems are non-linear to some extent, at least over portions of their operational range, so that linear methods of analysis are at best an approximation and many at worst produce results that are positively misleading. Linear methods are normally used, of course, because they can usually be expected to provide a good first estimate of behaviour, because they are much more fully developed than non-linear methods and because they are in general very much simpler in application. However, even quite simple practical control systems are apt to be inherently so nonlinear that a linear analysis cannot be used at all, and it is appreciated today that the introduction even of simple non-linearities (Ex: fouling) may improve the performance of a system beyond that attainable with the most sophisticated linear synthesis *(Macmillan, 1962)*.

General methods for the design of nonlinear systems are not available but a number of methods based on approximate solutions have been developed. Of particular mention are the following methods of design:

- The Phase-Plane Method
- Piecewise Linear Methods
- The Describing Function Technique
- Lyapunov Stability Analysis

The last of these techniques is the only one to have been used to any extent by Chemical Engineers. It is a geometrical tool and a number of simple geometrical methods have been proposed to assure stability. The work described in this thesis only uses Lyapunov's second method.

2.2 Stability in the Sense of Lyapunov

One of the most important events in the theory of stability of dynamic systems was the publication in 1892 of Lyapunov's famous paper in a Russian journal. Translated into French in 1907, its application for control problems was not discovered until 1944; this was because the difficulties in studies of stability of nonlinear control problems were not understood and the work of *Lur'e (1951)* and *Letov (1955)* on this subject prepared the ground for systematic studies of these questions.

Developments in the west in the analysis of nonlinear systems occurred much later and were much less fruitful than Lyapunov's method *(Minorsky, 1962)*. In these works the nonlinear problem is usually considered to be almost linear or a problem of searching for approximate solutions of some form. The unifying concept of qualitative theory did not reach western control literature until the important paper of *Bertram and Kalman (1960)* was published. In the short time since the publication of these papers, a phenomenal interest has developed in the west in Lyapunov's method which is also known as the second or direct method.

The theory of stability was advanced by *V. M. Popov (1960)*, who showed that certain concepts of linear theory (such as the so-called frequency characteristics) can also be used in nonlinear theory under certain conditions which are frequently encountered in applications. The most interesting feature of his discovery is the fact that this new concept of stability is closely related to Lyapunov's second method. This was the situation towards the end of 1963. A review of developments with Lyapunov's method is given by Gurel and Lapidus (1969). The same authors (1968) review applications to chemical systems.

2.3 Lyapunov's Direct Method

The fundamental idea of Lyapunov's second method is as follows: instead of attacking the problem of stability on the basis of the variational equations, one tries to transform the differential equations to a form from which one can see directly (that is, without integration) whether its trajectory approaches the state of rest (the trivial solution) or not. If one succeeds in showing that the trajectories enter a certain region Ω surrounding the position of equilibrium and never leave it, one can assert that the equilibrium position (i.e. the unperturbed solution) is stable. If, moreover, one can show that the trajectory approaches the position of equilibrium for $t \to \infty$, the unperturbed solution is asymptotically stable.

The underlying idea of Lyapunov's second method is an obvious, and simple fact. If the initial motion is small and the subsequent motion is also small, the system is stable; if for small initial conditions the later motion is not small, the motion is unstable *(Berger and Perlmutter, 1964).*

2.4 Mathematical Interpretations

Lyapunov's direct method is extensively discussed in the applied mathematical literature by *LaSalle and Lefschetz (1961), Hahn (1963)* and *Letov (1962).* Briefly stated this method entails defining a positive definite function, the Lyapunov function, and it is the sign definiteness of the total time derivative of the Lyapunov function which determines the stability of a system.

Consider an autonomous system represented by the equation

$$\dot{x}_i = f_i(x_1, x_2, \ldots x_n) \qquad i = 1,2,\ldots n \tag{2.1}$$

where the origin is one of the equilibrium states

$$f_i(0) = 0 \qquad i = 1,2,\ldots n \tag{2.2}$$

The search for stability properties of the solution $x_i(x_{10}, x_{20} \ldots x_{n0}, t_0, t)$ is reduced to the search for a scalar function, $V(x_1, x_2, \ldots, x_n) > 0$, with the following properties

1. Outside the origin: $V(x_1, x_2, \ldots, x_n) > 0$
2. $V(0) = 0$
3. $V(x_1, x_2, \ldots, x_n)$ is continuous and has continuous first partial derivatives in an open region Ω about the origin (LaSalle and Lefschetz, 1961).
4. $\dot{V} = f_1 \partial V/\partial x_1 + f_2 \partial V/\partial x_2 + \ldots f_n \partial V/\partial x_n \leq 0 \in \Omega$

A function with the properties given above is a Lyapunov function. If such a function exists, the system is "stable in the sense of Lyapunov." If condition 4 is modified as follows

- $\dot{V} < 0 \in \Omega$ outside the origin.
- $V(0) = 0$

then the stability is asymptotic. The existence of a Lyapunov function is a sufficient condition for stability. Lyapunov's direct method involves a search for such a function.

In some applications, the region, may not include the entire region of interest. It is then very useful to determine the extent of asymptotic stability by giving an independent proof that all solutions remain in the region Ω.

Properties 1 and 2 require that the Lyapunov function be positive definite except when the state is at the origin. Property 2 indicates that V is in some rough sense a measure of the distance from the origin. The stability conditions state that V is decreasing toward zero or at worst not increasing with time.

There are two properties which are extremely important to note. Since there is no definite method available to construct a Lyapunov function representing a particular process, therefore, there can be no limit to the number of potential Lyapunov functions which can be considered. However, it is sufficient to have just one to ensure stability. The second point is closely related. It is that the existence of a Lyapunov function guarantees stability. But if none of the following conditions are satisfied by the function

$$\dot{V} \leq 0 \qquad x \neq 0$$

$$\dot{V} < 0 \qquad x \neq 0$$

then it does not say that the system is unstable; it simply says that the function under consideration is not a Lyapunov function. The search must continue for other candidates.

2.5 Construction of Lyapunov Function

The lack of a generally applicable guide to the construction of Lyapunov functions is the biggest drawback to the method's use. There have been attempts to generate successively general forms of Lyapunov functions by *Warden et al. (1964), Gurel and Lapidus (1965), Chen and Kinnen (1970), and Davison and Kurak (1970).* These approaches have not received a great deal of use. Numerous methods have been proposed in the literature to derive suitable Lyapunov functions to study the stability of nonlinear systems. These methods are written briefly as

- The method of canonical variables *(Lur'e 1951, Lur'e and Rozenvasser 1960, Letov 1955, 1962).*
- The method of squaring *(Krasovskii 1954).*
- The method of analogy with linear systems *(Malkin 1952, Barbasin 1960).*
- The method of separation of variables *(Barbasin 1960, 1961, Chin 1967).*
- The method of Zubov *(Zubov 1964).*
- The method of integration *(Ingwerson 1961, Ponzo 1965, Brockett 1966, Puri 1966, Huaux 1967).*
- The variable gradients method *(Schultz and Gibson 1962, 1963).*
- The method of Szego *(Szego 1962).*
- The initiating function method *(Mukherjee et al. 1972).*
- The Lagrange-Charpit method *(Miyagi and Taniguchi 1980).*
- The method of system energy *(Marino and Nicosia 1983).*
- The integral method *(Chin 1986).*
- Other methods *(Ku and Puri 1963, Kalman and Bertram 1960, Skidmore 1966).*

All these methods listed above are applied to derive suitable Lyapunov functions for several nonlinear problems related to electrical or mechanical engineering problems.

Some authors have tried to apply these methods in chemical engineering literature as well.

2.6 Krasovskii Forms

One standard form of Lyapunov function which has received wide use is that due to *Krasovskii (1963)*. In the chemical engineering literature it was applied to extraction units by *Koepcke and Lapidus (1961)* and to the CSTR by many other authors. Among the most useful applications are the works by *Leathrum et al. (1964), Berger and Perlmutter (1964), Luecke and McGuire (1965), Paradis and Perlmutter (1966), Stevens and Wanninger (1966), Berger and Lapidus (1968). Berger and Lapidus (1969)* have also considered the use of the Krasovskii form on the tubular reactor modeled by a series of continuous stirred tank reactors. In general the results of all these analyses have been rather conservative. The predicted stable range has been quite small as compared to the actual nonlinear system behaviour.

The basic features of Krasovskii's theorem can be outlined in a simple fashion if the nonlinear systems of equations can be represented in the form of equations 2.1 and 2.2 Then these will be subject to a theorem due to *Krasovskii (1954):*

> Let f have continuous first partial derivatives and its Jacobian matrix be given by $F(x) = \partial f_i / \partial x_j$. If $F'(x)$ is defined as
>
> $$F'(x) = F(x) + F^T(x) \tag{2.3}$$

and $F'(x)$ is negative definite, then the steady state $x_s = 0$ of the system is asymptotically stable in the large, and

$$V(x) = ||f(x)||^2 \tag{2.4}$$

is a Lyapunov function for the system.

In the course of proving this theorem *Kalman and Bertram (1960)* have shown that the sign of the derivative of V(x) depends on the sign definiteness of the matrix $F'(x)$. If the matrix $F'(x)$ is negative definite, then the scalar derivative of V(x) will be negative.

Another interesting feature of Krasovskii's method is that it proposes a Lyapunov function which describes closed surfaces *(Letov 1962)* in the n-dimensional space of the state variables. The proposed Lyapunov function is of the following form *(Hahn 1963)*

$$V(x) = f^T A f \tag{2.5}$$

where A is a constant positive symmetric matrix. Thus V(x) is a positive definite quadratic form in the derivatives of the state variables.

There are several important features concerning the above form of Lyapunov function. First, in chemical reactor stability studies where multiple equilibria states occur the region of asymptotic stability (RAS) is bounded and not global. The Lyapunov function defined by equation (2.5) permits determination of the bounded RAS because within the bounded region the derivative of V(x) must be negative definite and outside this region it may be positive definite. The bounded region is defined by the surface V(x) equal to a constant and these surfaces, V(x)= K, are closed in n-space. Another fortunate feature is that the closed surfaces, V(x)= K, are nested surfaces, and as the constant K of the surface increases the distance of the surface from the origin uniformly increases.

The quadratic forms of the function discussed above, used by Lyapunov and Krasovskii made the Lyapunov function a measure of the distance from the origin. An alternative norm of the state space was used by Rosenbrock (1963).

$$V = \sum_{j=1}^{N} | f_j | \tag{2.6}$$

where V is somewhat analogous to the Krasovskii norm with A=I. Equation (2.6) satisfies the conditions of a Lyapunov function for certain nonlinear systems.

2.7 Applications

The Lyapunov function can be used for certain naturally occurring systems of nonlinear simultaneous differential equations. The equations arise when there is a flow of some physical quantity such as heat, liquid flow, diffusion and chemical reaction. When these systems obey nonlinear equations their stability may not always be self evident, and it can be investigated by the use of Lyapunov function. Lyapunov's direct method is used to examine the stability of a chemical reactor and heat exchanger in this section.

2.7-1 CSTR

The need to determine a finite region of asymptotic stability (RAS) for nonlinear systems arises, for example, in the case of an exothermic reaction taking place within a CSTR. An exothermic type reactor operating at some steady state is subject to a number of disturbances which cause this condition to change. If following such a disturbance the reactor variables (temperature and concentration, for example) remain within some bounded range, the system is called "stable". If in addition the system approaches its steady state condition with increasing time, it is termed asymptotically stable. If on the other hand the system behaves such that a given disturbance produces a runaway (unbounded) response, it is called "unstable" with respect to that disturbance. The stability of a given reactor is in general dependent on its initial condition, on the form and magnitude of the disturbances and also on the inherent physics and chemistry of the system under study. Furthermore, these concepts can be extended to develop definitions for stability over larger regions. If a system's steady state is stable for inputs of any magnitude, that is if trajectories from any initial condition converge on a steady state, the system is called "globally asymptotically stable". In many cases of practical interest this behaviour can only be demonstrated for a restricted set of initial conditions. The system is then said to be asymptotically stable in a bounded region.

However, in addition to these definitions it is important to establish the stability limits of a region around each stable point such that one may predict the result of a finite perturbation. One way to approach this problem is to consider the direct solution or integration of the nonlinear system equations. However, this becomes more and more difficult as the number of variables increases. The numerical or linearized approach is limited in one important aspect: that the result can only provide information on local stability. For practical design a guarantee that a particular steady state is locally stable is not as useful as quantitative information showing stability over at least a region of interest because from local stability alone it is not possible to establish whether a small disturbance can produce instability. In this CSTR system, nonlinear kinetics are retained by using a Lyapunov function and equations are transformed in a suitable form in order to analyse the system by Krasovskii's theorem.

2.7-1.1 The System Equations

A well stirred tank reactor is considered in which a homogeneous reaction is taking place. The system is exothermic, and heat transfer takes place at the walls of the vessel. This system was discussed by *Berger and Perlmutter (1964)*, and has been selected to elaborate the application of a Lyapunov function and to provide a geometrical interpretation of the method. The equations representing the heat and material balance are

$$\rho V C_p \frac{dT}{dt} = \Delta H V r - U A_r (T - T_A) - \rho q C_p (T - T_0) \tag{2.7}$$

$$V \frac{dc}{dt} = -Vr - q(c - c_0) \tag{2.8}$$

where T and c are the state variables of the system.

These equations were transformed into a suitable form for further analysis by Krasovskii's theorem. Firstly, these equations were normalized and then transformed to form a system of equations in which the steady state has the vector coordinate equal to zero. The transformation equations are given in *Berger and Perlmutter (1964)*

Equations (2.7) and (2.8) after subsequent analysis reduce to

$$\frac{d\eta'}{dt} = \frac{r'}{c_0} - \frac{b}{a}\eta' \tag{2.9}$$

$$\frac{dy'}{dt} = -\frac{r'}{c_0} - \frac{1}{\tau}y' \tag{2.10}$$

where $r' = r - r_s$, $\eta' = \eta - \eta_s$ and $y' = y - y_s$ are the specific perturbations from the steady state point.

where η and y are the normalized temperature and concentration respectively.

Equations (2.9) and (2.10) combined with equation (2.4), give a Lyapunov function of the form

$$V(\eta', y') = \left(\frac{r'}{c_0} - \frac{b}{a}\eta'\right)^2 + \left(\frac{r'}{c_0} + \frac{1}{\tau}y'\right)^2 \tag{2.11}$$

In this set of equations the only nonlinear term is r which is a rate equation given by

$$r = Ae^{-Q/T}c^n \tag{2.12}$$

Also the rate term in the equations is considered as an implicit function of concentration and temperature, $r = r(T, c) = r(\eta', y')$.

Equations (2.9) and (2.10) can easily be treated with Krasovskii's theorem. Reducing these equations with Krasovskii's theorem the results may be further simplified using

Sylvester's inequalities *(Hohn, 1958)*. Sylvester's inequalities reduce equations (9) and (10) so that the elements of the system matrix of state variables must satisfy the following inequalities:

$$b - (\Delta HVQr/T^2) > 0 \qquad (2.13)$$

$$\frac{4}{a\tau}\left(b - \Delta HV\frac{Q}{T^2}r\right) + \frac{4bnr}{ac} > \left(\frac{\Delta HV}{a}\frac{Q}{T^2}r + \frac{nr}{c}\right)^2 \qquad (2.14)$$

Equations (2.13) and (2.14) together with equation (2.12) define two curves in the temperature - concentration plane. If these equations are combined with the Lyapunov function given by equation (2.11), they are sufficient to fix the RAS about an arbitrary steady state.

2.7-1.2 Geometrical Interpretations

In order to give a better understanding of the ideas explained above, a geometrical interpretation of the Lyapunov function has been given in the figure 2.1. The plot in the temperature and concentration plane explains the mathematical developments discussed above.

Equations (2.13) and (2.14) determine the two curves 1 and 2 respectively as shown in the T, c plane of figure 2.1. For a hypothetical Lyapunov function V=K, contours are drawn. Increasing the value of K, would increase the value of V, resulting in a larger area covered by a contour in the T, c plane. Inequalities (2.13) and (2.14) are satisfied under the curves 1 and 2, and above those curves they are contradicted. At any point in

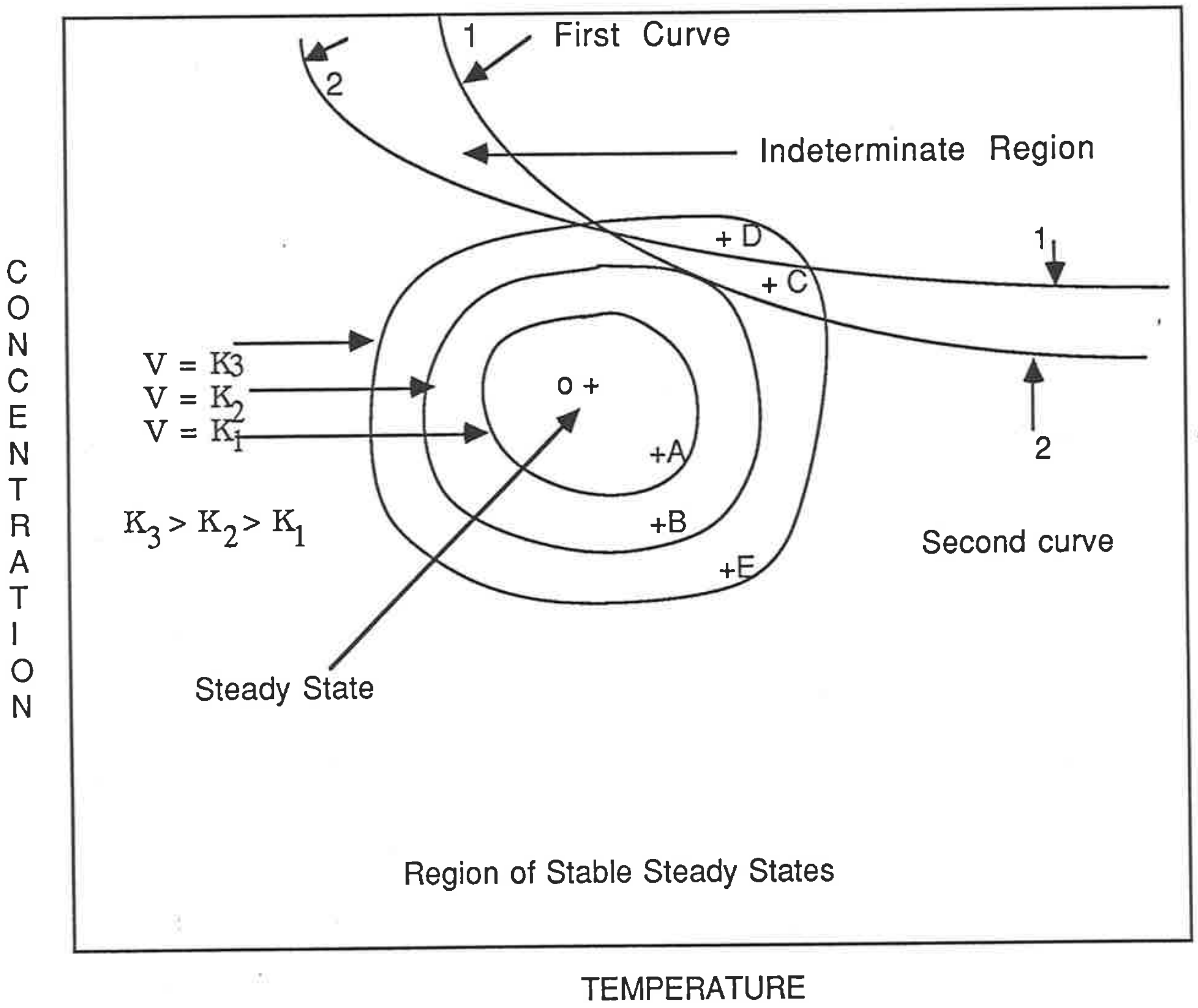


Figure 2.1 Stability Regions in the T - c Plane

the region of the plane which lies below both lines $\dot{V}(x)$ will be negative. Therefore any region which is below the curves and within a contour satisfies all the requirements of the LaSalle and Lefschetz theorem (1961) and is a region of asymptotic stability.

Depending on the values of K, the stability regions for a particular Lyapunov function shown in fig. 2.1 could be larger. The larger the value of K satisfying the condition of Lyapunov function, the less conservative will be the prediction of the stability region.

Figure 2.1 shows that the curve $V = K_1$ gives an RAS which includes point A. It shows that a disturbance to this point will ultimately vanish, and the system will return to its steady state. The curve $V = K_2$ shows that the same idea is valid for the point B. Also the area shown by the contour $V=K_2$ is the largest possible RAS for the particular Lyapunov function. If for example, $V=K_3$ is considered, then the contour encloses areas in the plane for which $\dot{V}$ is indeterminate in sign. Points C and D, for example, are in a region of indeterminate behaviour as regards this Lyapunov function. The behaviour of the trajectory from point E is also indeterminate. Although E is in the region of locally stable states, it cannot be included in the RAS. It might be of interest to find another Lyapunov function for which an RAS includes points which are in the indeterminate region.

