Nonlinear Modelling and Analysis of Chemical Process Systems

Ashley C. Burston

A dissertation submitted to the Faculty of Engineering, University of the Witwatersrand, Johannesburg, in fulfilment of the requirements for the degree of Master of Science in Engineering.

University of the Witwatersrand, Johannesburg, September 1996

Declaration

I declare that this dissertation is my own, unaided work, except where otherwise acknowledged. It is being submitted for the degree of Master of Science in Engineering in the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination in any other university.

Signed this [illegible] day of [illegible] 19[illegible]

Ashley C. Burston.

Abstract

This research outlines a methodology for constructing chemical system models using unit operations as the building blocks. Order reduction of the nonlinear models produced is also addressed. A nonlinear analysis methodology based on bifurcation theory is presented. Bifurcation theory is introduced from an engineering perspective. Finally a nonlinear design technique is illustrated using a CSTR model. Throughout the dissertation, a simple example is used to illustrate the various methodologies.

Acknowledgements

I would like to thank my supervisor Dr Brian Wigdorowitz for his support and insight, also for the many hours spent reading and rereading the manuscript. I gratefully acknowledge the chemical engineering assistance I received from Craig McGregor, especially the derivations for the CSTR unit model and the numerical values he worked out for the simple mixing system. I would also like to thank Andrew Gaylard for improving the Unix environment where I was working and providing many invaluable tips, and computer tools.

I would like to thank SASOL for their continued financial support of this research.

Finally I would like to thank my parents and my fiancé for their encouragement and support.

I dedicate this to my Lord and Saviour Jesus Christ who has gifted me with the ability and the opportunity to complete this work.

Contents

List of Figures

List of Tables

Chapter 1

Introduction

Process modelling and analysis involves the construction of a model for the process in question and the analysis of that model to ensure :

1. The model dynamic behaviour in the operating region of interest corresponds to the process being modelled.
2. The dynamic behaviour of the model in (1) is properly understood.

This means that while a model should as accurately as possible reproduce known behaviours of the plant in the operating region of interest, it should also be possible to use it as a tool for predicting behaviour. These behaviours should be verified using simulation and experimentation.

The research has the following aims:

- To present a methodical approach to process modelling for control (process systems are often complex). Control is often seen as an after thought which is done at the end of a project. The need to produce process control models as part of the design process is emphasized in this dissertation.
- To implement some of the nonlinear bifurcation techniques which have been developed over the last thirty years [22] [24]. The usefulness of bifurcation theory, to predict unexpected and counter intuitive behaviour of the plant is investigated.

Nonlinear modelling of chemical processes can be divided into two types, modelling for design and modelling for control [15]. Almost all chemical models are nonlinear. [5] and [12] are excellent examples of nonlinear modelling of chemical processes for

design. Especially [12], whose *Circulation Loop Reactor* only works because of its exploitation of a nonlinear phenomenon. [9], [11] and [23] discuss nonlinear modelling and analysis for control. An interesting result presented in [11] is that a CSTR with a controller containing a time delay could be made chaotic.

A key method in engineering for nonlinear analysis is bifurcation analysis [24]. This involves the linearization and parameterization of nonlinear models [2]. All the equilibrium points of the chemical system in question must be found using continuation methods [22]. The nonlinear model is linearized around all of the possible equilibrium points and this information is used to detect changes in stability [18]. This information is then used to determine when to use more computationally intensive forms of nonlinear analysis [16] [23].

The approach adopted in this dissertation as detailed in Chapter 2, is to introduce two methodologies. The first is a nonlinear modelling methodology which addresses the problem of complexity. The second is a nonlinear analysis methodology which implements the theory of bifurcations to some extent. Using these two methods it is believed that many of the problems associated with nonlinear chemical process modelling and control can be solved. In the current literature there seems to be no uniform methodology for process modelling and control design. [12] presents a modelling methodology, but it is primarily a chemical design approach and requires their software.

A simple mixing system was used to illustrate how the methodologies should be implemented. It was shown that the model for the mixing system as a whole required 17 states to describe its dynamics. This model was found to be cumbersome. The model was reduced using decoupling and time scaling and it was shown that the model which described the essential dynamics of the system was second order. The reduced model was then analysed and the system was shown to exhibit limit cycle behaviour for certain values of the chemical process parameters. It was shown that the analysis methodology significantly reduces the time required to analyse the system when compared with simulation.

The research aims were addressed as follows :

Chapters 2-5 present the modelling methodology. Chapters 6-7 present the nonlinear analysis methodology. As a result of the application of the methodologies to the system example, the intial stages of a nonlinear model design technique were developed. The technique is presented in chapter 8.

Chapter 2

Overview

2.1 Current Approach to Process Modelling and Control

Industrial chemical process control is a field which is receiving increasing attention. The approaches currently used in this field are essentially no different from those used in the most fundamental classical control. The standard controller which is implemented in chemical processes is the PID (proportional-integral-differential) controller [15]. This is a simple linear controller which dates back to the earliest beginnings of process control.

The use of control theory in the chemical process area does not appear to be as advanced as in other areas. This is due to the fact that chemical systems are said to be more difficult to model than in other fields. The result of this reasoning is that when control systems are designed for chemical systems more controllers may be used than is actually necessary. Even the simplest chemical processes can contain ten or more controllers (usually PID). The justification of which is usually given as safety considerations. While the maxim, "rather safe than sorry" is a good one it is tremendously expensive as every control loop implies not only that you have a controller but expensive sensors and actuators, all of which have to be maintained throughout the life of the plant.

The designers of chemical process control systems often do not have accurate models of the process, so using experimental data, simple, trusted controllers are implemented. While this method of control is acceptable when you have no other way of approaching the problem, it can be highly inefficient as it results in very conservative designs (large safety margins have to be implemented). This approach has been

perpetuated with the use of fuzzy controllers. The idea is that with little knowledge of the plant one can achieve good controllers, this is a fallacy. The knowledge of the plant is simply presented in another way, namely rules. Not only are there too many control loops, they also result in systems which tend to be inefficient. With increasing global competition and international trade agreements, companies are continually demanding better efficiency from their processes.

The source of the problem with chemical process control is the lack of reliable dynamic process models [20]. The models that result from chemical processes are also often of high order even for relatively simple systems. There are several steps which need to be achieved in any field where control systems are going to be implemented. The first is to model the physical reality using a minimum of simplifying assumptions and any form of mathematical modelling which is appropriate. The next step is to convert those models into ordinary differential equations which are compatible with process control techniques.

The key to improving the current situation is to develop a method of modelling chemical processes which is simple and reliable. The development of models for individual unit operations is an important aspect of any attempt at chemical process modelling and is indeed a fundamental step. This has however already been addressed in the chemical engineering literature [19], at least for simple systems. The focus of this dissertation will be to develop a methodology for combining sets of simple chemical process units to form an overall model for a process. It will also focus on the nonlinear analysis of such systems with a view to reducing and simplifying such models. The end result will be a useful model for control design.

2.2 Nonlinear Process Modelling and Control

Nonlinear process modelling and control has been an intellectual backwater in engineering for many years. With the popularization of chaos and fractals, renewed interest in the field has begun to generate interesting research. The potential for advances in the way control is approached because of these changes should not be overlooked. While linear methodologies have in some areas stagnated, nonlinear process modelling and control still has to be "discovered". The focus of this section is nonlinear chemical process modelling and control.

Linear dynamic models are the most common form of dynamic chemical model available. Most static models of chemical systems are highly nonlinear [20] as this

is required for efficient design of the operating points. Dynamic models are usually linear because it is much easier to model a process at a set point for small perturbations than to model it for its entire range of operation. Consider a system made up of submodels. Linear models can be derived by formulating a complete nonlinear dynamic model of the system and then linearizing the system, about various operating points as is done in this dissertation [19]. Often however, it is easier to use several sets of linearized models which are constructed to work around the operating point to produce a dynamic model for the system. This results in the situation that the model is only valid for a particular operating region. This means that the model cannot be trusted for large variations of the states around the operating point (the neighbourhood of valid operation can also not be determined). It means that if the states are varied too much the control system behaviour is unpredictable.

When there is a lack of information about a particular chemical system the standard control modelling approach is to obtain step responses (or transfer functions using any available information) for the system around a particular operating point. It must be kept in mind that the important information for control engineers is the dynamic response of the plant. Using the step response information for several operating conditions a suitable linear model with respect to the application would be chosen and control design would proceed. In most situations this gives rise to acceptable controllers and the chemical process unit in question operates as is expected. Every so often, however, a chemical process will be difficult to control and give a nonlinear behaviour which makes a linear controller effective only within a small operating region. Due to the nature of chemical systems, which are often long straight line processes, this single nonlinear process can cause the entire process to fail.

The logical way of approaching this problem is to begin to use nonlinear models which relate to a particular process and devise online and off-line tests which enable the control engineer to determine the nonlinear structure of the dynamics of the system. This would mean that step response (and other) information would still be used, but interpreted in terms of a nonlinear model which is appropriate for a particular process (distillation column, CSTR, etc). Work has been done in the area of nonlinear parameter estimation [10] using bifurcation theory, but this relates to chemical process design modelling and not control modelling. It must always be kept in mind that while design models are useful as sources of information for the control engineer, they are not useful for designing the actual control system.

Nonlinear control modelling for chemical processes appears to be a neglected field.

Control modelling is discussed in [15] but from a linear perspective. Nonlinear models which are useful for control were developed in [19]. The nature of a nonlinear control model is different to a design model. A control model tends to focus on retaining physically meaningful states (that is states that can be measured). In design equations however the models are usually converted into a form which allows the system to be scaled up easily. This involves the use of special design nondimensional terms or "numbers" (*Biot number, Damköhler number, etc*). These are often used as the bifurcation parameters (see chapter 6 and [14]).

Work has actively been done in dynamic nonlinear design modelling in chemical engineering ove. the last decade. Some excellent work has been done in the area of nonlinear behaviour and bifurcations. In [14] an overview of the behaviours exhibited by a CSTR with a simple chemical reaction is given. This paper shows that it is possible to get limit cycle behaviour for certain parameter values. The analysis is however done in terms of nondimensional design parameters as opposed to measurable variables. Measurable variables could be derived from the design numbers but this introduces more complexity into the control problem. Another aspect is that often control models can be simplified by replacing distributed parameter models with lumped parameter models. A control model is designed around the inputs and the outputs with no concern as to how the variables vary between these points.

In [5] the behaviour of an *auto-thermal tubular packed bed reactor* is modelled and analysed using bifurcation analysis. In [12] the *circulation loop reactor* which has a limit cycle as its normal mode of operation is discussed. Again however the focus of the modelling is understandably on the design and analysis of the reactor.

A new approach which is suggested in this dissertation, is to design the control system of a nonlinear chemical unit, into the system from the start. What this involves is developing both the design and control models simultaneously at design time. This means that some of the control problems that could arise in a nonlinear system can be assessed and appropriate changes made. It also becomes possible to exploit nonlinear behaviour as was done in [12]. The method outlined in chapter 8 and in [7] give possible ways of achieving this. The theory in [21] supports this approach theoretically.

The field of nonlinear control systems is summarized in [1]. The book focuses on the theory of control and gives a summary of nonlinear concepts from that perspective. The examples in [1] are given in almost every engineering field except process systems. Examples of where nonlinear process control has been suggested are [8] and [9]. Interesting examples where chemical process controllers produce nonlinear

behaviour are given by [6] and [11].

The nonlinear analysis in this dissertation uses elements of bifurcation theory. [24] gives an overview of the theory while the numerical methods employed are similar to those described in [22]. [16] is an introduction to the field of nonlinear dynamics while [17] gives an introduction to chaos. Bifurcation theory for control has been applied (as opposed to only being postulated) in the aeronautical control field [13].

In conclusion, the field of process control needs to be increasingly updated with respect to the current developments in chemical process design. The rapid advances that are occurring in the field of nonlinear dynamics have a profound effect on how process analysis and design [4] and process control design should be approached. This is because control design revolves around the dynamic behaviour of a system. The advantages of exploiting increased understanding of nonlinear dynamics have to be realized so that chemical processing companies can remain competitive.

2.3 Proposed Methodology

The method proposed in this dissertation involves two steps. The first is the construction of a model for a chemical system by interlinking known models of each of the components. The second is the analysis of those models using elements of linearization analysis [2] and bifurcation theory. The aim is to not only work towards a reliable modelling methodology but also to practically apply nonlinear analysis techniques.

The construction of models from first principles is not the focus of the dissertation but was a neccessary step as no unit models existed in the format required for easy linking. Existing models where adjusted for this purpose. What this means is that no models were developed from partial differential equations but where derived using existing ordinary differential equation models.

The methodology can be broken down into the following constituent parts :

Model Construction

- Construction of models for individual units from physical principles.
- Conversion of models into ordinary differential equation (state space) format.
- Construction of system equations by linking the individual models for each

unit operation.

Analysis and Model Order Reduction

- Model order reduction using decoupling, time scaling and physical reasoning.
- Limitation of the states and parameters (the dimension of the state-parameter space is made finite).
- Analytical calculation of obvious equilibrium points.
- Numercial calculation of remaining equilibrium points.
- Linearisation around equilibrium points and bifurcation analysis for the ranges of parameter values given.
- Identification of quasiperiodic and other forms of behaviour using simulation.

This methodology is defined as model development by [15]. Figure 2.1, taken from [15] gives the place of this methodology in the process control development cycle. The method is part of the *develop process model* section shown in figure 2.1. It involves two of the attached items in the diagram, that is computer simulation and physical and chemical principles. Plant data, while being useful for verification is not used to develop the models or even tune their parameters. Methods to achieve this will have to be investigated in further work.

The analysis methodology itself can be broken down into the following seven steps :

1. Limit states and parameters to some finite state-parameter space using physical reasoning and plant information.
2. Examine equations for any obvious analytical solutions for the position of the equilibrium points.
3. Visualize the magnitude of the vector field to determine the location of possible equilibrium points (this information is used to choose starting points for the numerical algorithms).
4. Solve numerically for the equilibrium points for different parameter values.
5. Linearize the system at all of the equilibrium points found in the previous step and find the pole positions in the s-plane.

6. Determine the bifurcation points and the types of bifurcations.

7. Simulate in the unstable regions to determine global stability behaviour.

The analysis methodology is shown in figure 2.2. The technique is similar to that used by [12] when they simulated the behaviour of a circulation loop reactor. This reactor's operation depends on the existence of a limit-cycle to operate. The reactor was simulated using the DIVA [12] package which uses various methods to reduce the partial differential equations into high order ordinary differential equations which are then analysed for stability. The bifurcation information about the system is then obtained using the movement of the poles in the s-plane. The difference between their method and this dissertation is that they started with partial differential equations which they converted using numerical methods to ordinary differential equations (which are of a very high order). This work starts with pre-developed sets of ordinary differential equations which have been verified.

2.4 Philosophy of Approach

The importance of having a set philosophy of approach [3] to the problem cannot be over estimated. The simplest principle of reasoning is that if your premise is incorrect, so will your conclusions be incorrect, no matter how well you argue from your false premise. There is a possibility that if you argue from a wrong premise incorrectly, that you may accidentally come to a true conclusion. The reverse however will in all probability occur.

This same argument can be applied to control theory. If you have a badly defined problem (model) and hence can only set up an approximate set of specifications based on general rules, you will at best get an adequate solution (not a highly efficient one). To use one of the current catch words of control engineering to restate this more elegantly : A fuzzy model leads to fuzzy specifications which in turn will lead to fuzzy performance.

The key idea on which the work here is founded is this : To get better performance and reliability from a chemical process, you have to know more about that chemical process. There are two areas to which this philosophy of approach is being applied. The first of these areas is the actual modelling of industrial chemical processes. The second area is the analysis of the nonlinear models which many chemical processes produce.

The aim is to develop both areas sufficiently to enable others to refine and develop methods which ultimately should have an impact on the way chemical process control is approached. The methodologies should be implemented before the specification stage of control design. Setting up specifications requires an accurate model and understanding of what the model represents. Hopefully this research will help towards providing a clearer picture of chemical processes and their behaviour.

One of the important steps taken in this research was to move away from general models (such as the linear second order prototype) and move towards definite models which are associated with a particular component (unit operation). This means that the types of nonlinearities which will be encountered in the state space equations will be limited by the physical characteristics of chemical processes. This ensures that the time spent analyzing nonlinear systems will be useful as it applies directly to some existing system.

There are many related issues, all of which are of importance within process control. These however will have to be neglected for the sake of focusing on the primary problems of obtaining a model and then analyzing the behaviour of the model (which may be chaotic). The belief is that as analysis proceeds on a variety of systems, patterns will emerge which can be exploited to enhance understanding of nonlinear systems in general and chemical processes in particular.

The questions that motivated this research are :

- Is there a need for the tremendous amount of control implemented on current chemical processes?
- What impact does our improved understanding of nonlinear systems have on engineering processes? (Could it reduce the amount of control apparently required?)
- Can linear models be trusted to model chemical processes with the presence of inevitable parameter variations?
- Is it possible to make the analysis of chemical systems as straight forward as the analysis of many electrical systems?

Designers of control systems are often drawn towards black-box approaches. The reason is that these approaches make the attractive, yet impossible claim that with little or no knowledge of the plant, efficient control can be achieved.

The belief held in this dissertation is that if process modelling became more accessible to control engineers through the development of sets of rules and tables, more engineers would find it practical to use and white-box models would become more common in chemical process control. This line of thought is followed throughout this work.

The aim of this section is to provide a philosophical basis for this research and for future work.

2.5 Object Oriented Approach

The movement in recent years towards object oriented programming has caused the philosophy of approaching complexity to become more developed. This is particularly applicable to the field of nonlinear dynamics. The inherent complexity of continuous nonlinear dynamical systems has resulted in an avoidance of the topic in many research fields. The author however believes that approaching the topic in a specific way, which will be outlined, will prove tremendously rewarding in the future.

The approach which the author has come to believe in is the approach used by software engineers when faced with the incredible complexity that characterises modern software projects. The chief concept which has been formalised to a greater degree than ever before for complex systems is the concept of abstraction. This has been formalised into two concepts, objects and classes. An object is a specific instance of a phenomenon or behaviour which the researcher is looking for.

An example would be a chemical reactor with certain ranges of flow rates and chemical reaction rates. This is a specific physical object and is by no means general. It does however belong to a broader class of things called chemical reactors and hence the nonlinear equations which describe the behaviour of the reactor also belong to their own general class. Most equations encountered in these chemical systems can be solved numerically but often specific numerical values for parameters are difficult or impossible to measure and can only be obtained by inference. This means that it would be useful to have an idea of how general classes of chemical units behaved for ranges of parameter values and also which parameters are important. This kind of information could not only be useful for those trying to control and debug existing systems but also to those designing chemical process systems.

An "Object Oriented" approach to nonlinear research opens up the field, because

it breaks down the inherent complexity into small enough chunks for researchers to handle. This approach is nothing new but has always been practised implicitly. Recognising what we have been naturally drawn to conclude by experience through use of a formal technique is a step forward in any field. The further qualification which applies to engineering research is that the objects which are used to develop the classes must be firmly rooted in physical reality. This rather than being a hindrance to discovery, is a help as it ensures that all the research conducted is relevant and that years of research are not wasted on creating practically useless abstractions. It is interesting to note that physical systems' equations exhibit symmetry which is not necessarily true of arbitrary equations.

In this research, being able to limit the type of nonlinear systems discussed by using chemical units is highly advantageous as it ensures that the research remains narrow enough so that results can be obtained. It also means that everything that is discovered has practical implications and hence the research is automatically more useful to practising engineers.

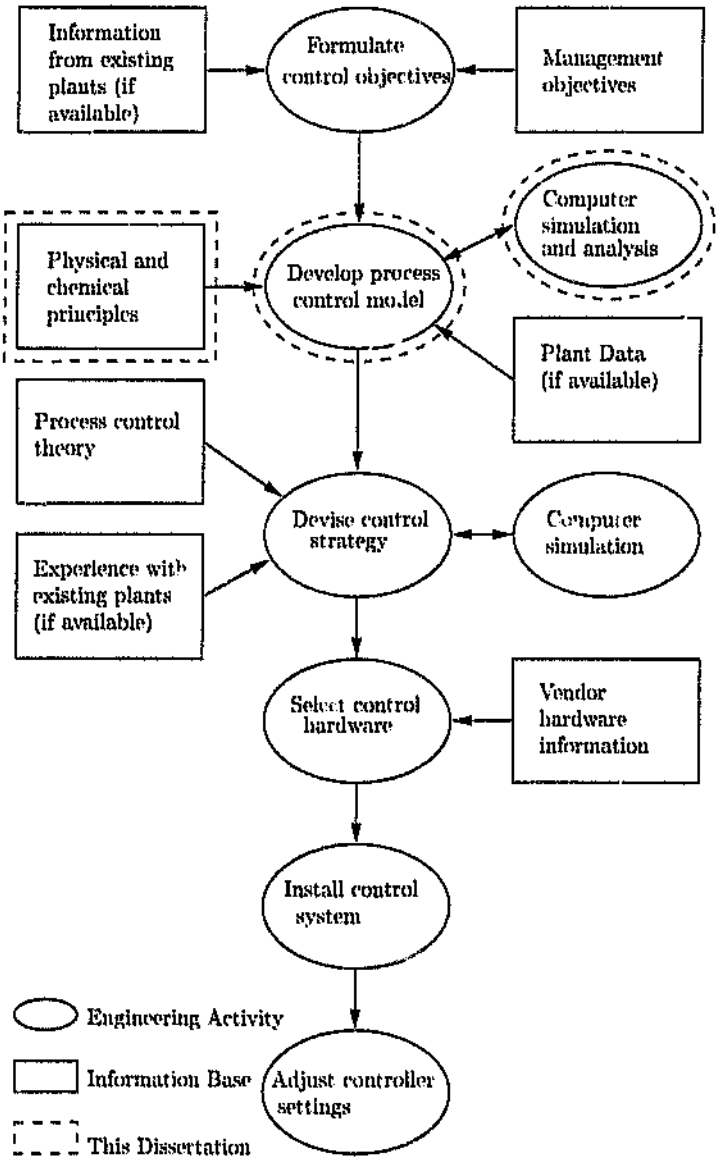


Figure 2.1: Major Steps in Control System Development

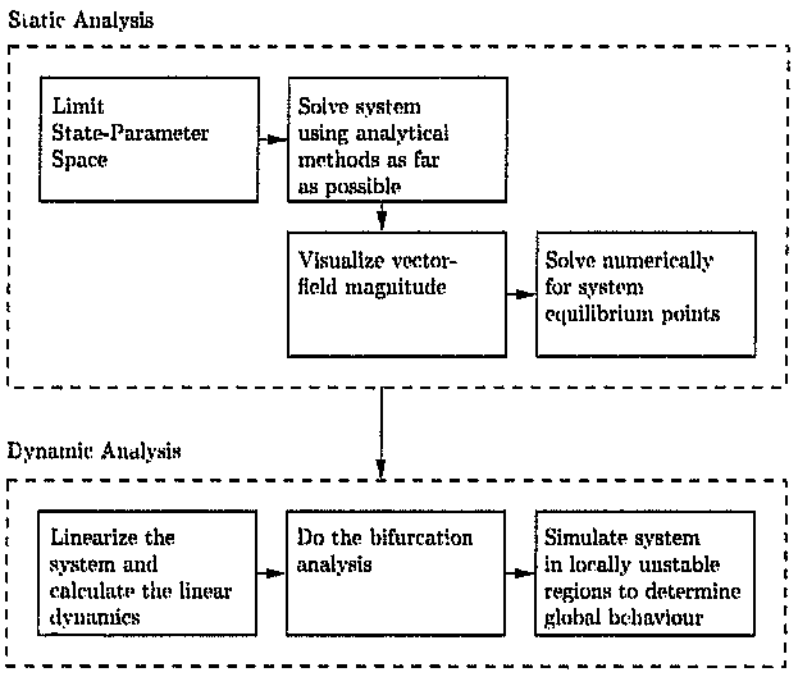


Figure 2.2: Analysis Methodology

Chapter 3

Unit Operation Models

3.1 Introduction

Industrial chemical processes consist of sets of unit operations in the same way that electrical circuits consist of electronic components. The chemical unit operations are often much more complex than their electronic counterparts but can still be linked together to form more complex systems. The aim of the control engineer is to obtain ordinary differential equations for unit operations which are based on physical principles.

An important point to be made is that although for electrical and even mechanical systems there exists a vast resource of modelling tools for control, there has been very little equivalent work done in the area of chemical engineering. Accurate static models exist, however these are of little use to the control engineer who wishes to design the controller to give certain dynamic characteristics. Static models are also of limited usefulness when nonlinear behaviour is encountered. As is the case with electrical systems, a systematic and modular approach has to be developed for constructing models. In circuit analysis, there are many such techniques which can easily be computerised and used to analyse complex systems. If for chemical engineering such a system can be developed, even apparently intractable chemical engineering problems can be analysed by using a very simple and repetitive methodology which can be carried out by a computer.

The most important step is to build up a library of accurate ordinary differential equation models for every conceivable unit operation. This is beyond the scope of this dissertation although the techniques for going about such a task will be discussed. A standard format for models will also be suggested to ensure compatibility with future work. Once a sufficient library of unit operations has been developed,

other unit operations can be developed by combining existing library units. These modules can then be linked together on the basis of information contained in a process instrumentation diagram for the plant to be modelled. The other information, such as the type of chemical reactions occurring in each unit can then also be entered into the model and libraries of reactions could also be constructed. Although ordinary differential equations have limitations in terms of the types of systems they can model, this is much better than using empirical data and assuming some kind of linear system.