2.7-1.3 Results and Discussions

The numerical example given by *Berger and Perlmutter (1964)* has been considered for the analysis with a view to obtaining the largest RAS for the given Lyapunov function. Numerical data may be found in Appendix A. The method entails determining the $\dot{V}(x) = 0$ curve and placing it on the T, c plane. For this purpose the Lyapunov function

STABILITY ANALYSIS OF A CSTR

BY THE METHOD OF LYAPUNOV

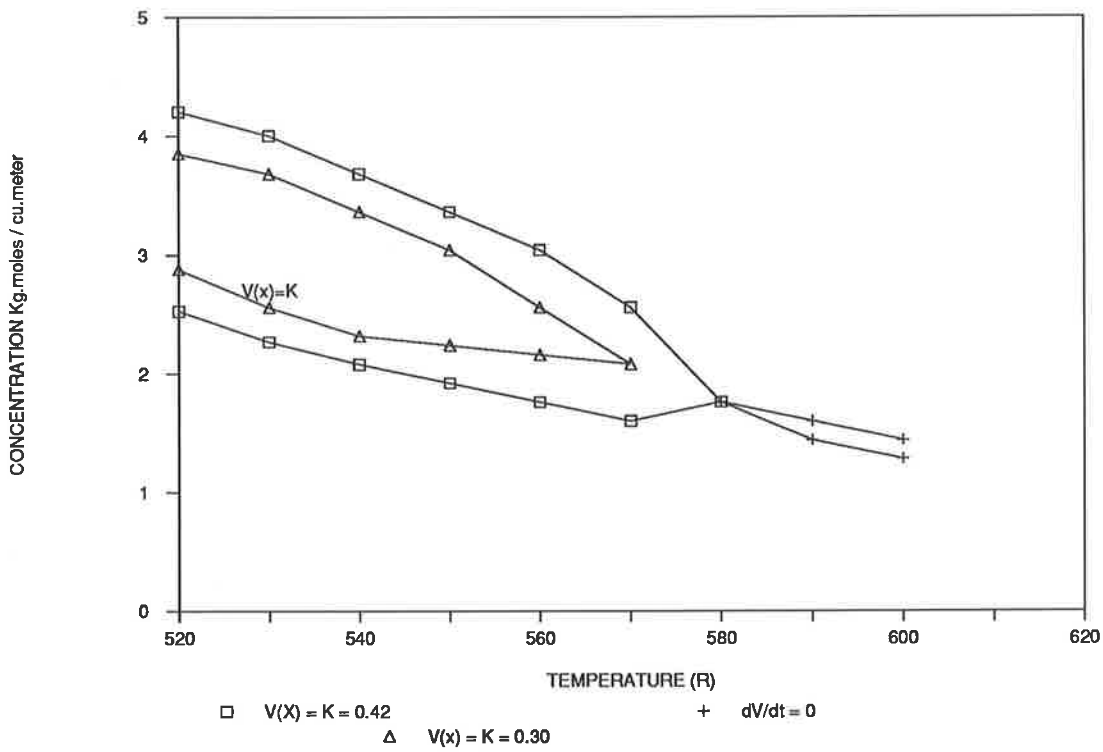


Figure 2.2 Region of Largest Asymptotic Stability of a CSTR

V given by equation (2.11) was differentiated with respect to time and the values of the variables were put in the derivative form of Lyapunov function. Then beginning at a very small value of the Lyapunov constant K the closed curves of V(x)=K were also put on the plot. The constant K is increased until the closed Lyapunov curve just touches the curve $\dot{V}(x)=0$, determining the largest RAS. Therefore, within the closed curve V(x) = K, $\dot{V}(x)<0$. On the closed curve $\dot{V}(x)=0$ at only one point, and it will be less than zero at all other points. Figure 2.2 shows that for a Lyapunov function K=0.42, the largest region of asymptotic stability is obtained since the curve $\dot{V}(x)=0$ intersects the closed curve. However, for K=0.30 the closed surface obtained does not intersect the curve $\dot{V}(x)=0$ which means that everywhere upon the closed surface the value of $\dot{V}(x)$ will be less than zero.

Table 2.1 gives the stability range for disturbances in temperature and concentration. It is apparent from this table that the Lyapunov function K=0.42 yields the largest RAS where the system will exhibit asymptotic stability for disturbances in temperature as great as $\pm 30°R$ and in composition as large as ± 1.44 Kg.moles/cu.meter.

Table 2.1 Stability Range for Disturbances in Temperature and Concentration

Lyapunov Function $V(x)=K$	Steady state Temp. $°R$	Disturbance in Temp. $°R$	Disturbance in Conc. $Kg.moles/m^3$
0.30	550	± 20	± 0.80
0.42	550	± 30	± 1.44

2.7-2 Heat Exchanger

Lyapunov's second method is applied to a shell and tube heat exchanger with condensation of vapours on the shell side. For this situation, we always expect to have a nonlinear heat release curve. The system of heat exchangers is usually considered to be continuous and its behaviour is expressed by partial differential equations. However in order to apply the second method of Lyapunov, the continuous system is divided into small elements within which conditions can be considered uniform.

Figure 2.3 shows the heat exchanger system. The exchanger has been divided into n sections where the rth element occupies the length between sections at s and $s+\delta s$. Two streams of liquid are flowing through the exchanger with constant flow rates. Within each element conditions are assumed uniform. In the rth element, masses H_r and H'_r with temperatures θ_r and θ'_r exchange heat at the rate W_r per unit time. W_r is considered to be some function of θ_r and θ'_r.

A lumped model of a heat exchanger given by Rosenbrock (1962) is considered which gives the following energy balance equations around the rth section:

$$\frac{d}{dt}(H_r C_p \theta_r) = LC_p\theta_{r-1} - LC_p\theta_r + W_r \qquad (2.15)$$

$$\frac{d}{dt}(H'_r C'_p \theta'_r) = L'C'_p\theta'_r - L'C'_p\theta'_{r-1} - W_r \qquad (2.16)$$

where $(C_p = c)$ and $(C'_p = c')$ are the specific heats of the liquids in the two streams. All the values of specific heats are assumed to be independent of time. If we identify variables of the system with the equations of the form

$$\dot{x} = f(x) \qquad f(0) = 0 \qquad (2.17)$$

then the two-dimensional state vector x can be expressed as follows

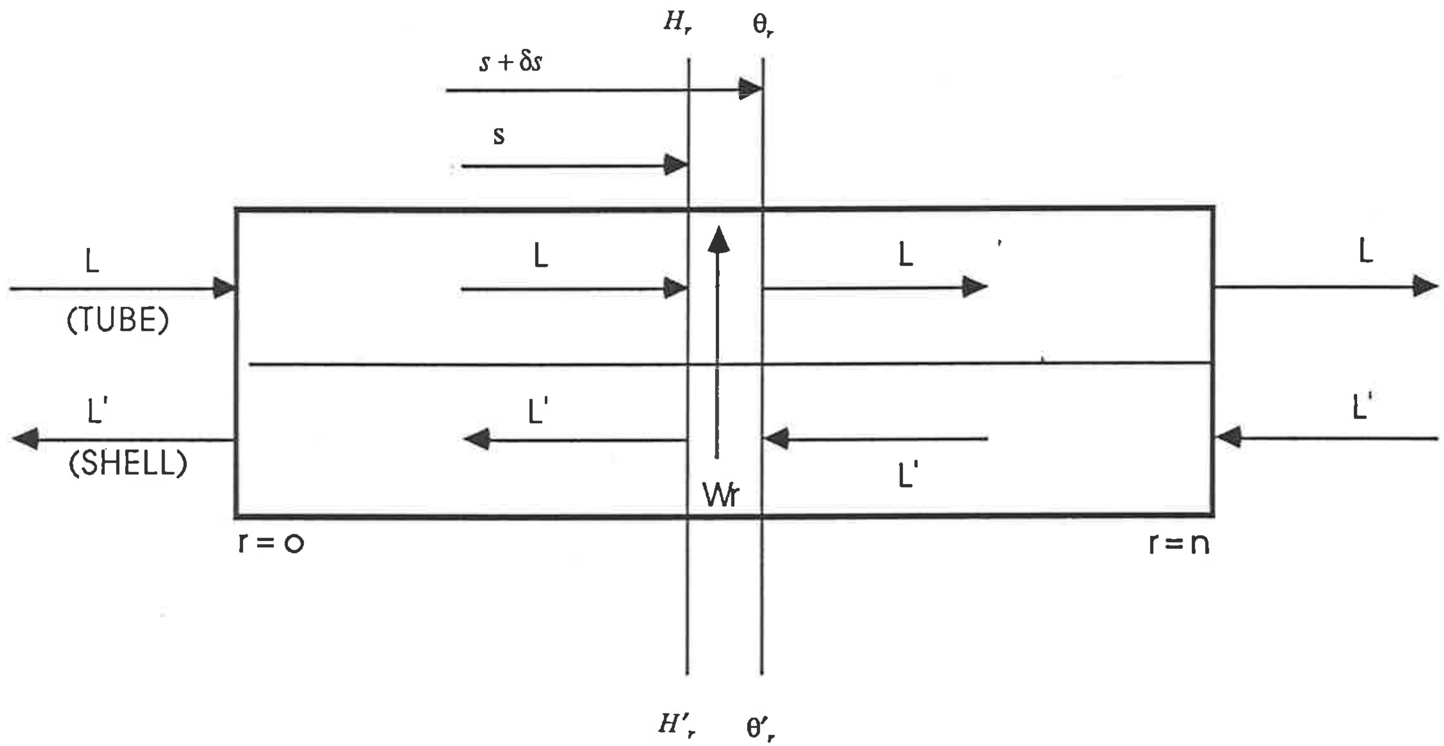


Figure 2.3 System of Heat Exchanger

$$x_i = x_{2r} = H_r C_p \theta_r \qquad r = 0,1,\ldots..n$$
$$= x_{2r+1} = H'_r C'_p \theta'_r \qquad i = 0,1,\ldots..2n+1 \tag{2.18}$$

The set of equations (2.15) and (2.16) combined with (2.18) gives the following equations

$$\dot{x}_{2r} = L\frac{x_{2r-2}}{H_{r-1}} - L\frac{x_{2r}}{H_r} + W_r\left\{\frac{x_{2r}}{cH_r}, \frac{x_{2r+1}}{c'H'_r}\right\} \tag{2.19}$$

$$\dot{x}_{2r+1} = L'\frac{x_{2r-1}}{H'_{r-1}} - L'\frac{x_{2r+1}}{H'_r} - W_r\left\{\frac{x_{2r}}{cH_r}, \frac{x_{2r+1}}{c'H'_r}\right\} \tag{2.20}$$

These equations have steady state solutions at $x_{2r} = x_{2r+1} = 0$ and the nonlinear heat flux is an implicit function $W_r = f(\theta_r, \theta'_r)$.

Equations (2.19) and (2.20) can be analysed by Krasovskii's theorem. If the heat flux is treated as an implicit function of the two inlet temperatures of the process streams such as $W_r = W_r(\theta_r, \theta'_r) = W_r(x_{2r}, x_{2r+1})$, then the Jacobian matrix is written as

$$F(x) = \begin{pmatrix} -\dfrac{\left(cL - \frac{\partial W_r}{\partial \theta_r}\right)}{cH_r} & \dfrac{\frac{\partial W_r}{\partial \theta'_r}}{c'H'_r} \\ -\dfrac{\frac{\partial W_r}{\partial \theta_r}}{cH_r} & -\dfrac{\left(c'L' + \frac{\partial W_r}{\partial \theta'_r}\right)}{c'H'_r} \end{pmatrix} \tag{2.21}$$

In order to satisfy Krasovskii's theorem, it is necessary to ensure that the Jacobian matrix F(x) represented by equation (2.21) satisfies the condition that

$$F'(x) = F(x) + F^T(x) \tag{2.22}$$

is negative definite. Then the steady state $x_{2s} = 0$ of the system is asymptotically stable in the large, and

$$V(x) = \| f(x) \|^2 \tag{2.23}$$

is a Lyapunov function for the system.

In the equation (2.22), $F^T(x)$ is the transpose of F(x) and is given by

$$F^T(x) = \begin{pmatrix} -\dfrac{\left(cL - \dfrac{\partial W_r}{\partial \theta_r}\right)}{cH_r} & -\dfrac{\dfrac{\partial W_r}{\partial \theta_r}}{cH_r} \\ \dfrac{\dfrac{\partial W_r}{\partial \theta'_r}}{c'H'_r} & -\dfrac{\left(c'L' + \dfrac{\partial W_r}{\partial \theta'_r}\right)}{c'H'_r} \end{pmatrix} \tag{2.24}$$

Therefore, the matrix $F'(x)$ can be calculated from equations (2.21) and (2.24) and is given by

$$F'(x) = \begin{pmatrix} -2\dfrac{\left(cL - \dfrac{\partial W_r}{\partial \theta_r}\right)}{cH_r} & -\dfrac{\dfrac{\partial W_r}{\partial \theta_r}}{cH_r} + \dfrac{\dfrac{\partial W_r}{\partial \theta'_r}}{c'H'_r} \\ -\dfrac{\dfrac{\partial W_r}{\partial \theta_r}}{cH_r} + \dfrac{\dfrac{\partial W_r}{\partial \theta'_r}}{c'H'_r} & -2\dfrac{\left(c'L' + \dfrac{\partial W_r}{\partial \theta'_r}\right)}{c'H'_r} \end{pmatrix} \tag{2.25}$$

The condition that $F'(x) < 0$ can be restated as $-F'(x) > 0$. The converted matrix is given by

$$-F'(x) = \begin{pmatrix} 2\dfrac{\left(cL - \dfrac{\partial W_r}{\partial \theta_r}\right)}{cH_r} & \dfrac{\dfrac{\partial W_r}{\partial \theta_r}}{cH_r} - \dfrac{\dfrac{\partial W_r}{\partial \theta'_r}}{c'H'_r} \\ \dfrac{\dfrac{\partial W_r}{\partial \theta_r}}{cH_r} - \dfrac{\dfrac{\partial W_r}{\partial \theta'_r}}{c'H'_r} & 2\dfrac{\left(c'L' + \dfrac{\partial W_r}{\partial \theta'_r}\right)}{c'H'_r} \end{pmatrix} \tag{2.26}$$

In order to prove that the matrix $-F'(x)$ is positive definite its elements must satisfy Sylvester's inequalities (Hohn 1958), given by the following equations

$$\left(cL - \frac{\partial W_r}{\partial \theta_r}\right)\frac{1}{cH_r} > 0 \tag{2.27}$$

$$4\left(cL - \frac{\partial W_r}{\partial \theta_r}\right)\frac{1}{cH_r}\left(c'L' + \frac{\partial W_r}{\partial \theta'_r}\right)\frac{1}{c'H'_r} - \left(\frac{\partial W_r}{\partial \theta_r}\frac{1}{cH_r} - \frac{\partial W_r}{\partial \theta'_r}\frac{1}{c'H'_r}\right)^2 > 0 \tag{2.28}$$

These inequalities determine the two curves in the heat flux - temperature plane. Inequalities (2.27) and (2.28) can be interpreted in a simplified form as

$$\frac{\partial W_r}{\partial \theta_r} = -UA < 0 \tag{2.29}$$

$$\frac{\partial W_r}{\partial \theta'_r} = UA > 0 \tag{2.30}$$

These inequalities are always satisfied except for very high rates of heat transfer as an increase in local temperature difference between the two liquids will in most circumstances increase the local rate of heat transfer (Rosenbrock 1962).

The sign of the derivative of the Lyapunov function $\dot{V}(x)$ is fixed by the sign definiteness of the matrix $F'(x)$ with reference to a theorem due to Krasovskii (1954). If in a region of the heat flux - temperature plane these inequalities are satisfied, then $\dot{V}(x)$ is negative in that region.

In order to check the other conditions for asymptotic stability in a bounded region it is necessary to examine the Lyapunov function for this system for the largest possible region $V(x) < K$ that lies within the region in which $\dot{V}(x) < 0$. Therefore the set of equations (2.19), (2.20) and (2.23), gives the following Lyapunov function of the form

$$V(x_{2r}, x_{2r+1}) = \left(\frac{W_r}{cH_r} - \frac{L}{H_r}x_{2r}\right)^2 + \left(\frac{W_r}{c'H'_r} - \frac{L'}{H'_r}x_{2r+1}\right)^2 = K \qquad (2.31)$$

where the variables x_{2r}, x_{2r+1} are implicit in $W_r(x_{2r}, x_{2r+1})$ and K is a Lyapunov constant. Replacing the variables of equation (2.18) in equation (2.31) a simplified form of Lyapunov function is obtained

$$V(H_r c\theta_r, H'_r c'\theta'_r) = (W_r - Lc\theta_r)^2 + (W_r + L'c'\theta'_r)^2 = K \qquad (2.32)$$

where $W_r = f(\theta_r, \theta'_r)$.

The Lyapunov function given by equation (2.32) is solved for W_r, which gives a quadratic equation of the form

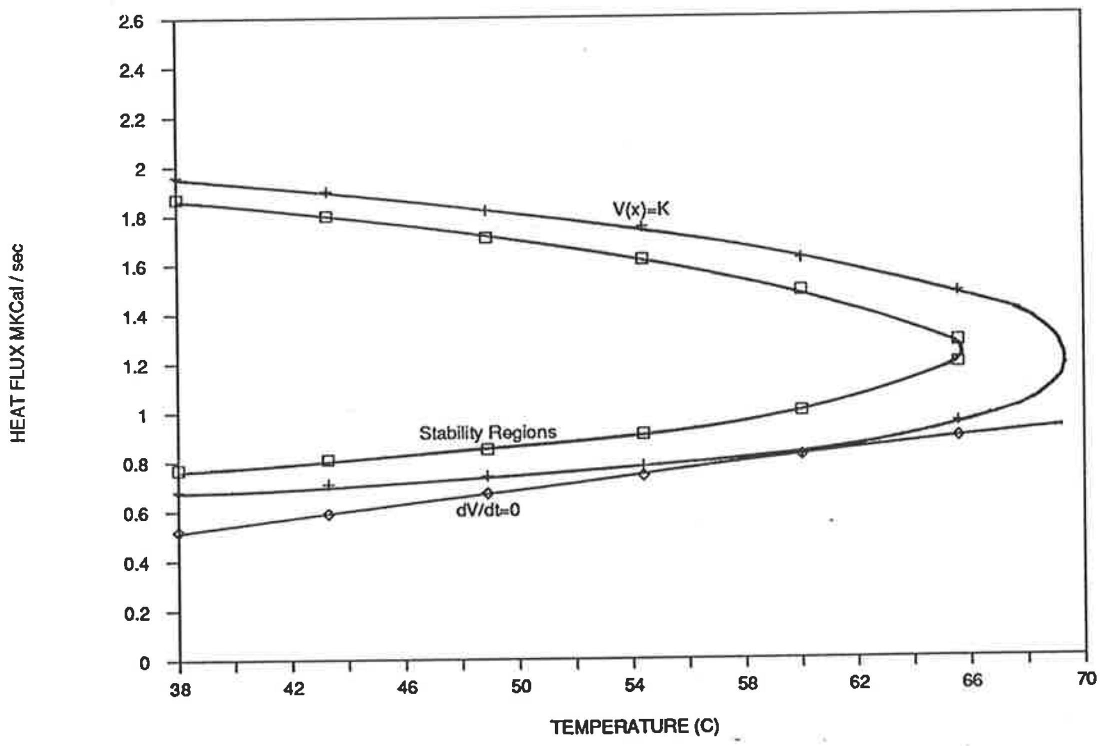
$$W_r^2 - W_r(Lc\theta_r - L'c'\theta'_r) + \frac{1}{2}\{(Lc\theta_r)^2 + (L'c'\theta'_r)^2\} - \frac{K}{2} = 0 \qquad (2.33)$$

2.7-2.1 Results and Discussions

The equation (2.33) gives for a value of $K = 5.58 \times 10^6$, two values of heat flux. Figure 2.4 shows the plot of V(x)=K curve. The curve $\dot{V}(x) = 0$ was also determined and placed on the Temperature-Heat Flux plane. The value of K was increased gradually to 5.80×10^6 until the V(x)=K curve touches the curve $\dot{V}(x) = 0$, determining the largest RAS for the given conditions in the heat exchanger. It should be pointed out that in figure 2.4 the stability regions drawn satisfy specific processing conditions for a particular value of a Lyapunov function. If conditions change due to some problems in operations, for instance due to fouling in heat exchanger, then the stability regions obtained will be

STABILITY ANALYSIS OF A HEAT EXCHANGER

BY THE METHOD OF LYAPUNOV



□ $K = 5.58 \times 10^6$ + $K = 5.80 \times 10^6$ ◇ $\dot{V}(x) = 0$

Figure 2.4 Region of Largest Asymptotic Stability of a Heat Exchanger smaller in shape as compared to one shown in the figure 2.4 due to reduction in heat transfer coefficient. This fact can also be demonstrated from the stability regions drawn in figure 2.4 which shows the stability regions for vapours condensing from a temperature of $66°C$ to $38°C$. However, if fouling takes place in the exchanger it will tend to increase the outlet temperature of vapours, thereby decreasing the condensation range of temperature and this decreasing effect in condensation will shrink the stability regions. Since it is always possible to find a stability region in a heat exchanger even in the case of fouling, the stability problem of heat exchangers in industrial operation does not seem to pose much difficulty. However, it will be interesting to study the stability criteria of a system with a feed effluent heat exchanger and an exothermic CSTR. In this type of situation, feed effluent heat exchange may lead to serious stability problems *(Stephanopoulos, 1984)*.

It has been shown analytically in Appendix A that the derivative of a Lyapunov function is always negative in the case of a heat exchanger, and that the inequalities given by equations (2.29) and (2.30) are always satisfied.

2.8 Conclusions

It is appreciated today that since chemical processes are nonlinear in their behaviour, a linear analysis of control gives an approximation only and the consideration of nonlinearities in the process is essential to enhance its performance. Lyapunov's second method does provide information on the stability analysis of nonlinear system but the construction of Lyapunov function for a particular chemical process is still a challenging research area. There are some forms of Lyapunov functions due to Krasovskii which provide an insight into the stability of chemical processes like CSTR and heat exchanger.

However, the mathematical results developed so far to study the stability criteria have limited applications due to the following constraints

- When there is a flow of two or more interacting quantities, the results cannot be applied. On multicomponent distillation, for example, the results have not been applied effectively (Rosenbrock, 1960).

- The results cannot be applied when a flow depends upon conditions in other sections.

- The results cannot be applied also to the systems in which both the potential and kinetic energy are stored.

Nevertheless, an attempt has been made in this Chapter to show that it is possible to obtain the stability regions for a CSTR and a heat exchanger provided a suitable Lyapunov function is constructed. Stability of a chemical process is also important for dynamic operability point of view. If at an initial design stage a thorough analysis of stability can be made with the methods discussed in this Chapter, it will be of great help in the operability analysis of the process system. For example, if a plant is unstable it may be rejected at an early design stage before making an extensive studies with regards to dynamic operability. Therefore, in the proceeding Chapters a dynamic operability studies is carried out to understand the dynamic behaviour of the two systems discussed in this Chapter.

CHAPTER 3

DYNAMIC PROCESS OPERABILITY AND SENSITIVITY ANALYSIS

A good theory must be useful to process control engineers and should be developed to accommodate the needs and skills of the potential users..... It was once said that only Frank Lloyd Wright can design a house for a family without asking about the number of children, or the family budget.

W . Lee and V . W . Weekman.

This chapter deals with analysing constraints on dynamic operability imposed by process design and control system design. It also gives an overview of dynamic operability analysis to provide an insight into the methodology developed for operability analysis.

The effect of physical constraints on dynamic operability can be measured by making use of singular value analysis techniques, hence some important aspects of singular value analysis have also been discussed. The significance of the condition number, which quantifies the sensitivity of the system with respect to uncertainties in the matrix (modelling errors), is also highlighted.

Since the singular values depend on the scaling of the system, i.e. the physical dimensions which are used in defining the variables and the equations, a method of optimum scaling of the transfer function matrix has also been discussed.

All these techniques have been applied to a CSTR with exothermic reaction and a Heat Exchanger in the following chapters.

3.1 Introduction

Dynamic process operability is defined as the ability of the plant to perform satisfactorily under conditions different from the nominal design conditions. The plant should be able to make the transition from operating conditions to stand-by or shutdown conditions without violating its environmental or safety constraints.

Dynamic process operability has a wide range of application, covering a broad field of process and control topics from efficient normal operation to startup and shutdown. It also includes considerations such as safety, reliability and profitability. For a particular process, dynamic operability analysis involves adjustment to changes in operating conditions such as product quality, product distribution and demand, energy conservation aspects and changes in feedstocks.

Most of the time process design work has been carried out without having much interaction with the control system design. General practice today depends heavily on detailed dynamic simulations, empirical overdesign and trial and error methods to encounter dynamic operability problems. But due to the complexity of integrated plants it is desired that an engineer be able to assess and improve the dynamic operability characteristics with more rigorous techniques.

The main objectives that should be kept in mind in order to achieve better operability of a chemical plant include the following

- A plant should recover from disturbances as quickly as possible.

- It should be capable of fast and smooth switchover from one set of operating conditions to another.

- It should be feasible (economical) for different ranges of feed conditions and other plant conditions.

- During equipment failure it should still be able to operate safely.

- There should not be any problem during startup and shutdown of the plant.

Figure 3.1 shows a simple representation of the design and operation of a chemical plant. This figure consists of the process design and the control system design within which several alternatives should be taken into account before a final plant design is decided. Furthermore, each of the factors described in figure 3.1 imposes different constraints on the system which limit the dynamic operability of the final design. The main idea for any dynamic operability study is then to be able to identify these constraints, quantify their efforts, and propose design changes to remove them.

Details of these factors and other fundamental constraints on dynamic operability have been addressed in literature by *Arkun (1986), Grossmann* and *Morari (1983)* and *Morari (1983)*. Here a brief overview on dynamic operability analysis is given in order to provide an insight into the methodology developed for operability analysis.

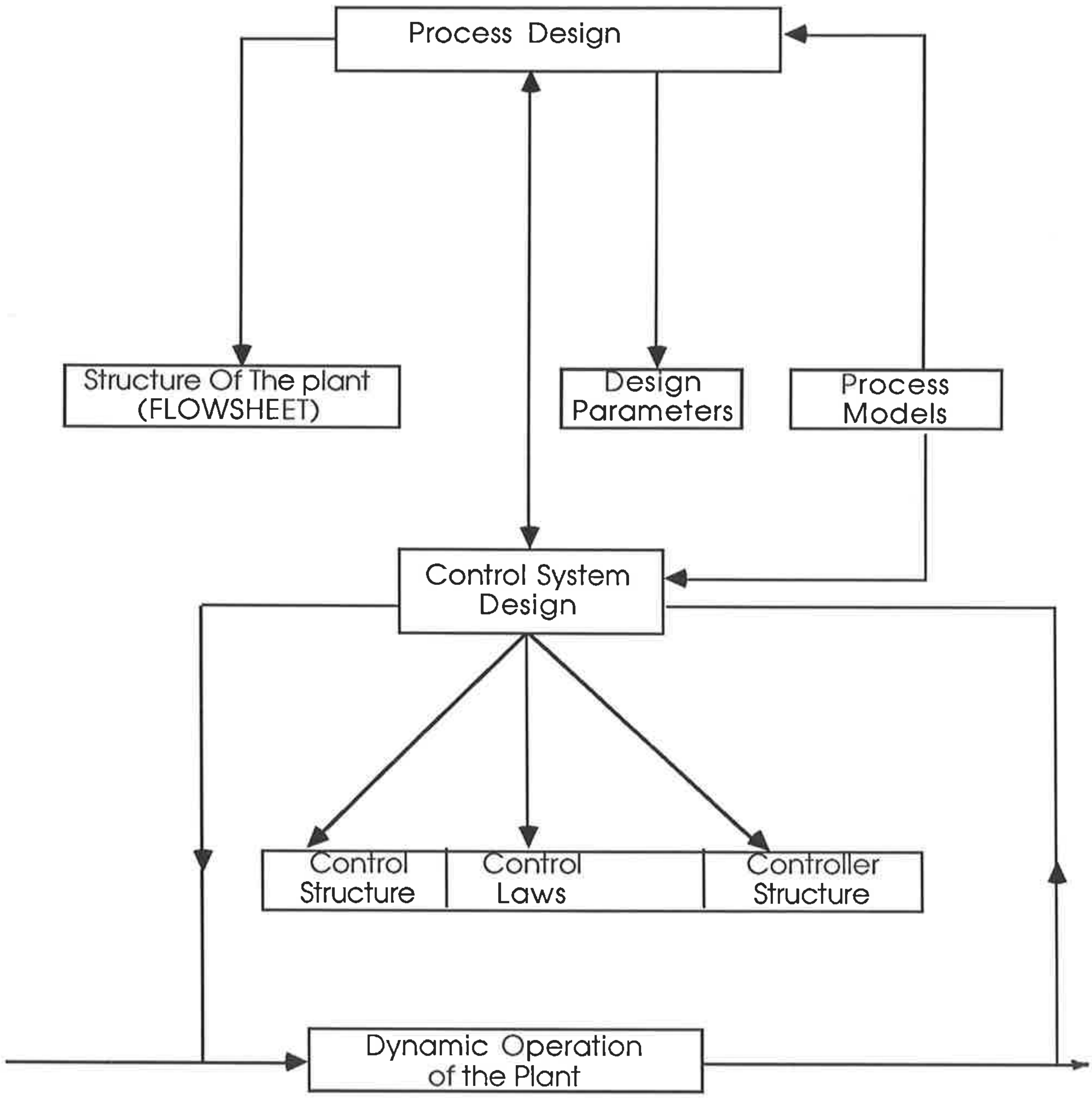


Figure 3.1 Representation of the Design and Operation of a Chemical Plant

3.2 Dynamic Operability Analysis - An Overview

A rational scheme based on frequency-domain decoupling was developed by *Buckley (1964)*. More formal attempts have been made to develop a framework for control synthesis *(Govind and Powers, 1982; Morari, 1980)*, but these techniques remain to be fully tested. In multivariable control systems, considerable progress has been made *(Bruns, 1982; Garcia and Morari, 1982 a and 1982 b; Lau et al., 1982)*, but this is only a part of the entire control system synthesis problem. Progress has also been made in the flowsheeting requirements to meet a range of operating conditions. The work of *(Grossmann and Sargent, 1978; Marselle et al., 1982; Morari, 1982 a and 1982 b)* provide milestones in this area. *Lenhoff and Morari (1982)* provided an interesting study of the tradeoff between optimal flowsheets and controllability. The variable control structure strategies developed by these authors can be considered as methodologies designed to provide more flexibility in the plant by either altering the control system or changing the process interconnections. The final aim of these strategies is to increase the performance and the reliability of the system.

Many methods are also developed for the design of regulatory control structure problems in which the measurements, the manipulated variables, and their interconnections are synthesized to regulate the process. These methods range from a relatively simple criterion such as static relative gain array (Bristol, 1966) and its dynamic extensions *(Tung and Edgar, 1977; Witcher and McAvoy, 1977; Gagnepain and Seborg, 1982)* to sophisticated computer aided methods using interactive graphics such as the direct Nyquist array *(Jensen et al., 1983) and* singular value analysis *(Lau et al., 1985)*. The review papers of *Ray (1982) and Stephanopoulos (1982)* give detailed discussions on this topic.

Singular value analysis was proposed by *Doyle (1982)* to study the stability and performance of control systems in the presence of uncertainty. The method offers opportunities to treat several different uncertainty descriptions in a nonconservative way *(Skogestad and Morari, 1985)*.

The development of synthesis of control policy, that is taking the process from a current operating condition to the new operating condition was carried out in a different ways. *Arkun and Stepanopoulos (1980)* addressed the synthesis of control policy in the form of steady-state optimizing control, *Bamberger and Isermann (1978); Prett and Gillette (1980); Garcia and Morari (1981)* studied it as on-line optimizing control and *Kao (1980); Brooks (1979)* considered the synthesis of control as a start-up control policy.

A new representation called Internal Model Control (IMC) has been introduced by *Morari (1983)*. IMC provides the right theoretical basis for the analysis of dynamic operability during process design and constitutes a powerful framework for the synthesis of control systems. *Morari et al., 1985* evaluated the operability characteristics of several given designs by comparing their robustness indices. Also *(Palazoglu et al., 1985)* suggested that starting from a given region, one can evolve to designs with better operability by conducting a sensitivity analysis in terms of the pertinent design variables, and making design modifications. The key to the robustness analysis is that it introduces new ways for characterizing the structure of the model/plant mismatch, and estimating the associated model error matrix and its magnitude bound.

Process simulation for operability analysis requires a lot of time, particularly in going from the steady-state to dynamic problems. A multipurpose simulation programme was developed *(Perkins and Sargent 1982)* to perform steady-state and dynamic simulation for the same set of models. It also interfaces directly with a state-space control system design package.

Most chemical companies are now making quantitative operability analysis part of their engineering procedures *(Tippets, 1982; White, 1982)*. The quantitative operability analysis refers to the system simulation approach to operations analysis under conditions of uncertainty.

3.3 Singular Value Analysis

The effect of physical constraints on dynamic operability can be measured by making use of singular value analysis techniques *(Klema and Laub, 1980)*.
In the structural analysis of multivariable systems, singular value analysis plays a vital role. The method is a powerful and computationally efficient tool for analysing matrix system *(Noble and Daniel 1977; Forsythe et al.,1977)*. Recent development shows its applications in systems engineering (*Doyle* and *Stein, 1981; Safanov et al., 1981; Cruz, et al., 1981*; *Postlewaite et al., 1981)*. These studies are based upon particular feedback controllers and consider some form of closed loop matrix operators. Many sources in the literature describe the physical interpretations (*Weber* and *Brosilow, 1972*; *Morari, 1982*; *Lau et al., 1985)* of singular value analysis.

3.3.1 Mathematical Interpretations

Essentially, singular value analysis allows us to express a general matrix in terms of a dyadic expansion or three decomposition matrices as in equation (3.2).

$$S_m = \sum_{i=1}^{r} \sigma_i Z_i V_i^+ = Z\Lambda V^+ \tag{3.1}$$

where S_m is the steady state version of the system matrix defined by *Rosenbrock (1970)* and

$$Z = (z_1 z_2 \ldots\ldots\ldots z_r z_{r+1})$$

= Left singular value decomposition matrix

$$V^+ = (v_1^+ v_2^+ \ldots\ldots\ldots v_r^+ v_{r+1}^+)$$

= Right singular value decomposition matrix

$$\Lambda = diag(\sigma_1, \sigma_2, \ldots\ldots\ldots, \sigma_r, 0)$$

=Diagonal matrix of singular values.

Singular value analysis application to the system of an (m x n) transfer function matrix G(s) leads to the equation (*Noble* and *Daniel, 1977).*

$$G(s) = Z(s)\Lambda(s)V^+(s) \qquad (3.2)$$

This representation provides the basic structure for the method used to analyse the CSTR and Heat Exchanger system by singular values in the proceeding chapters.

The manipulated variables are less likely to be saturated by load changes for those process designs whose minimum singular values are large over a large frequency range *(Morari, 1983)*. Singular Values (also known as principal gains) of the transfer function matrix may be used to evaluate stability margins for multiinput/multioutput (MIMO) systems in the same manner as the amplitude ratio is used in SISO systems.

The singular value depends only on the process design and is independent of the particular controller used.It is easy to compute and is utilized as a dynamic operability measures.

Doyle and *Stein, (1981)* and *Smith et al., (1981)* have adopted SVD to the loop selection in a steady state system. *Morari (1982)* used the SVD to quantify the control performance attainable in a process and interpreted implementability and sensitivity of the plant, concepts which quantify the resiliency of the plant, in terms of the norms of the transfer function operator.

3.3.2 Process Control Properties Provided by SVA

It has been shown that the condition number of a system can be used as a measure of sensitivity of control performance to modelling error and as such is a measure of controllability *(Morari, 1983)*. It is also a measure of robustness, i.e., the ability to guarantee a set of fixed outputs y given errors in the process model G since for the linear system

$$Gu = y \tag{3.3}$$

errors in u may be estimated as

$$\frac{||\delta u||}{||u||} \leq \gamma(G) \frac{||\delta G||}{||G||} \tag{3.4}$$

where γ is the condition number of the matrix G *(Perkins and Wong, 1985)* and

$$\gamma(G) = ||G|| \; ||G^{-1}|| \tag{3.5}$$

The analysis comes directly from analysing the singular values of the matrix G since the condition number of a matrix is defined as:

$$\gamma(G) = \frac{\sigma^*(G)}{\sigma_*(G)} \tag{3.6}$$

where σ^* and σ_* denote the maximum and minimum singular values, respectively.

Since the condition number is a measure of the sensitivity of the system to modelling errors, it is desirable that this number should be as small as possible. The smaller the condition number, the more it will tolerate a larger uncertainty before going unstable. This also indicates that when the condition numbers are low, higher gain for the feedback filter is allowed, thus improving the dynamic performance.

Perkins and Wong (1985) studied the dynamic behaviour of a model representing the double effect distillation of methanol with three different configurations. They have observed by plotting the minimum condition numbers as a function of frequency that one of the configurations is influenced by the large values of condition numbers at high frequencies whereas the best configuration seems to be the one having low condition numbers at high frequency.

Joseph and *Brosilow (1978)* used the singular values to select measurement structures for inferential control. The magnitude of the minimum singular value is a measure of the minimum distance to the nearest singular matrix and hence also a measure of the invertibility of the system. Therefore, the minimum singular value may be interpreted physically as an indicator of control effort required to reject a disturbance. Thus $\sigma_*(G)$ gives a measure of potential difficulties when implementing feedback control *(Morari, 1982)*

Consider a system matrix given by

$$S_m = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{3.7}$$

where A is a linearized state transition matrix, B is a linearized input matrix and C is defined as a measurement matrix and the four coefficient matrices are those of the standard linear state space equations. The system description can be formulated as

$$S_m \begin{pmatrix} x \\ \hline u \end{pmatrix} = \begin{pmatrix} 0 \\ \hline y \end{pmatrix} \tag{3.8}$$

The transfer function matrix G(s) is then related to the matrix (3.8) in the following way

$$G(s) = -CA^{-1}B + D(s) \tag{3.9}$$

and its dynamic version is written as

$$G(s) = C(sI - A)^{-1}B + D(s) \tag{3.10}$$

If $D(s) \equiv 0, \quad then G(s) \to 0 \quad as \quad s \to \infty$ and G(s) is then said to be strictly proper. D=0 for most systems, since the measurements rarely are influenced by the manipulated variables.

Lau and *Jensen (1985)*, described a method for evaluating the controllability of a process by SVA using the system matrix. By plotting contours of the minimum singular value and the condition number of the steady state system matrix over the feasible range, defined by the state and constraint equations, they visualized the sensitivity and operability of the process system.

3.4 Dynamic Analysis of System Matrix

The steady-state expression of the system matrix is given by equation (3.7), whereas its dynamic version is given by the following formula:

$$\begin{pmatrix} A - sI & B \\ C & 0 \end{pmatrix} \tag{3.11}$$

Steady-state analysis has been applied to a CSTR system by *Lau and Jensen (1985)* as a preliminary tool to identifying critical points in the feasible operating region. The steady-state matrix represented by equation (3.7) provides information on how the outputs of the system will be effected due to changes in the inputs. However, S_m does not supply information on how the output variables change with respect to time and it does not reflect the dynamic characteristics of the system. This situation is best represented by transfer function of the system given by equation (3.10) or by the dynamic version of the state space matrix represented by the equation (3.11).

This study is based on a dynamic analysis of the open loop transfer function and state space matrices. Open loop analysis refers to the system itself, that is the reactor without the addition of controllers. This approach provides insight into important closed loop system properties such as stability *(Postlewaite et al., 1981)*, sensitivity *(Weber, 1972)*, and invertibility *(Morari, 1981)*. Again $\sigma_*(G)$ gives a measure of potential difficulties when implementing feedback control but as a function of the frequency of the disturbance.

3.5 The Effect of Scaling

Singular values depend on the scaling of the system. By selecting an appropriate scaling method the condition number of the scaled system may be reduced from the original values. If D_1 and D_2 are diagonal scaling matrices then

$$\gamma(A) \neq \gamma(D_1 A D_2) \tag{3.12}$$

Perkins and Wong (1985) suggested comparing transfer function matrices only on the basis of the optimal condition number in the maximum norm as defined by *Bauer (1963)* which is an upper bound on the optimal condition number in the 2-norm. *Lau and Jensen (1985)* take into consideration a series of scaling procedures for the state space matrix. They investigated the effects of scaling on the analysis by scaling the steady-state system matrix with empirical methods, equilibration, and geometric scaling. They have also demonstrated that the scaling of the variables and equations can drastically change the contours of sensitivity and invertibility.

Taking the optimally scaled condition number of the state space matrix is inappropriate, however. The optimal condition number of a matrix S is given by the maximum eigen value π of the matrix

$$|S||S^{-1}| \tag{3.13}$$

where the modulus represents taking the absolute values of elements. It can be shown that the optimal ∞ – norm condition number of the matrix P, $\gamma_\infty^*(P)$, for strictly proper (D = 0) square system is given by

$$\gamma_\infty^*(P) = \max[\gamma_\infty^*(B), \gamma_\infty^*(C)] \tag{3.14}$$

i.e, $\gamma_\infty^*(P)$ is independent of A for this class of systems.

If the matrix S_m of equation (3.7) is denoted by P, then its inverse would be given by

$$P^{-1} = \begin{pmatrix} 0 & C^{-1} \\ B^{-1} & -B^{-1}AC^{-1} \end{pmatrix} \tag{3.15}$$

The eq. (3.15) has been derived in Appendix A.

The matrix $|P||P^{-1}|$ is therefore

$$|P||P^{-1}| = \begin{pmatrix} |B||B^{-1}| & |A||C^{-1}| + |B||B^{-1}AC^{-1}| \\ 0 & |C||C^{-1}| \end{pmatrix} \tag{3.16}$$

The maximum eigenvalue of this matrix, $\pi(|P||P^{-1}|)$, is, therefore, the maximum of $\pi(|B||B^{-1}|)$ and $\pi(|C||C^{-1}|)$.

Eigenvalues of eq. (3.16) do not depend on the system matrix A, therefore, the optimal ∞- norm condition number of P is independent of A. The condition number of this matrix is inappropriate as it does not reflect the controllability of the process and the optimal scaling of this matrix removes important information from the analysis.

Therefore in the next chapters optimal scaling method is applied only to transfer function matrices whereas the state-space matrices are treated without being scaled.

3.6 Conclusions

The main important conclusion that may be drawn from the survey of dynamic operability studies is that operability must be considered early in the process design work. Due to the trend toward increased mass and energy recycling in processes, the entire plant must be taken into consideration as a whole rather than as a collection of individual unit operations.

A plant design for optimum economic performance at nominal design conditions is usually not sufficient to ensure a successful design. Likewise, a plant design to meet the energy conservation aspects does not necessarily guarantee safe operation. The objective of ensuring good operability characteristics is often of greater importance due to uncertainties and changing conditions that are normally encountered during plant operation.

The general concepts of oversizing the equipment for feasibility of steady-state operation for a range of different feed conditions and avoiding long dead times for dynamic operability are not the best solutions to the problems faced these days. There is a great need for much more rigorous techniques for the assessment and improvement of the dynamic operability characteristics of chemical plants. The actual solution to the problems lies in correctly quantifying the dynamic operability of the problem, understanding easily the area of trouble shooting on the plants, process monitoring and improving the dynamic operability of the process design and the control system design systematically.

Since the steady state analysis of the system matrix does not give information on how the output variables change with respect to time, therefore, a dynamic analysis of the system matrix is essential to look into the dynamic characteristics of the system.

Since the singular values are scale dependent, a method of optimal scaling is also essential to compare the transfer function matrices. However, the condition number of the scaled state space matrix is not a reliable measure of controllability as scaling policies can remove important information from the analysis.

Finally, since chemical processes are nonlinear, sensitivity conclusions based on the condition number of the linear system will only be valid in a small region around the operating point at which the linearization was derived. It will be very useful to develop nonlinear methods to assess the effect of constraints on dynamic operability of chemical plants.

CHAPTER 4

DYNAMIC MEASURES OF SENSITIVITY AND OPERABILITY OF A CSTR

"The Nature alone has the power to expand a body in all directions so that it remains unruptured and preserves completely its previous form."

Galen, On the Natural Faculties

In this chapter a study of a CSTR system is carried out making use of irreversible, first order, exothermic reaction kinetics having nonlinear modelling equations. This system expected to have more control difficulties than the endothermic system studied by *Lau and Jensen (1985)*. The dynamic characteristics of the system are investigated for the model linearised at several steady states over a range of frequencies for different operating conditions. It has been observed that a system design for one steady state may not be the best at another steady state from a dynamic point of view because of its nonlinear behaviour. System control measures, sensitivity, and invertibility are evaluated over a wide range of operating conditions which are of practical importance for a particular processing unit. The control potential of the system is established by analysing the singular values (also known as principal gains) of the steady state system matrix and extending it to include dynamics of the system.

The condition numbers of both unscaled and optimally scaled transfer function matrices of the CSTR at different operating conditions have also been taken into consideration. The optimal scaling procedure has not been applied to state-space matrices as the condition number of the scaled state-space matrix is not a reliable indication of the controllability of the system.

It appears by studying the sensitivity and invertibility contours that optimal economic performance is obtained in a region of high conversion and high temperature, but it may not be feasible to operate the reactor at the optimum conditions because the system is much more difficult to control under those conditions.

It has been observed that the singular value plots drawn in the case of CSTR analysis remain constant at low frequencies and decrease linearly at high frequencies. Furthermore, the sensitivity of the system deteriorates in a high frequency range.

4.1 Introduction

Most of the existing control theory is applicable only to linear systems with constant coefficients, but the great majority of practical process control problems involve nonlinear systems.

Systems described by nonlinear differential equations are very common in the process industries and have models of the general form

$$\frac{dx}{dt} = f(x,u,d) \qquad x(t_0) = x_0 \tag{4.1}$$

$$y = h(x,u) \tag{4.2}$$

where

x(t) is an n vector of states,

u(t) is an m vector of controls,

d(t) is a k vector of disturbances,

y(t) is an l vector of measured outputs.

When

$$f = Ax + Bu + \Gamma d \tag{4.3}$$

$$h = Cx + Du \tag{4.4}$$

the nonlinear system given by equations (4.1) and (4.2) reduce to a linear problem.

4.2 Ray, Uppal and Poore CSTR Model

Material and energy balances for the first order, exothermic, irreversible reaction $A \rightarrow B$, in a well mixed stirred tank reactor lead to the following modelling equations *(Ray et al. 1974)*.

$$V\frac{dc_A}{dt'} = F(c_{Af} - c_A) - Vk_0 \exp\left\{-\frac{E}{RT}\right\} c_A \tag{4.5}$$

$$\rho C_p V \frac{dT}{dt'} = F\rho C_p (T_f - T) + V(-\Delta H) k_0 \exp\left\{-\frac{E}{RT}\right\} c_A - hA(T - T_c) \tag{4.6}$$

The quantity $V\rho C_p$ represents the thermal capacity of the reacting fluid alone. Similarly V is the reaction volume.