The construction of process modules which are based on unit operations has some interesting results. Firstly it becomes clear that certain aspects of chemical systems remain the same. The structure of the equations to be expected are consistent in certain respects. There are however certain areas of the equations where non-standard structures can enter the system. These areas are the chemical kinetics (the reaction rates) and types of reactions occurring. These can all be contained in a simple modelling system. Certain rules for modelling need to be decided upon and adhered to religiously to ensure consistency.

The following sections will illustrate the construction of such models and justify a simple set of rules which can be used to create modular unit operation models.

3.2 Simple Tank

3.2.1 Description

The incompressible fluid (liquid) tank is the simplest unit operation. It is simply described by a mass balance equation and an energy equation. This model assumes no change of state is occurring in the tank. The model does however take changes in temperature of the liquid in the tank into account.

3.2.2 Assumptions

- No changes of state or chemical reactions occur.
- The densities inside the tank are assumed to be constant which makes $C_p = C_v$ and permits the use of enthalpies in the derivation instead of internal energies [19].
- The model will only hold for incompressible fluids (liquids).

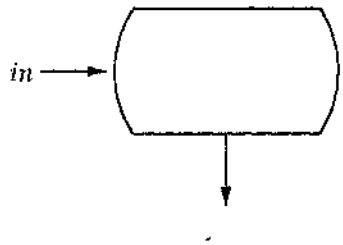


Figure 3.1: Liquid Tank (one input, one output)

- The mass of the metal walls is assumed to be negligible so that the "thermal" inertia of the metal can be ignored.
- The heat transfer between the process temperature T and the external surroundings which have a temperature T_S is described by an overall heat transfer coefficient where $Q = UA_H(T - T_S)$.
- [illegible] has a constant cross-sectional area over its entire height.
- The incoming pipe is above the surface of the liquid.
- The outgoing pipe is at the bottom of the tank.

3.2.3 Variable Descriptions

$A = tank\ cross-sectional\ area$	Constant	m^2
$A_H(V) = 2(V\sqrt{\frac{\pi}{A}} + A) = heat\ transfer\ area$	Function	m^2
$C_p = heat\ capacity\ of\ liquid$	Constant	J/kgK
$F_{in} = total\ incoming\ flowrate$	Input	m^3/s
$F_{out} = ouput\ flowrate$	Input	m^3/s
$g = gravitational\ acceleration$	Constant	m/s^2
$p = pressure\ at\ the\ output$	Output	kPa
$p_s = pressure\ at\ the\ liquid\ surface$	Constant	kPa
$T = tank\ temperature$	Output	K
$T_S = temperature\ of\ surroundings$	Constant	K
$V = volume\ of\ liquid\ in\ the\ tank$	Output	m^3
$U = overall\ heat\ transfer\ coefficient$	Constant	W/m^2K
$\rho = liquid\ density$	Constant	kg/m^3

3.2.4 Dynamic Model

continuity equation

$$\frac{dV}{dt} = F_{in} - F_{out} \tag{3.1}$$

energy equation

$$\frac{d(VT)}{dt} = F_{in}T_{in} - F_{out}T - \frac{UA_H(V)}{\rho C_p}(T - T_S) \tag{3.2}$$

3.2.5 Constitutive Relationships

$$p = p_s + \rho g \frac{V}{A} \tag{3.3}$$

3.2.6 Equilibrium Points

$$F_e = F_{ine} = F_{oute} \tag{3.4}$$

$$V_e = Constant \tag{3.5}$$

$$T_e = \frac{\rho C_p F_e T_{ine} + UA_H(V)T_S}{\rho C_p F_e + UA_H(V)} \tag{3.6}$$

Note that equation 3.2 is derived in appendix D. The subscript e denotes an equilibrium value.

3.2.7 Dynamic Response

By solving for the poles at the equilibrium points we can get a very good idea of how the system responds dynamically. Solving for the dynamic response is not a standard process but varies from problem to problem. The dynamics are often predicted using a mixture of physical and mathematical reasoning.

The first dynamic equation 3.1 gives a pole at the origin. Equation 3.2 gives rise to an additional pole which means the system is first order in terms of the temperature. Since no source of energy is found in the tank (ie there are no reactions or heating elements), and only one heat storage element occurs in the tank (the liquid itself) the behaviour is first order. Therefore the pole will appear on the real axis.

The rate of heat transfer is dependant on the area of heat transfer. The area available for heat transfer increases as the volume of liquid in the tank increases. This can clearly be seen from the formula for A_H. This however does not mean that the pole will move further into the left hand plane as the volume of liquid increases because the "thermal inertia" of the liquid has to be taken into account. The greater the volume of liquid in the tank, the slower it will cool down or heat up. Due to the nature of tanks (even those with small volumes - the smaller the tank volume, the smaller the heat transfer area), this effect is the dominant one and hence as the volume of fluid in the tank decreases, the liquid cools down or heats up at a faster rate. Hence as volume decreases, the pole moves further into the left hand plane.

The tank system is inherently stable for the simple reason that there are no energy sources within the tank and the system is dissipative by nature (heat is dissipated to the surroundings).

The following pole plot gives a qualitative view of the characteristic dynamics of the tank.

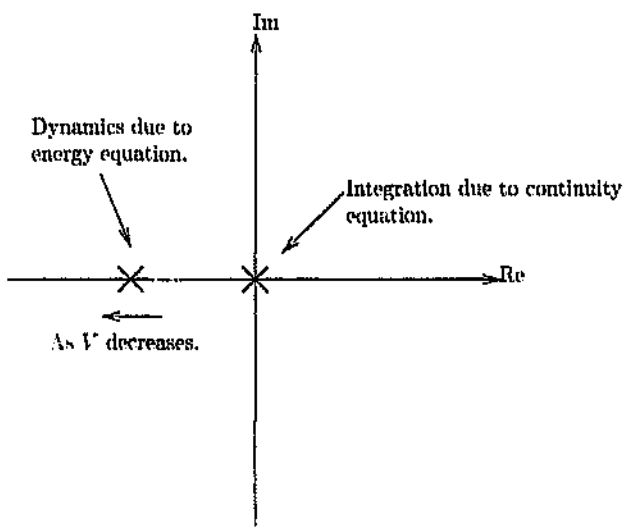


Figure 3.2: s-plane Diagram of Tank Dynamics

To obtain a quantitative picture of the dynamics, the range of values of the system parameters and inputs has to be quantified and the poles calculated using numerical methods.

3.2.8 Standard Control

The control that is used on tanks is essentially safety equipment which will not allow the tank to be emptied below a certain level or become overfilled. Although that kind of equipment is essential in real world systems, it is irrelevant in the current study which is focusing on the dynamics of the system from a process control perspective. The implicit assumption made is that the tank is never in one of those critical states in this work.

3.2.9 Observations

An important aspect this simple model brings out is that for every different set of combinations of inputs and outputs, a separate unit has to be developed. For instance a tank with two inputs and two outputs will have a different set of equations. For the equations to hold which only include flows and volumes, the densities of all the liquids flowing in and out have to be the same. This means that the model only holds for a homogeneous fluid in the tank. Hence, these tank models can only be used for liquids which are sufficiently similar.

3.3 Continuous Stirred Tank Reactor

3.3.1 Description

The continuous stirred tank reactor is quite an advance when compared to the simple tank. Not only are chemical reactions catered for but so are changes in temperature as a result of the reaction and the external conditions. Another aspect of this model is it includes a cooling jacket as part of the reactor. The chemical reaction which is assumed for this reactor is very simple and in most real world situations would be far more complex. The number of reactions occuring determines the order of the reaction kinetics part of the equation. In this case there is one reaction and hence one state is used for the chemical reaction.

3.3.2 Assumptions

- The chemical reaction is assumed to be : $\mathbf{A} \rightleftharpoons \mathbf{B}$.
- The forward reaction is exothermic with heat of reaction λ.

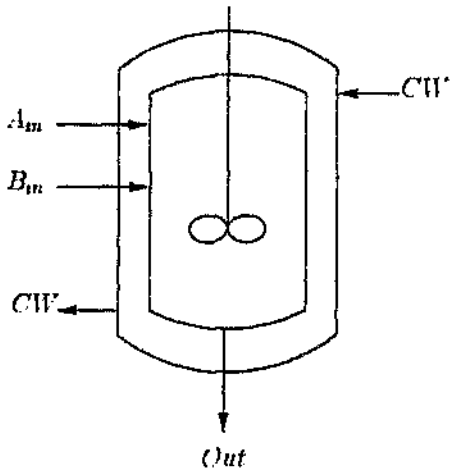


Figure 3.3: CSTR (two inputs, one output)

- The densities inside the reactor are assumed to be constant which makes $C_p = C_v$ and permits the use of enthalpies in the derivation instead of internal energies [19].
- The model will only hold for incompressible fluids (liquids).
- The water is added to the jacket at a rate of F_J and the volume V_J of water in the jacket is assumed to be constant.
- The jacket water is assumed to be perfectly mixed.
- The mass of the metal walls is assumed to be negligible so that the "thermal inertia" of the metal can be ignored.
- The heat transfer between the process temperature T and the cooling water which has a temperature T_J is described by an overall heat transfer coefficient where $Q = UA_H(T - T_J)$.
- The tank has a constant cross-sectional area over its entire height.
- The incoming pipes are above the surface of the liquid.
- The outgoing pipe is at the bottom of the tank.

3.3.3 Var'able Descriptions

A = *cross – sectional area of tank*	Constant	m^2
$A_H(V) = 2(V\sqrt{\frac{\pi}{A}} + A)$ = *heat transfer area*	Function	m^2
C_p = *heat capacity of process liquids*	Constant	J/kgK
C_A = *fracti.nal concentration of A in output*	Output	
C_{Ain} = *incoming fractional concentration of A*	Input	
$f(C_A, T)$ = *reaction rate*	Function	$1/s$
F_{Ain} = *incoming flowrate of A*	Input	m^3/s
F_{Ain} = *incoming flowrate of B*	Input	m^3/s
F_{in} = *total incoming flowrate of A and B*	Input	m^3/s
F_{out} = *output flowrate*	Input	m^3/s
g = *gravitational acceleration*	Constant	m/s^2
p = *pressure at the output*	Output	kPa
p_s = *pressure at the liquid surface*	Constant	kPa
T = *reactor temperature*	Output	K
$T_{in} = \frac{1}{2}(T_{Ain} + T_{Bi}{}^{\backslash}$ = *Average temperature of A & B mixed*	Input	K
T_S = *temperature of surroundings*	Constant	K
V = *volume of reactants and products in the tank*	Output	m^3
U = *overall heat transfer coefficient*	Constant	W/m^2K
λ = *heat of reaction*	Constant	J/kg
ρ = *density of reactor liquids*	Constant	kg/m^3
C_J = *heat capacity of cooling water*	Constant	J/kgK
F_J = *cooling water output flowrate*	Input	m^3/s
T_{Jin} = *incoming temperature of cooling water*	Input	K
T_J = *temperature of cooling water in jacket*	Output	K
V_J = *volume of cooling water in jacket*	Constant	m^3
ρ_J = *density of cooling water*	Constant	kg/m^3

3.3.4 Dynamic Model

total continuity equation

$$\frac{dV}{dt} = F_{in} - F_{out} \tag{3.7}$$

component continuity equation

$$\frac{d(VC_A)}{dt} = F_{in}C_{Ain} - F_{out}C_A - Vf(C_A, T) \tag{3.8}$$

reactor energy equation

$$\frac{d(VT)}{dt} = F_{in}T_{in} - F_{out}T - \frac{\lambda V}{\rho C_p} f(C_A, T) - \frac{UA_H(V)}{\rho C_p}(T - T_J) \quad (3.9)$$

jacket energy equation

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}(T_{Jin} - T_J) + \frac{UA_H}{V_J \rho_J C_J}(T - T_J) \quad (3.10)$$

3.3.5 Constituitive Relationships

$$F_{in} = F_{Ain} + F_{Bin} \quad (3.11)$$

$$p = p_s + \rho g \frac{V}{A} \quad (3.12)$$

3.3.6 Equilibrium Points

$$F_e = F_{ine} = F_{oute} \quad (3.13)$$

$$V_e = Constant \quad (3.14)$$

$$0 = F_{in}C_{Ain} - F_{out}C_A - Vf(C_A, T) \quad (3.15)$$

$$0 = F_{in}T_{in} - F_{out}T - \frac{\lambda V}{\rho C_p} f(C_A, T) - \frac{UA_H(V)}{\rho C_p}(T - T_J) \quad (3.16)$$

$$0 = \frac{F_J}{V_J}(T_{Jin} - T_J) + \frac{UA_H}{V_J \rho_J C_J}(T - T_J) \quad (3.17)$$

These equations have to be solved simultaneously using numerical methods once all of the parameters and ranges of inputs have been defined for the CSTR. All the equilibrium points for T, C_A and T_J must be obtained.

Note that equations 3.8-3.10 are derived in appendix D. The subscript e denotes an equilibrium value.

3.3.7 Dynamic Response

Without solving the numerical equations for a particular reactor it is more difficult to predict the type of dynamics that will occur than it was with the tank. It is however possible, from mathematics and physics, to obtain a good idea of the type of behaviour to expect and also to know what aspect of the reactor is critical in determining the type of dynamics that can occur.

At every equilibrium point, there will be a pole at the origin in the $s-plane$. This is due to the integrating action of the tank as defined by equation 3.7. Equations 3.8 and 3.9 are inextricably linked by the chemical reaction as the first gives the concentration of the chemicals and the second their temperature. As the chemical reaction proceeds, the concentration will change and heat will be generated causing changes in the temperature. Because these two states are so tightly linked oscillatory behaviour is a definite possibility.

We know that a single bi-directional chemical reaction occurs within the reactor which results in another system state, VC_A. This state is linked to the state VT and hence the interaction between the temperature of the reaction and the concentration of the products could result in oscillatory transients or even sustained oscillations of the temperature and concentration. This is dependent on the nature of the chemical reaction and catalytic effects as well as the effectiveness of the cooling jacket.

The final set of dynamics to be considered are the fluctuations of the temperature of the liquid in the cooling jacket (see equation 3.10). Since one of the poles of the system is the result of the integrating effect of the tank and hence falls on the origin of the $s-plane$, this means that three poles remain to be placed. Because poles that have a complex component come in conjugate pairs (due to the differential equation having real coefficients), at least one pole will have to fall on the real axis.

Hence if oscillitory behaviour is going to occur, two of the states will make a complex conjugate pair and the third will act as a first order system (ie it will appear on the real axis). The remaining pole is the pure integration (equation 3.7) which results in a pole at the origin. Figure 3.4 shows a block diagram of a linear system which could represent the CSTR at an equilibrium point.

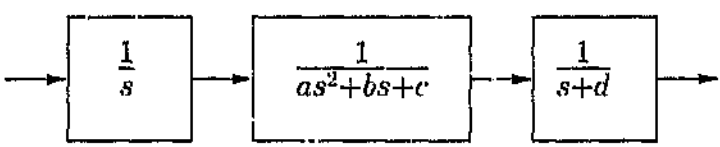


Figure 3.4: Linear System Block Diagram for the CSTR

Taking into account the fact that the transfer of energy is predominantly from the CSTR to the cooling water, the dynamics of the cooling water is usually first order, leaving the only two states whose dynamics remain to form a conjugate pair of poles in the $s-plane$ as the concentration and temperature. Hence, the only part of the CSTR equations which can give second order transient dynamics or steady state

oscillatory behaviour is the chemical reaction.

3.3.8 Standard Control

The standard control that is used by chemical process engineers to control a CSTR, usually consists of volume control and temperature control. If the volume control of the system is strong this results in the integration pole been moved far into the lefthand plane. Essentially the aim of volume control is to maintain the set point and reject the disturbance of changing input flow rates. The actuator is the output product control valve. If the integration pole (the one related to the volume) is moved far enough into the left hand of the $s-plane$ then the continuity equation can be ignored as the volume will essentially remain constant at all times. Hence the equations can be simplified and the only remaining dynamics are those caused by temperature and the chemical kinetics.

The temperature control uses the flow rate of cooling water through the cooling jacket as the means of controlling the temperature. Temperature control is more expensive than volume control as it requires a complete redesign of the reactor (the cooling jacket is part of the reactor). If the cooling jacket size could be reduced and the temperature is less controllable, the reactor could conceivably be produced at a lower cost.

If the cooling jacket control system is successful in controlling the temperature of the reactor then the dynamic caused by temperature will usually be far into the left hand plane and appear on the real axis. This is due to the fact that the cooling process will have a damping effect (it dissipates energy).

The dynamics which will probably be specified when doing a control design will be those related to the temperature and concentration (states VC_A and VT). These would be controlled using the cooling water and an attempt must be made by the control engineer to achieve a fast rise time while avoiding excessive overshoot. The specifications would be decided on by using the model and other chemical engineering information.

3.3.9 Extra Information

Most chemical reactions are of much higher order than one, especially the organic chemical reactions found in petro-chemical systems. The theory relating to chemical

kinetics is the study of the dynamic interaction of chemicals with time and usually the equations are expressed in terms of concentrations for liquids. The rule for chemical reactions is that you have one new state for every reaction. So for one reaction, you have one state (ie the dynamics are first order), for two reactions you have two states and hence second order behaviour. So if you have three reactants with the form of the equation $A \rightleftharpoons B \rightleftharpoons C$ then you have two reactions and hence they result in a second order differential chemical kinetic equation.

3.4 Simple Pump and Valve

3.4.1 Description

The pump is the standard means of propelling process fluids from one place to another. There are many different physical configurations of pumps, all of which are suited to particular circumstances. The most common form of pump in chemical process industries is the centrifugal pump. The fluid is assumed to be incompressible (ie liquid). The model presented here includes the control valve as part of the model. Most pumps in chemical process systems are accompanied by a control valve. Simply leave out the equation for u and set $\nu = 1$ if no valve is present.

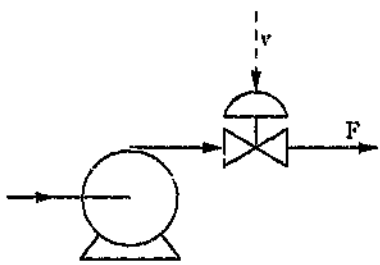


Figure 3.5: Pump

3.4.2 Assumptions

- No changes of state or chemical reactions occur.
- The model will only hold for incompressible fluids (liquids).
- The dynamics introduced by the motor and pump rotor are ignored.

- The mass of the metal walls are assumed to be negligible so that the 'thermal inertia" of the metal can be ignored.
- The heat transfer between the process temperature T and the surroundings which have a temperature T_S is described by an overall heat transfer coefficient where $Q = U A_H (T - T_S)$.
- The viscosity is dependent on temperature only.
- The densities inside the pump are assumed to be constant which makes $C_p = C_v$ and permits the use of enthalpies in the derivation instead of internal energies [19].
- Hydrodynamic effects are assumed to be negligible.

3.4.3 Variable Descriptions

$A = pipe\ cross-sectional\ area$	Constant	m^2
$A_H = heat\ transfer\ area$	Constant	m^2
$C_p = heat\ capacity\ of\ liquid$	Constant	J/kgK
$F = flowrate$	Output	m^3/s
$L = length\ of\ pipe$	Constant	m
$P_p(F,r) = pump\ characteristic\ surface$	Function	kPa
$P_s(F,u) = system\ characteristic\ surface$	Function	kPa
$r = normalized\ power\ input$	Input	
$T_1 = instantaneous\ liquid\ temperature$	Output	K
$T_2 = delayed\ output\ liquid\ temperature$	Output	K
$T_{in} = incoming\ liquid\ temperature$	Input	K
$T_S = temperature\ of\ surroundings$	Constant	K
$u = linear\ normalised\ valve\ appeture$	State	
$U = overall\ heat\ transfer\ coefficient$	Constant	W/m^2K
$v = linear\ normalized\ valve\ input$	Input	
$\mu(T) = liquid\ viscosity$	Function	kg/ms
$\rho = liquid\ density$	Constant	kg/m^3
$\tau_v = valve\ time\ constant$	Constant	$1/s$
$\tau = delay\ from\ input\ to\ output$	Output	s

3.4.4 Dynamic Model

continuity equation

$$\frac{dF}{dt} = \frac{A}{\rho L}[P_p(F,r) - P_s(F,u)] \tag{3.18}$$

energy equation

$$\frac{dT_1}{dt} = \frac{F}{V}(T_{in} - T_1) - \frac{UA_H}{V\rho C_p}(T_1 - T_S) \tag{3.19}$$

valve time response equation

$$\frac{du}{dt} = \frac{1}{\tau_v}(v - u) \tag{3.20}$$

3.4.5 Constitutive Relationships

$$\tau = \frac{LA}{F} \tag{3.21}$$

$$T_2(t) = T_1(t - \tau) \tag{3.22}$$

$$\tag{3.23}$$

3.4.6 Equilibrium Points

The following equations need to be solved simultaneously to get the equilibrium points:

$$F_e \tag{3.24}$$

by solving

$$P_p(F,r) = P_s(F,u) \tag{3.25}$$

$$T_1(t) = k_1 T_{in} + k_2 T_S \tag{3.26}$$

$$u = v \tag{3.27}$$

where

$$k_1 = \frac{UA_H}{UA_H + F\rho C_p}$$

$$k_2 = \frac{F\rho C_p}{UA_H + F\rho C_p}$$

Note that equations 3.18-3.20 are derived in appendix D. The subscript e denotes an equilibrium value.

3.4.7 Dynamic Response

The dynamic response of the pipe and pump is usually very much faster than any of the other chemical processes. The dynamics are all essentially of a first order type (that is the poles appear on the real axis). The dynamics which have the most impact on the entire chemical system when a control loop is implemented around two units joined by a pump and pipe is the variable transport delay. This feature of the dynamics is very difficult to model in a nonlinear system[1] and causes a great deal of difficulty with stability when using feedback control.

3.4.8 Standard Control

A simple proportional controller is used with the pump and its associated control valve. This essentially linearizes the system and can even further improve the dynamic response (make it faster).

3.5 Proportional-Integral Controller

3.5.1 Description

The proportional-integral controller is a common feature in chemical processes. It uses some type of input obtained directly or indirectly from measurement equipment and sends a control signal to an actuator (usually a control valve). The measuring instrument can be nonlinear.

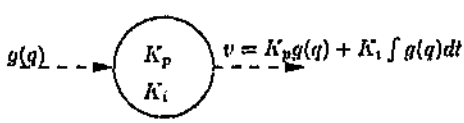


Figure 3.6: PI Controller

3.5.2 Assumptions

- Noise is assumed to be negligible.

[1] It is possible to use high order delay differential equations which are cumbersome and computationally intensive.

- The sensor is assumed to have no dynamics but may be non-linear.

3.5.3 Variable Descriptions

$g(q) = nonlinear\ sensor\ output$	Function
$K_i = integrator\ gain$	Constant
$K_p = proportional\ gain$	Constant
$q = variable\ sensor\ is\ measuring$	Input
$v = output\ of\ PI\ controller$	Output
$w = integrated\ sensor\ output$	State

3.5.4 Dynamic Model

integrator equation

$$\frac{dw}{dt} = g(q) \tag{3.28}$$

3.5.5 Constitutive Relationships

$$v = K_p g(q) + K_i w \tag{3.29}$$

3.5.6 Equilibrium Points

$$g(q) = 0 \tag{3.30}$$

3.5.7 Dynamic Response

The controller on its own results in a single pole at the origin although when used as part of a feedback loop it will have a low pass filter effect (a lag controller).

3.6 Conclusion

The development of unit operation models has proved to be an intricate task. There is however much that has been learned from the process. The fact that a great deal of

information can be gleaned about the behaviour of the unit just by creating a model for it is very important. This information needs to be documented in a standard format which can be used again and again by practicing engineers. In this way their time can be used more effectively in the analysis of the effects of linking the model to other units. If a large enough library of unit models could be built it would shed a great deal of light on the control design process. The process control engineer would be able to approach apparently intractable chemical engineering problems with a great deal more confidence and hence build a model which could predict possible failure modes, instead of relying on a black box approach.

Although nonlinear analysis of the system is the ultimate aim in this dissertation, it would be totally worthless without a logical and transparent model development strategy.

Chapter 4

System Model Construction

4.1 Introduction

The approach that is taken in this chapter is one of illustration. A model for a simple mixing system is modelled using the units described in chapter 3. The linking procedure is illustrated by the combination of the chemical process units. A standard numbering technique is also suggested, again by illustration. From the resulting model, initial information about the system is drawn.

The aim of developing a model of this form is to enable model order reduction and nonlinear analysis. Also it allows for the analysis of the interaction between different units.

4.2 System Example

The following system combines the units described so far into a simple chemical process. This process involves the mixing of two liquid reactants which then react to produce one of the original reactants. Essentially this reaction is an auto catalytic reaction where the desired product is one of the reactants. The chemical reaction is described by the equation $\mathbf{A} \rightleftharpoons \mathbf{B}$.

The units have been given the following numbers:

1. Tank A
2. Tank B

3. Pump and pipe A

4. Pump and pipe B

5. CSTR

6. Product pump and pipe

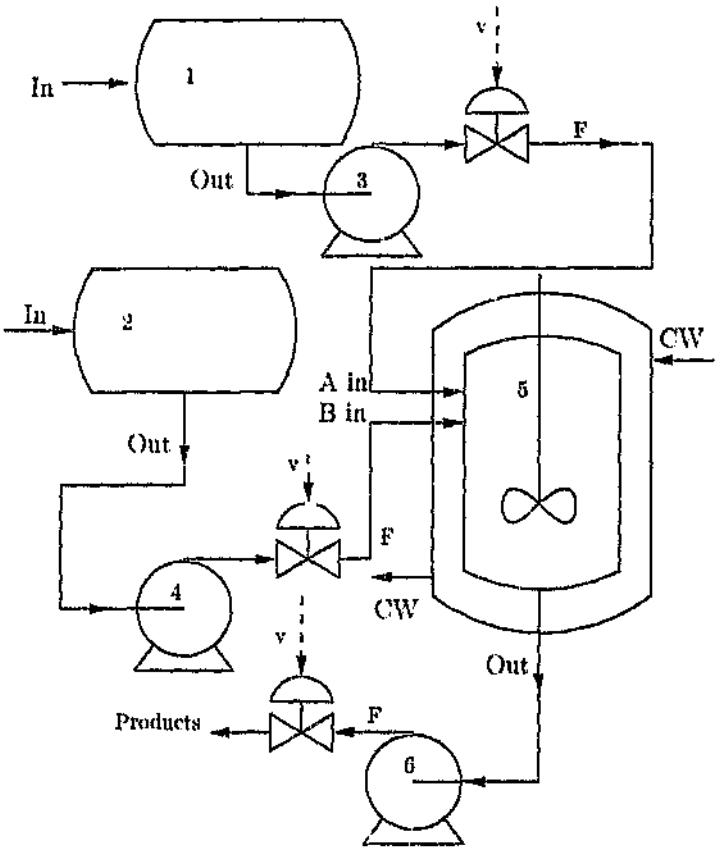


Figure 4.1: Simple Mixing Process

4.3 Linking

A package would normally be used but is not necessary in this dissertation since the methodology is being illustrated. It is helpful to write out all of the dynamic models of the units that make up the system as one model. The unit model equations are given in chapter 3.

$$\frac{dV_1}{dt} = F_{in1} - F_{out1} \tag{4.1}$$

$$\frac{d(V_1T_1)}{dt} = F_{in1}T_{in1} - F_{out1}T_1 - \frac{U_1A_{H1}}{\rho_1C_{p1}}(T_1 - T_{S1}) \tag{4.2}$$

$$\frac{dV_2}{dt} = F_{in2} - F_{out2} \tag{4.3}$$

$$\frac{d(V_2T_2)}{dt} = F_{in2}T_{in2} - F_{out2}T_2 - \frac{U_2A_{H2}}{\rho_2C_{p2}}(T_2 - T_{S2}) \tag{4.4}$$

$$\frac{dF_3}{dt} = \frac{\Delta p_3(\tau_3)A_3\eta_3(u_3)}{\rho_3L_3} + \frac{(p_{out3} - p_{in3})A_3\eta_3(u_3)}{\rho_3L_3} - \frac{g\Delta h_3A_3\eta_3(u_3)}{L_3} - \frac{\mu_3(T_3)F_3}{\rho_3A_3\eta_3(u_3)} \tag{4.5}$$

$$\frac{dT_3}{dt} = \frac{F_3}{V_3}(T_{in3} - T_3) - \frac{U_3A_{H3}}{V_3\rho_3C_{p3}}(T_3 - T_{S3}) \tag{4.6}$$

$$\frac{du_3}{dt} = \frac{1}{\tau_{v3}}(v_3 - u_3) \tag{4.7}$$

$$\frac{dF_4}{dt} = \frac{\Delta p_4(\tau_4)A_4\eta_4(u_4)}{\rho_4L_4} + \frac{(p_{out4} - p_{in4})A_4\eta_4(u_4)}{\rho_4L_4} - \frac{g\Delta h_4A_4\eta_4(u_4)}{L_4} - \frac{\mu_4(T_4)F_4}{\rho_4A_4\eta_4(u_4)} \tag{4.8}$$

$$\frac{dT_4}{dt} = \frac{F_4}{V_4}(T_{in4} - T_4) - \frac{U_4A_{H4}}{V_4\rho_4C_{p4}} \tag{4.9}$$

$$\frac{du_4}{dt} = \frac{1}{\tau_{v4}}(v_4 - u_4) \tag{4.10}$$

$$\frac{dV_5}{dt} = F_{in5} - F_{out5} \tag{4.11}$$

$$\frac{d(V_5C_{A5})}{dt} = F_{in5}C_{Ain5} - F_{out5}C_{A5} - V_5f_5(C_{A5}, T_5) \tag{4.12}$$

$$\frac{d(V_5T_5)}{dt} = F_{in5}T_{in5} - F_{out5}T_5 - \frac{\lambda_5V_5}{\rho_5C_{p5}}f_5(C_{A5}, T_5) - \frac{U_5A_{H5}}{\rho_5C_{p5}}(T_5 - T_{J5}) \tag{4.13}$$

$$\frac{dT_{J5}}{dt} = \frac{F_{J5}}{V_{J5}}(T_{Jin5} - T_{J5}) + \frac{U_5A_{H5}}{\rho_{J5}C_{J5}}(T_5 - T_{J5}) \tag{4.14}$$

$$\frac{dF_6}{dt} = \frac{\Delta p_6(\tau_6)A_6\eta_6(u_6)}{\rho_6L_6} + \frac{(p_{out6} - p_{in6})A_6\eta_6(u_6)}{\rho_6L_6} - \frac{g\Delta h_6A_6\eta_6(u_6)}{L_6} - \frac{\mu_6(T_6)F_6}{\rho_6A_6\eta_6(u_6)} \tag{4.15}$$

$$\frac{dT_6}{dt} = \frac{F_6}{V_6}(T_{in6} - T_6) - \frac{U_6A_{H6}}{V_6\rho_6C_{p6}} \tag{4.16}$$

$$\frac{du_6}{dt} = \frac{1}{\tau_{v6}}(v_6 - u_6) \tag{4.17}$$

The above set of equations gives no idea as to how they are linked together. Thus the next step is to link together the appropriate variables based on the layout of the physical system. We accomplish this by making a list of all the variables that are either directly or indirectly equivalent.

$F_{out1} = F_3$	
$p_{in3} = p_{out1}$	$p_{out1} = p_{in1} + \frac{\rho g V_1}{A_1}$
$p_{out3} = p_{in5}$	
$T_{in3} = T_1$	
$T_{in5} = T_3$	
$F_{Ain5} = F_3$	
$F_{out2} = F_4$	
$p_{in4} = p_{out2}$	$p_{out2} = p_{in2} + \frac{\rho g V_2}{A_2}$
$p_{out4} = p_{in5}$	
$T_{in4} = T_2$	
$T_{Bin5} = T_4$	
$F_{Bin5} = F_4$	
$F_{out5} = F_6$	
$p_{in6} = p_{out5}$	$p_{out5} = p_{in5} + \frac{\rho g V_5}{A_5}$
$T_{in6} = T_5$	
$\rho = \rho_1 \simeq \rho_2 \simeq \rho_3 \simeq \rho_4 \simeq \rho_5 \simeq \rho_6$	
$F_{in5} = F_{Ain5} + F_{Bin5}$	
$T_{in5} = C_{Ain5}T_{Ain} + (1 - C_{Ain5})T_{Bin}$	$C_{Ain5} = \frac{F_{Ain5}}{F_{in5}}$

4.4 System Dynamic Model

$$\frac{dV_1}{dt} = F_{in1} - F_3 \tag{4.18}$$

$$\frac{d(V_1T_1)}{dt} = F_{in1}T_{in1} - F_3T_1 - \frac{U_1A_{H1}}{\rho_1C_{p1}}(T_1 - T_S) \tag{4.19}$$

$$\frac{dV_2}{dt} = F_{in2} - F_4 \tag{4.20}$$

$$\frac{d(V_2T_2)}{dt} = F_{in2}T_{in2} - F_4T_2 - \frac{U_2A_{H2}}{\rho_2C_{p2}}(T_2 - T_S) \tag{4.21}$$

$$\frac{dF_3}{dt} = \frac{\Delta p_3(\tau_3)A_3\eta_3(u_3)}{\rho_3L_3} + \frac{(p_{in5} - p_{out1})A_3\eta_3(u_3)}{\rho_3L_3} - \frac{g\Delta h_3A_3\eta_3(u_3)}{L_3} - \frac{\mu_3(T_3)F_3}{\rho_3A_3\eta_3(u_3)} \tag{4.22}$$

$$\frac{dT_3}{dt} = \frac{F_3}{V_3}(T_1 - T_3) - \frac{U_3A_{H3}}{V_3\rho_3C_{p3}}(T_3 - T_S) \tag{4.23}$$

$$\frac{du_3}{dt} = \frac{1}{\tau_{v3}}(v_3 - u_3) \tag{4.24}$$

$$\frac{dF_4}{dt} = \frac{\Delta p_4(\tau_4)A_4\eta_4(u_4)}{\rho_4L_4} + \frac{(p_{in5} - p_{out2})A_4\eta_4(u_4)}{\rho_4L_4} - \frac{g\Delta h_4A_4\eta_4(u_4)}{L_4} - \frac{\mu_4(T_4)F_4}{\rho_4L_4\eta_4(u_4)} \tag{4.25}$$

$$\frac{dT_4}{dt} = \frac{F_4}{V_4}(T_2 - T_4) - \frac{U_4 A_{H4}}{V_4 \rho_4 C_{p2}}(T_4 - T_S) \tag{4.26}$$

$$\frac{du_4}{dt} = \frac{1}{\tau_{v4}}(v_4 - u_4) \tag{4.27}$$

$$\frac{dV_5}{dt} = F_3 + F_4 - F_6 \tag{4.28}$$

$$\frac{d(V_5 C_{A5})}{dt} = F_3 - F_6 C_{A5} - V_5 f_5(C_{A5}, T_5) \tag{4.29}$$

$$\frac{d(V_5 T_5)}{dt} = (F_3 + F_4)(C_{Ain5} T_3 + C_{Bin5} T_4) - F_6 T_5 - \frac{\lambda_5 V_5}{\rho_5 C_{p5}} f_5(C_{A5}, T_5) - \frac{U_5 A_{H5}}{\rho_5 C_{p5}}(T_5 - T_{J5}) \tag{4.30}$$

$$\frac{dT_{J5}}{dt} = \frac{F_{J5}}{V_{J5}}(T_{Jin5} - T_{J5}) + \frac{U_5 A_{H5}}{\rho_{J5} C_{J5}}(T_5 - T_{J5}) \tag{4.31}$$

$$\frac{dF_6}{dt} = \frac{\Delta p_6(r_6) A_6 \eta_6(u_6)}{\rho_6 L_6} + \frac{(p_{out6} - p_{out5}) A_6 \eta_6(u_6)}{\rho_6 L_6} - \frac{g \Delta h_6 A_6 \eta_6(u_6)}{L_6} - \frac{\mu_6(T_6) F_6}{\rho_6 A_6 \eta_6(u_6)} \tag{4.32}$$

$$\frac{dT_6}{dt} = \frac{F_6}{V_6}(T_5 - T_6) - \frac{U_6 A_{H6}}{V_6 \rho_6 C_{p5}}(T_6 - T_S) \tag{4.33}$$

$$\frac{du_6}{dt} = \frac{1}{\tau_{v6}}(r_6 - u_6) \tag{4.34}$$

4.5 System Constituitive Relationships

$$C_{Ain5} = \frac{F_3}{F_3 + F_4} \tag{4.35}$$

$$C_{Bin5} = \frac{F_4}{F_3 + F_4} \tag{4.36}$$

$$p_{out1} = \frac{\rho g V_1}{A_1} + p_{in1} \tag{4.37}$$

$$p_{out2} = \frac{\rho g V_2}{A_2} + p_{in2} \tag{4.38}$$

$$p_{out5} = \frac{\rho g V_5}{A_5} + p_{in5} \tag{4.39}$$

4.6 Assumptions

The following assumptions are made within the equations. The other assumptions are defined for each unit in chapter 3.

$\rho \simeq \rho_1 \simeq \rho_2 \simeq \rho_3 \simeq \rho_4 \simeq \rho_5 \simeq \rho_6$	Assume densities remain approximately constant throughout.
$p_{in1} = p_{in2} = p_{in5}$	Constant at atmospheric pressure.
$C_{p1} = C_{p3}$	Constant for tank and pipe.
$C_{p2} = C_{p4}$	Constant for tank and pipe.
$C_{p5} = C_{p6}$	Constant for CSTR and output pipe.
$T_S = T_{S1} = T_{S2} = T_{S3} = T_{S4} = T_{S5} = T_{S6}$	Assume the temperature of the surroundings is the same for all the units.
$T_{in5} = C_{Ain5}T_3 + C_{Bin5}T_4$	The reactants mix on entry into the CSTR and reach an average temperature between the two.
$A_H = Constant$	All the units have constant heat transfer areas which do not vary with liquid volume.

4.7 Variable Descriptions

The following variables now have new meaning due to the fact that the units are now part of a larger system. The rest of the variables are described in the original variable descriptions in chapter 3.

4.7.1 Inputs

F_{in1}	Flow into tank A.	m^3/s
T_{in1}	Temperature of liquid flowing into tank A.	K
F_{in2}	Flow into tank B.	m^3/s
T_{in2}	Temperature of liquid flowing into tank B.	K
r_3	Normalised pump power input for component A.	
v_3	Normalised control valve signal for component A.	
r_4	Normalised pump power input for component B.	
v_4	Normalised control valve signal for component B.	
F_{J5}	Flow rate of cooling water.	m^3/s
T_{Jin5}	Incoming temperature of cooling water.	K
r_6	Normalised pump power input for output mixture.	
v_6	Normalised control valve signal for output mixture.	

4.7.2 Outputs

The states of the system are not always in the desired form, so they have to be converted into a usable form. The table shown below gives the outputs of the system in terms of the states of the system. These outputs are the variables of the system which can be measured physically.

V_1	Volume of liquid in tank A	m^3
$T_1 = \frac{(V_1 T_1)}{V_1}$	Temperature of liquid flowing out of tank A.	K
V_2	Volume of liquid in tank B.	m^3
$T_2 = \frac{(V_2 T_2)}{V_2}$	Temperature of liquid flowing out of tank B.	K
F_3	Flow rate of component A.	m^3/s
T_3	Temperature of component A just before the CSTR.	K
F_4	Flow rate of component B.	m^3/s
T_4	Temperature of compone[illegible] before the CSTR.	K
$C_{A5} = \frac{(V_5 C_{A5})}{V_5}$	Fraction of component A [illegible]ut stream.	
$C_{B5} = 1 - C_{A5}$	Fraction of component B in output stream.	
V_5	Volume of liquid in the CSTR.	m^3
$T_5 = \frac{(V_5 T_5)}{V_5}$	Temperature of the liquids flowing out of the CSTR.	K
F_6	Flow rate of the output products.	m^3/s
T_6	Temperature of the output products.	K

4.8 State Space Equations

The next step is to convert all of the equations into a form which can be easily used in mathematical analysis. This requires that constants be condensed into single variables, the states be identified by numbers rather than letters and the system of equations be subdivided in such a way as to facilitate mathematical analysis.

$$\dot{x}_1 = a_1 x_? + b_1 u_1 \tag{4.40}$$

$$\dot{x}_2 = f_1 x_5 \frac{x_2}{x_1} + f_2 \frac{x_2}{x_1} + g_1 u_1 u_2 + k_1 \tag{4.41}$$

$$\dot{x}_3 = a_2 x_8 + b_2 u_3 \tag{4.42}$$

$$\dot{x}_4 = f_3 x_8 \frac{x_4}{x_3} + f_4 \frac{x_4}{[illegible]} + [illegible] \tag{4.43}$$

$$\dot{x}_5 = f_5 \frac{h_2(x_6) x_5}{h_3(x_7)} + f_6 h_3(x_7) + f_7 h_3(x_7) + f_8 x_1 h_3(x_7) + f_9 h_1(u_5) h_3(x_7) \tag{4.44}$$

$$\dot{x}_6 = a_3x_6 + f_{10}x_5\frac{x_2}{x_1} + f_{11}x_5x_6 + k_3 \tag{4.45}$$

$$\dot{x}_7 = a_4x_7 + b_3u_6 \tag{4.46}$$

$$\dot{x}_8 = f_{12}\frac{h_5(x_9)x_8}{h_6(x_{10})} + f_{13}h_6(x_{10}) + f_{14}h_6(x_{10}) + f_{15}x_3h_6(x_{10}) + f_{16}h_4(u_7)h_6(x_{10}) \tag{4.47}$$

$$\dot{x}_9 = a_5x_9 + f_{17}x_8\frac{x_4}{x_3} + f_{18}x_8x_9 + k_4 \tag{4.48}$$

$$\dot{x}_{10} = a_6x_{10} + b_4u_8 \tag{4.49}$$

$$\dot{x}_{11} = a_7x_5 + a_8x_8 + a_9x_{15} \tag{4.50}$$

$$\dot{x}_{12} = a_{10}x_5 + f_{19}x_{15}\frac{x_{12}}{x_{11}} + f_{20}x_{11}h_7\left(\frac{x_{12}}{x_{11}}, \frac{x_{12}}{x_{11}}\right) \tag{4.51}$$

$$\dot{x}_{13} = a_{11}x_{14} + f_{21}x_5\left[\frac{x_5x_6}{x_5 + x_8} + \frac{x_8x_9}{x_5 + x_8}\right] + f_{22}x_8\left[\frac{x_5x_6}{x_5 + x_8} + \frac{x_8x_9}{x_5 + x_8}\right] + f_{23}x_{15}\frac{x_{13}}{x_{12}} + f_{24}x_{11}h_7\left(\frac{x_{12}}{x_{11}}, \frac{x_{12}}{x_{11}}\right) + f_{25}\frac{x_{13}}{x_{11}} \tag{4.52}$$

$$\dot{x}_{14} = a_{12}x_{14} + f_{26}\frac{x_{13}}{x_{11}} + f_{27}u_9x_{14} + g_1u_9u_{10} \tag{4.53}$$

$$\dot{x}_{15} = f_{28}\frac{h_9(x_{16})x_{15}}{h_{10}(x_{17})} + f_{29}h_{10}(x_{17}) + f_{30}h_{10}(x_{17}) + f_{31}x_{11}h_{10}(x_{17}) \quad f_{31}h_8(u_{11})h_{10}(x_{17}) \tag{4.54}$$

$$\dot{x}_{16} = a_{13}x_{16} + f_{32}x_{15}\frac{x_{13}}{x_{11}} + f_{34}x_{15}x_{16} + k_5 \tag{4.55}$$

$$\dot{x}_{17} = a_{14}x_{17} + b_5u_{12} \tag{4.56}$$

$$\tag{4.57}$$

The constants used in the previous set of equations are defined in the following table.

$a_1 = -1$ $a_2 = -1$ $a_3 = \frac{-U_3 A_{H3}}{V_3 \rho C_{p3}}$ $a_4 = \frac{-1}{\tau_{v4}}$

$a_5 = \frac{-U_5 A_{H5}}{V_5 \rho C_{p5}}$ $a_6 = \frac{-1}{\tau_{v4}}$ $a_7 = 1$ $a_8 = 1$

$a_9 = -1$ $a_{10} = 1$ $a_{11} = \frac{U_5 A_{H5}}{\rho C_{p5}}$ $a_{12} = \frac{-U_6 A_{H6}}{\rho_{J6} C_{J6}}$

$a_{14} = \frac{-U_6 A_{H6}}{V_6 \rho C_{p6}}$ $a_{15} = \frac{-1}{\tau_{v6}}$ $b_1 = 1$ $b_2 = 1$

$b_3 = \frac{-1}{\tau_{v4}}$ $b_4 = \frac{1}{\tau_{\rho l_0}}$ $b_5 = \frac{F_{J5}}{V_{J5}}$ $b_6 = \frac{1}{\tau_{v6}}$

$f_1 = -1$ $f_2 = \frac{-U_3 A_{H3} T_3}{\rho C_{p3}}$ $f_3 = -1$ $f_4 = \frac{-1}{\rho C_{p2}}$

$f_5 = \frac{-1}{\rho A_3}$ $f_6 = \frac{-g \Delta h_3 A_3}{L_3}$ $f_7 = \frac{A_3 p_{a0}}{\rho L_3}$ $f_8 = \frac{-g A_3}{L_4 A_1}$

$f_9 = \frac{A_3}{\rho L_3}$ $f_{10} = \frac{1}{V_3}$ $f_{11} = \frac{-1}{V_4}$ $f_{12} = \frac{-1}{V_5}$

$f_{13} = \frac{-g \Delta h_4 A_4}{L_4}$ $f_{14} = \frac{A_4 p_{a0}}{\rho L_4}$ $f_{15} = \frac{-g A_4}{L_4 A_2}$ $f_{16} = \frac{A_4}{\rho L_4}$

$f_{17} = \frac{1}{V_4}$ $f_{18} = \frac{-1}{V_4}$ $f_{19} = -1$ $f_{20} = -1$

$f_{21} = 1$ $f_{22} = 1$ $f_{23} = 1$ $f_{24} = \frac{-A_5}{\rho C_{p5}}$

$f_{25} = \frac{-U_5 A_{H5}}{\rho C_{p5}}$ $f_{26} = \frac{U_5 A_{H5}}{\rho_{J5} C_{J5}}$ $f_{27} = \frac{1}{V_{J5}}$ $f_{28} = \frac{-1}{\rho A_6}$

$f_{29} = \frac{-g \Delta h_6 A_6}{L_6}$ $f_{30} = \frac{A_6 p_{a0}}{\rho L_6}$ $f_{31} = \frac{-\rho}{L_6}$ $f_{32} = \frac{A_6}{\rho L_6}$

$f_{33} = \frac{1}{V_6}$ $f_{34} = \frac{-1}{V_6}$ $g_1 = 1$ $g_2 = 1$

$g_3 = \frac{1}{V_{J5}}$ $h_1(u_5) = \Delta p_3(r_3)$ $h_2(x_6) = \mu_3(T_3)$ $h_3(x_7) = \eta_3(u_3)$

$h_4(u_7) = \Delta p_4(r_4)$ $h_5(x_9) = \mu_4(T_4)$ $h_6(x_{10}) = \eta_4(u_4)$ $h_7\left(\frac{x_{12}}{x_{11}}, \frac{x_{13}}{x_{11}}\right) = f_5(C_{J5}, T_5)$

$h_8(u_{10}) = \Delta p_6(r_6)$ $h_9(x_{16}) = \mu_6(T_6)$ $h_{10}(x_{17}) = \eta_6(u_6)$ $k_1 = \frac{U_3 A_{H3} T_3}{\rho C_{p3}}$

$k_2 = \frac{U_5 A_{H5} T_5}{\rho C_{p5}}$ $k_3 = \frac{U_5 A_{H5} T_5}{V_{J5} C_{p5}}$ $k_4 = \frac{U_6 A_{H6} T_6}{V_6 \rho C_{p6}}$ $k_5 = \frac{U_6 A_{H6} T_6}{V_{J6} \rho C_{p6}}$

$u_1 = F_{in1}$ $u_2 = T_{in1}$ $u_3 = F_{in2}$ $u_4 = T_{in2}$

$u_5 = r_3$ $u_6 = v_3$ $u_7 = r_4$ $u_8 = v_4$

$u_9 = F_{J5}$ $u_{10} = T_{Jin5}$ $u_{11} = r_6$ $u_{12} = v_6$

$x_1 = V_1$ $x_2 = V_1 T_1$ $x_3 = V_2$ $x_4 = V_2 T_2$

$x_5 = F_3$ $x_6 = T_3$ $x_7 = a_3$ $x_8 = F_4$

$x_9 = T_4$ $x_{10} = a_4$ $x_{11} = V_5$ $x_{12} = V_5 C_{45}$

$x_{13} = V_5 T_5$ $x_{14} = T_{J5}$ $x_{15} = F_6$ $x_{16} = T_6$

$x_{17} = a_6$

Where the coefficients, variables and functions according to their types are :

a	linear state coefficients
b	linear input coefficients
f	nonlinear state coefficients
g	nonlinear input coefficients
h	functional relationships
k	constant values
u	input variables
x	state variables

The system should now be linearized and changed into the form :

$$\Delta\dot{\mathbf{x}} = \mathbf{A}(\mathbf{x_0}, \mathbf{u_0})\Delta\mathbf{x} + \mathbf{B}(\mathbf{x_0}, \mathbf{u_0})\Delta\mathbf{u} \tag{4.58}$$

This results in an A matrix of 17 by 17 which is sparse in the sense that the majority of the coefficients are zero. The next step would be to analytically solve for the eigenvalues which are of great importance in model order reduction and bifurcation analysis.

Solving for eigenvalues analytically is not feasible for large complex systems. An alternative to this approach is to put in the numerical values or ranges of values and solve the equations numerically. This approach however is too cumbersome as it results in 17 eigenvalues which are not directly linked to the dynamics of any particular part of the system. This makes model order reduction unnecessarily difficult.

Once the entire system has been constructed and analysed for interelationships between the states it can be decoupled into functionally separate units. The most successful practical approach is to obtain the numerical values or ranges of values for the system concerned and apply them to each unit separately. The dynamics of each of the units is evaluated and the models are simplified depending on the speed of the dynamics required in the overall model by the engineer. For process control, the high speed dynamics are often ignored and that is what will be done in this work, however, they could be included if the problem required them to be present. The control usually used for each unit that has been described is also included in the analysis of the dynamics.

4.9 Conclusion

The linking of the example illustrates three things. Firstly that the systems constructed by linking unit operation models are large and unwieldy. The second point is that there is generally no analytical solution for most systems created this way as they are nonlinear. The third realization results in that even solving the equations numerically is practically useless information because the solution of the linearization process which gives the system poles at different equilibrium points are not linked explicitly with the system parameters.

The solution to this problem is to decouple the system into smaller manageable subsystems and analyse each one separately and then compare them to each other. This is is discussed in the succeeding chapters.

Chapter 5

Model Order Reduction

5.1 Decoupling Units

5.1.1 Decoupled Units

As illustrated in chapter 4, the systems created by linking the models for various units together are extremely complicated. The order of the resulting set of differential equations is too high for practical analysis of the system. It is therefore necessary to reduce the order of the system. Their are two ways of doing this. The simplest method which is illustrated here is decoupling the units by comparing the speed of their dynamics and looking for obvious independence of state variables. Each unit must be examined and it must be determined whether the speed of the dynamics in that unit will be comparable to the speed of dynamics of units to which it is connected. Also each state must be examined for dependencies and those which are negligible in comparison to the rest of the dependencies can be ignored.