We define the following dimensionless quantities:

$$x_1 = \frac{c_{Af} - c_A}{c_{Af}}$$

= Reactant Concentration.

$$x_2 = \frac{T - T_f}{T_f}\gamma$$

= Reactant Temperature.

$$\gamma = \frac{E}{R}T_f$$

= Activation Energy.

$$\beta = \frac{(\rho C_p)_T}{\rho C_p} = \frac{hA}{F\rho C_p}$$

= Heat Transfer Coefficient.

$$Da = k_0 e^{-\gamma}\frac{V_{\max}}{F_0}$$

= Damkohler Number

$$u_1 = \frac{F_f}{F_0}$$

= Feed Flow Rate

$$u_2 = \frac{T_c - T_f}{T_f}\gamma$$

= Cooling Temperature.

$$B = (-\Delta H)c_{Af}\frac{\gamma}{\rho C_p T_f}$$

= Heat of Reaction.

$$t = t'\frac{F}{V}$$

= Time

After substituting these dimensionless quantities in equations (4.5) and (4.6), the modelling equations of the CSTR take the following form:

$$\frac{dx_1}{dt} = -x_1 + Da(1 - x_1)\exp\left\{\frac{x_2}{1 + \frac{x_2}{\gamma}}\right\} + u_1 = f_1(x_1, x_2, u_1) \qquad (4.7)$$

$$\frac{dx_2}{dt} = -x_2(1 + \beta) + BDa(1 - x_1)\exp\left\{\frac{x_2}{1 + \frac{x_2}{\gamma}}\right\} + \beta u_2 = f_2(x_1, x_2, u_2) \qquad (4.8)$$

4.3 Linearization of CSTR Modelling Equations

For dynamic analysis of nonlinear systems there are many methods which can be used to solve the system, such as:

- Simulation of nonlinear system on an analog or digital computer and computing its solution numerically.
- Transforming the nonlinear system into a linear one by an approximate transformation of its variables (if possible).

- Developing a linear model that approximates the dynamic behaviour of a nonlinear system in the neighbourhood of specified operating conditions.

Developing a linear model that approximates the dynamic behaviour of a nonlinear system in principle is always feasible. Linearization of the CSTR system is carried out by the last method written above. The problem under discussion is to linearise system equations (4.7) and (4.8) with many variables.

Expanding the nonlinear functions $f_1(x_1, x_2, u_1)$ and $f_2(x_1, x_2, u_2)$ into a Taylor's series around the steady state of interest, we obtain a system which takes the following general form of linear differential equations

$$\frac{dx}{dt} = Ax + Bu \tag{4.9}$$

$$y = Cx \tag{4.10}$$

where system matrices A, B, and y are written as

$$A = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix}_{x_1 = x_{1s},\, x_2 = x_{2s}} \tag{4.11}$$

$$B = \begin{pmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{pmatrix}_{u_1 = u_{1s},\, u_2 = u_{2s}} \tag{4.12}$$

$$y = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{4.13}$$

where

A = Linearized State Transition Matrix.

B = Linearized Input Matrix.

y = Measurement Matrix.

Therefore in order to write A, the following derivatives were calculated from the CSTR modelling equations.

$$\frac{\partial f_1}{\partial x_1} = -1 - Da \exp\left\{\frac{x_2}{1+\frac{x_2}{\gamma}}\right\} \tag{4.11a}$$

$$\frac{\partial f_1}{\partial x_2} = Da \frac{(1-x_1)}{\left(1+\frac{x_2}{\gamma}\right)^2} \exp\left\{\frac{x_2}{1+\frac{x_2}{\gamma}}\right\} \tag{4.11b}$$

$$\frac{\partial f_2}{\partial x_1} = -BDa \exp\left\{\frac{x_2}{1+\frac{x_2}{\gamma}}\right\} \tag{4.11c}$$

$$\frac{\partial f_2}{\partial x_2} = -(1+\beta) + BDa \frac{(1-x_1)}{\left(1+\frac{x_2}{\gamma}\right)^2} \exp\left\{\frac{x_2}{1+\frac{x_2}{\gamma}}\right\} \tag{4.11d}$$

Replacing these four derivatives back in the equation (4.11), the linearized state transition matrix A takes the following form

$$A = \begin{pmatrix} -1 - Da\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} & Da\dfrac{(1-x_{1s})}{\left(1+\frac{x_{2s}}{\gamma}\right)^2}\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} \\ -BDa\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} & -(1+\beta)+BDa\dfrac{(1-x_{1s})}{\left(1+\frac{x_{2s}}{\gamma}\right)^2}\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} \end{pmatrix}_{x_1=x_{1s},x_2=x_{2s}} \quad (4.14)$$

where x_{1s} and x_{2s} are solutions of steady state equations. x_{1s} is the dimensionless reactant concentration and x_{2s} is the dimensionless reactant temperature and the system matrices B and C are written as follows:

$$B = \begin{pmatrix} 1 & 0 \\ 0 & \beta \end{pmatrix} \quad (4.15)$$

$$C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (4.16)$$

where B and C are the input and output matrices respectively.

4.4 Application to CSTR Model

Modelling equations (4.7) and (4.8) of a CSTR have two measured variables, the reactant concentration and the temperature of the reactor. The two manipulated variables are feed flow rate and the cooling water flow rate as shown in figure 4.1. Using equations (4.7) and (4.8) and the measured variables, the following 4x4 steady-state system matrix was calculated

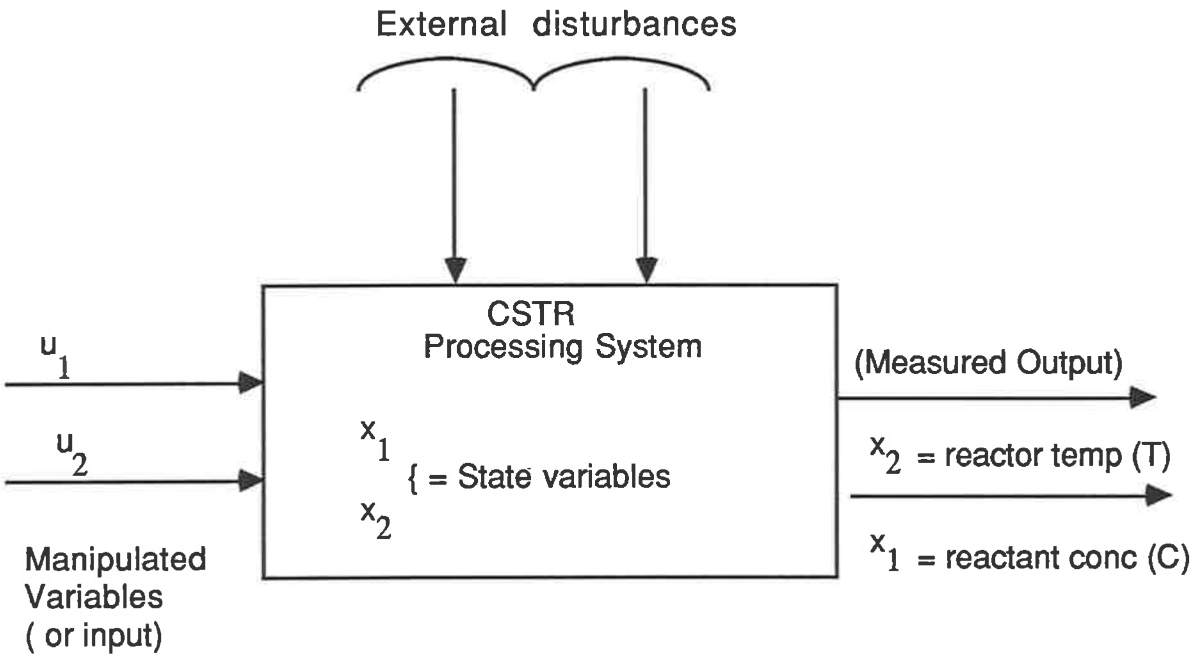


Figure 4.1 Input and output variables around CSTR system

$$S_m = \begin{pmatrix} -1 - Da\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} & Da\dfrac{(1-x_{1s})}{\left(1+\frac{x_{2s}}{\gamma}\right)^2}\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} & 1 & 0 \\ -BDa\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} & -(1+\beta)+BDa\dfrac{(1-x_{1s})}{\left(1+\frac{x_{2s}}{\gamma}\right)^2}\exp\left\{\dfrac{x_{2s}}{1+\frac{x_{2s}}{\gamma}}\right\} & 0 & \beta \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad (4.17)$$

For dynamic analysis, the system matrix represented by equation (4.17), was substituted in equation (3.9) and parameter values were estimated from figure 4.2 which was drawn by taking into consideration the influence of the parameters discussed by *(Ray at El. 1974)* on the types of dynamic behaviour in a CSTR. They have observed during the studies of dynamic behaviour of the reactor that for small values of γ, the activation energy, higher values of B, the heat of reaction, and β, the heat transfer coefficient are obtained. They suggested that for multiplicity and limit cycle behaviour a much more exothermic reaction would be required. The physical implications of these results suggest that it is possible to achieve more stable and less exotic operation by accomplishing the necessary cooling through increasing the value of β.

Since the model was linearised at several steady state conditions therefore the values for each steady state condition were estimated by figure (4.2) which is drawn for one steady state case. However, parameter estimation for other steady state conditions can also be made by the simple formula (Ray et al. 1974)

$$B = \frac{(1+\beta)^3}{\beta} \qquad (4.18)$$

The 4x4 system matrix given by equation (4.17) was then solved for different frequencies (ω). Figure 4.3 shows the singular values σ_i (i=1, ... 4) of 4x4 system matrix as functions of frequency on a log-log plot, while figure 4.4 gives the corresponding condition number as a function of frequency. The graphical representation is similar to that employed in Bode plots and the singular values are multivariable analogs to the gain in an SISO system.

4.5 Results and Discussions

Dynamic analysis of the CSTR system matrix (4.17) was also performed at different operating conditions. The analysis carried out for the range of conversion x_{1s}=(0.3 ,..., 0.9) and temperature x_{2s}=(2 ,..., 5) and the results of the analysis are presented in table 4.1. In a practical situation there usually is a maximum temperature constraint, *(Arkun, 1979)* and therefore the region of temperature $x_{2s} > 5$ has not been included in the analysis.

Analysis of the unscaled state space matrix is shown by the two figures 4.5 and 4.6. This matrix has not been scaled optimally, as the optimally scaled condition number of the state space matrix does not reflect the controllability of the process.

Figures 4.5 and 4.6 show the sensitivity and invertibility of the system. At low temperatures, the sensitivity of the system is poor for a wide range of frequencies and increases sharply at high frequencies. Therefore, large control efforts will be needed in the feedback control scheme. Another interesting feature is that the condition number does not deteriorate so significantly in the region of high temperature (x_{2s}=5) and high frequency ($\omega = 100$) in comparison with other steady state conditions shown in figure 4.5. A further increase in frequency shows that all the contours converge to a one point in the plane where the condition number is very high giving an indication of difficulties in control.

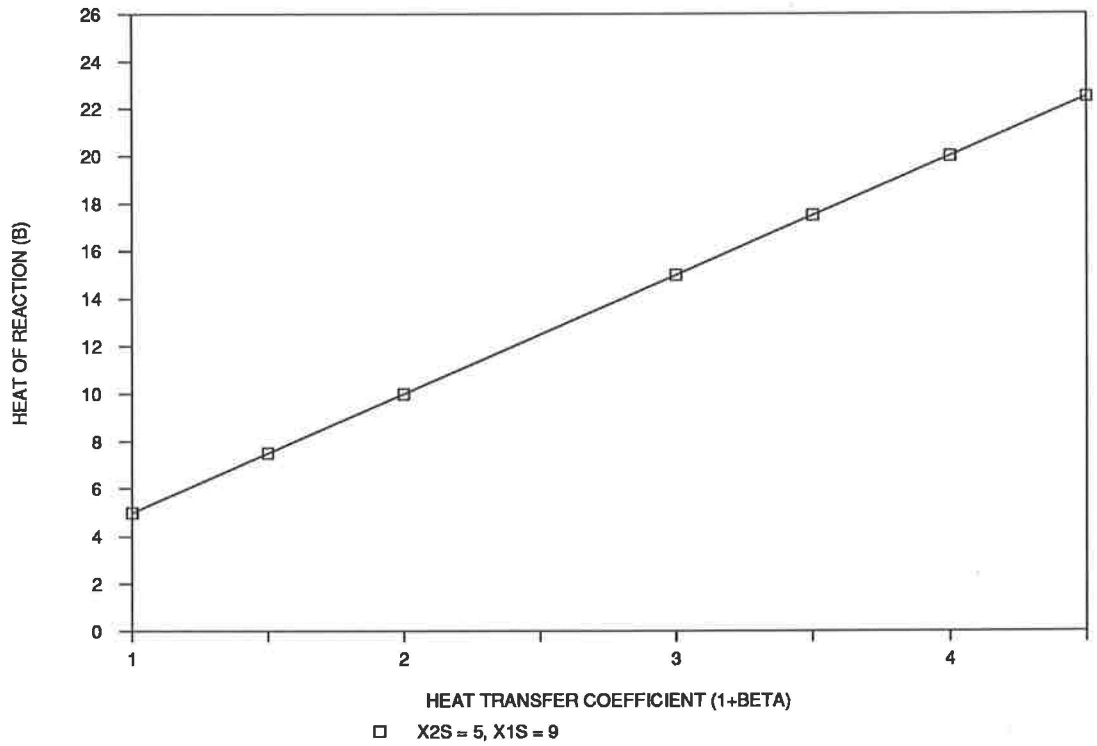
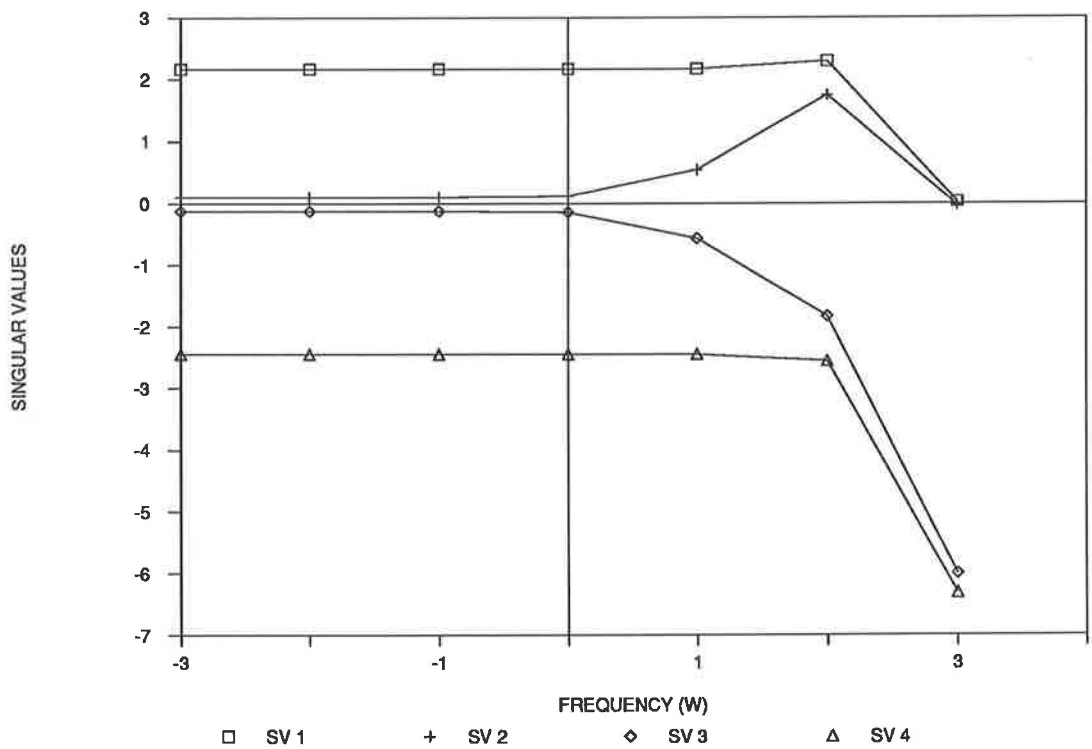


Figure 4.2 Heating Profile of a CSTR

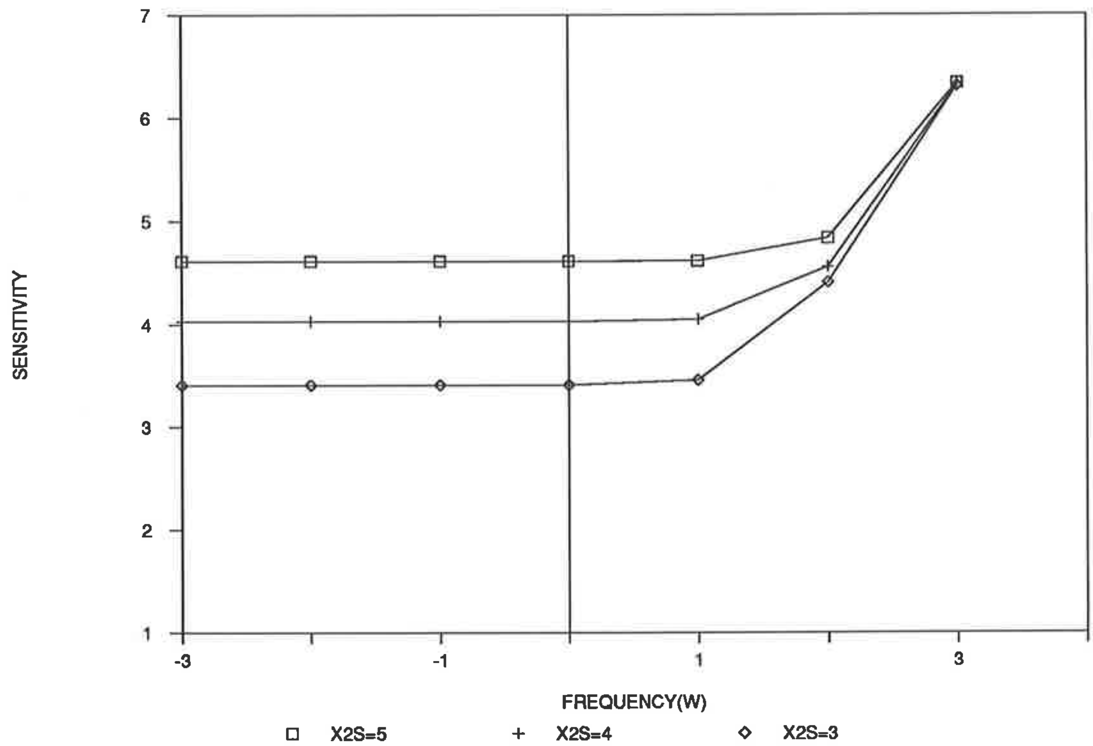
In Parameter Space (Ray and Uppal)



Conversion = 0.9, Temperature = 5

Figure 4.3 Singular Value Analysis

DYNAMIC ANALYSIS OF A CSTR



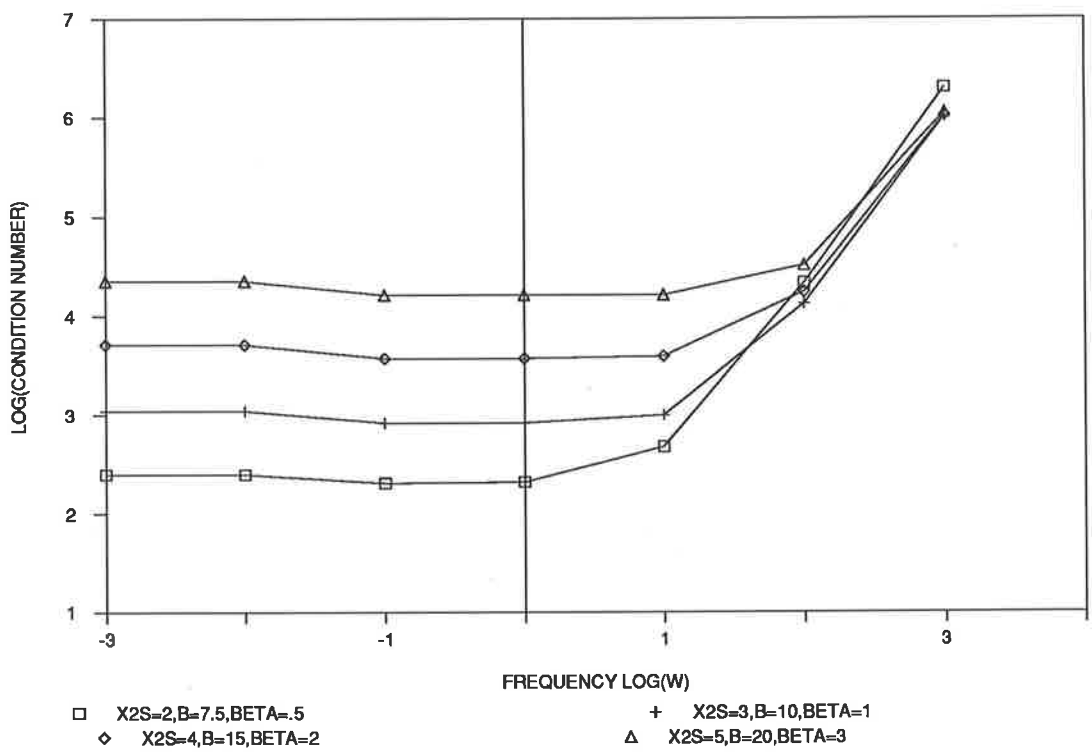
Conversion = 0.9

Figure 4.4 Frequency - Sensitivity Analysis

Table 4.1 Sensitivity and Singular Value Analysis

	BETA=.5	B=7.5	BETA=1	B=10	BETA=2	B=15	BETA=3	B=20
FREQ. (W)	SV(MIN)	COND.NR	SV(MIN)	COND.NR	SV(MIN)	COND.NR	SV(MIN)	COND.NR
0.001	0.0446	252.80	0.0301	1.10E+3	0.0197	5.11E+3	0.0115	2.24E+4
0.01	0.0446	252.80	0.0301	1.10E+3	0.0197	5.11E+3	0.0115	2.24E+4
0.1	0.0494	206.31	0.0349	823.30	0.0231	3.69E+3	0.0135	1.61E+4
1	0.0491	209.47	0.0348	825.24	0.0231	3.69E+3	0.0135	1.61E+4
10	0.0341	477.63	0.0315	1.01E+3	0.0223	3.88E+3	0.0134	1.64E+4
100	0.0050	2.12E+4	0.0087	1.33E+4	0.0098	1.72E+4	0.0079	3.25E+4
1000	0.0005	2.01E+6	0.00099	1.03E+6	0.00099	1.05E+6	0.00099	1.12E+6

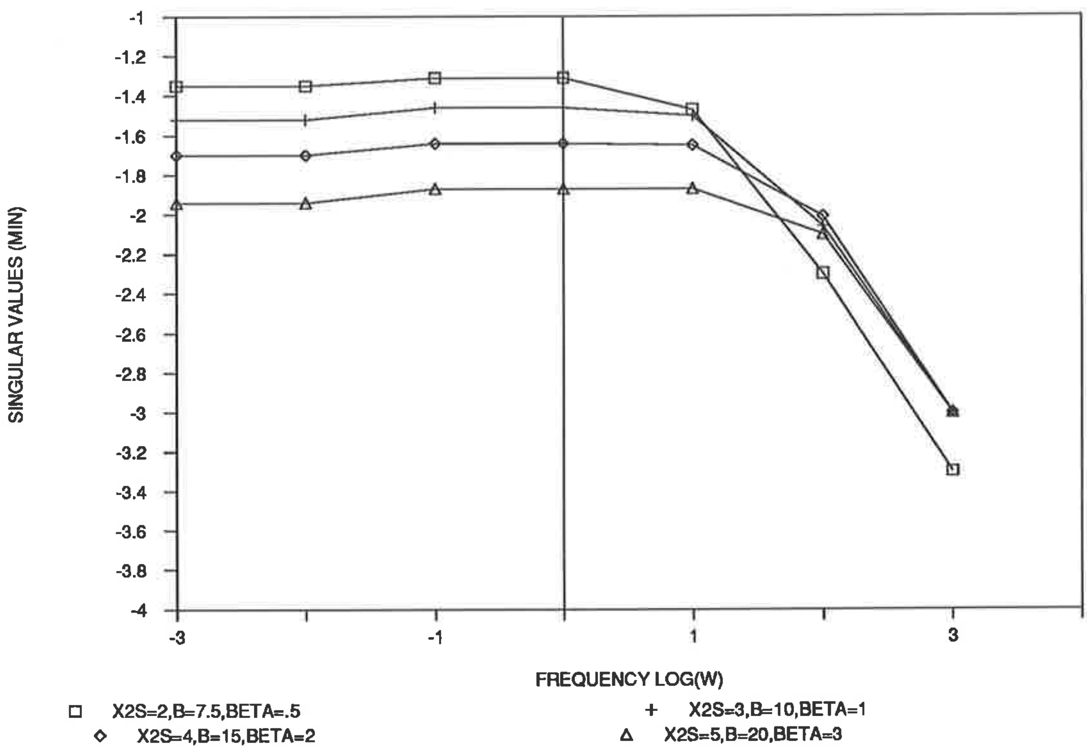
DYNAMIC ANALYSIS OF A CSTR



Conversions = 0.3, 0.5, 0.7, 0.9

Figure 4.5 Analysis of Unscaled State Space Matrix

DYNAMIC ANALYSIS OF A CSTR



Conversions = 0.3, 0.5, 0.7, 0.9

Figure 4.6 Analysis of Unscaled State Space Matrix

It is possible to obtain optimal economic performance in a region of high temperature and conversion, but due to exothermicity of the reaction, the operation becomes more sensitive and would likely pose more difficulties in reactor control. *Lau and Jensen (1985)*, arrived at the same conclusion when they treated an exothermic second order polymerization CSTR model. Although their analysis is based on the steady-state system, it gives sufficient information to identify critical points in the feasible region of operation. Figure 4.5 also illustrates that at low temperatures and high frequency region, a small perturbation in the system causes a large deviation in its response.

For example, the reactor was operated at some steady-state condition with temperature, x_{2s}=3 and heat of reaction, B=10, a small change in operating condition brought the temperature down to x_{2s}=2 and B=7.5, bringing the system into a high sensitivity region. Therefore, it would be more advantageous to operate the system at a suboptimal condition in exchange for better controllability. It is also evident, however, that in order to arrive at a feasible region, the operating route passes through a region of higher sensitivity.

The condition numbers of both unscaled and optimally scaled transfer function matrices of the CSTR are determined and plotted. Figures 4.7 and 4.8 give the variation of condition numbers with respect to frequencies on a log-log plot. As x_{2s}, the reactor temperature increases from 2 to 5, conversion and heat of reaction also increase, thereby increasing yield. The highest value of x_{2s} corresponds to the most economic operating conditions under normal circumstances. It is of interest to see whether increasing yield and therefore profitability, affects controllability, and also whether controllability assessments based on a linear analysis made at the lower steady state design rating provide erroneous conclusions at higher yields.

At low frequencies while the optimally scaled condition number indicates that high

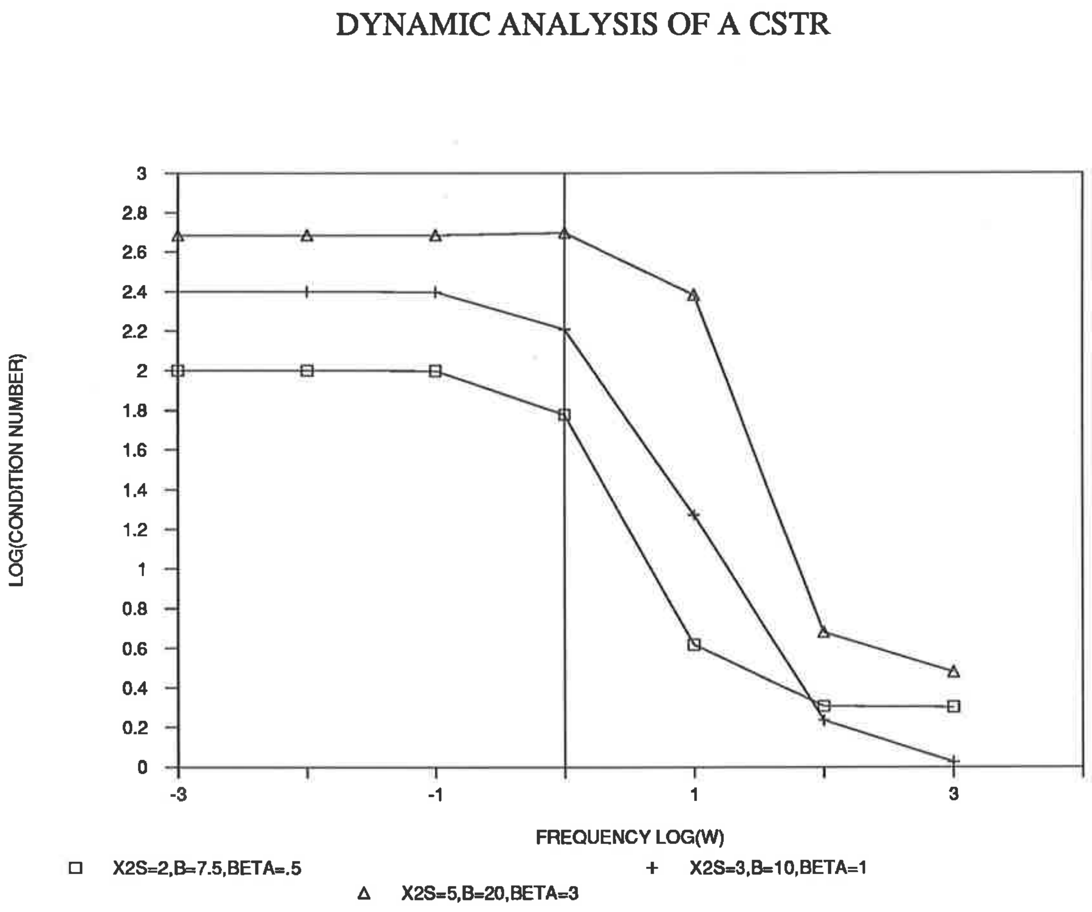


Figure 4.7 Analysis of an Unscaled Transfer Function Matrix

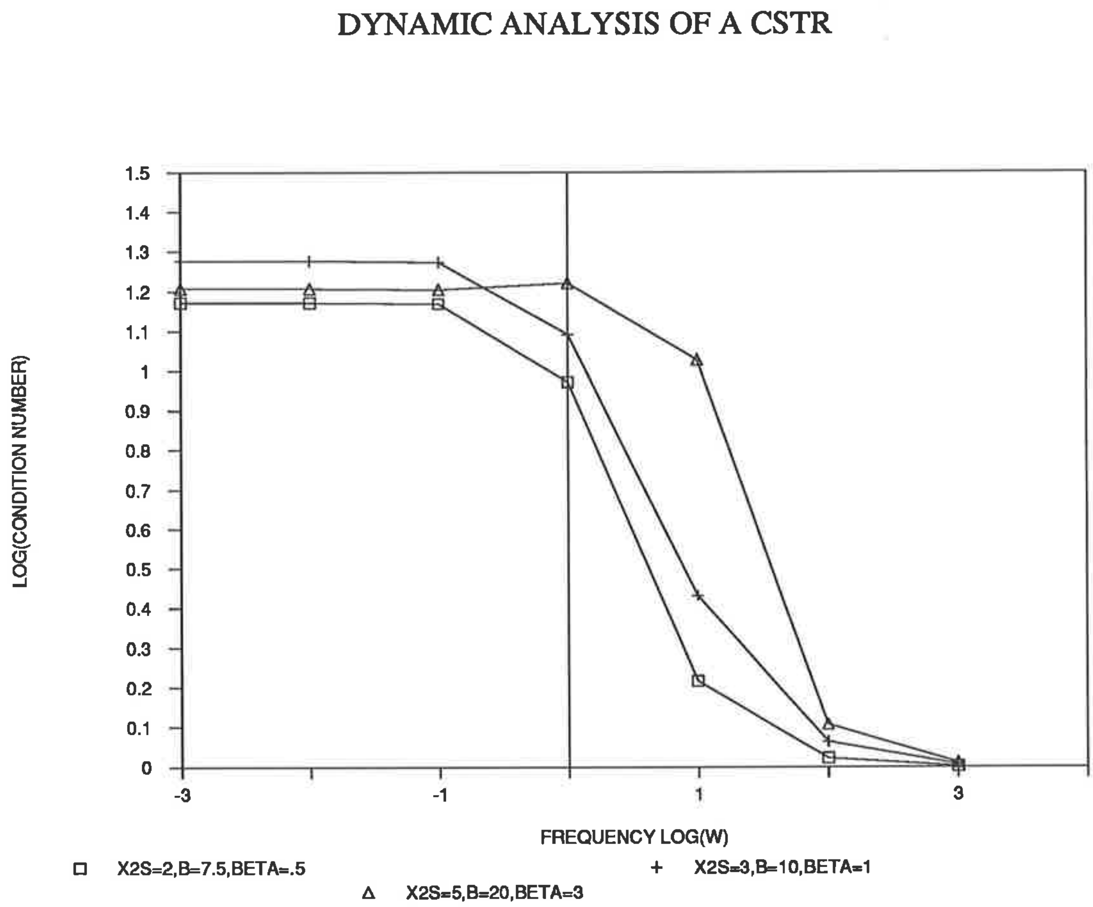


Figure 4.8 Analysis of an Optimally Scaled Transfer Function Matrix

temperature and conversion provide no extra control problems the unscaled results do not agree. This indicates that as expected scaling must be taken into account in some way. The optimal scaling of *Perkins and Wong (1985)* seems to be the most appropriate procedure for comparing sets of conditions which have differing scales.

It can also be seen from figure 4.5, that the condition number increases with higher frequencies in contrast to the transfer function matrix condition number, shown by figures 4.7 and 4.8. This is because the matrix G contains $(sI-A)^{-1}$ in its product (equation 3.10).

The state space condition numbers converge to one curve while the condition numbers of the transfer function matrix have more variation between the operating points. The conclusions drawn from figure 4.7 at intermediate frequencies cannot be drawn from figure 4.8.

4.6 Conclusions

In this Chapter, attempts have been made to investigate how seriously nonlinearities in the CSTR system mar controllability assumptions made on the basis of linearisations. System control measures, sensitivity, and invertibility are evaluated at different steady state over the range of operating conditions.

The optimal scaling procedure was carried out for the transfer function matrix and the results then compared with the unscaled analysis. The analysis showed that the CSTR at high throughputs has a significantly higher condition number under certain conditions thereby providing unpredicted difficulties for a system design at low yields. It has been shown also that the condition number of the scaled state space matrix is not a reliable measure of controllability. It masks potential problems with nonlinearities, and although it is scale dependent, scaling policies can remove important information from the analysis. In Chapter 3 it has been shown why such information is being removed from the analysis.

CHAPTER 5

DYNAMIC OPERABILITY AND SENSITIVITY ANALYSIS OF A DISTRIBUTED SYSTEM

> *"... always from a definition or rough sketch of whatever presents itself to the mind; strip it naked and look at its essential nature, contemplating the whole through its separate parts, and these parts in their entirety."*
>
> *Marcus Aurelius, Meditations*

In this Chapter, dynamic operability and sensitivity analyses are carried out on a heat exchanger model with fouling conditions. The shell and tube heat exchanger is a condenser with condensation taking place on the shell side.

The dynamic characteristics of the system are investigated for the model linearised at several steady-states over a range of frequencies for different operating conditions. The analysis is performed at three different cases: when the exchanger is clean, with moderate fouling and with a high fouling. Results are interpreted graphically. Also, the condition numbers of both unscaled and optimally scaled transfer function matrices at different operating conditions have been obtained and tabulated for comparison.

It has been shown that although the optimal scaling method reduces condition numbers of transfer function matrix to very small values, their plots have the same profile as obtained in the unscaled case.

5.1 Introduction

In all processes which have heat, mass, or momentum transfer there must be gradients in spatial directions. There are some processes which are specifically designed to take advantage of gradients along the axis of flow. The most common examples representing these type of processes are the tubular reactor, the shell and tube heat exchanger, and packed mass exchange columns.

Such physical systems are usually regarded as continuous and their behaviour is expressed as partial differential equations. The general situation, however is that in which variables such as flow rate, temperature, pressure and composition are not only distributed in spatial dimensions but also vary with time.

The most common approach to solve partial differential equations, which is suitable to computer simulation, is that of converting the partial differential equations into multiple sets of simultaneous, ordinary differential equations, for which there is only one independent variable, usually time. The continuous system is divided into small elements within which conditions are considered uniform. However, most methods discretize the spatial variable and then solve for the dependent variable at the grid points.

5.2 Heat Exchanger Model

A heat exchanger model given by *Rosenbrock (1962)* is considered for the dynamic operability and sensitivity analysis. This model has been discussed in detail in Chapter 2.

If the heat flux rate is treated as an implicit function of the two inlet temperatures of the process streams such as $W_r = W_r(\theta_r, \theta'_r) = W_r(x_{2r}, x_{2r+1})$, then the Jacobian matrix, A' is written as

$$A' = \begin{pmatrix} -\dfrac{\left(cL - \frac{\partial W_r}{\partial \theta_r}\right)}{cH_r} & \dfrac{\frac{\partial W_r}{\partial \theta'_r}}{c'H'_r} \\ -\dfrac{\frac{\partial W_r}{\partial \theta_r}}{cH_r} & -\dfrac{\left(c'L' + \frac{\partial W_r}{\partial \theta'_r}\right)}{c'H'_r} \end{pmatrix} \tag{5.1}$$

and the system matrices B' and C' take the the following form

$$B' = \begin{pmatrix} \dfrac{L}{H_r} & 0 \\ 0 & \dfrac{L'}{H_{r'}} \end{pmatrix} \tag{5.2}$$

$$C' = \begin{pmatrix} 1 & 0 \\ 0 & \dfrac{1}{c'} \end{pmatrix} \tag{5.3}$$

A' is the state transition matrix, B' is the input matrix and C' is the measurement or output matrix. The two outlet variables (y) are the outlet temperatures, the state variables (x) are the inlet temperatures and the manipulated variables (u) are the flowrates.

Since condensation is taking place on the shell side and heat is transferred from shell to tube the inequalities

$$\frac{\partial W_r}{\partial \theta_r} = -UA < 0 \tag{5.4}$$

$$\frac{\partial W_r}{\partial \theta'_r} = +UA > 0 \tag{5.5}$$

where r = 0, 1, ... n are always satisfied except for very high rates of heat transfer as an increase in local temperature difference between the two liquids will in most cases increase the local rate of heat transfer *(Rosenbrock 1962)*.

In order to form a state space matrix of the heat exchanger system, system matrices A', B' and C' were substituted in the equation (3.7).

After replacing the above values in equation (3.7) the following 4x4 state-space system matrix was obtained

$$S_m = \begin{pmatrix} -\dfrac{\left(cL - \frac{\partial W_r}{\partial \theta_r}\right)}{cH_r} & \dfrac{\frac{\partial W_r}{\partial \theta'_r}}{c'H'_r} & \dfrac{L}{H_r} & 0 \\ -\dfrac{\frac{\partial W_r}{\partial \theta_r}}{cH_r} & -\dfrac{\left(c'L' + \frac{\partial W_r}{\partial \theta'_r}\right)}{c'H'_r} & 0 & \dfrac{L'}{H_{r'}} \\ 1 & 0 & 0 & 0 \\ 0 & \dfrac{1}{c'} & 0 & 0 \end{pmatrix} \tag{5.6}$$

For dynamic analysis, the system matrix given by equation (5.6) was substituted in equation (3.9).

5.3 Dynamic Analysis with Fouling

In industry fouling is a major problem. Plant operation is also affected by fouling. Effects of fouling come as a source of additional fuel costs, maintenance costs, use of antifoulants, plant downtime, reduced throughput etc. In industrial practice, a variety of approaches can be adopted to mitigate the effects of fouling. Which method is followed depends on the type and severity of fouling encountered. In some cases, the asymptotic value of fouling may be such that the problem can be tolerated, provided that the exchanger is initially oversized, and an appropriate bypass installed. However, if fouling is heavy, and the bypass used to control fouling is also used as a process controller, it may eventually become inoperative. Therefore these difficulties due to fouling make it necessary to consider fouling aspects in the operability and sensitivity analysis of heat exchanger.

In the case of scaling of cooling tower water, if the fouling resistance-time relationship reaches an asymptote, the effect of surface temperature may be determined by the following formula *(Knudsen, 1984)*

$$(R_f)_\infty = C \exp(-E/RT_s) \tag{5.7}$$

where E is the activation energy, C is a constant, R is the gas constant, $(R_f)_\infty$ is the asymptotic fouling resistance and T_s is the absolute temperature at the surface of the deposit.

The effect of fouling on the heat transfer coefficient of an exchanger, is generally taken into account by the formula

$$\frac{1}{U} = \frac{1}{U_0} + R_f \tag{5.8}$$

where U_0 and U are the overall heat transfer coefficients in clean and fouled cases respectively. The fouling factor R_f can be selected either from commercial data or TEMA (1978).

Fouling is considered to be a transient process. Therefore, exchangers designed to incorporate the equation (5.8) are initially oversized, which reflect poorly on the dynamic operability of the network *(Morari and Grossmann, 1984)*. If operation is at a constant heat duty, fouling has the effect of increasing the overall temperature driving force, thereby lowering the heat transfer. Fouling results in lower cold stream and higher hot stream outlet temperatures.

Sensitivity of heat exchangers to fouling was discussed by *Fryer (1986)*, who derived linearised equations to study the sensitivity of the network. In this Chapter, a sensitivity analysis using the system matrix is also performed taking into consideration the fouling equation (5.8) which introduces a nonlinearity.

5.4 Results and Discussions

The process configuration for a typical condenser is shown in figure 5.1. Process conditions are given in Appendix C. A dynamic analysis of the 4x4 system matrix was performed for different frequencies. Analysis of the unscaled state space matrix is shown by figure 5.2. This figure indicates that in the case of heat exchanger analysis the condition number varies linearly without being influenced by the variation in frequencies. Again, this matrix has not been scaled optimally for the same reasons as explained in Chapter 4, in the case of the CSTR analysis.

The condition number of both unscaled and optimally scaled transfer function matrices of the heat exchanger has been determined and plotted. Figures 5.3 and 5.4 give the variation of condition numbers with respect to frequencies in both the cases, whereas tables 5.1 and 5.2 provide a comparison of the magnitude of the condition numbers. Since the heat exchanger is sensitive to fouling *(Fryer et al. 1987)* and poses some problems of control, therefore, the analysis is performed at conditions without fouling, with a moderate amount of fouling, and with high fouling.

Table 5.1 shows the condition numbers of optimally scaled matrices. It can be observed that condition numbers vary slightly ($\gamma = 1.18$ *to* 1.27) at a high frequency from the clean

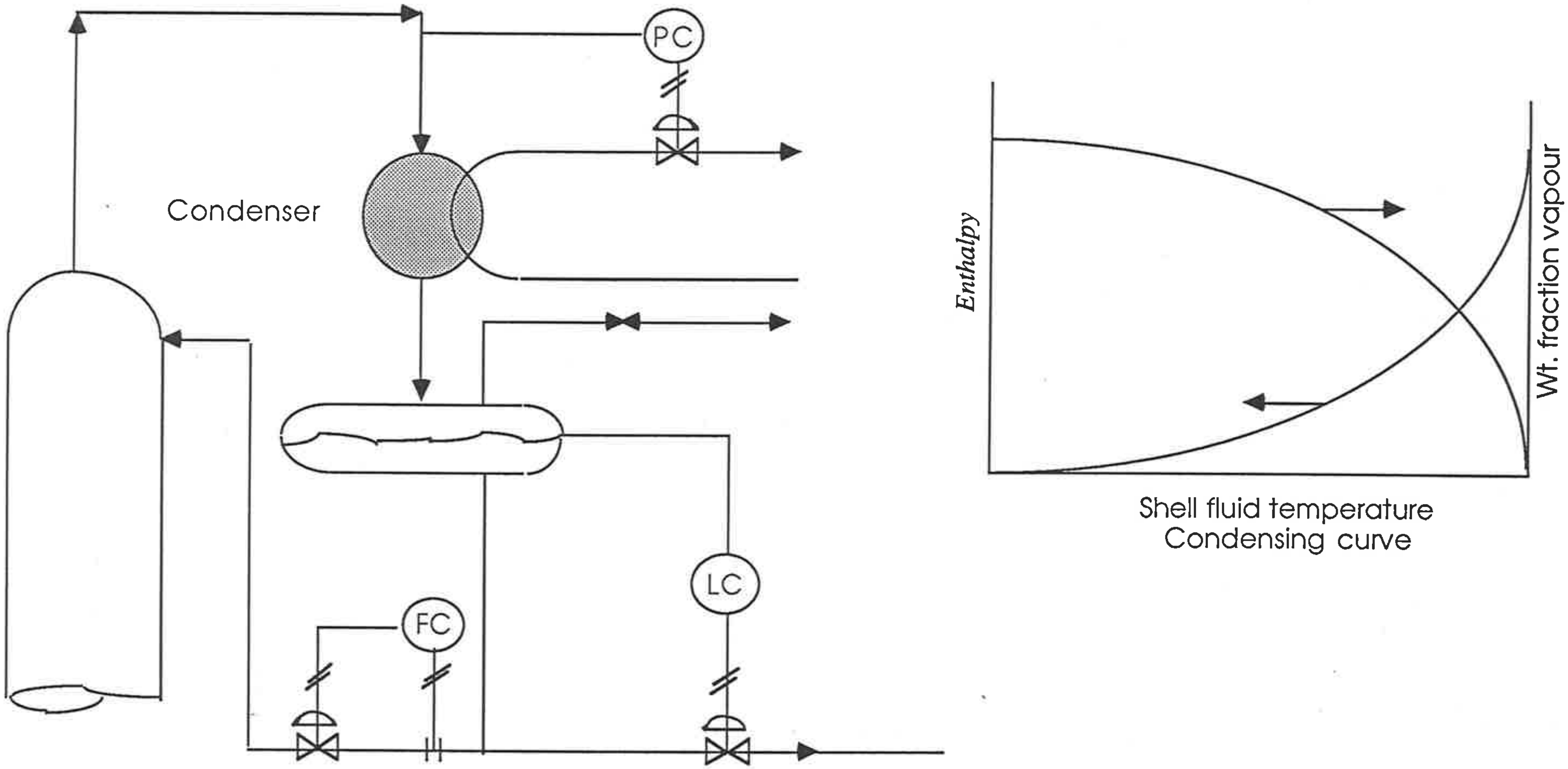


Figure 5.1 Process Configuration for Typical Condenser

case to the high fouling case. Since the values of condition numbers are very small in all these cases, it suggests that fouling in heat exchangers does not affect controllability significantly.