If the speed of the dynamics of a system is a number of times faster or slower than that of a system to which it is inter-connected, then the effect of the inter-connection of the units can be modelled, either by an instantly changing variable or by a constant value respectively. The instantly changing variable is used in the case of dynamics that are very much faster and the constant value is used in the case of dynamics that are very much slower.

An important question that needs to be addressed is how much feedback there is between two units. If for instance the back-pressure down a pipe has an appreciable effect on the flow rate out of a certain unit, it may effect the volume in that unit and hence we would not be able to decouple those units and analyse them separately.

Decoupling in chemical process systems is influenced by the transport methods used to get products or reactants from one point to another. In most instances the flow rate of a substance, whether it be solid, liquid or gas is regulated using some form of feedback controller. Hence in chemical process systems the equations can be decoupled using physical reasoning.

An example of this method of decoupling is the case of liquid transport. The pipe and the pump with its associated control valve often form a buffer between connected units. This is due to the fact that the pump offsets any back-pressure because of its feedback controller. This effectively means that all liquid units can be modelled as being conected together by set flow rates with pure delays. The temperture of the liquid however is not decoupled from the other unit, while the pressures are. The temperature is transferred with a loss dependent on the amount of time the liquid spends in the pipe. The amount of time that the liquid spends in the pipe is dependent on the flow rate. Thus in the liquid systems used in the system example the pressure is decoupled, while the temperature is only decoupled in the reverse direction.

The fact that the temperature is not completely decoupled is not a major problem because it does not feed back into the previous unit (ie there is no term for the downstream unit's temperature in the unit's model — unlike for pressure). Hence if we define coupling to mean that the variable appears in both the models of the units in question, then temperature is by definition already decoupled. We have ignored the dynamics associated with changes in temperature in the pipe for the sake of simplicity.

Equations 3.18 through 3.20 give a possible dynamic model for a pipe and a pump including a control valve. The set of state-space equations is third order. If a proportional controller is used to maintain the flow at a constant rate then the equations become:

$$\frac{dF}{dt} = \frac{A}{\rho L}[P_p(F,r) - P_s(F,u)] \tag{5.1}$$

$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) - \frac{UA_H}{V\rho C_p}(T - T_S) \tag{5.2}$$

$$\frac{du}{dt} = \frac{1}{\tau_v}((F^* - F)K - u) \tag{5.3}$$

The following block diagram shows the structure of the simple proportional controller

.

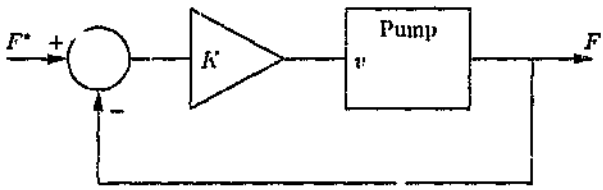


Figure 5.1: Block Diagram of Proportional Controller for Pump

F^* is the flow rate set-point and K is the gain of the proportional controller. It can reasonably be assumed that the system is stable for a large enough value of K which ensures that the steady state error is negligible. Thus the system is statically decoupled as any back-pressure will have very little effect on the flow rate equilibrium point. This will of course only be true if the pump is powerful enough to provide the required pressure rise. To ensure dynamic decoupling (dynamic decoupling is insensitivity to sudden changes in pressure), the pump must be able to respond sufficiently quickly to changes in pressure. The dynamics of the associated control valve also have to be taken into account. For the pump-control valve pair to dynamically decouple the units, it must respond much faster to the change in pressure than the process or reaction does.

Usually the system is designed in such a way that the pump and control valve end up with dynamics which are very much faster than those of the process (except in the case of explosions). Thus the complex model presented in section 4.4 is simplified to the following static model. Note the variable delay.

A = *pipe cross – sectional area*	Constant	m^2
F = *flowrate*	Output	m^3/s
k_F = *flowrate constant*	Constant	
k_n = *heat transfer constants*	Constant	
L = *length of pipe*	Constant	m
$P_p(F,\tau)$ = *pump characteristic surface*	Function	kPa
$P_s(F,u)$ = *system characteristic surface*	Function	kPa
T_1 = *instantaneous liquid temperature*	Output	K
T_2 = *delayed output liquid temperature*	Output	K
T_{in} = *incoming liquid temperature*	Input	K
T_S = *temperature of surroundings*	Constant	K
v = *normalised linear valve input*	Input	
τ = *delay from input to output*	Output	s

$$Fc \tag{5.4}$$

by solving

$$P_p(F, r) = P_s(F, n) \tag{5.5}$$

$$T_1 = k_1 T_m + k_2 T_S \tag{5.6}$$

$$\tau = \frac{LA}{F} \tag{5.7}$$

$$T_2(t) = T_1(t - \tau) \tag{5.8}$$

where

$$k_1 = \frac{UA_H}{UA_H + F\rho C_p}$$

$$k_2 = \frac{F\rho C_p}{UA_H + F\rho C_p}$$

The pump and the control valve are designed for normal operating conditions. In cases when pressures rise so quickly that the pump and the valve can no longer dynamically decouple the units, the appropriate safety valves need to be installed to protect upstream and downstream units from damage.

Another possible approach to the problem of dynamic decoupling is to design the system in such a way that less high speed decoupling is required. This would require that at the design stage, the system would be designed in such a way so as to allow a degree of dynamic coupling. The effects of hi coupling could be predicted using nonlinear modelling and bifurcation theory as outlined in chapter 6. Systems could even be designed to produce certain types of nonlin ar behaviour if it had some kind of advantage (superior mixing properties, etc). An example of a possible way this could be achieved are discussed in chapter 8.

Now that we have illustrated the problems encountered when linking units via liquid transport we are ready to illustrate the process of decoupling.

The decoupling of the simple mixing system presented in chapter 4 can be done by making use of the simplified model of the pump developed in equations 5.4-5.8. The result of replacing the dynamic model with the static model, effectively decouples all of the units. The reason this happens can be seen by looking at figure 4.2 in chapter 4 and noticing that all the units are joined using the pipe and pump. By then combining that information with the facts outlined above concerning the controlled pipe and pump, one can see that every unit is decoupled from every other unit in terms of their input and output pressures. The temperatures of the fluids in the system are only propagated foward, that is there is no feedback path in the example

system.

This results in only the CSTR having a more complex model than a simple integration or a first order lag with a delay (ie it is the only unit worth analysing). The result is that the CSTR can be modelled as a separate entity to the other units and their impact can then be assessed at a later stage. If a control loop encompassed both one of the tanks and the CSTR for some reason, then the time delay of the liquid flowing along the pipe would have to be taken into account. For linear systems this is relatively simple but for nonlinear systems it creates a great deal of difficulty as there is no equivalent nonlinear tool to the Laplace transform as used in linear systems[1]. The result of decoupling is essentially that the entire mixing system can be treated as just a CSTR.

5.1.2 Closely Coupled Units

The following section describes a system consisting of two units which are coupled in such a way that their mathematical models are very difficult to separate. The system shown is isothermal.

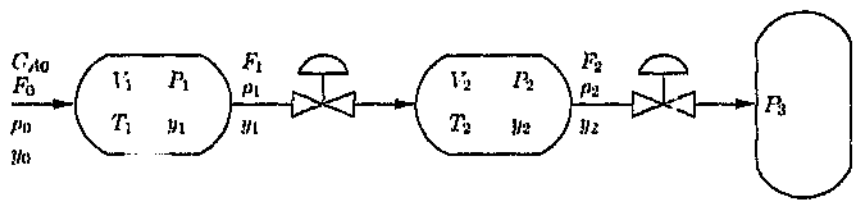


Figure 5.2: Isothermal Gas Pressurized CSTRs

The two gas pressurized tanks are joined together by a short length of pipe and a valve. The feed gas is pumped into the first chamber where it decomposes into another gas. It then passes through the pipe and valve into the second tank where it further decomposes. The final product passes through a second pipe and valve into a storage tank which is held at constant pressure.

The following analysis is used to develop the model for this system. The gas pressurized reactor is not one of the units modelled in chapter 3. The result is that the methodology for constructing complex system models from individual units is not

[1]This does not mean that delays can not be achieved in nonlinear systems by means of delay differential equations. These equations however are usually very high order and hence cumbersome to use as opposed to Laplace transforms.

followed, but the model is developed from a model given in [19].

The following relationships are adapted from [19].

$$F_1 = C_{V1}\sqrt{\frac{P_1 - P_2}{\rho_1}} \tag{5.9}$$

$$F_2 = C_{V2}\sqrt{\frac{P_2 - P_3}{\rho_2}} \tag{5.10}$$

$$\rho_1 = \frac{M_1 P_1}{RT_1} = [y_1 M_A + (1 - y_1)M_B]\frac{P_1}{RT_1} \tag{5.11}$$

$$\rho_2 = \frac{M_2 P_2}{RT_2} = [y_2 M_A + (1 - y_2)M_B]\frac{P_2}{RT_2} \tag{5.12}$$

$$C_{A1} = \frac{P_1 y_1}{RT_1} \tag{5.13}$$

$$C_{A2} = \frac{P_2 y_2}{RT_2} \tag{5.14}$$

The variables are defined as follows :

F_n	flows through the system	m^3/s
y_n	mole fractions of reactant A in the system	
ρ_n	densities in the system	kg/m^3
P_n	pressures in the system	kPa
R	gas constant	
T_n	temperatures in the system	K
V_n	volumes of the tanks	m^3
M_n	average molecular weights	
M_A	molecular weight of reactant A	
M_B	molecular weight of reactant B	
C_{Vn}	valve sizing coefficients [2]	

The following assumptions where made about the system in order to simplify it :

- The system is assumed to be isothermal.
- The relationship between the rate of flow through the control valve and pressure was assumed to be $F = C_V\sqrt{\frac{P_1 - P_2}{\rho}}$.
- The reaction is assumed to be of the form $2A \rightleftharpoons B$.

[2] These are the control inputs to the system as they change as the aperture of the valve is increased or decreased.

The total continuity equations are written as follows :

$$V_1 \frac{d\rho_1}{dt} = \rho_0 F_0 - \rho_1 F_1 \tag{5.15}$$

$$V_2 \frac{d\rho_2}{dt} = \rho_1 F_1 - \rho_2 F_2 \tag{5.16}$$

The component continuity equations are expanded as follows :

Step 1

$$V_1 \frac{dC_{A1}}{dt} = F_0 C_{A0} - F_1 C_{A1} - V_1 f_1(C_{A1}) \tag{5.17}$$

$$V_2 \frac{dC_{A2}}{dt} = F_1 C_{A1} - F_2 C_{A2} - V_2 f_2(C_{A2}) \tag{5.18}$$

Step 2

$$\frac{V_1}{RT_1}\frac{d}{dt}(y_1 P_1) = F_0 C_{A0} - \frac{P_1 y_1}{RT_1} C_{V1}\sqrt{\frac{P_1 - P_2}{\rho_1}} - V_1 f_1\left(\frac{P_1 y_1}{RT_1}\right) \tag{5.19}$$

$$\frac{V_2}{RT_2}\frac{d}{dt}(y_2 P_2) = F_1 C_{A1} - \frac{P_2 y_2}{RT_2} C_{V2}\sqrt{\frac{P_2 - P_3}{\rho_2}} - V_2 f_2\left(\frac{P_2 y_2}{RT_2}\right) \tag{5.20}$$

Finally writing out the entire dynamic model :

$$\frac{d\rho_1}{dt} = \rho_0 \frac{F_0}{V_1} - \rho_1 \frac{F_1}{V_1} \tag{5.21}$$

$$\frac{d\rho_2}{dt} = \rho_1 \frac{F_1}{V_2} - \rho_2 \frac{F_2}{V_2} \tag{5.22}$$

$$\frac{d}{dt}(y_1 P_1) = C_{A0} RT_1 \frac{F_0}{V_1} - \frac{P_1 y_1}{V_1} C_{V1}\sqrt{\frac{P_1 - P_2}{\rho_1}} - RT_1 f_1\left(\frac{P_1 y_1}{RT_1}\right) \tag{5.23}$$

$$\frac{d}{dt}(y_2 P_2) = \frac{P_1 y_1}{V_1} C_{V1}\sqrt{\frac{P_1 - P_2}{\rho_1}} - \frac{P_2 y_2}{V_2} C_{V2}\sqrt{\frac{P_2 - P_3}{\rho_2}} - RT_2 f_2\left(\frac{P_2 y_2}{RT_2}\right) \tag{5.24}$$

The two units (the two pressurized gas reactors) could be considered as separate entities. The model which was constructed to represent these tanks, however, reveals that they are ultimately linked via their pressures. Because the pressures in the tanks vary as the reactions proceed, the rates of flow, F_1 and F_2 vary. This affects the concentration of the products and hence the reaction rate. It becomes clear that the tanks are closely coupled units and cannot be analysed separately.

This system illustrates the fact that sometimes it is impossible and perhaps even undesirable to decouple units. It would increase the capital cost of building the gas system if a pump and a control valve with its associated control system were placed in between the two units. If the model is a reasonably true reflection of the physical system and if the model can be properly understood for all the regions of operation, then physical decoupling could be made uneccessary. There could be other important reasons to decouple the system which must of course be taken into account.

Although a system such as this, may not be able to be decoupled, it may still be possible to reduce the order of the state-space model (See section 5.2).

5.2 Model Order Reduction

5.2.1 Scaling

Scaling is essentially a process whereby a model's order is reduced or the number of variables involved is reduced. Scaling is used to simplify partial differential equations and to help in the process of creating sets of ordinary differential equations. The resulting equations are easier to solve but still produce sufficiently accurate results. This process is used extensively in simplifying chemical engineering models which usually result in high order partial differential equations.

Since the model equations in this dissertation are already assumed to be ordinary differential equations, it follows that scaling, if it has to be done, has already taken place. There is however one form of scaling which is still applied in this dissertation (time scaling) which is discussed in section 5.2.2. A simple introduction which is by no means exhaustive, is outlined here (see [20] for a detailed treatment of the subject).

Scaling essentially consists of two steps :

1. The process of non-dimensionalization.
2. The removal of "irrelevant" terms.

The equations have to first be converted into a form where the terms can be compared. To do this, the variables have to be normalized by dividing them by their

maximum expected value, so that the value of the transformed variable will always be near one. The coefficients that result from the original equation and the normalisation or non-dimensionalisation process determine which terms outweigh other terms and hence the equations can be reduced. The process itself is described in more detail in [20].

Scaling however has a weakness in that the models are sometimes very sensitive to small changes in a variable. This results essentially from an over-estimation of the maximum value of a variable in the normalization process. Hence although the scaling process helps to reduce models, it does have a serious weakness in that it requires prior knowledge of the ranges of variable values.

This problem is partly offset by the use of simulation on the original equations and then comparing the results.

There remains however a distinct possiblity that once a system has been scaled and even tested at a set of general operating points the model could be totally wrong. This can ultimately, only be corrected by physical experimentation.

5.2.2 ODE Model Order Reduction

Once a simplified ordinary differential equation has been obtained via the process of decoupling and scaling, the resulting set of ordinary differential equations can be reduced using time scaling. This could have already been done in the scaling process, but often it is better to leave the time scaling until the system control can be determined (control has a profound effect on the time constants of the system).

To use the chemical engineering methods for time scaling (which involve approximate estimates of the residence times for reactors, etc) is considered less effective than the standard control engineering techniques of linearization and $s-plane$ analysis at the extremes of the parameter values. For example it is uneccessary to 'normalize' the time variables, as long as we have an idea of which processes are faster and which processes are slower, and we need then decide (on the basis of our control objectives) which are the dynamics which will be included in the model.

The set of differential equations which will be used to illustrate the process of model order reduction are equations 5.25-5.28. They were obtained from the mixing system detailed in chapter 4 after the system was decoupled in section 5.1.

$$\frac{dV}{dt} = F_{in} - F_{out} \tag{5.25}$$

$$\frac{d(VC_A)}{dt} = F_{in}C_{Ain} - F_{out}C_A - Vf(C_A,T) \tag{5.26}$$

$$\frac{d(VT)}{dt} = F_{in}T_{in} - F_{out}T - \frac{\lambda V}{\rho C_p}f(C_A,T) - \frac{UA_H(V)}{\rho C_p}(T - T_J) \tag{5.27}$$

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}(T_{Jin} - T_J) + \frac{UA_H(V)}{V_J\rho_J C_J}(T - T_J) \tag{5.28}$$

This set of equations is described in section 3.3. The equations can be simplified in the following manner :

1. The fact that the volume is usually held constant by the use of feedback control is assumed true in this case.

2. The dynamics of the temperature of the water in the cooling jacket are shown to be much faster than the dynamics of the temperature of the process liquids and hence the dynamics of the jacket can be ignored.

The first point depends on the fact that the volume of the tank is reasonably large compared to the flow rate and hence is insensitive to changes in the output flowrate for short periods of time. This is the low-pass filtering effect of an integration. This combined with feedback control designed to keep the system at a constant volume results in an essentially constant volume which is quite insensitive to disturbances.

The second point depends on the fact that the volume of the cooling water in the jacket is very much smaller than the volume of the liquids in the tank. This means that the cooling water will take a much shorter time to heat up or cool down than the liquid in the tank. Hence the dynamics associated with the heating and cooling of the cooling water are much faster than the dynamics associated with the heating and cooling of the process liquids. Because the dynamics of the cooling water temperature are so much faster than those of the reactants, they can be treated as an instantly changing quantity for all practical purposes.

The following technique can be used to determine whether it is valid to assume that the jacket dynamics are negligible for a particular system. The parameter ranges shown in table 5.1 where chosen based on those obtained in section 7.2.4.

The approximate speed of the dynamics should be calculated for extreme values of the parameters. If more confidence in the results is required, more points should

Parameter	Range
C_{Ain}	$[0, 1]$
F_{in}	$[5 \times 10^{-6}, 1.5 \times 10^{-5}]\ m^3/s$
F_{Jin}	$[1 \times 10^{-5}, 3 \times 10^{-5}]\ m^3/s$
T_{in}	$[310, 330]\ K$
T_{Jin}	$[300, 320]\ K$
V	$[0.1, 0.2]\ m^3$

Table 5.1: CSTR Parameter Ranges for Scaling

be used. The analysis has to be done for a linearized system, with nonlinearity accounted for by using a range of parameters. A second order linear system can be represented as follows :

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} a & q \\ \bar{q} & \bar{a} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} b_1 & b_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \tag{5.29}$$

The poles of the system can be determined using the formula :

$$g(s) = det(s\mathbf{I} - \mathbf{A}) \tag{5.30}$$

where

$$\mathbf{A} = \begin{bmatrix} a & q \\ \bar{q} & \bar{a} \end{bmatrix} \tag{5.31}$$

This results in the following polynomial in s, the roots of which are the poles of the system :

$$g(s) = s^2 - (a + \bar{a})s - q\bar{q} \tag{5.32}$$

$$p_{1,2} = \frac{1}{2}\left\{(a + \bar{a}) \pm \sqrt{(a + \bar{a})^2 - 4(a + \bar{a})q\bar{q}}\right\} \tag{5.33}$$

The aim here is to analyse the interelationship between the cooling jacket and the reactor temperature dynamics. This can be done by taking all of the equations in the reactor model which contain direct references to the cooling water temperature.

Looking at equations 5.25 through 5.28, the only equations with direct references to the variable T_J are :

$$\frac{dT}{dt} = \frac{F_{in}}{V}T_{in} - \frac{F_{out}}{V}T - \frac{\lambda}{\rho C_p}f(C_A, T) - \frac{UA_H(V)}{V\rho C_p}(T - T_J) \quad (5.34)$$

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}(T_{Jin} - T_J) + \frac{UA_H(V)}{V_J\rho_J C_J}(T - T_J) \quad (5.35)$$

These equations must now be analysed to establish the relative speed of their dynamics in order to prove that the system can be decoupled. Equations 5.34 and 5.35 must be linearized. It is important to keep in mind that when equations are linearized, we assume that it is done around some equilibrium point. The actual position of the equilibrium point is not that important here as only an estimate of the dynamics is required to establish whether the dynamics are sufficiently different to justify decoupling. This means that only a range within which the equilibrium point would appear needs to be supplied and usually this information is known by the designers of the CSTR. It is important to remember that in the linearized equations all the state variables and inputs become perturbations around a set point.

The linearized form of the jacket and reactor energy equations is shown below (We assume $F = F_{in} = F_{out}$ holds — reactor fluid volume is held constant) :

$$\frac{dT}{dt} = \frac{F}{V}T_{in} - \frac{F}{V}T - \frac{\lambda}{\rho C_p}\frac{\partial f}{\partial C_A}\bigg|_{C_{Ae},T_e} C_A + \frac{\lambda}{\rho C_p}\frac{\partial f}{\partial T}\bigg|_{C_{Ae},T_e} T - \frac{UA_H(V)}{V\rho C_p}(T - T_J) \quad (5.36)$$

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}(T_{Jin} - T_J) + \frac{UA_H(V)}{V_J\rho_J C_J}(T - T_J) \quad (5.37)$$

C_A can be considered an input because it is not directly related to T_J. This results in a second order system, which is linearized in equations 5.36 and 5.37. We now need to determine the positions of the poles for all of the parameter ranges. The equations need to be converted into the form given for the standard second order system shown in equation 5.29.

Table 5.2 gives the values of the constants required for the solution of this problem (taken from appendix A and chapter 8) :

Equation 5.38 is used to calculate the heat transfer

Constant	Value
α	$\frac{1}{3}$
β	30
δ_1	$\frac{1}{2}$
δ_2	320
γ	2.667×10^{-4}
U	400
$\rho = \rho_J$	1000
$C_p = C_J$	4200
V_J	0.05
λ	-7.56×10^8
A	0.3

Table 5.2: Constant Values for Scaling

$$\begin{aligned} A_H(V) &= 2(V\sqrt{\frac{\pi}{A}} + A) \\ \text{where A} &= \text{CSTR cross} - \text{sectional area} \end{aligned} \tag{5.38}$$

$$\begin{bmatrix} \dot{T} \\ \dot{T}_J \end{bmatrix} = \begin{bmatrix} -\frac{F}{V} - \frac{\lambda}{\rho C_p}\frac{\partial f}{\partial T}\Big|_{C_{Ae},T_e} - \frac{UA_H(V)}{V\rho C_p} & \frac{UA_H(V)}{V\rho C_p} \\ \frac{UA_H(V)}{V_J\rho_J C_J} & -\frac{UA_H(V)}{V_J\rho_J C_J} - \frac{F_J}{V_J} \end{bmatrix} \begin{bmatrix} T \\ T_J \end{bmatrix} + \begin{bmatrix} b_1 & b_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \tag{5.39}$$

T uts to the equations are not considered as they have no impact on the position of the poles of the system (they do however effect the position of the zeroes). By comparing equation 5.39 and 5.29 the following relationships can be determined.

$$a = -\frac{F}{V} - \frac{\lambda}{\rho C_p}\frac{\partial f}{\partial T}\Big|_{C_{Ae},T_e} - \frac{UA_H(V)}{V\rho C_p} \tag{5.40}$$

$$\tilde{a} = -\frac{UA_H(V)}{V_J\rho_J C_J} - \frac{F_J}{V_J} \tag{5.41}$$

$$q = \frac{UA_H(V)}{V\rho C_p} \tag{5.42}$$

$$\tilde{q} = \frac{UA_H(V)}{V_J\rho_J C_J} \tag{5.43}$$

Therefore we now have to determine the variations of the states, inputs and functions which effect the position of the poles. This involves calculating the maximum variation of the chemical reaction for the variables, T and C_A. The variables C_A and T are simply limited using the reasoning outlined in section 7.2.1 to $C_A = [0, 1]$ and $T = [270, 370]$.

The only nonlinear part of the problem is the chemical reaction partial derivative. The maximum and minimum value of the chemical reaction coefficient for the entire range of C_A and T needs to be calculated. The first step is to calculate the formula for $\frac{\partial f}{\partial T}$.

$$f(C_A, T) = \frac{\alpha\gamma}{2}\left[-\left(\frac{C_A - \delta_1}{\alpha}\right)^2\left(\frac{T - \delta_2}{\beta}\right) + \left(\frac{C_A - \delta_1}{\alpha}\right) + 2\left(\frac{T - \delta_2}{\beta}\right)\right] \tag{5.44}$$

thus

$$\frac{\partial f}{\partial T} = \frac{\gamma}{2\alpha\beta}\left\{-{C_A}^2 + 2C_A\delta_1 - \delta_2^2 + 2\alpha^2\right\} \tag{5.45}$$

The first thing that can be observed from equation 5.45 is that the temperature has only linear terms which result in the fact that only C_A remains in the partial derivative. This means that the only variable which will cause a change in the slope of the reaction rate is C_A. Now what has to be determined is the maximum and the minimum value of the reaction rate slope. This can be done by equating $\frac{d}{dC_A}\frac{\partial f}{\partial T}$ to zero in order to obtain the maxima and minima. This equation is quadratic so we only expect one minimum or maximum point. The numerical values for α, β, γ and δ_1 are found in chapter 8. The results are as follows :

$$\frac{d}{dC_A}\frac{\partial f}{\partial T} = \frac{\gamma}{2\alpha\beta}\left\{-2C_A + 2\delta_1\right\} \tag{5.46}$$

hence the maximum occurs at

$$C_A = \delta_1 = \frac{1}{2} \tag{5.47}$$

hence the maximum is

$$\frac{\partial f}{\partial T} = \frac{\gamma\alpha}{\beta} \tag{5.48}$$

substituting in the values of (5.49)

$$C_A = [0, 1]$$

$$for\ C_A = 0\ :\ \frac{\partial f}{\partial T} = \frac{\gamma}{2\alpha\beta}(-\delta_1^2 + 2\alpha^2) \tag{5.50}$$

$$for\ C_A = 1\ :\ \frac{\partial f}{\partial T} = \frac{\gamma}{2\alpha\beta}(-\delta_1^2 + 2\delta_1 + 2\alpha^2 - 1) \tag{5.51}$$

Parameter	Range
$\frac{\partial f}{\partial T}$	$[-3.704 \times 10^{-7}, 2.963 \times 10^{-6}]$
F	$[5 \times 10^{-6}, 1.5 \times 10^{-5}]$
V	$[0.1, 0.2]$
F_J	$[1 \times 10^{-5}, \, \times 10^{-5}]$

Table 5.3: CSTR Parameter Ranges for Scaling (Simplified)

we know

$$\delta_1 = \frac{1}{2} \tag{5.52}$$

hence the minimum is

$$\frac{\partial f}{\partial T} = \frac{\gamma}{2\alpha\beta}\left(2\alpha^2 - \frac{1}{4}\right) \tag{5.53}$$

The numerical results for the variation of $\frac{\partial f}{\partial T}$ are :

$$\frac{\partial f}{\partial T} = [-3.704 \times 10^{-7}, 2.963 \times 10^{-6}] \tag{5.54}$$

Table 5.3 gives the variations of the relevant parameters :

Using the information in tables 5.1, 5.2 and 5.3 concerning all of the system parameters and states we get figure 5.3 which gives the variation in the position of the poles.