Figures 5.3 and 5.4 show that the profile of the curves in both cases is the same, indicating that the optimal scaling in this case does not provide extra information. However, it seems likely in this case that since nonlinearities are not significant in the heat exchanger model, the conditioning based on a linear analysis would be sufficiently accurate even in the case of high fouling.

5.5 Conclusions

Dynamic operability and sensitivity analyses of a heat exchanger with fouling considerations carried out in this Chapter. Fouling in heat exchangers though a problem does not seem to affect controllability significantly.

The optimal scaling method although reducing condition numbers of transfer function matrix to a very small values have their plots with the same profile as obtained in the unscaled case.

Although the fouling process can be controlled in practice by the use of additives and cleaning methods, the cost of such methods is considerable. Also the idea of oversizing the heat exchanger to overcome the fouling problem leads to the operability problem in the network. Since individual exchangers interact with each other in the network, they are more sensitive to fouling, therefore, it would perhaps be more useful to set up a mathematical model representing the fouled heat exchanger network and to analyse it to see the effects of fouling on it. The networks whose response is not acceptable may be rejected at an early stage. *Fryer et al. 1987*, have studied the operability problems and simplicity of control schemes in the heat exchangers where fouling on the tube side takes place due to milk deposits. However, much work is still be needed for the investigation of dynamic operability of fouled heat exchangers.

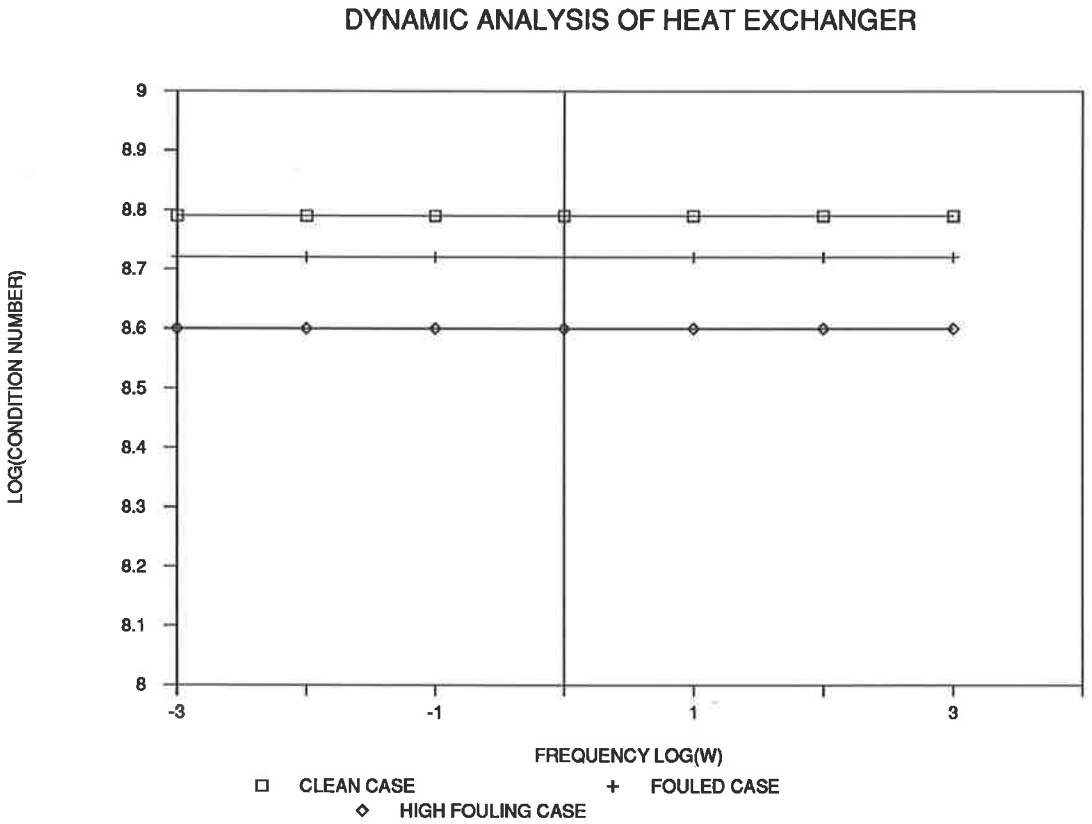


Figure 5.2 Analysis of an Unscaled State Space Matrix

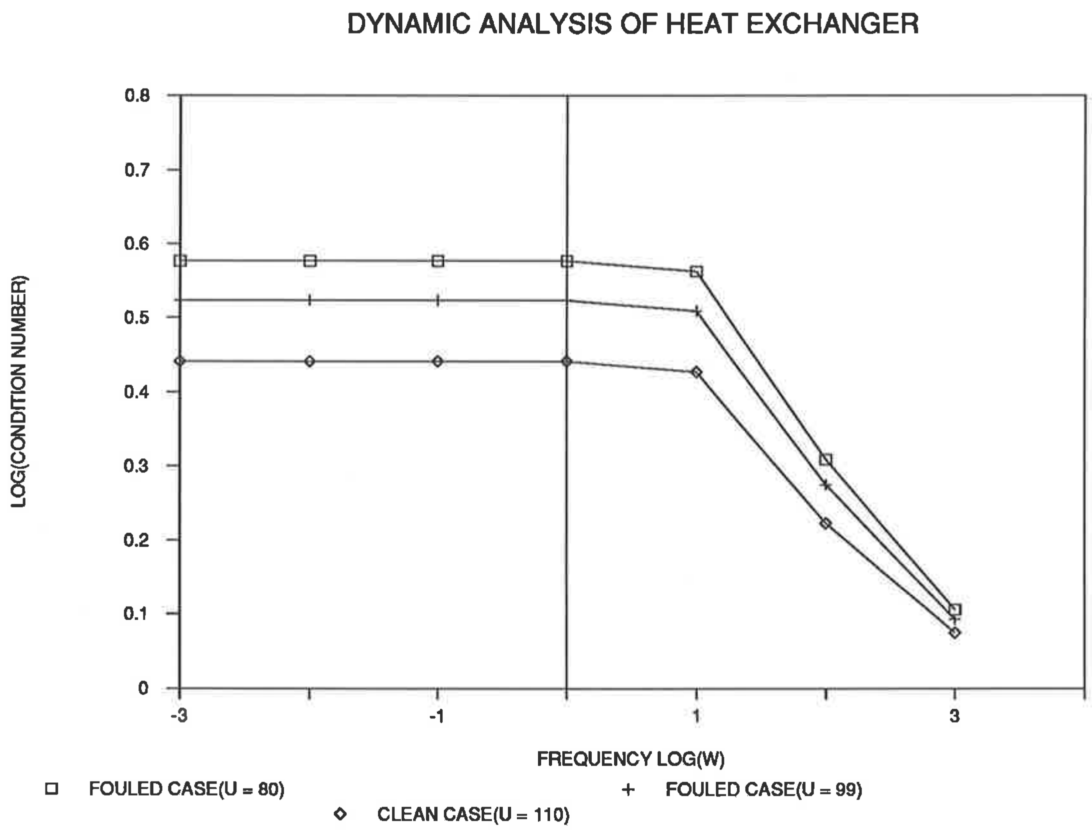


Figure 5.4 Analysis of an Optimally Scaled Transfer Function Matrix

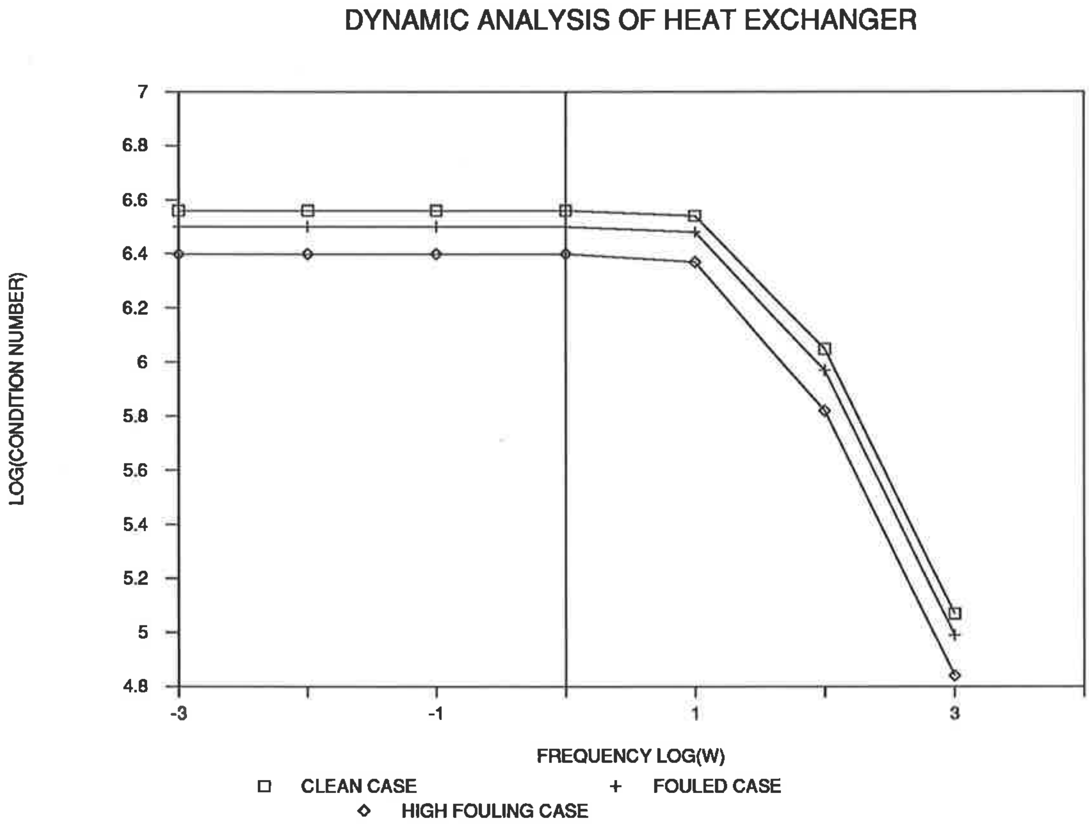


Figure 5.3 Analysis of an Unscaled Transfer Function Matrix

DYNAMIC ANALYIS OF A HEAT EXCHANGER

Table 5.1 Condition Numbers of the Optimally Scaled Matrix

$$G = C(sI - A)^{-1}B + D$$

	HIGH FOULING		FOULED CASE		CLEAN CASE	
FREQ	γ	$\log(\gamma)$	γ	$\log(\gamma)$	γ	$\log(\gamma)$
-3	3.774	0.577	3.334	0.523	2.759	0.441
-2	3.774	0.577	3.334	0.523	2.759	0.441
-1	3.774	0.577	3.334	0.523	2.759	0.441
0	3.773	0.577	3.333	0.523	2.758	0.441
1	3.654	0.563	3.230	0.509	2.671	0.427
2	2.035	0.309	1.883	0.275	1.667	0.223
3	1.275	0.106	1.240	0.093	1.188	0.075

DYNAMIC ANALYIS OF A HEAT EXCHANGER

Table 5.2 Condition Numbers of Unscaled Matrix

$$G = C(sI - A)^{-1}B + D$$

	HIGH FOULING		FOULED CASE		CLEAN CASE	
FREQ	γ	$\log(\gamma)$	γ	$\log(\gamma)$	γ	$\log(\gamma)$
-3	3.61×10^6	6.560	3.16×10^6	6.500	2.54×10^6	6.400
-2	3.61×10^6	6.560	3.16×10^6	6.500	2.54×10^6	6.400
-1	3.61×10^6	6.560	3.16×10^6	6.500	2.54×10^6	6.400
0	3.61×10^6	6.560	3.16×10^6	6.500	2.54×10^6	6.400
1	3.45×10^6	6.540	3.06×10^6	6.480	2.40×10^6	6.370
2	1.12×10^6	6.050	5.97×10^5	5.970	7.05×10^5	5.820
3	1.18×10^5	5.070	1.01×10^5	4.990	7.35×10^4	4.840

CHAPTER 6

DYNAMIC SIMULATION

"It must be remembered that the object of the world of ideas as a whole is not the portrayal of reality.... this would be an utterly impossible task.... but rather to provide us with an instrument for finding our way about in the world more easily."

Hans Vaihinger,
Philosophy of "As If"

6.1 Introduction

The development of a computer program by *(Perkins and Sargent, 1982)*, called SpeedUp is the most dedicated and ingenious work in the area of dynamic simulation of chemical processes. SpeedUp is a process simulation system which can be used for both steady-state and dynamic simulation of chemical processes. It also includes facilities for optimizing process conditions.

The need for development of a dynamic simulation package was due to increasing interest in control system design, hazard analysis and operability studies. Dynamic simulation has evolved quite independently of the activity in steady-state flowsheeting since its roots are in digital simulators of analogue computers hence the forms of the models and data requirement are usually different for the two systems. In 1979, a new package called SpeedUp was developed at Imperial College which incorporated dynamic simulation. It solves differential and algebraic equations used in the models. Using the same program for steady-state and dynamic simulation results in greater efficiency for the user, since much of the data for both types of simulation of the same process is common. Also the same models can be used in SpeedUp for steady-state and dynamic simulation of units.

The system is interactive though an option is available for running portions in batch mode. It is also modular so that the user can change not only data and operating conditions but also the level of sophistication of the models for the various parts of the plant.

6.2 Main Features

The main features of SpeedUp are briefly highlighted below to give an idea of how useful the program is

- It solves steady-state process simulation or design problems.
- Given limiting conditions, it uses an objective function to optimize steady-state solutions.
- For graphical display of the results of dynamic simulations, it is possible to interface SpeedUp to a plotting package.
- It operates from a library of steady-state and dynamic models.

- It creates an environment where processes of any kind may be simply described as sets of equations and procedures, and where the problem description may be modified and updated easily.

6.3 SpeedUp Description

SpeedUp contains all the information entered in problem descriptions on the SpeedUp database. Data for the input file may be written outside SpeedUp and can be stored on the data base from within SpeedUp, or it may be edited directly from the database by using the editor within SpeedUp. Individual sections of the problem may also be edited from within the SpeedUp executive using the editor.

The whole system interfaces with a databank which comprises design data for process models and physical properties. The library includes standard flowsheeting models such as heat exchangers, compressors and distillation columns. It also contains a library of FORTRAN subroutines used by the executive. It is also possible to add more information to the databank.

Since dynamic simulation is the main object of study here only those sections are discussed giving details which are used to specify the dynamic simulation problem. The following sections must be defined to set up a problem:

FLOWSHEET	A process FLOWSHEET, describing the connections between the various units.
MODEL	The modelling equations representing each of the unit-types occurring in the process.

UNIT	The design specifications for each unit, stating which models are used to model particular processes and giving values for parameters used within those models.
OPERATION	The operating strategies to be followed during the simulation, by setting or initializing the values of variables occurring in the process.
DECLARE	The types of streams and variables are defined and upper and lower bounds and initial guesses for variable types are set. The components are identified by name or number.
TITLE	A title section describing the problem may be included.
OPTIONS	An option section is required in order to specify numerical routines to be used, giving printout levels and tolerances.

For dynamic problems, the basic structure of the model remains unchanged. Dynamic aspects may be introduced by the help of equation or procedures. Dynamic equations determine the rate of change of variable with respect to time and are denoted by preceding that variable with a dollar symbol which enjoys the same status as that of the operator d/dt.

6.4 Methods for Solving Nonlinear Equations

Mathematically speaking, the steady-state simulation problem can be represented as the solution of a large, sparse set of nonlinear equations. A review of the numerical techniques is given for such problems by *Sargent (1980)*.

One of the best recent studies is that of *Hiebert (1980)*. The conclusions from that study are that a number of robust and efficient codes are available for solving "well-scaled" problems. However, there are some problems with these codes in some situations. To overcome these difficulties, methods were developed and their details can be found in *Paloschi (1981)*. Much work has also been done on numerical performance of Newton-like algorithms for the direct solution of sparse systems of nonlinear equations. Details of different methods can be found in *Bogle and Perkins (1988)*.

6.5 Numerical Methods for Dynamic Simulation

Numerical techniques in SpeedUp are available to solve a set of coupled ordinary differential equations and nonlinear algebraic equations. Two integration methods, one explicit* and one implicit, are supplied to solve such problems. Methods like Runge-Kutta and linear multistep (Adams) methods fall into the first class. Implicit methods are required for stiff problems because of their increased stability. The Backward differentiation formula proposed by *Gear (1971)* falls into this category.

*At present there are no explicit methods in SpeedUp to solve DAE systems.

Since the implicit methods have extended stability regions, stable solutions may be generated for truly unstable problems. However, this must be recognised when using these methods, and in the case of unstable problems explicit methods are preferred since they usually detect solution growth *(Perkins and Sargent, 1982)*.

6.6 Dynamic Problems

Two examples discussed in previous Chapters, namely a CSTR and a heat exchanger, were selected from the literature and dynamic simulations were performed using the SpeedUp simulation package to verify the results obtained in the dynamic operability analysis. Detailed problem descriptions set up in SpeedUp input language may be found in Appendix D.

6.6.1 Simulation of a CSTR

Dynamic simulation of a CSTR was performed using the set of a nonlinear differential equations (4.7) and (4.8). These equations were written in the model section of SpeedUp.

An operation section was used in order to give different operating conditions for which this model was solved. Initial conditions were provided to give a starting solution. Given below is an example of the OPERATION section used to solve the problem of a CSTR. In dynamic simulation, it is permissible to make certain variables arbitrary functions of time, either using standard functions or using conditional statements.

OPERATION

SET WITHIN CSTR

Da = 0.2

Beta = 0.5

Gamma = 20

B = 7.5

U_1 = If T > 5

THEN

1.1

ELSE

0

ENDIF

U_2 = 0

INITIAL WITHIN CSTR

$$X_1 = 0.1$$

$$X_2 = 1.0$$

These conditions were varied to see the influence of operating conditions on the performance of reactor.

6.6.1.1 Results and Discussions

Figure 6.1 shows response to step changes in reactor temperature obtained by dynamic simulation using SpeedUp at different operating conditions. The simulation results suggest that at high temperature, a small perturbation in the reactor brings it to a very high temperature region where reactor control might cause some problems. Although, it may be possible to obtain better economic return in that region, but due to control problems the best option seems to be to operate the reactor at a slightly lower temperature for the sake of a better control.

Figures 6.1 and 6.2 show that at dimensionless temperature x_{2s} equal to 5, although conversion x_{1s} is very high (0.92) the reactor is pushed to x_{2s} greater than 7 before settling down to normal operating temperature. However, when x_{2s} equals 4, the conversion is still equal to 0.88 and the reactor temperature is greater than 5. The second option is better with regards to reactor control.

Since there is a maximum temperature constraint (x2s <5) in a practical situation (Arkun, 1979), it is more practical and easy to control the reactor if its temperature overshoot remains within the control limits. The response to a step change at (x2s=4,B=15) in figure 6.1 is better than (x2s=5,B=20) with regards to better control as the reactor operates most of the time within the temperature constraints.

Figure 6.3 shows that two different responses to step changes in temperature were obtained when the reactor was operated at x_{2s} equal to 5. Keeping the other conditions

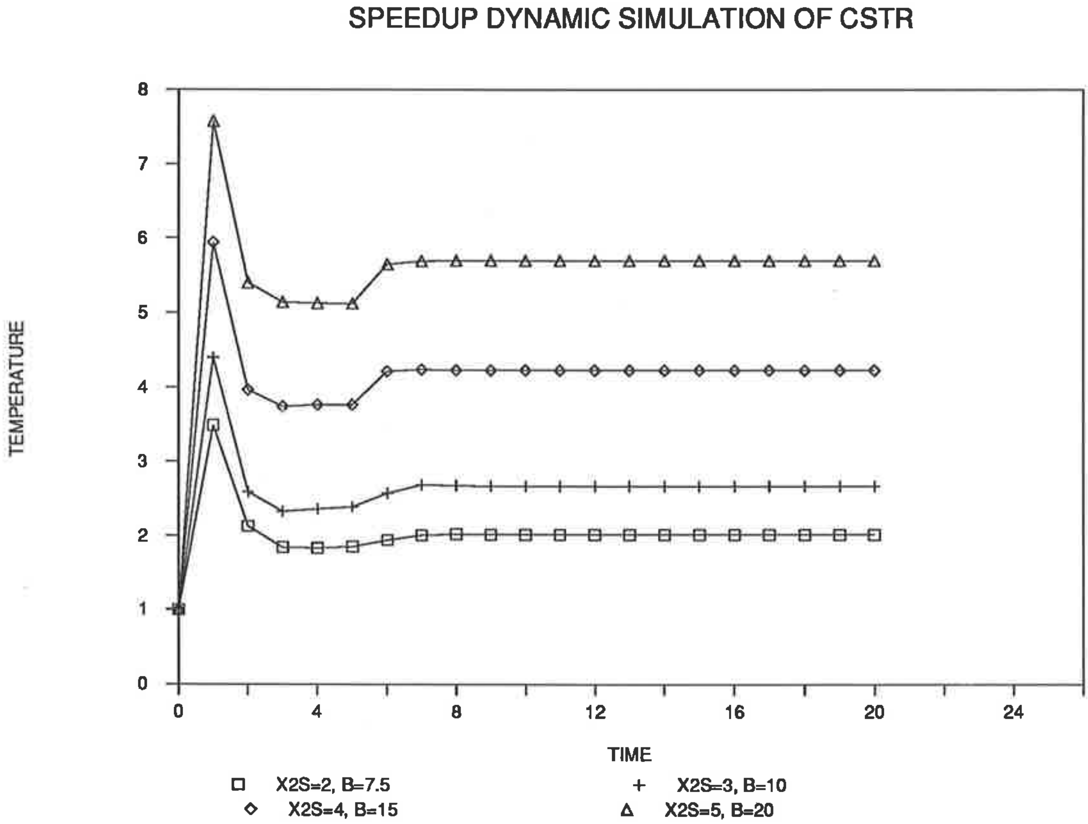


Figure 6.1 Response to Step Changes in Reactor Temperature

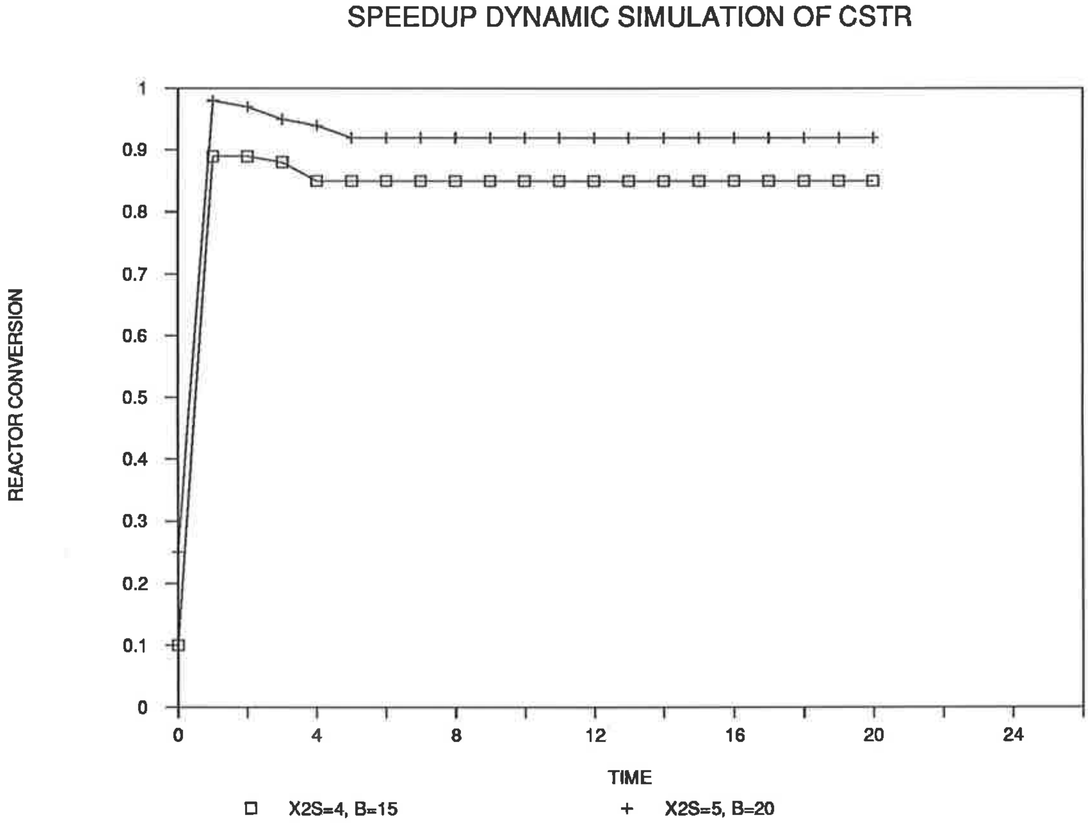


Figure 6.2 Response to Step Change in Reactor Temperature

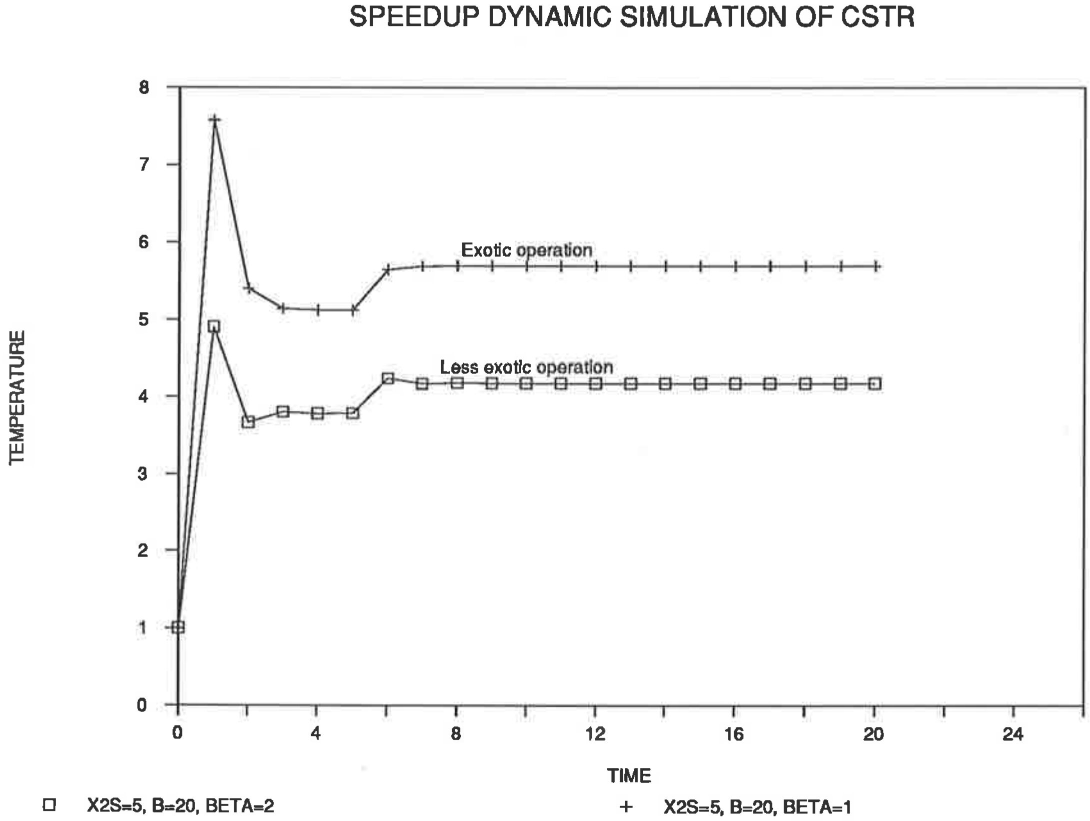


Figure 6.3 Response to Step Changes in Reactor Temperature

(Influence of Operating Conditions)

constant in the reactor a dynamic simulation was performed at two different values of heat transfer coefficient β. When β is equal to 2, less exotic operation is observed and exotic operation is achieved when the value of β is equal to 1.

These simulation results are in agreement with *Ray et al. (1974)*, who suggested that it is possible to achieve more stable and less exotic operation by accomplishing the necessary cooling through increasing the value of β, the heat transfer coefficient.

6.6.2 Simulation of a Fouled Heat Exchanger

In practical situations, the most severe limitations on heat exchanger performance may be the formation of fouling deposits on the heat transfer surfaces which impede heat transfer and increase the pressure drop. The fouling within a heat exchanger, in which the temperatures of the tubes and shell side fluids vary in a complex manner, will not be uniform. Deposition will be concentrated in regions of highest temperature when the fouling is due to reaction, or the lowest flowrate. The value of R_f obtained from the operation of such an exchanger will thus be a lumped parameter, representing an average condition.

Fryer and Slater (1986) have discussed a computational technique for the dynamic simulation of heat exchanger performance in the presence of tube side chemical reaction fouling. In that analysis, they have observed that deposit accumulation obeys the familiar *Taborek (1972)* form of kinetics. The technique employs the method of characteristics to integrate simultaneously the constitutive enthalpy balance equations and the fouling rate equations. Temporal and spatial variations of temperatures through the exchanger have also been taken into consideration by the same authors.

In chemical processes, fouling commonly takes place over a longer time scale. *Sundaram and Froment (1979)* considered influence of coke accumulation on the walls of the furnace tubes in thermal gasoline cracking plants. He described a simulation procedure in which gas temperature profiles in furnace tubes were maintained constant during fouling. Industrially, fouling simulations may be employed in two different ways: to aid in the design of new plant, or in the redesign, for more efficient operation of old plant.

Many experimental studies have been made of the effects of fouling on industrial equipment. In general the fouling factor may increase, at either a constant or a falling rate. The period of fouling may be preceded by one in which the heat transfer coefficient is unchanged, or may increase slightly: an induction period. In many cases fouling eventually reaches an asymptote.

In SpeedUp, the dynamic simulation of a fouled heat exchanger was carried out using the modelling equations (5.14) and (5.15). However, since in practical situation fouling takes place gradually, it is desirable to use a model reflecting the variation of fouling with respect to time. For this purpose a fouling resistance-time relationship can be developed in the form of

$$R_f = (R_f)_\infty (1 - e^{Bt}) \tag{6.1}$$

and it is possible to determine values of constants $(R_f)_\infty$ and B by the help of nomograph developed by Zanker (1978).

6.6.2.1 Results and Discussions

The dynamic simulation of a heat exchanger was performed using the set of equations described in Chapter 2. Initially, it is assumed that the heat exchanger is placed in operation in the clean condition. A sudden change in water flowrate is introduced during the simulation runs in order to see the effect of these changes on the outlet temperature of the heat exchangers. These sudden changes may occur in practical situations on many occasions: for instance, an operational mistake, pump failure, impurities in water circulating in the tubes, etc. Figure 6.4 shows response to step change in flowrate. This figure suggests that when the exchanger is clean a change in the water flowrate does not affect the heat exchanger target temperature significantly. When the exchanger is clean ($R_f = 0$) conditions are such that the excess area in the heat exchanger is not used, and is subjected to fouling.

Figures (6.5) and (6.6) show the simulation of heat exchangers carried out for two different cases, one which represents moderate fouling (U=90) and the other with high fouling (U=80). In the two types of exchangers, the hot stream outlet temperature is greater in the case of counter current exchanger. From the overall results of dynamic simulation, given in table 6.1, it can be seen that for equal amount of fouling, co-current exchangers have the best response, since they are able to compensate for the effects of fouling.

Table 6.1 Effect of Fouling on the Exchanger

Type of Exchanger	Drift in Outlet Temp.(K) (Hot Stream)	$\frac{1}{U_0}+R_f$
Co-Current	326.9-321.9	0.012
Counter Current	328-321.9	0.012
Co-Current	329-321.9	0.013
Counter Current	331-321.9	0.013

Figures 6.7 and 6.8 show the dynamic response to a step change in flowrate in the case of two different types of exchangers. It can be seen from the figures that dynamic effects due to fouling in both the cases are not very significant. These results are in agreement with the operability analysis of fouled heat exchanger in Chapter 5 where the

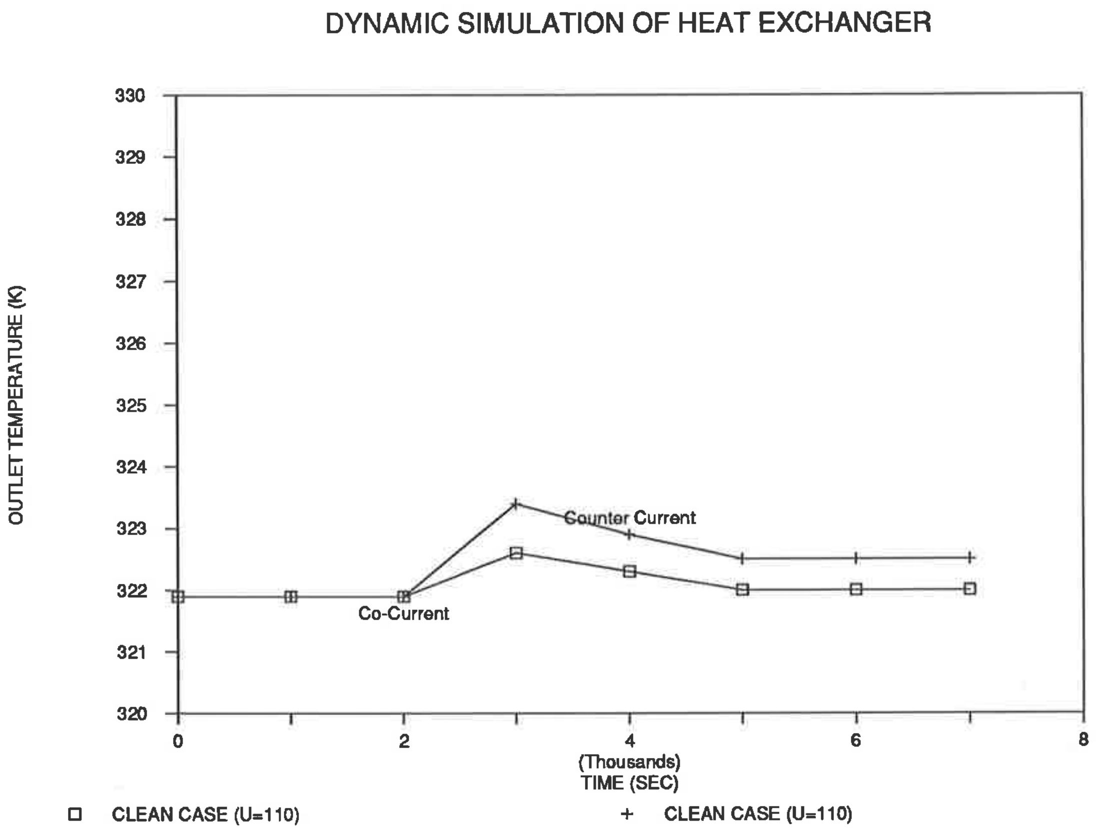


Figure 6.4 Response to Step Change in Flowrate

Variation in Hot Stream Outlet Temperature for a Co-Current and Counter Current Exchanger

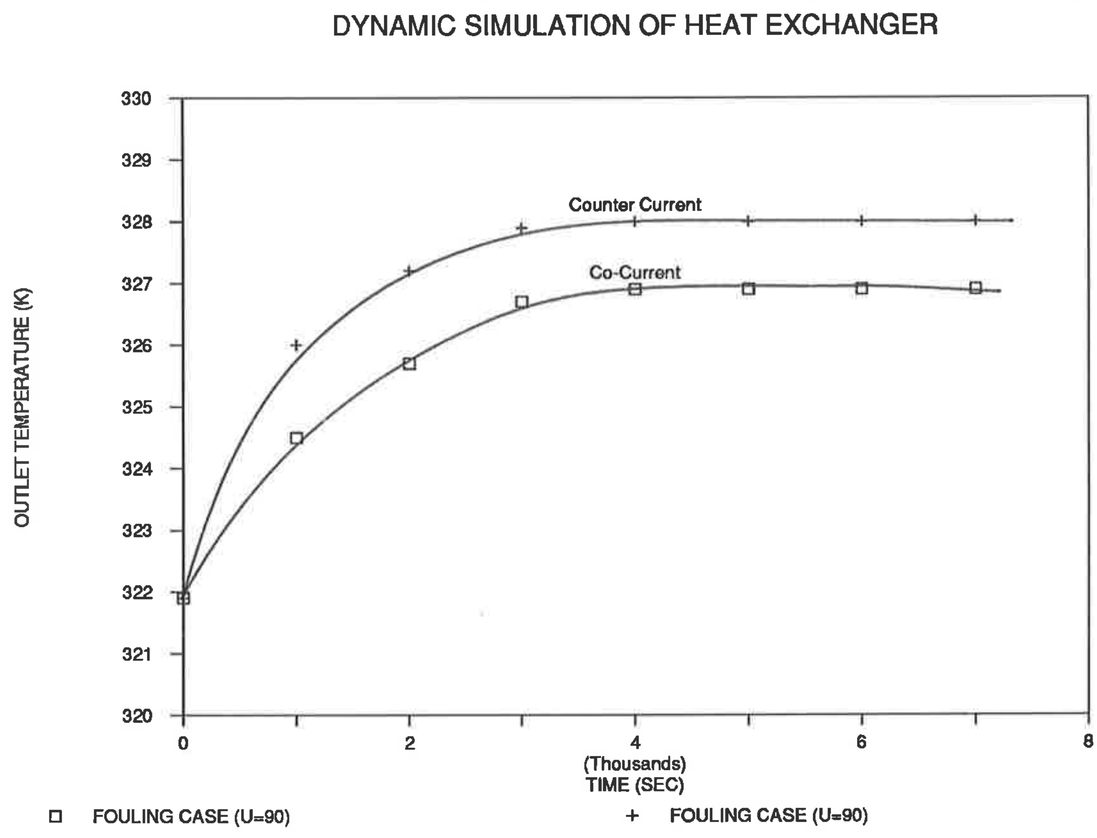


Figure 6.5 Response to Step Change in Flowrate

Variation in Hot Stream Outlet Temperature for a Co-Current and Counter Current Exchanger

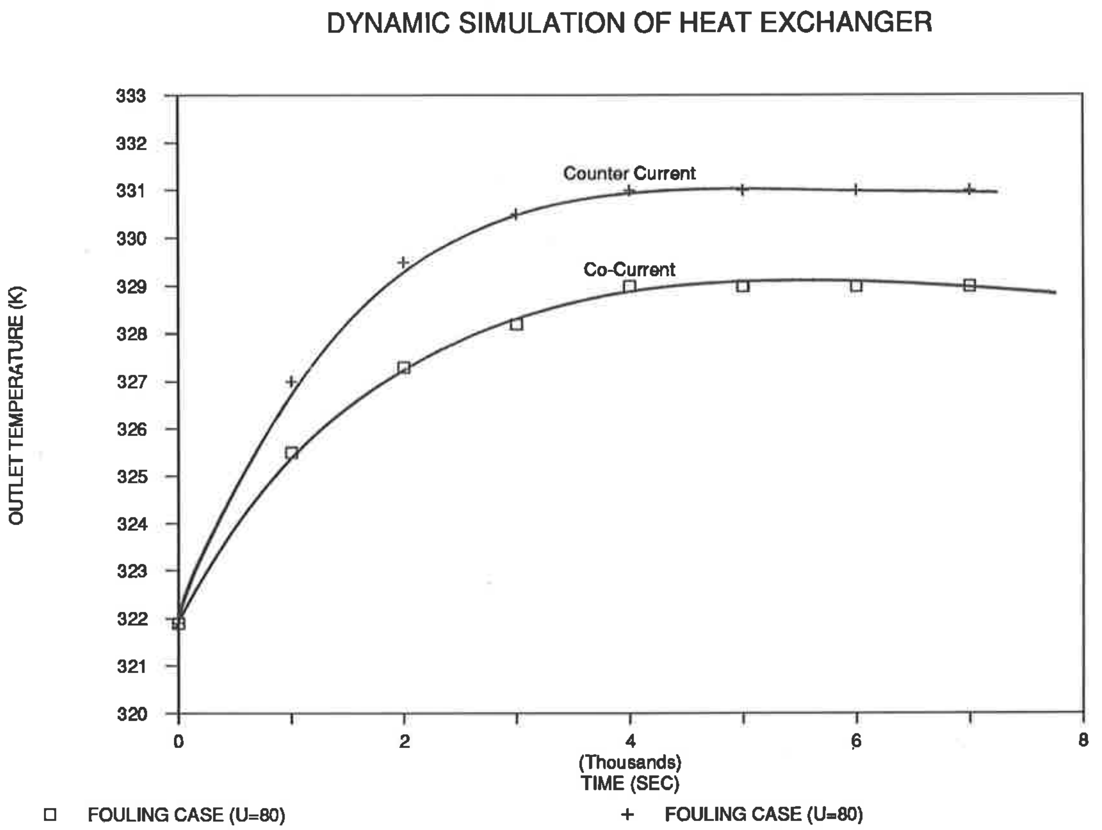


Figure 6.6 Response to Step Change in Flowrate

Variation in Hot Stream Outlet Temperature for a Co-Current and Counter Current Exchanger

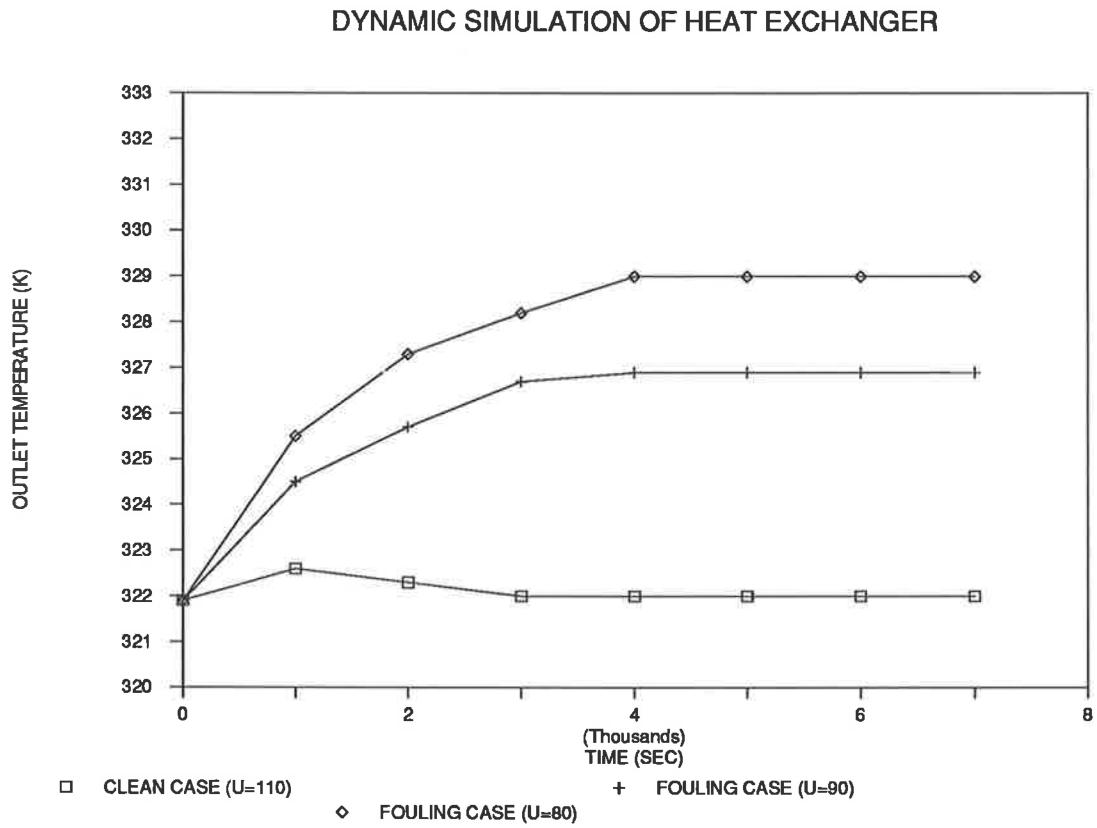


Figure 6.7 Response to Step Change in Flowrate

Variation in Hot Stream Outlet Temperature for a Co-Current Exchanger

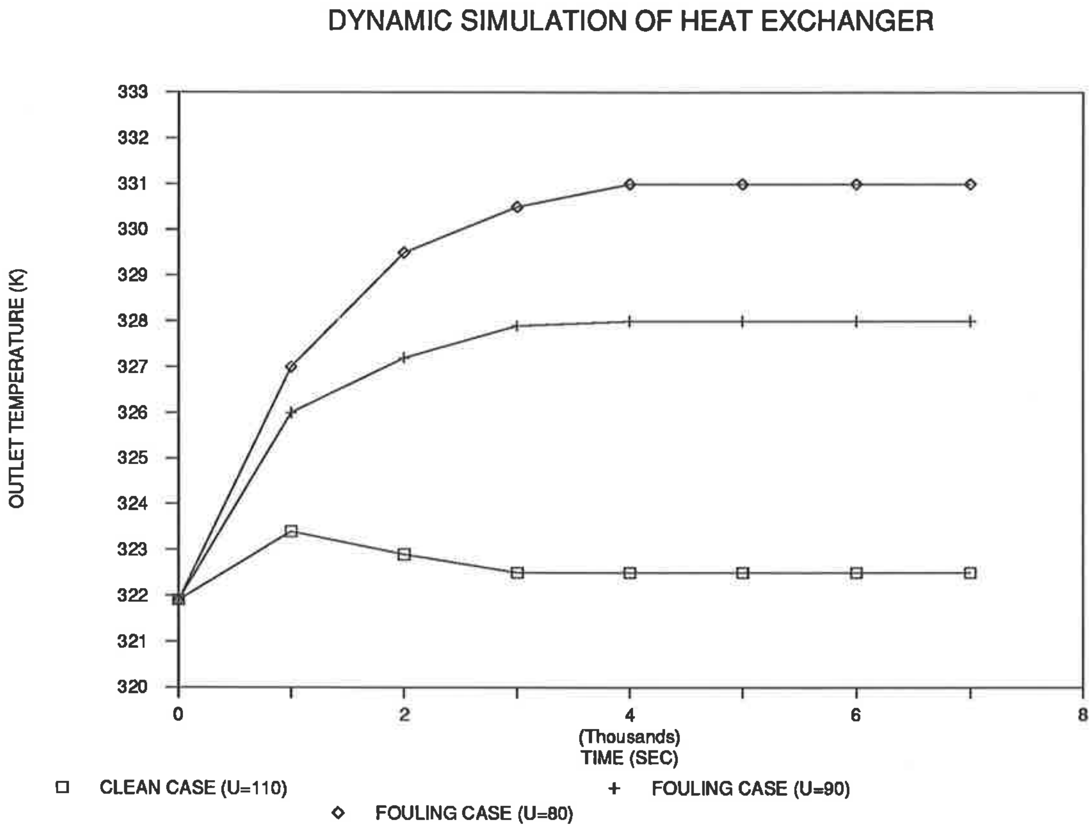


Figure 6.8 Response to Step Change in Flowrate

Variation in Hot Stream Outlet Temperature for a Counter-Current Exchanger condition numbers obtained from the system matrix were very small even in the high fouling case which suggested that fouling in heat exchanger does not affect controllability significantly.