The smallest ratio of the time constants of the jacket and reactor temperature dynamics was found to be 12. The MATLAB function **jacket.m** (see appendix B) was used to draw the picture and obtain the ratio. The zeroes shown in the pole-zero map are irrelevant and should be ignored. Due to the fact that the jacket temperature dynamics have been shown to be much faster than the reactor dynamics, they can safely be ignored.

Using the reasoning outlined so far, equations 5.25 through 5.28 can be reduced to the following dynamic form :

$$V\frac{dC_A}{dt} = F_{in}C_{Ain} - F_{out}C_A - Vf(C_A, T) \tag{5.55}$$

$$V\frac{dT}{dt} = F_{in}T_{in} - F_{out}T - \frac{\lambda V}{\rho C_p}f(C_A, T) - \frac{UA_R(V)}{\rho C_p}(T - T_J) \tag{5.56}$$

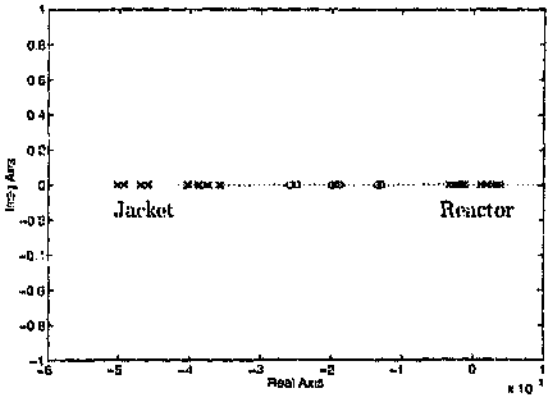


Figure 5.3: Reactor - Jacket Dynamics

and the following constituitive relationships :

$$F = F_{in} = F_{out} \tag{5.57}$$

$$T_J = \frac{1}{k_1 + k_2}(k_1 T_{Jin} + k_2 T) \tag{5.58}$$

where

$$k_1 = F_J \rho_J C_J$$

$$k_2 = U A_H(V)$$

This reduces the CSTR from a fourth order system to a second order system which is more easy to analyse. It will not always be possible to reduce the order of a system, but for every reduction in order of the system there is a corresponding saving in the amount of calculation to be performed.

The CSTR is now a second order nonlinear problem, which although not analytically tractible in many cases, does reduce the amount of numerical calculations substantially.

Chapter 6

Bifurcation Theory

6.1 Introduction

Bifurcation refers to a sudden change in the solution of a system of equations. When the system of equations represents a model it is referred to as a change in behaviour of the system being modelled. There are essentially two types of bifurcations, static and dynamic bifurcations. The types of dynamic systems can also be broken down into two groups, discrete and continuous. The models used in this dissertation are all continuous as most chemical processes are modelled using continuous time models (partial or ordinary differential equations).

Static bifurcations occur in a continuous differential equation when an equilibrium point appears or disappears as a system parameter is varied. This can be illustrated using Duffings equation.

$$\dot{x_1} = x_2 \tag{6.1}$$

$$\dot{x_2} = x_1 - x_1^3 - x_2 + \mu \tag{6.2}$$

where μ is the model parameter

The position of the equilibrium point can be drawn for μ vs x_1. Figure 6.1 is constructed by considering the equilibrium points of equations 6.3 and 6.4.

$$x_1^3 - x_1 - \mu = 0 \tag{6.3}$$

$$x_2 = 0 \tag{6.4}$$

Solving equation 6.3 for x_1 as μ is varied in the range $[-0.5, 0.5]$, gives the bifurcation diagram shown in figure 6.1.

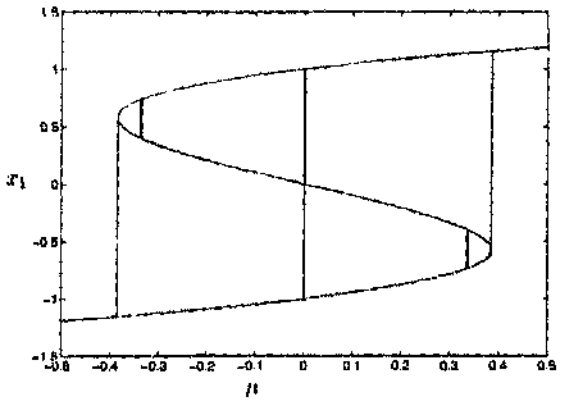


Figure 6.1: Equilibrium diagram showing a Static Bifurcation

Figure 6.1 shows that for different values of μ, the number of equilibrium points changes. For instance, in the range $[-0.37, 0.37]$, for instance the dynamic system has three equilibrium points whereas in the range $(-\infty \ -0.37]$ the dynamic system has one equilibrium point. This can be seen in the diagram by drawing a vertical line at the relevant value of μ and noting the number of times it is crossed by the equilibrium point curve.

The important thing to note is that at some point the three equilibrium points abruptly disappear and are replaced by a single equilibrium point. This is known as a static bifurcation. When doing the bifurcation analysis of a chemical system, this is the first set of information that is required.

The next type of bifurcations that occur are dynamic bifurcations. These do not result in the appearance or disappearance of an equilibrium point but rather in a change of dynamic behaviour around the equilibrium point in question. That is, the stability of the equilibrium point changes when a dynamic bifurcation occurs. There are many different types of dynamic bifurcation which can occur, some of these are illustrated in section 6.3.

The van der Pol equation, given by equations 6.5 and 6.6 illustrates the concept of a dynamic bifurcation.

$$\dot{x}_1 = x_2 \tag{6.5}$$

$$\dot{x}_2 = \mu(1 - x_1^2)x_2 - x_2 \tag{6.6}$$

From 6.5 and 6.6 with $\dot{x}_1 = 0$ and $\dot{x}_2 = 0$, it can clearly be seen that for all values of μ the number of equilibrium points remains the same, namely, the point $(0, 0)$. No new equilibrium points appear and the existing equilibrium point never disappears. However the behaviour of the system is affected by the change in μ. If the stability of the linearized system is analysed at the equilibrium point it is found that the path traced out by the poles of the linearized system for a changing μ is shown in figure 6.3.

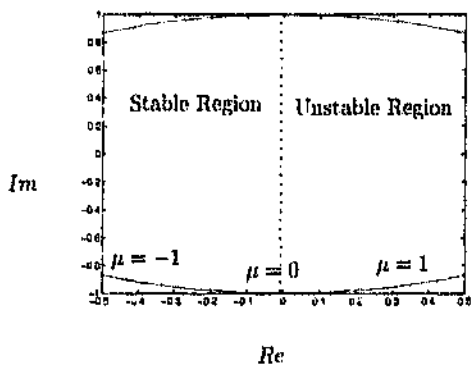


Figure 6.2: Dynamic Bifurcation Diagram

The relationship between the stability and the parameter μ can be clearly shown by plotting the real part of the poles vs μ. Figure 6.3 gives this relationship.

The examples given in this section clearly show the difference between static and dynamic bifurcations :

1. In static bifurcations the number of equilibrium points changes after the bifurcation occurs.

2. In dynamic bifurcations, the same number of equilibrium points exist on either side of the centre manifold (before and after the bifurcation occurs) as μ changes. However the qualitative dynamic behaviour of the system changes.

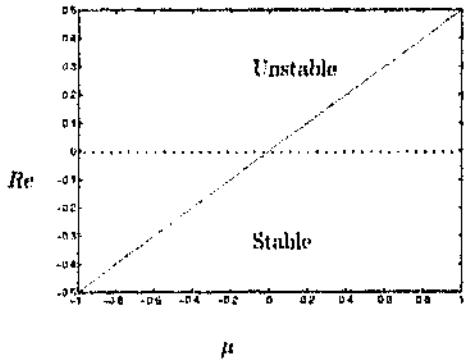


Figure 6.3: Parameter Stability Relationship

We can also see how important bifurcations are, and how they radically affect the behaviour of continuous dynamic systems.

6.2 Centre Manifold Theory

Center manifold[1] theory examines the characteristics of a system at the critical point for dynamic bifurcations. The critical point occurs when changing a system parameter has caused the system to become marginally stable around an equilibrium point. Marginal stability is usually structurally unstable[2]. By finding the equilibrium points of a nonlinear system, linearizing the system around each of those equilibrium points and observing how the eigenvalues of the linearized systems change with changes in system parameters, it is possible to determine when the system is on the centre manifold and how it is behaving. This is very important information because, "the nature of the bifurcation is determined by the dynamics on the centre manifold at the bifurcation point." — [24]

The system is on the centre manifold when the real part of the poles of the linearized system (at a particular equilibrium point) are zero. This means that the poles are on the imaginary axis. The poles are usually[3] on the threshhold of crossing

[1] A centre manifold is a manifold of a nonlinear dynamic system and is analogous to a linear subspace for linear systems (for a definition of invariant manifolds, see [24]).

[2] A system is structurally unstable if an infinitesimal change in a parameter changes the system stability (see [26]).

[3] Sometimes systems can have poles that move from the lefthand plane onto the axis and then back into the lefthand plane or vice versa (see [24])

the imaginary axis with the system becoming unstable (or stable). Note that the system dynamic behaviour in the neighbourhood of an equilibrium point may be unstable, while the global system dynamic behaviour could be stable. This is because a nonlinear system can have unstable equilibrium points but still remain globally stable (that is the output remains finite as time goes to infinity). This is only true as long as the initial conditions are not on the unstable manifold.

For nonlinear systems there are two kinds of stability, global and local stability. In linear systems these two are exactly the same but in nonlinear systems they can be separated. The reason for this is that in a linear system the structure of the vector field for the entire state space can be determined by examining the local behaviour of the linear system at its single equilibrium point. In nonlinear systems however, this is not true as there could be several equilibrium points or some other form of behaviour such as a limit cycle which makes it impossible to predict global behaviour by using analysis of a single equilibrium point (local stability analysis).

A nonlinear system can become locally unstable but remain globally stable. This happens when a system begins to spontaneously oscillate as a parameter changes (as in the case of the van der Pol equation). The oscillations remain bounded as time proceeds and hence the system is still stable even though it is locally unstable at an equilibrium point. Figure 6.4 shows the output of the van der Pol oscillator where the system is locally unstable at the equilibrium point $(0, 0)$.

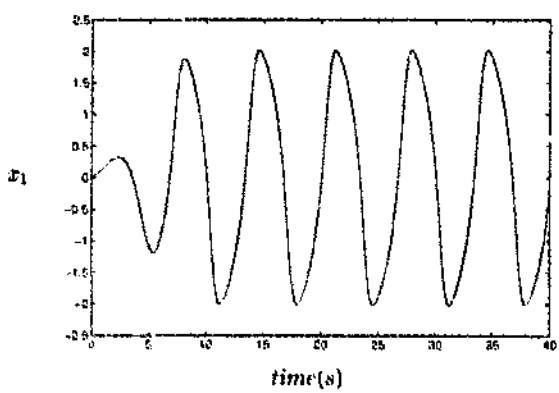


Figure 6.4: Output of the van der Pol Oscillator ($\mu = 1$)

There are certain conditions that emerge from centre manifold theory that are important to determining whether a dynamic bifurcation *could* lead to stable oscillatory

or chaotic behaviour. These are neccessary but not sufficient conditions for oscillatory and chaotic behaviour. There are strict mathematical conditions which can be applied to a system on the centre manifold. They are not dealt with here due to the fact that the focus of this dissertation is the application of the mathematical conditions in a useful and practical way. The mathematical conditions can be found in [24].

6.3 Review of Second Order Behaviour

Once the static analysis of the system is complete we know how the equilibrium points of the system change as parameters and inputs change. This is very useful information but it is not complete as we would have no idea how long a particular process system will take to reach its steady state or whether the system is inherently stable or unstable.(The next step is to gain insight into how the system responds as time proceeds.)

The system must be linearized at all of the equilibrium points. This provides information about the local stability of the equilibrium points. It is however possible to use the information about local stability to form a qualitative picture of the global stability. By determining how a behaviour will effect the local stability of an equilibrium point, it is possible to identify when a nonlinear behaviour might be occurring and use other methods (for example simulation or Lyapunov analysis [23]) to verify its existence.

For any form of nonlinear ordinary differential equations, there are a finite number of ways the system can behave. This does not mean that this finite set of behaviours cannot occur in infinite varieties and combinations, but the behaviours themselves definitely fall into a finite set of classes, based on the order of the differential equations and the types of nonlinearity present. An example would be a system with multiple equilibrium points. The classes of behaviour would be finite (stable/unstable foci, nodes and saddles) while the way these were combined could be infinitely variable.

The following paragraphs and diagrams give a breakdown of the types of behaviour which can occur for second order systems. The list is not completely exhaustive but covers the most common behaviours. Second order systems are very important because parameters tend to effect poles as pairs (ie two poles will move in a linked way for a change in a parameter). More than two poles may move (in high order

systems), but they will very often also move as pairs. The exception is a single pole which always stays on the real axis.

The first type of behaviour encountered is a second order system with a stable equilibrium point which is a node (figure 6.5). It is the equivalent of having two first order systems coupled together. The opposite kind of behaviour (from a stability point of view) is the unstable node(figure 6.6).

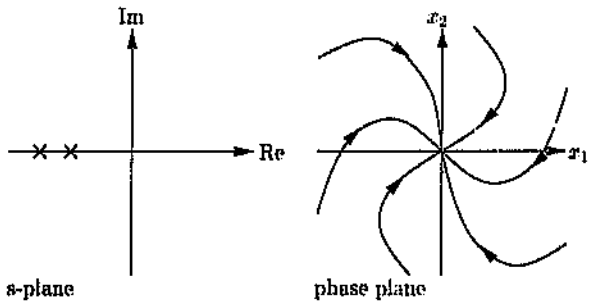


Figure 6.5: The Stable Equilibrium Point (Node)

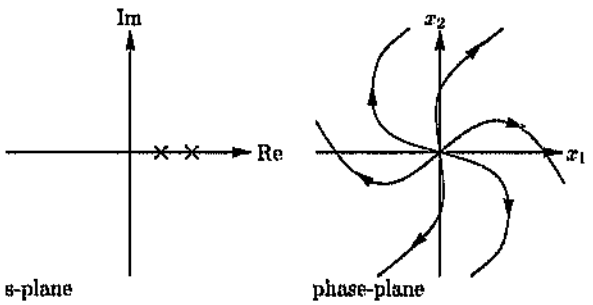


Figure 6.6: The Unstable Equilibrium Point (Node)

The second type of behaviour that a second order system exhibits is a stable or unstable focus. A focus only occurs in second or higher order systems as it requires the interaction of two states (see figures 6.7 and 6.8).

A combination of stable and unstable (called non-stable) equilibrium points is the saddle which attracts a state when in one region of the phase plane but repels it when in a different region. This is shown in figure 6.9.

The final form of second order behaviour which can occur in linear second order

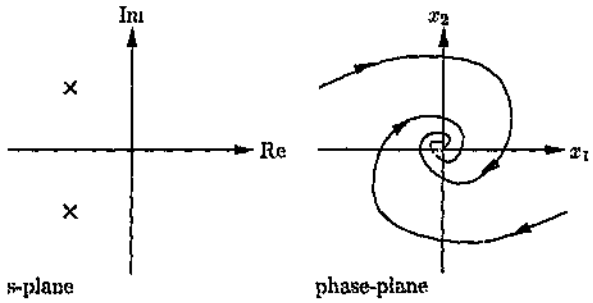


Figure 6.7: The Stable Equilibrium Point (Focus)

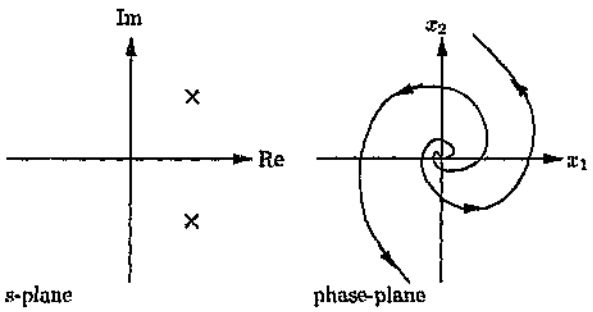


Figure 6.8: The Unstable Equilibrium Point (Focus)

systems is the centre. A centre is usually a structurally unstable behaviour in linear systems. Hamiltonian systems however, are structurally stable on the centre manifold. A fricitionless pendulum is an example of a hamiltonian system (because hamiltonian systems are not dissipative which is rare in normal engineering problems). The centre behaviour consists of a sustained oscillation with an amplitude determined by the initial conditions. It has no set amplitude of oscillation as the limit cycle does. Figure 6.10 illustrates this behaviour (for several initial conditions).

In addition the dynamic behaviour that can only occur in a *nonlinear* second order system are the stable and unstable limit cycle, as well as multiple equilibrium points.

Multiple equilibrium points are essentially any combination of the equilibrium points given so far. It must be kept in mind that only certain kinds of equilibrium points can exist together. A way to illustrate this idea is to imagine two unstable equilibrium points in the phase plane. By making a qualitative drawing of the possible trajectories of the system in the phase plane, one will realize that a third equilibrium

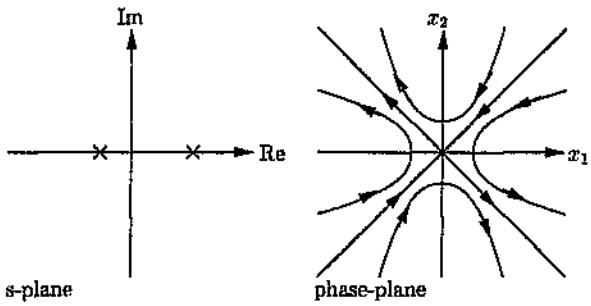


Figure 6.9: The Non-Stable Equilbrium Point (Node) or Saddle

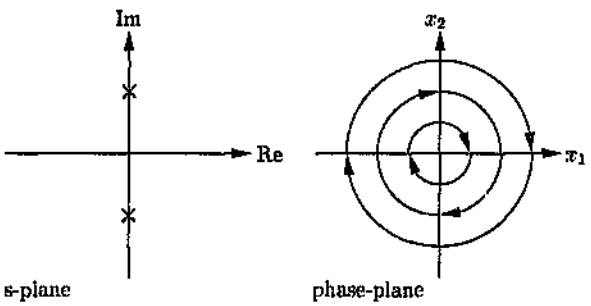
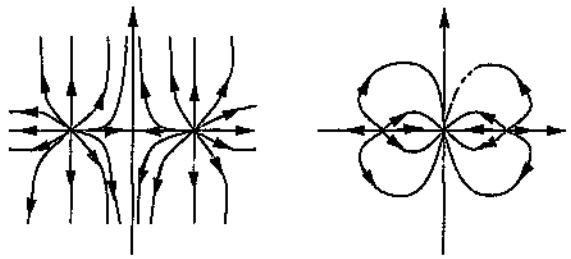


Figure 6.10: The Centre

point (of different stability) must exist for the system to exist (it becomes m thematically impossible to create a system with only two unstable or stable equilibrium points — hence such a system cannot exist). Figure 6.11 shows two cases of multiple equilibrium points (the $s-plane$ diagrams are the same as those for the single equilibrium points already described).

The limit cycle is similar to the centre in that it results in a sustained oscillation. The difference however between the limit cycle and the centre is that while the centre will oscillate at an amplitude dependent on the initial conditions, the limit cycle has a set amplitude which is independent of the initial conditions. A frictionless pendulum would be an example of a system which could be modelled by a set of equations which exhibit centre behaviour (the greater the initial force, the greater the amplitude of the resulting oscillations).

A limit cycle however is a form of dynamic equilibrium. Figure 6.12 shows the phase plane representation of a possible limit cycle. The s-plane illustrates a possible



2 Unstable Points & Saddle 2 Unstable & 1 Stable Point

Figure 6.11: Multiple Equilibrium Points

position of the poles of the nonlinear system when linearized about the equilibrium point. The unstable form of the limit cycle is similar to the stable limit cycle in structure but has the following differences. The s-plane has the poles in the left hand plane and the system flow moves in the opposite direction in the phase-plane. Thus an unstable limit cycle intitially looks like a stable equilibrium point.

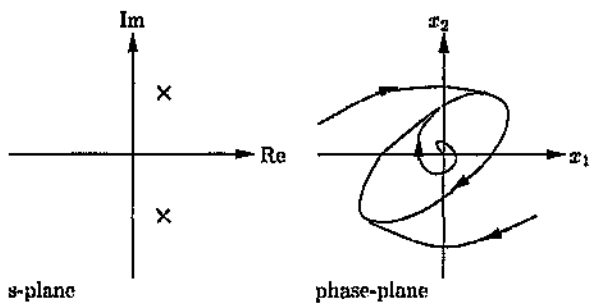


Figure 6.12: The Stable Limit Cycle

The weakness of the method presented in this dissertation is that the linearized analysis is only valid in a *local neighbourhood* of the equilibrium point. The size of the neighbourhood is not specified. This is an important weakness as it means that it is possible to have a system which appears stable but may become unstable for certain sets of initial conditions. The reason that this happens is shown in figure 6.13. A way to detect whether this is occuring is to be very careful (that is simulate the system for a range of initial conditions) whenever eigenvalues cross the imaginary axis.

The simplest way to test for this is to ensure that at least one simulation is done for the stable equilibrium point at an extreme value of initial conditions. This may be

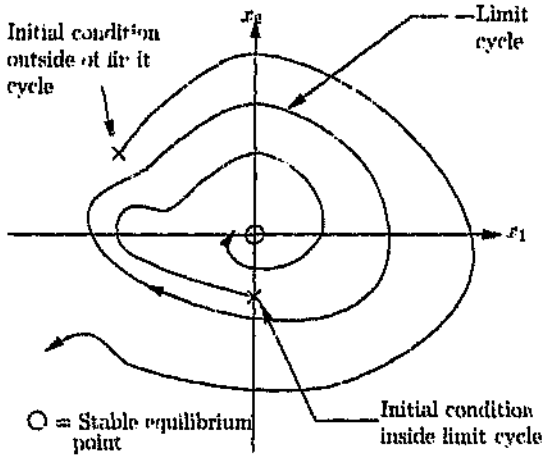


Figure 6.13: Unstable Limit Cycle Showing Regional Instability

increased to several if this behaviour is suspected for the system being analysed. An alternative is to use Lyapunov function analysis if it is possible to derive or obtain a Lyapunov function for the system. This approach however will not be discussed in this dissertation.

Higher order systems are essentially collections of poles as either linked pairs or poles on their own. This means that by observing the movement of poles in the s-plane, the poles that are important from a stability point of view can be determined. All that matters from a bifurcation point of view are the poles which move across the imaginary axis (the nonlinear system behaviour on the centre manifold). Essentially, qualitative dynamic behaviour of the system is determined by the behaviour on the centre manifold. All that the higher order system allows is the possibility of more interesting forms of nonlinear behaviour. The bifurcations however are still very similar. Hence the information that is obtained for the second order system is very helpful for higher order sys s and the methodology will work exactly the same for any order system (within reason, that is, it is limited by your ability to manage a large amount of information).

6.4 Identifying Bifurcations

To identify bifurcations we rely on the behaviour of the system on the centre manifold (see section 6.2). Obtaining this information directly is often tedious and also

takes specialized information to interpret (see [24] for mathematical methods). Another approach is not to bother solving for the case when the system is on the centre manifold, but rather to look at the behaviour of the system on either side of the centre manifold. The chances of the system behaving qualitatively differently for parameter variations increases as the parameter variations are increased. Thus the variation in the parameter should be kept small with respect to changes in the behaviour. This means that the amount the poles move for a given change in parameter should be kept small.

Once it has been ascertained that a system's stability has changed as a parameter was varied, then the type of bifurcation can be determined by observing the system before and after the bifurcation. Usually, either one real or two complex conjugate poles will cross the imaginary axis simultaneously (although it is possible to construct examples for which this does not occur). This means that the behaviour of second order systems becomes very important for all orders of systems (except obviously first order systems).

Once the bifurcation has been classified as either static or dynamic then it is further classified using the charts shown in figures 6.14 and 6.15. Note that there are some bifurcations which are not covered here but developing more chart entries should not be too complex. Often the more complex bifurcations represent structurally unstable cases valid only for a singular value of a parameter and hence can be ignored for practical purposes.