Figure (6.9) explains the simulation results in more details. It may be observed from this figure that as fouling resistance becomes higher than the value used in the design, the drift in outlet temperature becomes more severe which may affect the operability problem in two ways. On one hand an increase in the process outlet temperature may cause difficulties in the operation and on the other hand water usage becomes greater than the design value to control the outlet temperature and therefore a significant cost penalty is incurred due to increased friction losses which will reflect poorly on the profitability of the process.

6.7 Conclusions

Simulation results of a CSTR are in agreement with the dynamic operability analysis carried out in Chapter 4. It has been found during simulation that when the reactor is operated at a high temperature, a small perturbation in the reactor brings it to a very high temperature region where it seems that as predicted from large condition numbers much more effort will be required to control the reactor. Simulation results also show that the best option seems to be to operate the reactor at a slightly lower than the design temperature for the sake of a better control.

Simulation of a fouled heat exchanger reveals that as dynamic effects due to fouling are not very pronounced, fouling in the heat exchanger does not seem to affect controllability significantly. However, a severe drift in hot stream outlet temperature due to fouling in counter-current heat exchanger highlighted by the simulation, can be minimised by the usual methods followed in the industries.

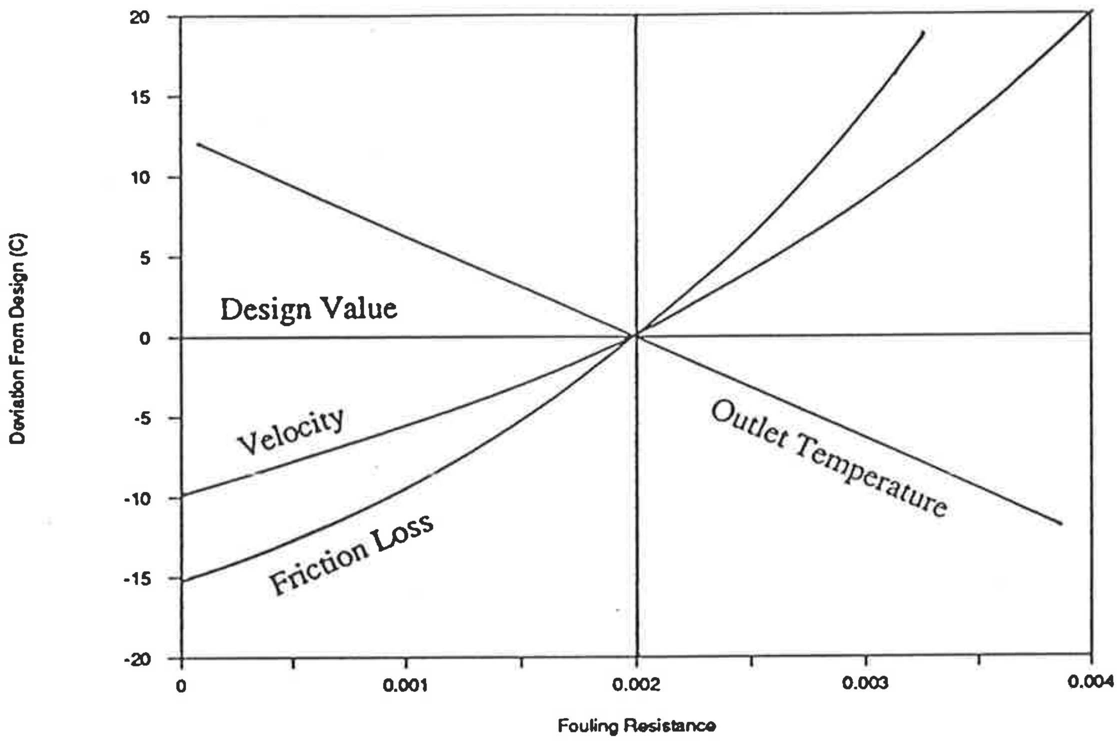


Figure 6.9 Effect of Fouling Resistance on Outlet Temperature

CHAPTER 7

GENERAL CONCLUSIONS

The purpose of the work described in this thesis has been to study the methods for assessing dynamic operability of nonlinear process systems. Dynamic operability is defined as the ability of the plant to perform satisfactorily under conditions different from the nominal design conditions. In order to study dynamic operability of a nonlinear process it is desirable that the process should be stable. If at an initial design stage a thorough analysis of stability can be made with the methods discussed in the thesis, it will be of great help in the operability analysis. For instance, if a plant is unstable it may be rejected at an early design stage before making an extensive studies with regards to dynamic operability. Operability must also be considered early in the process design work. Dynamic simulation plays an important role as it can be used to see whether the results obtained by operability analysis are in agreement with the simulation.

In order to investigate the stability of nonlinear processes considered in this thesis the Lyapunov second method has been utilized. This method gives information on the stability of a system by transforming the differential equations without integrating them to a form from which one can see directly whether the system is stable in a region of interest. Application of Lyapunov's second method to CSTR and heat exchanger systems has shown that the method is useful for stability analysis of nonlinear systems provided a suitable function of Lyapunov is constructed for a particular chemical system. In the analysis it has been shown that the stability regions can be obtained for each steady state conditions by the help of a Lyapunov function. When the method is applied to a heat exchanger, it has been shown that if fouling takes place in the exchanger it will tend to increase the outlet temperature of vapour, thereby decreasing the condensation range of temperature which shrinks the stability regions.

Dynamic operability and sensitivity measures of a CSTR and heat exchanger were carried out by making use of the condition number of the system. The condition number of a system can be used as a measure of sensitivity of control performance to modelling error and as such is a measure of controllability. Although the optimal economic performance of an exothermic reactor is obtained in a region of high conversion and high temperature, the singular value analysis has shown that it may not be feasible to operate the reactor at the optimum conditions because the system is much more difficult to control under those conditions. The system control measure of sensitivity is also evaluated for the model linearised at several steady state conditions over the range of frequencies. The analysis reveals that a system design for one steady state may not be the best at another steady state for a dynamic point of view because of its nonlinear behaviour

Since the singular values are scale dependent, ie; the physical dimensions which are used in defining the variables and the equations, a method of optimal scaling is taken into consideration for the transfer function matrix and the results then compared with the unscaled analysis. At low frequencies while the optimally scaled condition number indicates that high temperature and conversion provide no extra control problems the unscaled results do not agree. This indicates that scaling must be taken into account in some way. The optimal scaling procedure of *Perkins and Wong (1985)* seems to be the most appropriate procedure for comparing sets of conditions which have differing scales. It has also been shown that the condition number of the scaled state space matrix is not a reliable measure of controllability. It masks potential problems with nonlinearities, and although it is scale dependent, scaling policies can remove important information from the analysis. In the case of the heat exchanger, dynamic operability and sensitivity analysis have shown that the fouling does not seem to affect controllability significantly.

Dynamic simulation of a CSTR has verified the operability analysis, suggesting that at high temperatures, a small perturbation in the reactor brings it to a very high temperature region where reactor control might cause some problem. Simulation results also show that the best option is to operate the reactor at a slightly lower temperature for the sake of a better control.

Dynamic simulation of heat exchangers undergoing fouling has shown that as fouling increases in a heat exchanger, the drift in the outlet temperature becomes more severe which affects the operability of the system. However, it has been shown that since the condition numbers obtained by the optimal scaling methods are very small in the case of heat exchanger analysis, the drift in temperature due to fouling highlighted by the simulation should cause difficulties in control. Since in practical situations fouling takes place gradually, it is suggested that a model which reflects the variation of fouling with respect to time should be utilized for the simulation in order to cope with the fouling problems in a better way.

The methods utilized in the thesis for assessment of stability and dynamic operability of nonlinear systems provide a suitable way of looking into the nonlinearities of the system. It is therefore suggested that these methods should be taken into consideration for analysing the system with nonlinearities as this approach enhances the dynamic performance of the process considerably.

Nomenclature

A_r = reactor area

a = constant $=\rho V C_p$

b = constant $=UA_r + \rho q C_p$

C_p = specific heat

c = concentration

F = Jacobian matrix

f = autonomous vector function

ΔH = heat of reaction

K = Lyapunov constant

n = order of reaction

Q = activation energy

q = volumetric flow rate

r = rate of reaction/unit vol.

T = temperature

t = time

U = overall heat transfer coefficient

V = reactor volume

V(x) = Lyapunov function

x = general state vector

y = normalized concentration $=c/c_0$

η = normalized temperature $=\rho C_p T/\Delta H c_0$

ρ = density

τ = time constant $=V/q$

subscripts and superscripts

s = steady state

0 = initial condition

T = transpose of a matrix

|| || = norm of a vector

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APPENDIX A

Consider the Lyapunov function of the the following form as discussed in Chapter 2

$$V(x_{2r}, x_{2r+1}) = x_{2r}^2 + x_{2r+1}^2 \tag{1}$$

where the two dimensional state vector x can be expressed as follows

$$\begin{aligned} x_{2r} &= H_r C\theta_r \qquad r = 0,1,\ldots n \\ x_{2r+1} &= H'_r C'\theta'_r \end{aligned} \tag{2}$$

Taking the first derivative of Lyapunov function with respect to time, the following expression is obtained

$$\frac{dV}{dt} = \dot{V} = 2\left\{x_{2r}\frac{dx_{2r}}{dt} + x_{2r+1}\frac{dx_{2r+1}}{dt}\right\}$$

$$= 2\left\{x_{2r}\left(W_r - \frac{L}{H_r}x_{2r}\right) + x_{2r+1}\left(-W_r - \frac{L'}{H'_r}x_{2r+1}\right)\right\}$$

$$= 2\left\{x_{2r}W_r - \frac{L}{H_r}x_{2r}^2 - \frac{L'}{H'_r}x_{2r+1}^2 - W_r x_{2r+1}\right\}$$

$$= 2\left\{-\frac{L}{H_r}x_{2r}^2 - \frac{L'}{H'_r}x_{2r+1}^2 - W_r(x_{2r+1} - x_{2r})\right\}$$

$$= -2\left\{\frac{L}{H_r}x_{2r}^2 + \frac{L'}{H'_r}x_{2r+1}^2 + W_r(X_{2r+1} - x_{2r})\right\}$$

This derivative is always negative (property 4 of Chapter 2), if the following inequality is true

$$\frac{L}{H_r}x_{2r}^2+\frac{L'}{H'_r}x^2x_{2r+1}>W_r(x_{2r+1}-x_{2r}) \tag{3}$$

Replacing the values from the eqution (2), the inequality becomes

$$\frac{L}{H_r}(H_rC\theta_r)^2+\frac{L'}{H'_r}(H'_rC'\theta'_r)^2>W_r(H'_rC'\theta'_r-H_rC\theta_r) \tag{4}$$

Derivation of eq. (3.15)

In order to get the form given by equation (3.15), first consider the system matrix given by equation:

$$S_m=\begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{3.7}$$

For strictly proper system D=0, the inverse of P is given by

$$P^{-1}=\begin{pmatrix} 0 & C^{-1} \\ B^{-1} & \rho \end{pmatrix} \tag{3.7.1}$$

However the value of ρ is unknown in equation (3.7.1). To get this value we should first calculate PP^{-1}

$$PP^{-1}=\begin{pmatrix} A & B \\ C & 0 \end{pmatrix}\begin{pmatrix} 0 & C^{-1} \\ B^{-1} & \rho \end{pmatrix}=\begin{pmatrix} I & AC^{-1}+B\rho \\ 0 & I \end{pmatrix} \tag{3.7.2}$$

From equation (3.7.2) it implies that

$$AC^{-1}+B\rho=0$$

$$\rho=-B^{-1}AC^{-1}$$

replacing the value of ρ in equation (3.7.1), we obtain the following form of equation (3.15):

$$P^{-1}=\begin{pmatrix} 0 & C^{-1} \\ B^{-1} & -B^{-1}AC^{-1} \end{pmatrix}$$

Numerical Example for a CSTR

$A = 10^8\ hr^{-1}$

$\rho = 641\ Kg/m^3$

$Q' = 1.21 \times 10^4\ °R$

$U = 24.4\ Kcal/m^2h°C$

$A_r = 4.65\ m^2$

$V = 0.71\ m^3$

$C_p = 0.5\ Kcal/Kg°C$

$T_0 = T_A = 520\ °R$

$\Delta H = 2.24 \times 10^4\ Kcal/Kg.mole$

$q = 0.71\ m^3/hr$

$C_0 = 3.20\ Kg.mole/m^3$

APPENDIX B

Operating Conditions for a CSTR

All the quantities used in the analysis are dimensionless, other informations on these quantities and their nomenclature are provided in Chapter 4.

Case 1

$x_{2s}=2$

$x_{1s}=0.3$

$\beta=0.5$

$\gamma=20$

B =7.5

Da=0.2

Case 2

$x_{2s}=3$

$x_{1s}=0.5$

$\beta=1$

$\gamma=20$

B =10

Da=0.2

Case 3

$x_{2s}=4$

$x_{1s}=0.7$

$\beta=2$

$\gamma=20$

B =15

Da=0.2

Case 4

$x_{2s}=5$

$x_{1s}=0.9$

$\beta=3$

$\gamma=20$

B =20

Da=0.2

APPENDIX C

Process Conditions for a Condenser

	Shell Side	Tube Side
Flow	100,000 LB/hr (13.58 Kg/sec)	800,000 Lb/hr (108.64 Kg/sec)
Temperature	150 - 100 F (65.56-37.8) C	80 - 100 F (26.66-37.8) C
Sp. gravity (V/L)	0.01 / 0.5	- / 1.0
Sp. Heat (V/L)	0.4 / 0.6 [Kcal/Kg C]	- / 1.0 [Kcal/Kg C]

Surface Area	4406 ft^2 (409.5m^2)
Heat Transfer Coefficient (Clean)	110 $Btu/hr.ft^{2\circ}F$ (625 $W/m^{2\circ}C$)
Tube Length	20 ft (6.1m)

APPENDIX D

SpeedUp Input for a CSTR

```
FLOWSHEET
 INPUT 1 OF CSTR IS FEED

****

MODEL  CSTR
  SET NOCOMP
  TYPE
        X1,X1DASH AS DIMLESS_CONVERSION
        X2,X2DASH AS DIMLESS_TEMP
        DA,BETA,GAMMA,B AS DIMLESS_NUMBER
        U1 AS FLOWRATE
        U2 AS  TEMPERATURE
  STREAM
     INPUT 1 U1,U2
  EQUATION
     $X1DASH = -X1 + DA *(1.-X1)* EXP(X2/(1.+(X2/GAMMA))) + U1;
     $X2DASH = -X2*(1.+BETA)+B*DA*(1-X1)*EXP(X2/(1.+(X2/GAMMA)))
              +BETA*U2;

     X1=X1DASH;
     X2=X2DASH;

****

UNIT CSTR IS A CSTR

****

OPERATION
     SET WITHIN CSTR
       DA =        0.2
       BETA =       0.5
       GAMMA =        20
       B =          7.5
       U1 =    IF T>5
               THEN
                1.1
               ELSE
                0
               ENDIF
       U2 =          0

      INITIAL WITHIN CSTR

       X1 =          0.1
       X2 =          1

****
```

```
DECLARE
   TYPE
     DIMLESS_NUMBER        = 0:0:25
     DIMLESS_TEMP          = 1:0:10
     DIMLESS_CONVERSION       = 0.1:0:1
     FLOWRATE              = 0:0:1
     TEMPERATURE           = 3:0:1E4
   STREAM  MAINSTREAM
     SET NOCOMP = 1
     TYPE FLOWRATE ,TEMPERATURE

****

OPTIONS
     EXECUTION
     PRINTLEVEL = 4
     TARGET = TERMINAL
****
```

SpeedUp Input for a Heat Exchanger

```
FLOWSHEET
INPUT 1 OF HEAT_EXCHANGER IS FEED 1
INPUT 2 OF HEAT_EXCHANGER IS FEED 2
OUTPUT 1 OF HEAT_EXCHANGER IS PRODUCT 1
OUTPUT 2 OF HEAT_EXCHANGER IS PRODUCT 2

****

MODEL HEAT_EXCHANGER      # TWO STREAM HEAT EXCHANGER  #
SET NOCOMP
TYPE
LT,LS,FLOW_IN_1, FLOW_IN_2    AS ARRAY(NOCOMP) OF FLOWRATE,
FLOW_OUT_1, FLOW_OUT_2  AS ARRAY(NOCOMP) OF FLOWRATE,
XNT,XNS,TEMP_IN_1, TEMP_IN_2    AS TEMPERATURE,
XNTT,XNSS,TEMP_OUT_1, TEMP_OUT_2  AS TEMPERATURE,
CT,CS,SPEC_HEAT_IN_1, SPEC_HEAT_IN_2  AS SPECIFIC HEAT,
TEMP_CHANGE_1, TEMP_CHANGE_2  AS DELTA,
HNT,HNS, MASS_WEIGHT_IN_1, MASS_WEIGHT_IN_2  AS MASS,
A AS AREA,
U AS HEAT_TRANS_COEF,
WN AS DUTY,
LMTD AS LOG_MEAN_TEMP
RESULT
TEMP_IN_1, TEMP_OUT_1, TEMP_IN_2, TEMP_OUT_2,
HEAT_TRANS_COEF
STREAM
INPUT 1 FLOW_IN_1, TEMP_IN_1
INPUT 2 FLOW_IN_2, TEMP_IN_2
OUTPUT 1 FLOW_OUT_1, TEMP_OUT_1
OUTPUT 2 FLOW_OUT_2, TEMP_OUT_2
EQUATION
```

```
# MASS BALANCE #
FLOW_IN_1 = FLOW_OUT_1 = LT;
FLOW_IN_2 = FLOW_OUT_2 = LS;
# TEMPERATURE RELATIONSHIP #
TEMP_IN_1 + TEMP_CHANGE_1 = TEMP_OUT_1 = XNTT;
TEMP_IN_2 + TEMP_CHANGE_2 = TEMP_OUT_2 = XNSS;

# ENERGY BALANCE #
WN = U * AREA * LMTD;
$XNTT = ((LT*CT)/(HNT*CT))*(XNTT-XNT)+WN/(HNT*CT);
$XNSS = ((LS*CS)/(HNS*CS))*(XNS-XNSS)-WN/(HNS*CS);
****

UNIT HEAT_EXCHANGER IS A HEAT_EXCHANGER
****

OPERATION
SET WITHIN HEAT_EXCHANGER
FLOW_IN_1 = 800,000
FLOW_IN_2 = 100,000
TEMP_IN_1 = 80
TEMP_IN_2 = 170
LMTD = 32.75
CT = 1
CS = 0.5
AREA = 4406
WN = 16000000
HNT = 15.30
HNS = 18596

INITIAL WITHIN HEAT_EXCHANGER
        XNTT = 100
        XNSS = 120
****

DECLARE
TYPE
FLOWRATE = 1000 : 0 : 10E8 UNIT="LBS/HR",
TEMPERATURE = 100 : 0 : 500    UNIT ="DEGREE F",
HEAT_TRANS_COEF = 50 : 0 : 200     UNIT = "BTU/SQR.FT*HR*F",
LOG_MEAN_TEMP = 20 : 0 : 55
AREA = 4000 : 0 : 5000        UNIT = "SQR.FT",
MASS = 30 : 0 : 20000      UNIT = "LBS",
DELT = 3 : 0 : 30
DUTY = 16E6 :-1E20:1E20  UNIT = "BTU/hr"
****

OPTIONS
EXECUTION
PRINTLEVEL = 2
TARGET = TERMINAL
****
```