Once the bifurcation has been classified as accurately as possible using the information obtained from the linearization process it can be analysed using different numerical methods. If there is confusion as to what kind of bifurcation it is (as in the case of the Hopf bifurcation), the system will have to be simulated at a set of appropriate parameter values. The cases where there could be confusion are those where global stability has to be determined. The method of linearizing at the equilibrium points, while being a powerful technique, can never determine the global stability characteristics of a system. As has been shown however, it can be a useful tool for reducing the amount of simulation which has to be done to determine global stability. What this essentially means is that while the engineer can narrow down the search for nonlinear behaviour using this method, simulation, along with other related methods (for example Lyapunov function analysis, Lyapunov exponents) remain the only way of characterizing complex behaviour.

Once the bifurcations that a system exhibits have been defined it becomes possible to design the system in such a way so as to either exploit or avoid certain nonlinear

behaviours which would never have been considered before. The analysis can also be performed on existing systems and used to predict what will happen if the operating point were adjusted because of changing requirements.

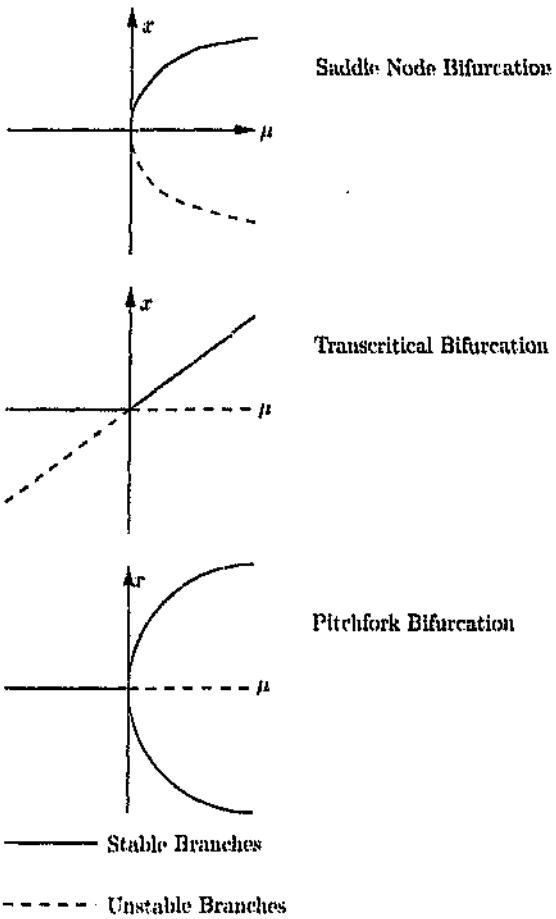


Figure 6.14: Chart of Simple Static Bifurcations

Figures 6.14 and 6.15 give two charts for classifying bifurcations, these were created using information from [18] and [24]. The diagrams in the chart are called bifurcation diagrams. Bifurcation diagrams represent the equilibrium surface of a system for change in a single parameter μ, that is they graphically represent the solution to the problem $\dot{\mathbf{x}}(\mu) = 0$. Stable surfaces (lines in the case of equilibrium points) are represented as solid while unstable surfaces are dotted.

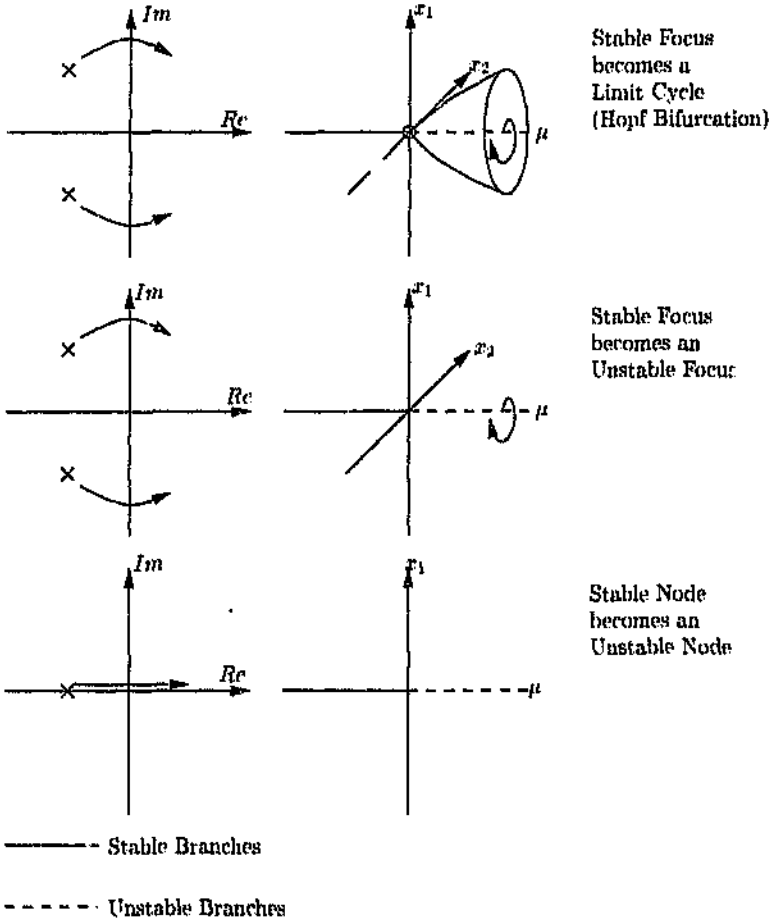


Figure 6.15: Chart of Simple Dynamic Bifurcations

6.5 Conclusion

The theory outlined in this chapter gives a synopsis of the practical ideas which have emerged from nonlinear theory, especially the branch that deals with sudden changes in behaviour, bifurcation theory. The theory uses linear theory to begin to interpret the more complex nonlinear behaviours. The aim is to use nonlinear theory to narrow down the search by excluding well understood behaviours and hence reduce the amount of detailed analysis (simulation, etc).

Chapter 7

Nonlinear Analysis

7.1 Overview

This chapter discusses the analysis methodology by making use of the system example (see chapter 4). The methodology is illustrated in figure 7.1.

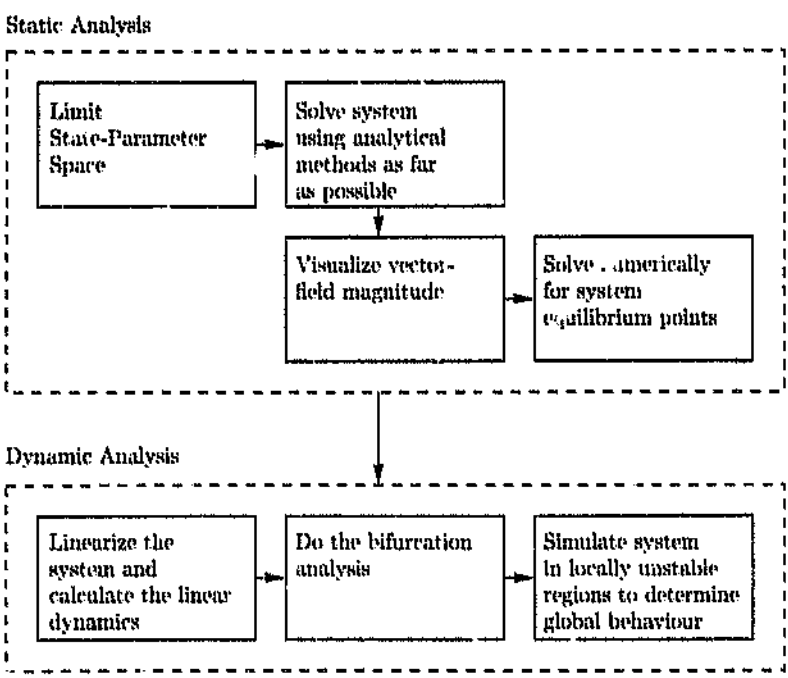


Figure 7.1: Analysis Methodology

7.2 Static Analysis

7.2.1 Limiting the State-Parameter Space

Limiting the state parameter space is another way of saying that all the variables, including both states and parameters are limited to some $m+n$ dimensional space, where m is the number of states (the order of the dynamic model) and n is the number of variable parameters. The states and parameters have to be limited to a set of ranges to make analysis feasible. That is, analysis can often not be performed for infinite ranges of variables. In almost every engineering problem (if not every problem), the ranges of values of the parameters will be limited to some finite range.

Limiting the ranges of the values of the states and parameters results in some $m+n$ dimensional volume being filled in the state-parameter space. For example, in a three dimensional state-parameter space, the limitation of the parameters would result in a rectangular parallelepiped volume if all the states and variables were varied between constant limits. Within that volume, equilibrium points could be found for varying parameter values.

In the case where the system has two states and one parameter ($m=2$ and $n=1$), the equilibrium points would describe arcs in the state parameter space. This is because, as the parameter is varied, the position of the equilibrium points could change continuously. It is also feasible for equilibrium points to appear and disappear as the parameter is varied. The equilibrium points could also move in a discontinuous manner.

The state parameter space must be divided into discrete points, so that analysis can proceed. The vector field, formed by the state equations is visualized in different ways for the changing parameters using numerical methods. The use of numerical methods requires that the problem be discretized. This process is further discussed in section 7.2.3.

The way that the ranges of the parameters and states are determined using physical reasoning is based on practical limitations. This process would be different for every different type of problem. It is however a relatively simple process, as it does not require a high degree of accuracy but just "ball-park" values. As long as all the realistic behaviours of the system will be contained within the state-parameter space, then the ranges assigned to the variables are sufficient.

To illustrate how this process would usually be carried out, the following example

is given based on the simplified model of section 5.2. The simplified model obtained for the CSTR was :

$$\frac{dC_A}{dt} = \frac{F}{V}C_{Ain} - \frac{F}{V}C_A - f(C_A,T) \tag{7.1}$$

$$\frac{dT}{dt} = \frac{F}{V}T_{in} - \frac{F}{V}T - \frac{\lambda}{\rho C_p}f(C_A,T) - \frac{UA_H(V)}{\rho C_p V}\left[T - \frac{1}{F_J\rho_J C_J + UA_H(V)}(F_J\rho_J C_J T_{Jin} + UA_H(V)T)\right] \tag{7.2}$$

Thus there are two states (C_A and T) and 6 variable parameters (C_{Ain}, F, F_J, T_{in} and T_{Jin}, V) as well as 3 constant parameters (C_p, U and λ). All the parameters could be seen as variable parameters, as many of them will change over very long periods of time. The ones that have been chosen as variable parameters are those which would be inputs. These can then be varied and the resulting response of the system determined. Step responses[1] to changes in these parameters can also be determined.

The ranges of the states and the variable parameters need to be defined so that analysis can proceed. Table 7.1 gives the ranges decided upon and a short justification. As can be seen, it is remarkably simple to establish reasonable ranges for the variables for this example. At this stage we also define the constant parameters (which obviously don't have a range). The values used come from the system example given in appendix A.

The resulting ranges of the variables were obtained using simple reasoning which significantly reduces the complexity of the problem. No longer are we trying to solve a problem with 2 state variables and 6 variable parameters over an infinite range of values. We are now limited to a very specific region. As seen in table 7.1, defining the limitations on one variable will often result in the ranges of other variables with the same physical dimensions also having the same range.

Only one more definition is required to continue the analysis to the next stage and that is the rate function, $f(C_A,T)$.

[1]The one parameter that it would be incorrect to do a step response for, is V (volume). This is because the volume couldn't change instantly without an infinite difference in the input and output flow rate. It would be wrong to change the input and output flow rate separately from each other for this model because it violates a basic assumption on which the model is based. This is a good example of how the modelling engineer should always be aware of what assumptions were used to create the model and never violate them. The model becomes invalid for this experiment.

[2]Note : When $F_J = 0$ the CSTR model will give results as though no energy is dissipated to the surroundings.

Variable	Range	Reason
C_A	$[0, 1]$	Fractional concentrations can't be negative or greater than 1.
T	$[270, 370]$	Freezing point and boiling point of process liquids.
F	$[0, 1]$	$1\ m^3/s$ is the design flow rate of liquid through the input and output valves.
F_J [2]	$[0, 1]$	$1\ m^3/s$ is the design flow rate of liquid through the jacket input and output valves.
V	$[0, 0.2]$	0.2 is the maximum volume of the tank.
C_{Ain}	$[0, 1]$	Fractional concentrations can't be negative or greater than 1.
T_{in}	$[270, 370]$	Freezing point and boiling point of process liquids.
T_{Jin}	$[270, 370]$	Freezing point and boiling point of cooling water.
$A_H(V)$	$[0.6, 1.894]$	Heat transfer area for V.
C_p	$4200\ J/kgK$	Heat capacity of water.
U	$400\ W/m^2K$	Heat transfer coefficient.
λ	$-7.56 * 10^8\ J/kg$	Heat of reaction.

Table 7.1: CSTR Variable Ranges for Static Analysis

The rate equation 7.3 is defined so as to give a limit cycle (the most complex nonlinear behaviour possible with a second order system). See chapter 8 for how the rate function was obtained. The rate equation is not based on a particular chemical process but designed to give a limit cycle. It could be used as a measure against which chemical reaction rates could be tested, to see if they will exhibit this kind of nonlinear behaviour.

$$\begin{aligned} f(C_A,T) &= 4.445 \times 10^{-6} x_1^2 x_2 - 4.445 \times 10^{-6} x_1 x_2 - 1.4224 \times 10^{-3} x_1^2 + \\ &\quad 1.55575 \times 10^{-3} x_1 + 4.07455 \times 10^{-6} x_2 - 1.370535 \times 10^{-3} \end{aligned} \quad (7.3)$$

7.2.2 Analytical Solutions

Analytical solutions are almost impossible to get for most nonlinear problems. However, there is some information which can be obtained by simple analysis of the equations. Often, while all of the equilibrium points cannot be analytically determined, one or two may be easily determined analytically. This provides additional information, usually with minimal effort, which can help direct the process of numerical solution (choosing starting points, etc). Singularities can also be detected although they may not be able to be exactly located. This helps the analyst to gain insight into the reason for failures of numerical methods.

It is always important for the analyst to look at the system from an analytical point of view at the start, so as to detect any obvious solutions and possible sources of numerical error.

7.2.3 Visualizing the Equilibrium Points

Now that the ranges and values of all the expressions in the set of equations have been defined and some possible sources of problems or obvious solutions have been detected, analysis can proceed.

We begin by setting the values of the variable parameters to their median value. That is we set them to half-way between the limits. We then proceed to do the numerical analysis. The first step is to visualize the vector field (ie values of $f(C_A,T)$) in different ways to give an idea of where to look for equilibrium points. This could be done using a computer program but it is unneccessary to write a complex program

to do what a human being can do more effectively and efficiently (the human brain is the most effective pattern recognition element we have available to us).

The vector field must be converted into a form which can be visualized by a human being. If the dimension of the equations is too high, ways must be found of including that information in a graphical format. The engineer can then determine the equilibrium points to within some acceptable tolerance (say 5%). A computer algorithm can then be used to find the equilibrium points to a high degree of accuracy.

Computer algorithms need some starting point to work properly and hence the visualization step is essential. Note that at this stage of the process we are not concerned about whether the equilibrium points are stable or unstable. We are only interested in determining their location to some degree of accuracy. We are also interested in determining how they move in the state space as the parameters are changed. Their appearance and disappearance must also be taken into account (An equilibrium point can disappear as a parameter changes).

The system shown is easy to visualize because it is two dimensional in the state-space. The only information that is required about the vector field to determine where the equilibrium points are, is the magnitude of the field. Where the magnitude is zero, there is an equilibrium point. The magnitude of the vector field is represented graphically using colours and shades. The positions of the equilibrium points become easy to determine providing the resolution of the viewer of the vector field is high enough. The magnitude of the vector field is observed for one set of parameter values.

Figure 7.2 results from the following set of parameter values in table 7.2. Figure 7.2 is taken of the vector field for values of the state variables defined in table 7.1. The picture is used to find a set of starting points for the numerical analysis algorithms implemented in MATLAB (see appendix B).

From this picture (black indicates a low magnitude ($f(C_A, T) \approx 0$)) the approximate location of the equilibrium point can be determined. The rate function which is used for this example is equation 7.3. We can observe where the equilibrium point will most probably be (we can never be 100% sure until we do the numerical analysis). The approximate position of the equilibrium point is somewhere along a stretched out Z going from (0.360), through $(0.5, 320)$ and finishing at $(1, 280)$. We know

[3]Note : This value is not half way between the two extremes but at the maximum value. It is chosen this way because normally CSTRs are designed to operate at maximum value (with some extra volume for a safety margin). The volume can be decreased to see the effect of changing this parameter.

Variable	Value
C_{Ain}	0.5
F	0.1
F_J	0.01
T_{in}	320 K
T_{Jin}	320 K
	0.2 m^3

Table 7.2: Initial Static Analysis Parameter Starting Point

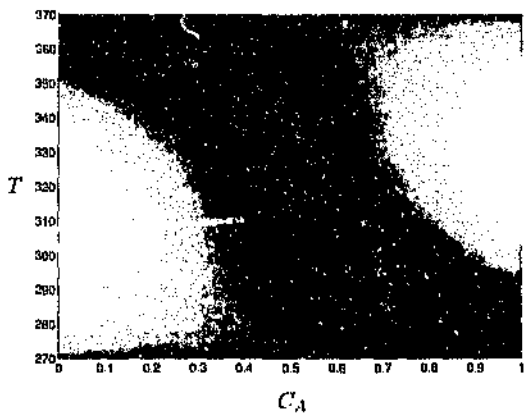


Figure 7.2: Vector field magnitude

there is one equilibrium point because we have a priori knowledge of the system (see chapter 8). Even if this were not the case, the values chosen for the starting p.int of the numerical analysis would be the same, in the centre of the diagram.

Note that at this stage nothing is said about the stability of the equilibrium point (or region). The process that is now followed is one of increasing and decreasing each of the parameters while holding the others constant at the original set point values (table 7.2) and observing the resulting changes in position of the ec alibrium point. The algorithm used, increases the chosen parameter a fraction of the overall distance (defined table 7.1) and then searches for the new position of the equilibrium point (using some standard numerical method). Once the new position of the equilibrium point has been determined, the procedure is repeated until the position of the equilibrium point has been established for the full range of that particular parameter (while holding the others constant). This process must then be repeated

for all the parameters (this is illustrated in section 7.2.4). Figure 7.3 gives a flow chart of the method outlined above. This method is essentially a simple continuation method for finding equilibrium points. One parameter is varied at a time while all the others are held constant.

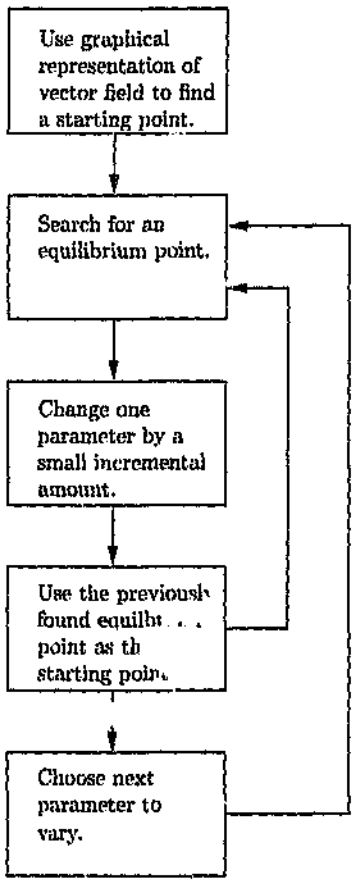


Figure 7.3: Flow Chart of Equilibrium Point Finding Algorithm

The information that is obtained in the process of determining the location of the equilibrium points must be stored as it will be very important in the next step of analysing the dynamic behaviour of the plant (this will be done at the equilibrium points).

The method presented here has several weaknesses. The most noticeable is that the entire state-parameter space is not analysed. This results in the danger that some behavioural change will "slip through the cracks". This can be reduced by

doing a more comprehensive analysis of the system which would be far more time consuming. This is recommended but has not been done because the aim of this work is to illustrate the methodology, not to comprehensively analyze a particular system.

7.2.4 Static Analysis of the System Example

The states and parameters of the model are limited to some finite parameter space using physical reasoning as per table 7.1. The first step is to examine the equations for any analytical equilibrium solutions which we may be able to obtain. Equations 7.1 and 7.2 must be set equal to zero.

$$0 = \frac{F}{V}C_{Ain} - \frac{F}{V}C_A - f(C_A, T) \tag{7.4}$$

$$0 = \frac{F}{V}T_{in} - \frac{F}{V}T - \frac{\lambda}{\rho C_p}f(C_A, T) - \frac{UA_H(V)}{\rho C_p V}\left[T - \frac{1}{F_J\rho_J C_J + UA_H(V)}(F_J\rho_J C_J T_{Jin} + UA_H(V)T)\right] \tag{7.5}$$

The first thing to note is that this reactor could be treated as a batch reactor by simply setting the flow rate to zero. The temperature could be controlled using the jacket cooling[4] water. The resulting set of equilibrium equations 7.6 and 7.7 with $F = 0$ are:

$$0 = -f(C_A, T) \tag{7.6}$$

$$0 = -\frac{\lambda}{\rho C_p}f(C_A, T) - \frac{UA_H(V)}{\rho C_p V}\left(1 - \frac{UA_H(V)}{F_J\rho_J C_J + UA_H(V)}\right)T - \frac{UA_H(V)F_J\rho_J C_J}{\rho C_p V(F_J\rho_J C_J + UA_H(V))}T_{Jin} \tag{7.7}$$

hence.

$$0 = 4.615 \times 10^{-6}C_A^2 T - 4.445 \times 10^{-6}C_A T - 1.4224 \times 10^{-3}C_A^2 + 1.555.5 \times 10^{-3}C_A + 4.07455 \times 10^{-6}T - 1.370535 \times 10^{-3} \tag{7.8}$$

$$T = T_{Jin} \tag{7.9}$$

[4]The cooling water could be heated and used to heat the reactor if that was required.

so that:

$$0 = (4.445 \times 10^{-6}T_{Jin} + 1.4224 \times 10^{-3})C_A{}^2 + (-4.445 \times 10^{-6}T_{Jin} + 1.55575 \times 10^{-3})C_A + (4.07455 \times 10^{-6}T_{Jin} - 1.370535 \times 10^{-3}) \quad (7.10)$$

The results from this equation must be in the range $C_A = [0, 1]$. Equation 7.10 can easily be solved using the general solution for quadratic equations. These results reveal that:

1. The position of the equilibrium points in a batch reactor of this sort are easily determined analytically.
2. From a static analysis point of view, the other parameters are of little importance (that is, they have little impact on the position of the equilibrium points). The parameters that were cancelled out (V,C_{Ain},T_{in}) have no impact on the position of the equilibrium points. This is helpful information because we should then expect that as the value of F decreases, these parameters will have less and less impact.
3. There will be between zero and two equilibrium points in the system (a quadratic equation can have a maximum of two roots).

Another important analytical step is to set certain variables or components of the equation to zero and observe the effects this has on the solution. This should be done while taking into account the physical reality of the situation.

If the volume is set to zero, we find that the equations become meaningless as they are divided by zero. This is consistent with the physical reality because without any liquid, there are no reactants and hence no reaction to be modelled. If however other variables or components are set to zero, several useful insights can be gained about the system being analysed. This was exactly what was done in the case of the batch reactor. The flow was set to zero. Now if the chemical reaction is set to zero, that is the reaction rate function $f(C_A, T)$ is set to zero then the CSTR is essentially a tank. This results in the following set of equations for equilibrium:

$$C_A = C_{Ain} \quad (7.11)$$

$$T = \frac{k_l k_1}{F(k_1 + k_2) + k_1 k_l} T_{Jin} + \frac{F(k_1 + k_2)}{F(k_1 + k_2) + k_1 k_l} T_{in} \quad (7.12)$$

Variable	Range	Reason
V	$[0.02, 0.2]$	Minimum volume allowed in the tank is 10% for safety reasons.

Table 7.3: Parameter Ranges Revisited

where

$$\begin{aligned} k_t &= \frac{UA_H}{\rho C_p} \\ k_1 &= F_J \rho_J C_J \\ k_2 &= UA_H \end{aligned}$$

The above result shows us that as the magnitude of $f(C_A, T)$ becomes less significant in comparison to the flow terms, the behaviour of the CSTR is more like a tank than a reactor. This is as would be expected using simple physical reasoning.

The next step is to visualize the equilibrium points. This is done using MATLAB. The equilibrium points are visualized for the median values of the parameters. It is however not always advantageous to use the median values for all of the parameters. This is because a parameter may be at one of the extremes during normal operation. In the case of the CSTR this is true for the volume of liquid in the system.

The vector field magnitude plot, shown in figure 7.2, is used as a starting point for the equilibrium point analysis of the system for changing parameter values. The ranges of some of the parameters are now revisited and refined for the next step of the analysis (ranges have already been defined in table 7.1): Figure 7.4 illustrates the solution obtained for the system example when each of the parameters are varied over their entire range while the other parameters are held constant. The diagram gives the position of the equilibrium points. The parameters not shown on this plot have no meaningful impact on the position of the equilibrium point over their entire range for this particular centre point [5]. This means that the equilibrium point stays at $(0.5, 320)$ as the other parameters are changed.

The problem with the above results is that several of the parameters were chosen in an arbitary way (the median of the extremes). The result is that the effect of some of the important control inputs (for instance the jacket flow rate) of the CSTR become irrelevant. Also the chemical reaction has a negligable impact which defeats the purpose of the CSTR.

[5]The "Centre Point" is the point defined by taking the median of all the parameter ranges.

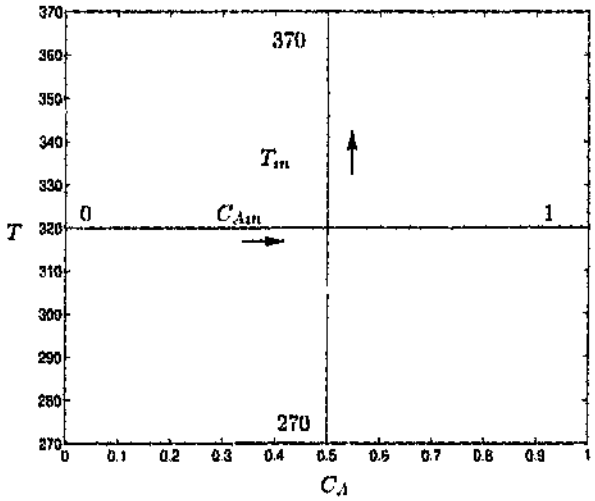


Figure 7.4: Equilibrium Point Movement

C_{Ain}	0.5
F_{in}	$1 \times 10^{-5}\ m^3/s$
F_{Jin}	$2 \times 10^{-5}\ m^3/s$
T_{in}	$320\ K$
T_{Jin}	$310\ K$
V	$0.15\ m^3$

Table 7.4: Design Set Point Parameter Values

When systems are designed however, a specific set of parameters is required for a particular type of reaction or product. These would be obtained through the traditional design disciplines used in chemical engineering. This dissertation will not concern itself with how the values are obtained. All that is required here is that there is some limitation of the state-parameter space and that these limits can be justified. Let us say, that for the sake of argument, a designer chooses the set of parameter values for the CSTR as per table 7.4.

In table 7.4 the flow rate is very small (in comparison to the size of the tank) and that the flow rate of the cooling jacket liquid is similar when compared to the incoming feed flow rate. The residence time of the tank $\left(t_{res} = \frac{V}{F_{in}}\right)$ varies around 250 minutes while the jacket residence time $\left(t_{res} = \frac{V_J}{F_{Jin}}\right)$ is 41 $\frac{2}{3}$ minutes.

C_{Ain}	$[0, 1]$
F_{in}	$[5 \times 10^{-6}, 1.5 \times 10^{-5}]\ m^3/s$
F_{Jin}	$[1 \times 10^{-5}, 3 \times 10^{-5}]\ m^3/s$
T_{in}	$[310, 330]\ K$
T_{Jin}	$[300, 320]\ K$
V	$[0.1, 0.2]\ m^3$

Table 7.5: Parameter Variation for Design Parameter Set Point

The chemical engineer then discovers that when the system will be implemented, due to various conditions that could occur in the plant, the following variations of the parameters (table 7.4) will occur as per table 7.5.

Using the static analysis methods outlined earlier, the following results are obtained for the position of the equilibrium point for changing parameter values. The analysis is not complete and a far more detailed study would be done in the case of an actual system, but the analysis presented is sufficient to demonstrate the concept. Figures 7.5 and 7.6 show how the equilibrium points in the CSTR move with changing parameter values. Figure 7.6 shows the area around the set point after it has been magnified several times.

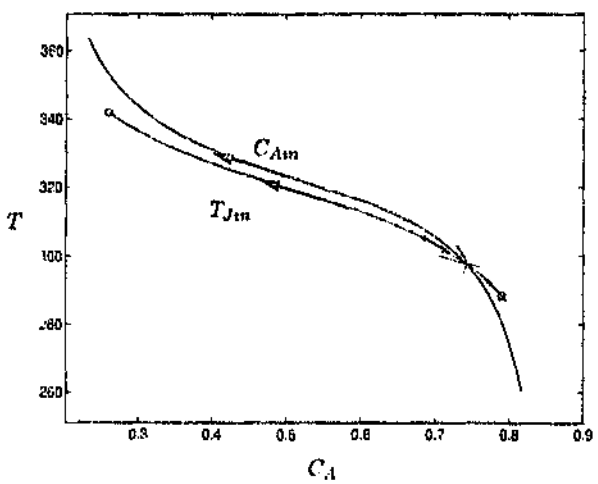


Figure 7.5: Static Equilibrium Points

The information given in figures 7.5 and 7.6 is incomplete in that it does not give the relationships between the parameters and the equilibrium points explicitly. This

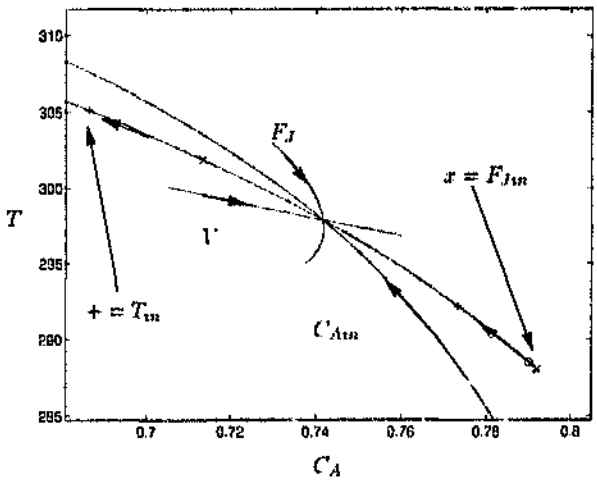


Figure 7.6: Static Equilibrium Points - Magnified

information is presented in appendix C.

7.3 Dynamic Analysis

7.3.1 Bifurcation Analysis

Bifurcation analysis is discribed in more detail in chapter 6. The field of bifurcation analysis is quite broad and there are several textbooks available on the subject (see [22] and [24]). A brief summary of what is used and how it is used is discussed here.

Bifurcation analysis in this context is observing the movement of the eigenvalues which result from the linearization of the system around the equilibrium points. The first step to achieving this is by finding all of the equilibrium points of the system for the different values of the system parameters. This information gives us the steady state behaviour of the plant as the parameters vary. It tells us what the ultimate ($t \rightarrow \infty$) output concentrations and temperatures will be as parameters are changed. This information does not however give us any idea of how the system will reach those steady states (equilibrium points). It does not ever tell us if the system will be stable or not.

Once the steady state information has been determined (see section 7.2.4), bifurcation analysis can proceed. This involves linearizing the system at all the relevant[6] equilibrium points. Using linear systems theory, the poles of the linear system can be determined for changing parameter values. This information is very useful because, depending on the number of equilibrium points, the changes in stability of the linear system can be used to give an idea of the global stability of the system. Although this information alone is not completely reliable, it helps to predict obvious changes in behaviour and once a particular region has been understood qualitatively, the entire region and its boundaries can be determined using this method. It is important to remember that bifurcation analysis has to be done in conjunction with other methods (such as simulation), to improve its reliability.

Section 6.4 gives details on how to interpret the results of linearized systems.

7.3.2 Interpreting Simulation Results

Once a region has been established as having some form of local instability, that is the poles of the linearized system cross the imaginary axes from the left hand of the s-plane into the right hand of the plane, simulation is required to determine the global stability behaviour. The results of the simulation have to be analysed by the engineer to determine (to some accuracy) the kind of behaviour which is occuring. It is important to remember that often engineers are more interested in determining the behaviour quickly and with some level of innaccuracy than conclusively proving that a behaviour is of one form or another. Usually it has very little impact on the practical situation whether, say for instance a system is chaotic or just exhibits a very complex form of limit cycle. Often both behaviours will result in similar output products if they look very similar to the naked eye. This section gives some examples of different kinds of behaviour and how to determine whether they are occuring.

The first kind of behaviour which needs to be understood is the globally unstable case. This will occur when the system becomes both locally and globally unstable simultaneously. This is a common form of behaviour and will often cause the simulation routine to fail and return some kind of appropriate message (for example arithmetic overflow). If the simulation time is sufficiently short, results may still be returned by the simulation. These will show exponential divergence from the initial point and have some very large values with respect to normal system results.

In the case of global instabilities, it is important to obtain an idea of the structure

[6] *Relevant* refers to equilibrium points that fall within the limits set in section 7.2.1.

of the phase space in the region of the local instability. In other words the way that the states change with time as they move away from the equilibrium point needs to be determined using simulations. This information is preferably displayed in a state space diagram. The diagrams used in section 6.3, illustrate how unstable and non-stable second order systems will look in the "phase plane". State space diagrams are important in showing all local equilibrium points as well as giving the engineer a better understanding of how the system behaves in the neighbourhood of these local equilibrium points.

The second type of behaviour that can be observed is multiple equilibrium points. This can be very confusing as the system appears to be stable while the equilibrium point in question is unstable. The reason for this is that there is another stable equilibrium point which is attracting the response. Figure 7.7 shows a phase plane multiple equilibrium point.

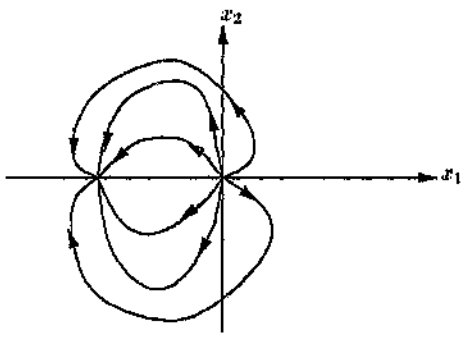


Figure 7.7: Phase Portrait of Two Equilibrium Points

There are many types of behaviours which can occur in nonlinear systems. Recognising them requires experience and a good working knowledge of the types of behaviour that can occur. This discussion is limited to second order systems and hence the only exclusively nonlinear behaviours mentioned here are limit cycles and multiple equilibrium points. Limit cycles are relatively easy to find as they are locally unstable equilibrium points or globally stable point. The system exhibits stable oscillatory behaviour as time proceeds if there is a limit cycle. Figures 7.12 and 7.13 are examples of how a limit cycle looks in the phase space and time domain. Chapter 6 gives a discussion of all the possible second order behaviours in greater detail.

C_{Ain}	0.5
F_{in}	$1 \times 10^{-5}\ m^3/s$
F_{Jin}	$2 \times 1^{-}\ m^3/s$
T_{in}	$320\ K$
T_{Jin}	$310\ K$
V	$0.15\ m^3$

Table 7.6: Design Set Point Parameter Values

7.3.3 Dynamic Analysis of the CSTR

Once the possible static behaviour of the system has been defined, we may proceed to analyse the system with a view to qualitatively[7] and to some extent quantitatively defining its behaviour. The system has six parameters and the design parameters assumed are shown in table 7.6.

The chemical reaction is assumed to result in the rate equation 7.13 for this analysis.

$$f(C_A,T) = \frac{\alpha\gamma}{2}\left[-\left(\frac{C_A-\delta_1}{\alpha}\right)^2\left(\frac{T-\delta_2}{\beta}\right)+\left(\frac{C_A-\delta_1}{\alpha}\right)+ 2\left(\frac{T-\delta_2}{\beta}\right)\right] \tag{7.13}$$

here

$$\begin{aligned}\alpha &= \tfrac{1}{3}\\ \beta &= 30\\ \delta_1 &= 0.5\\ \delta_2 &= 320\\ \gamma &= 2.667 \times 10^{-4}\\ \lambda &= -7.56 \times 10^{8}\end{aligned}$$

Substituting the parameters into equation 7.13 gives equation 7.14.

$$f(C_A,T) = 4.445 \times 10^{-6}C_A^2T - 4.445 \times 10^{-6}C_AT - 1.4224 \times 10^{-3}C_A^2 +$$

[7]The qualitative behaviour of the system means that you have a good idea of what to expect as you move into different regions of the parameter space. It does not however give you exact dynamic results (although you can work out approximate settling times, etc). To get exact results, simulation is required.

C_{Ain}	$[0, 1]$
F_{in}	$[5 \times 10^{-6}, 1.5 \times 10^{-5}]\ m^3/s$
F_{Jin}	$[1 \times 10^{-5}, 3 \times 10^{-5}]\ m^3/s$
T_{in}	$[310, 330]\ K$
T_{Jin}	$[300, 320]\ K$
V	$[0.1, 0.2]\ m^3$

Table 7.7: Parameter Variation for Design Parameter Set Point

$$1.55575 \times 10^{-3} C_A + 4.07455 \times 10^{-6} T - 1.370535 \times 10^{-3} \quad (7.14)$$

The parameters could vary for a number of reasons, which are not important here. What is important is that the effect on the dynamic behaviour caused by the variation of the parameters must be understood.

Table 7.7 gives the ranges over which the parameters are to be analysed. Figures 7.8 and 7.9 shows the dynamic behaviour of the system if the design values are chosen as the "centre" point around which all the other parameters are varied. Figures 7.8 and 7.9 show the path of the poles of the system created by linearizing around the equilibrium points determined in section 7.2.1. The picture shows that the solution of the dynamic problem results in a set of solutions which are all different (ie they do not overlap) except for (T_{in} and T_{Jin}). The $s - plane$ plot shows that for the parameter ranges decided upon, the system is essentially stable with a decreasing oscillation (that is most of the equilibrium points are stable foci).

There are two exceptions to this. The one is the variation with C_{Ain} which results in an unstable focus. And the second is the variation with T_{Jin} which results in an unstable focus. The unstable regions must be further investigated to check for nonlinear behaviour which is globally stable and for other equilibrium points which may have appeared.

Figures 7.11 through 7.16 show the simulation results that where obtained for the region of the parameter space investigated which contained the unstable foci. It indicates that within these regions limit cycles exist[8] .

Using all the information obtained from the static and dynamic analysis of the system, not only have the static characteristics of the system been determined, but also

[8]The bifurcation which produces this oscillatory behaviour is known as a hopf bifurcation (see section 6.4). This behaviour is described in detail in [24].

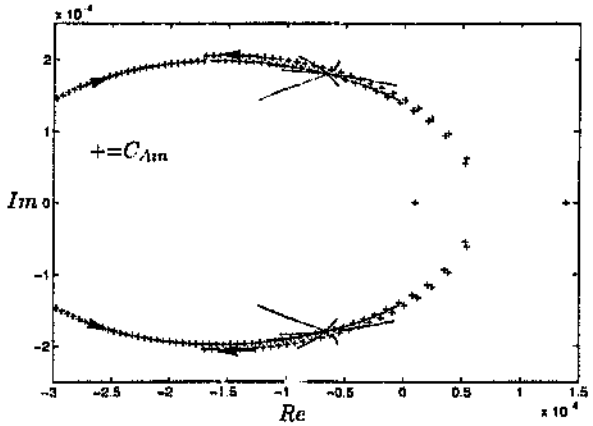


Figure 7.8: Pole Positions for Changing Equilibrium Points (C_{Ain})

the type of nonlinear behaviour for given parameter values. This type of analysis enables an engineer to predict the behaviour of a system without having to do an inordinate number of simulations [2] (which are very time consuming). The information given above is incomplete in that it does not give the relationships between the parameters and the pole positions explicitly. This information is presented in appendix C.

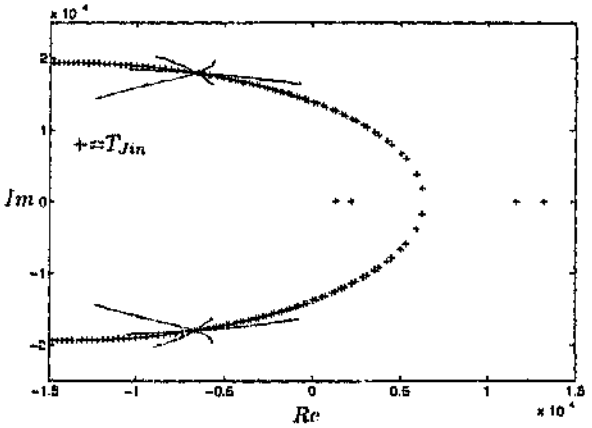


Figure 7.9: Pole Positions for Changing Equilibrium Points (T_{Jin})

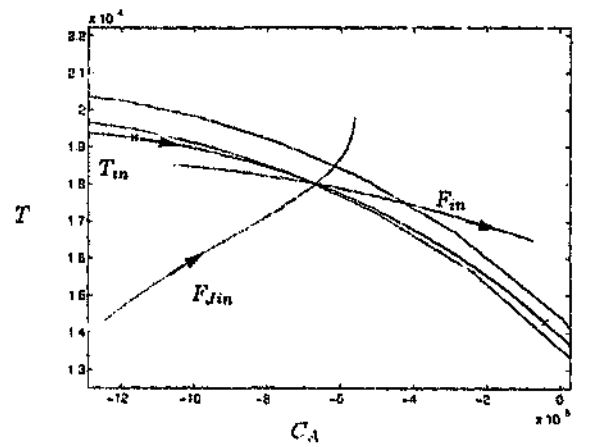


Figure 7.10: Pole Positions for Changing Equilibrium Points : Magnified

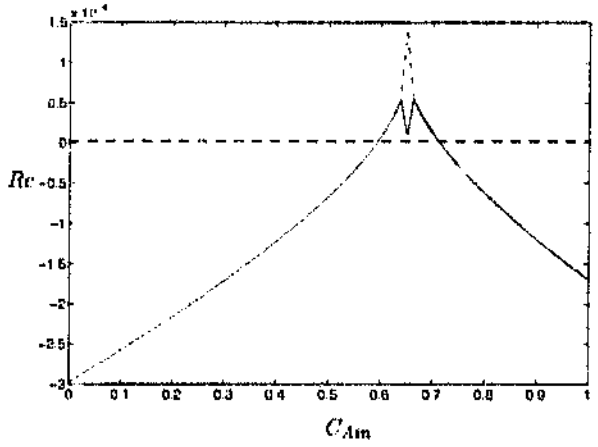


Figure ..11: Changes in stability versus C_{Ain}

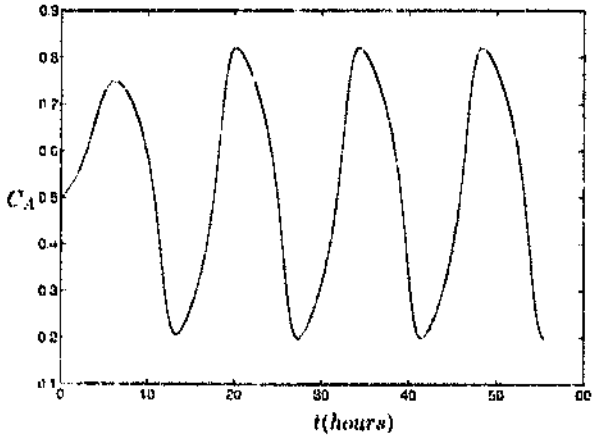


Figure 7.12: Time history for C_A at $C_{Ain} = 0.65$

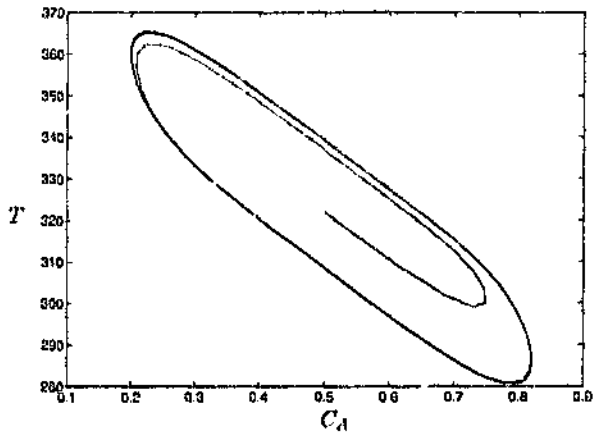


Figure 7.13: Phase Portrait for $C_{Ain} = 0.65$

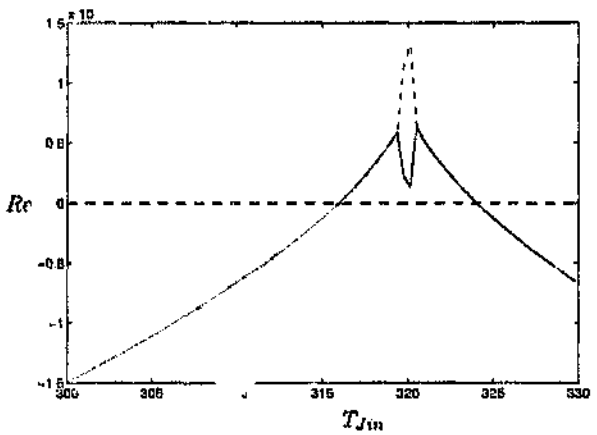


Figure 7.14: Changes in stability versus $T_{J...}$

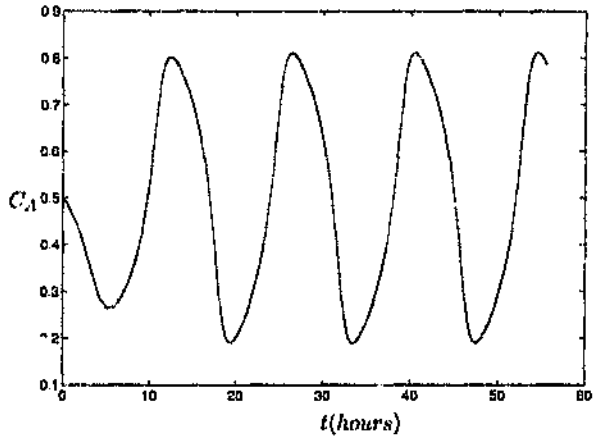


Figure 7.15: Time history for C_A at $T_{Jin} = 320K$

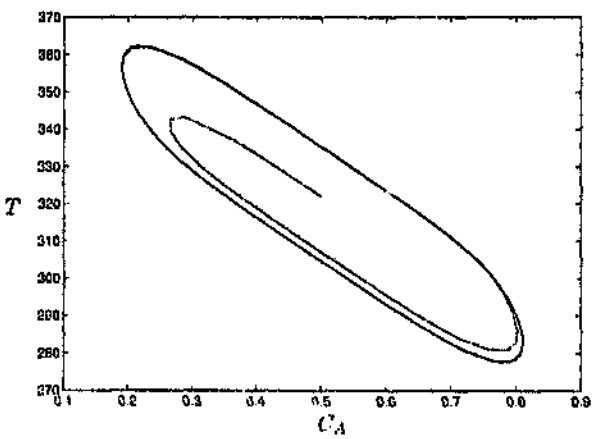


Figure 7.16: Phase Portrait for $T_{Jin} = 320K$

Chapter 8

A Nonlinear Design Technique

8.1 Introduction

The nonlinear design technique discussed evolved from the simple idea that the behaviour of an ordinary differential equation can be adjusted using simple transformations. Using these transformations to resize an equation to give the desired behaviour, followed by conforming a chosen chemical process into the same form (in this case a CSTR) is illustrated in this chapter.

8.2 Transforming Ordinary Differential Equations

There are many ways in which differential equations can be transformed. In this section, we will focus on three simple point transformations, translating the axes, scaling the size of the behaviour in the directions of the axes and changing the overall speed of the dynamics.

The equation used as an example is the general second order nonlinear ordinary differential equation. Assume that there are no inputs.

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} \tag{8.1}$$

The first point transformation is to translate the axes. This is done by simply substituting $\bar{x}_1 = (x_1 + \delta_1)$ and $\bar{x}_2 = (x_2 + \delta_2)$ into the equation. This has the effect of translating the axes to (δ_1, δ_2). The equation is transformed to the following :

$$\begin{bmatrix} \dot{\bar{x}}_1 \\ \dot{\bar{x}}_2 \end{bmatrix} = \begin{bmatrix} f_1(\bar{x}_1 - \delta_1, \bar{x}_2 - \delta_2) \\ f_2(\bar{x}_1 - \delta_1, \bar{x}_2 - \delta_2) \end{bmatrix} \tag{8.2}$$

The second transformation scales the behaviour of the system along each of the axes. This means that the behaviour can be stretched or reduced by a certain factor. Choosing α and β, the behaviour can be increased or reduced in size with respect to each axis. If we make $\bar{x}_1 = \alpha x_1$ and $\bar{x}_2 = \beta x_2$. Then $\frac{d\bar{x}_1}{dt} = \alpha \dot{x}_1$ and $\frac{d\bar{x}_2}{dt} = \beta \dot{x}_2$. Substituting $\bar{x}_1$ and $\bar{x}_2$ into equation 8.1 gives :

$$\begin{bmatrix} \dot{\bar{x}}_1 \\ \dot{\bar{x}}_2 \end{bmatrix} = \begin{bmatrix} \alpha f_1(\frac{\bar{x}_1}{\alpha}, \frac{\bar{x}_2}{\beta}) \\ \beta f_2(\frac{\bar{x}_1}{\alpha}, \frac{\bar{x}_2}{\beta}) \end{bmatrix} \tag{8.3}$$

The overall speed of the dynamics of the entire set of ordinary differential equations can be governed by multiplying every function by a constant. The constant γ will be used for this purpose. Let $\bar{t} = \frac{t}{\gamma}$. This results in the following set of equations :

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} \gamma f_1(x_1, x_2) \\ \gamma f_2(x_1, x_2) \end{bmatrix} \tag{8.4}$$

Finally if all the point transformations discussed so far are included in one set of equations, the following equations result :

$$\begin{bmatrix} \dot{\bar{x}}_1 \\ \dot{\bar{x}}_2 \end{bmatrix} = \begin{bmatrix} \alpha\gamma f_1(\frac{\bar{x}_1 - \delta_1}{\alpha}, \frac{\bar{x}_2 - \delta_2}{\beta}) \\ \beta\gamma f_2(\frac{\bar{x}_1 - \delta_1}{\alpha}, \frac{\bar{x}_2 - \delta_2}{\beta}) \end{bmatrix} \tag{8.5}$$

These results were developed for a second order system but could easily be generalized for any order of system.

8.3 Restructuring a Nonlinear Behaviour

The idea of this chapter, as stated in the introduction, is to use an existing set of nonlinear equations, whose behaviour is understood, to design a chemical process (in this case a CSTR) with similar behaviour.

The [illegible] used in this dissertation is the van der Pol oscillator equation 8.6 with $\mu = 1$ (see section 6.1).

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ \mu(1 - {x_1}^2)x_2 - x_1 \end{bmatrix} \tag{8.6}$$

This equation results in a limit cycle (see section 6.3). Equation 8.6 must now be transformed by looking at the form of the CSTR equations into which we want to transform the van der Pol oscillator. The transformed equation must preserve the limit cycle behaviour while including all the necessary structural requirements.

The reduced CSTR equations which are used here are taken from section 5.2.2. For convenience we restate them here :

$$\frac{dC_A}{dt} = \frac{F}{V}C_{Ain} - \frac{F}{V}C_A - f(C_A, T) \tag{8.7}$$

$$\frac{dT}{dt} = \frac{F}{V}T_{in} - \frac{F}{V}T - \frac{\lambda}{\rho C_p}f(C_A, T) - \frac{UA_H(V)}{\rho C_p V} \left[T - \frac{1}{F_J\rho_J C_J + UA_H(V)}(F_J\rho_J C_J T_{Jin} + UA_H(V)T)\right] \tag{8.8}$$

Equation 8.6 has to be adjusted to allow for terms in the chemical model which result in $\dot{x}_1$ being directly effected by x_1. It was found from simulation that by including a $-\frac{1}{2}x_1$ term, the limit cycle behaviour is preserved.

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} x_2 - \frac{1}{2}x_1 \\ (1 - {x_1}^2)x_2 - x_1 \end{bmatrix} \tag{8.9}$$

The equation has to be changed again so that both states in the equation contain a common term. This term represents the chemical reaction $f(C_A, T)$ which must exist in both equations. Notice that the sign of the existing terms in equation 8.9 have been changed and the coefficient of x_1 in equation 8.10 changed to $-\frac{3}{4}$. Equation 8.10 was found via an interactive process of simulation and experimentation with different values and structures. This involves changing the signs of certain terms, adding and removing terms and simulating to see if the behaviour of the system has qualitatively remained the same.

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{4}x_1 - \frac{1}{2}\left\{-{x_1}^2 x_2 + x_1 + 2x_2\right\} \\ -x_2 + \left\{-{x_1}^2 x_2 + x_1 + 2x_2\right\} \end{bmatrix} \tag{8.10}$$

Figure 8.1 shows the behaviour of equation 8.10 in the phase plane.

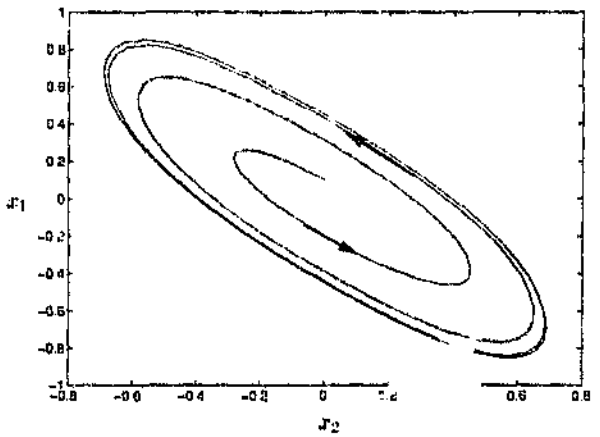


Figure 8.1: Behaviour of Equation 8.10

Equation 8.10 must then be transformed to a position in the phase plane which is compatible with the output that would be expected from a CSTR. This is done by applying the transformations given in section 8.2.

$$\begin{aligned} \dot{x}_1 &= \alpha\gamma\left\{-\frac{1}{4}\left(\frac{x_1-\delta_1}{\alpha}\right) - \frac{1}{2}\left[-\left(\frac{x_1-\delta_1}{\alpha}\right)^2\left(\frac{x_2-\delta_2}{\beta}\right) + \right.\right. \\ &\quad \left.\left.\left(\frac{x_1-\delta_1}{\alpha}\right) + 2\left(\frac{x_2-\delta_2}{\beta}\right)\right]\right\} \qquad (8.11) \\ \dot{x}_2 &= \beta\gamma\left(-\left(\frac{x_2-\delta_2}{\beta}\right) + \left[-\left(\frac{x_1-\delta_1}{\alpha}\right)^2\left(\frac{x_2-\delta_2}{\beta}\right) + \right.\right. \\ &\quad \left.\left.\left(\frac{x_1-\delta_1}{\alpha}\right) + 2\left(\frac{x_2-\delta_2}{\beta}\right)\right]\right\} \qquad (8.12) \end{aligned}$$

8.4 Designing Plant Behaviour

Equations 8.11 and 8.12 were chosen to give qualitatively similar dynamic behaviour to the CSTR governed by equations 8.7 and 8.8.

Let :

$$\begin{aligned} x_1 &= C_A \\ \dot{x}_1 &= \frac{dC_A}{dt} \\ x_2 &= T \\ \dot{x}_2 &= \frac{dT}{dt} \end{aligned}$$

Equating coefficients of equations 8.7 and 8.8 with those of equations 8.11 and 8.12 respectively, the following relationships result :

$$\frac{F}{V}C_{Ain} = \frac{\gamma\delta_1}{4} \tag{8.13}$$

$$\frac{F}{V}C_A = \frac{\gamma x_1}{4} \tag{8.14}$$

$$f(C_A,T) = \frac{\alpha\gamma}{2}\left[-\left(\frac{x_1-\delta_1}{\alpha}\right)^2\left(\frac{x_2-\delta_2}{\beta}\right)+\left(\frac{x_1-\delta_1}{\alpha}\right)+ 2\left(\frac{x_2-\delta_2}{\beta}\right)\right] \tag{8.15}$$

$$\gamma\delta_2 = \frac{F}{V}T_{in}+\frac{UA_H(V)F_J\rho_JC_J}{\rho C_pV(F_J\rho_JC_J+UA_H(V))}T_{Jin} \tag{8.16}$$

$$\gamma x_2 = \left(\frac{F}{V}+\frac{UA_H(V)}{\rho C_p}\left[1-\frac{UA_H(V)}{F_J\rho_JC_J+UA_H(V)}\right]\right)T \tag{8.17}$$

Using the relationships defined by 8.13 through 8.17, the following set of conditions can be derived. These have to be fulfilled for equations 8.7 and 8.8 to produce the nonlinear behaviour of equation 8.10 :

$$\gamma = \frac{4}{3}\frac{UA_H(V)}{\rho C_p}\left[1-\frac{UA_H(V)}{F_J\rho_JC_J+UA_H(V)}\right] \tag{8.18}$$

$$\frac{F}{V} = \frac{\gamma}{4} \tag{8.19}$$

$$\frac{\lambda}{\rho C_p} = -2\frac{\beta}{\alpha} \tag{8.20}$$

Provided the conditions are preserved, the parameters C_{Ain}, T_{in} and T_{Jin} can be given any value within physically realistic limits.

$$C_{Ain} = \delta_1 \tag{8.21}$$

$$\frac{1}{4}T_{in}+\frac{UA_H(V)F_J\rho_JC_J}{F\rho C_p(F_J\rho_JC_J+UA_H(V))}T_{Jin} = \delta_2 \tag{8.22}$$

These are remarkable results in that as long as the conditions given by equations 8.18 through 8.20 are fulfilled, the system's centre point (not neccessarily equilibrium) can be determined by changing the temperature and concentration of the incoming

stream. The flow rate however proves to be a vital parameter. This is because the whole system of equations relies on the flow rate being maintained at a particular value.

An important observation is that the ratio of the flow rate and the volume $\frac{V}{F}$ is a very important parameter (*residence time* $= \theta = \frac{V}{F} = \frac{1}{\gamma}$). The flow rate and the volume of liquid in the CSTR can be varied as long as the ratio between the flow rate and the volume is maintained.

The required CSTR system parameters for the calculation of γ are shown below :

$$\begin{aligned} C_p = C_J &= 4200 \\ \rho = \rho_J &= 1000 \\ V &= 0.15 \\ F_J &= 1 \times 10^{-5} \end{aligned}$$

The parameter values required to transform equation 8.10 into a physically realistic position in the phase plane are:

$$\begin{aligned} \alpha &= \frac{1}{3} \\ \beta &= 30 \\ \delta_1 &= 0.5 \\ \delta_2 &= 320 \end{aligned}$$

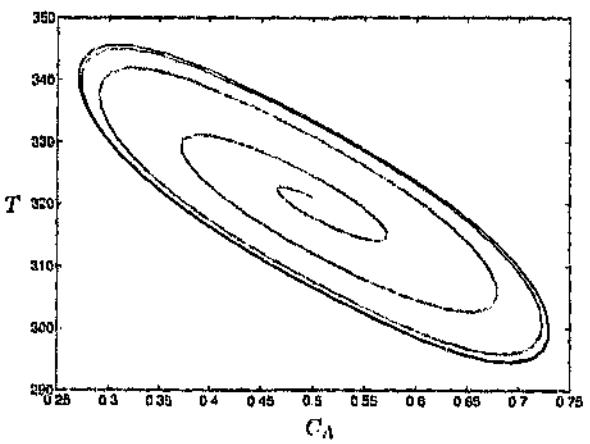


Figure 8.2: Trajectory of the System in the Phase Plane ($\gamma = 1$)

The value of γ can now be calculated using equation 8.18.

$$\gamma = 2.3522 \times 10^{-5}$$

The relationships defined by equations 8.18 through 8.20 give the following values for the system parameters F and λ :

$$F = 8.8209 \times 10^{-7}$$
$$\lambda = -7.56 \times 10^{8}$$

Figure 8.3 shows a time history plot for the resulting CSTR system.

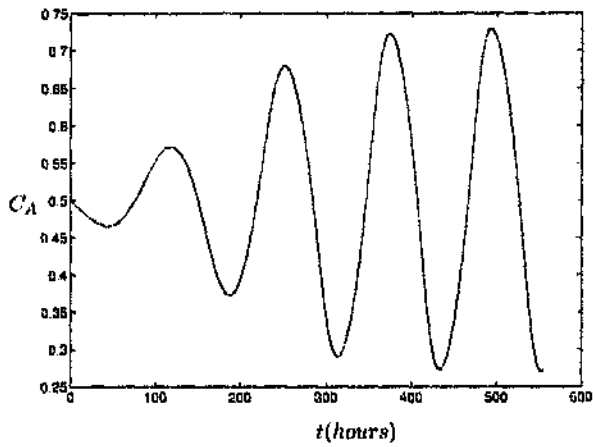


Figure 8.3: Time History of C_A for the CSTR ($\gamma = 2.3522 \times 10^{-5}$)

Figure 8.3 illustrates the fact that the system oscillates very slowly, approximately once every four days! This is a very long period of oscillation. What should now be done is to change the speed of the oscillation by using the system obtained so far as a starting point. We now change the chemical system parameters and observe the changes in behaviour. By changing each of the parameters and simulating the system to see which parameters increase the speed of the oscillation (ignoring the origional transformation conditions in equations 8.18 through 8.20) the following new parameters were obtained. It must be remembered that the chemical equation $f(C_A, T)$ is changed when F is varied (the equation 8.15 for $f(C_A, T)$ depends on γ). Using an iterative process of adjustment and simulation, the following results were obtained (the objective was to speed up the dynamics).

The new values of the parameters which have changed are :

$$F = 1.00 \times 10^{-5}$$
$$\gamma = 2.667 \times 10^{-4}$$

Figures 8.4 and 8.5 give the dynamic behaviour of the system after the parameters

have been adjusted.

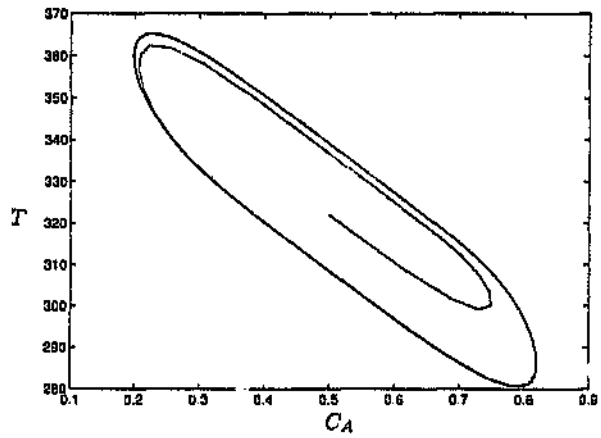


Figure 8.4: Phase Portrait of the Faster System

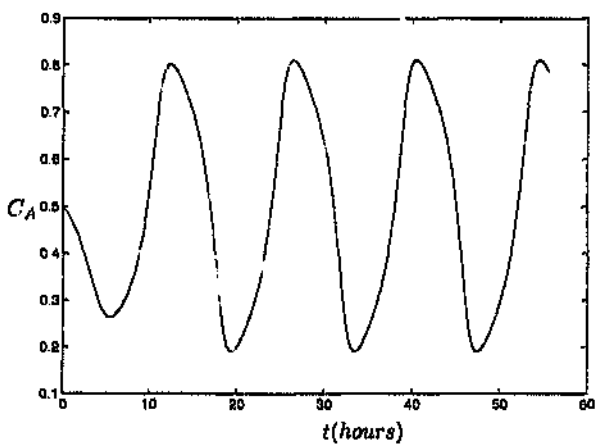


Figure 8.5: Time History of C_A for the CSTR ($\gamma = 2.667 \times 10^{-4}$)

The chemical reaction rate (equation 8.23) which is required for a system to exhibit the behaviour shown in figure 8.5 is obtained by substituting the values of the parameters into equation 8.15.

$$f(C_A,T) = 4.445 \times 10^{-6}x_1^2x_2 - 4.445 \times 10^{-6}x_1x_2 - 1.4224 \times 10^{-3}x_1^2 + 1.55575 \times 10^{-3}x_1 + 4.07455 \times 10^{-6}x_2 - 1.370535 \times 10^{-3} \quad (8.23)$$

8.5 Conclusion

The methodology followed in this chapter is described by the flowchart in figure 8.6.

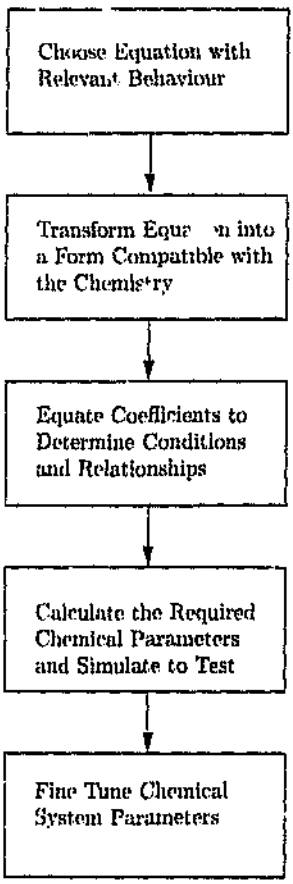


Figure 8.6: Nonlinear Design Methodology

The design method is effective in producing behaviours which do not often occur. This method illustrates a concept which the author believes is lacking from many attempts at understanding nonlinear systems. This idea is that the key to understanding nonlinear system design is to design systems which produce different types of behaviour and then to compare them with existing physical systems and note the similarities. In this case, a limit cycle was produced in a system which does not readily produce that kind of behaviour (see [14]).

Chapter 9

Conclusion

The research has been inherently challenging because of the multiple themes which are present. Each area covered in this research is in itself a whole field on its own. It was often difficult to limit the amount of content on each subject, but for the sake of completing the work it was necessary to limit the scope. This results in a simple set of concepts, all of which are linked together to form the central arguments:

1. It is possible to model chemical processes for control, they are not "too complicated".
2. Nonlinear theory is very useful for understanding nonlinear control models and increases our knowledge of the dynamics of a process, hence enhancing our ability to control it.

Thus we can see that while each section on its own may not give any original ideas, once put together they make a very important statement.

The modelling of unit operations for control brought out the fact that this area has been largely ignored and black box techniques have been used instead. It also caused the author to realize the differences between design models and control models. It made the author realize that control models focus on subtly different aspects of the same system. Design models emphasize the distributed parameters, for instance how a temperature varies with distance, while the control model only gives the dependence of the outputs on the inputs.

The linking of process models together brought out the need to modularize each of the unit models so that their inputs and outputs are compatible with each other. Immediately this meant that all of the unit models had to use the same basis of units. An important fact which emerged was the fact that doing bifurcation analysis

on a linked model numerically was practically useless because there was no way of attaching the state which caused an eigenvalue of the linearized system to the eigenvalue. This meant that while the system may well have been analyzed, we would not know which state or states caused which mode of the system.

Nonlinear chemical models are usually of high order and hence need to be simplified and reduced for control and system design. Reducing the order of the linked system thus became a vital step. Two methods were used for this purpose, the first was decoupling and the second was time scaling. The first involved determining the relationships between variables and showing that the effects of a variable were negligible and hence could be ignored. One of the important methods in this regard was to use the characteristics of the physical system. An important decoupling agent in the liquid process which was used to illustrate the problem was the pump, controller and control valve combination. This seems to be a standard method of decoupling the pressures of coupled liquid systems.

The second form of model order reduction was time scaling. Here a more rigorous method was employed involving numerical and analytical calculation. The dynamics of a subset of the system were analyzed and it was shown that the difference in time scales was large enough to justify order reduction. These methods need to be improved and applied to different problems in future work.

The aim of the chapter on bifurcation theory was to provide a necessary foundation in nonlinear theory while avoiding as much as possible the jargon associated with nonlinear systems. Some new terms were necessary as no equivalent term existed in the field of process control. The theory presented only details of second order behaviours as this was what was required for the system example. The theory needs to be expanded to include higher order systems while maintaining its simplicity and directness. It was felt that for the sake of reaching a wider audience of engineers it was necessary to sacrifice some of the intricacies of the nonlinear field. This is often done in engineering and is often decried by other academic disciplines.

The analysis methodology which is presented by way of an example is reasonably straight forward. It could be improved in three areas :

1. More reliable methods should be introduced which aid in the detection of multiple equilibrium points.
2. A formal method needs to be adopted for making sure that the bifurcation analysis is valid (an example would be in the case of an unstable limit cycle).

3. Methods need to be experimented with for predicting behaviour from local equilibrium points and the centre manifold.

Finally, a design method is presented. This essentially is outside the scope of the dissertation. It was however used to construct the example CSTR. It is an exciting part of the dissertation and holds great promise for the future. More nonlinear equations and more chemical processes need to be put through this method to help improve our understanding of nonlinearity in chemical processes.

Work which remains to be done has been mentioned above, but one final point remains. A very important aspect of process systems is transport delays. While this was mentioned in passing it remains to be solved. The direction that is suggested is the use of delay differential equations.

Hopefully this dissertation will go some way towards providing a foundation for future work in the area of nonlinear process modelling and control.

Appendix A

Physical Numerical Values

The following values were decided upon for the simple mixing system described in chapter 4.

Common Constants	
$C_p = C_{p1} = C_{p2} = C_{p3} = C_{p4} = C_{p5} = C_{p6} = 4200\ J/kgK$	Heat capacity of pure water
$p_{in1} = p_{in2} = p_{in5} = 101\ kPa$	Atmospheric pressure for the tanks and the CSTR at the liquid surface
$T_S = 298\ K$	Temperature of the surroundings
$\rho = 1000\ kg/m^3$	Density of pure water (reactants are aqueous solutions)

Tank A	**Unit 1**
$A_1 = 2.5\ m^2$	Cross-sectional area
$A_{H1} = 13.7\ m^2$	Heat transfer area
$F_{in1} = 1\ m^3/s$	Design input flow rate
$U_1 = 50\ W/m^2K$	Heat transfer coefficient
$V_1 = 5\ m^3$	Buffer tank volume

Tank B	**Unit 2**
$A_2 = 2.5\ m^2$	Cross-sectional area
$A_{H2} = 13.7\ m^2$	Heat transfer area
$F_{in2} = 1\ m^3/s$	Design input flow rate
$U_2 = 50\ W/m^2K$	Heat transfer coefficient
$V_2 = 5\ m^3$	Buffer tank volume

Pump A	**Unit 3**
$A_3 = 0.017\ m^2$	Cross-sectional area of pipe
$A_{H3} = 0.46\ m^2$	Heat transfer area of pipe
$L_3 = 100\ m$	Length of pipe
$\Delta p_3(r_3) = 5000(1 - (r_3 - 1)^2)\ kPa$	Change in pressure caused by pump
$U_3 = 100\ W/m^2K$	Heat transfer coefficient
$\eta_3(u_3) = 1 - (1 - u_3)^2$	Normalised nonlinear valve aperture
$\mu_3(T_3) = \frac{10^{-6}}{T_3}\ kg/ms$	Viscosity of water

Pump B	**Unit 4**
$A_4 = 0.017\ m^2$	Cross-sectional area of pipe
$A_{H4} = 0.46\ m^2$	Heat transfer area of pipe
$L_4 = 100\ m$	Length of pipe
$\Delta p_4(r_4) = 5000(1 - (r_4 - 1)^2)\ kPa$	Change in pressure caused by pump
$U_4 = 100\ W/m^2K$	Heat transfer coefficient
$\eta_4(u_4) = 1 - (1 - u_4)^2$	Normalised nonlinear valve aperture
$\mu_4(T_4) = \frac{10^{-6}}{T_4}\ kg/ms$	Viscosity of water

CSTR	**Unit 5**
$A_5 = 0.3\ m^2$	Cross-sectional area
$A_{H5} = 4.667\ m^2$	Heat transfer area
$F_{in5} = 2\ m^3/s$	Design total input flow rate
$f_5(C_{A5}, T_5) = -5 * 10^5 e^{\frac{-1000}{T_5}} C_{A5} + 5 * 10^8 e^{\frac{-8000}{T_5}} (1 - C_{A5})\ 1/s$	Rate function a possible reactio
$U_5 = 400\ W/m^2K$	Heat transfer coefficient
$V_5 = 0.2\ m^3$	Reactor volume
$V_{J5} = 0.05\ m^3$	Cooling jacket volume
$\lambda_5 = -3.36 * 10^8\ J/kg$	Heat of reaction

Pump : Products	**Unit 6**
$A_6 = 0.017\ m^2$	Cross-sectional area of pipe
$A_{H6} = 0.46\ m^2$	Heat transfer area of pipe
$L_6 = 100\ m$	Length of pipe
$\Delta p_6(r_6) = 5000(1 - (r_6 - 1)^2)\ kPa$	Change in pressure caused by pump
$U_6 = 100\ W/m^2K$	Heat transfer coefficient
$\eta_6(u_6) = 1 - (1 - u_6)^2$	Normalised nonlinear valve aperture
$\mu_6(T_6) = \frac{10^{-6}}{T_6}\ kg/ms$	Viscosity of water

Appendix B

Matlab Code

B.1 jacket.m

This MATLAB m-file is used to calculate the difference in the speed of the temperature dynamics of a reactor and its jacket.

The following MATLAB commands were used (at the MATLAB prompt >>) to call it and plot the various graphs :

```
>>jacket([-3.704e-7 2.936e-6],[5e-6 1.5e-5],[0.1 0.2],[1e-5 3e-5],2);
```

```
function r=jacket(dfdTr,Fr,Vr,FJr,n);

%A=jacket(dfdTr,Fr,Vr,FJr,n);
%dfdTr The reaction rate
%Fr The flow rate
%Vr Volume
%FJr Jacket flow rate
%n is the number of steps
%r is the smallest ratio of the dynamics in question

%constants
alpha=1/3;
beta=30;
gamma=2.667e-4;
U=400;
rho=1000;
```

```
rhoJ=rho;
Cp=4200;
CJ=Cp;
VJ=0.05;
lambda=-7.66e8;
AC=0.3;
B=[0 1]';
C=[1 1];
D=0;
r=1000;

hold off

for FJ=FJr(1):FJr(2)-FJr(1):FJr(2),
  for V=Vr(1):Vr(2)-Vr(1):Vr(2),
    for F=Fr(1):Fr(2)-Fr(1):Fr(2),
      for dfdT=dfdTr(1):dfdTr(2)-dfdTr(1):dfdTr(2),

%functions
AH=2*(pi/AC)^0.5*V+2*AC;
A=[-F/V-lambda/(rho*Cp)*dfdT-U*AH/(V*rho*Cp), U*AH/(V*rho*Cp);...
U*AH/(VJ*rhoJ*CJ), -U*AH/(VJ*rhoJ*CJ)-FJ/VJ];
pzmap(A,B,C,D);
hold on;
p=pzmap(A,B,C,D);
if abs(p(2)/p(1))<r;,r=abs(p(2)/p(1));,end;

      end;,
    end;,
  end;,
end;

hold off
```

B.2 vdpol1.m

This MATLAB m-file is used in conjunction with ode23 to simulate the system which is used as basis for the example CSTR system.

The following MATLAB commands were used (at the MATLAB prompt >>) to call it and plot the various graphs :

```
>>[t,y]=ode23('vdpol1',0,50000,[0.5 321],1e-5);
>>plot(y(:,1),y(:,2)); %Phase plot of concentration vs temperature
>>plot(t/3600,y(.,1); %Time history plot of concentration vs time (in hours)
```

Here is the MATLAB code :

```
function xdot=vdpol1(t,x);

%starting equation
%xdot(1)=-1/4.*x(1)-1/2.*(-x(1).^2.*x(2)+x(1)+2.*x(2));
%xdot(2)=-x(2)+(-x(1).^2.*x(2)+x(1)+2.*x(2));

%scaled & shifted equation
%2.*x(1) 1/10.*x(2)
alpha=1/2;
beta=20;
delta1=0.5;
delta2=320;
gamma=2.0909e-3;
d1=1;

xdot(1)=gamma*alpha.*(-1/4.*(x(1)-delta1)./alpha-1/2.*(-((x(1)...
        -delta1)./alpha).^2.*(x(2)-delta2)./beta+2.*(x(1)-...
        delta1)./alpha./2+(x(2)-delta2)./beta.*2));
xdot(2)=gamma*beta.*(-(x(2)-delta2)./beta+d1.*(-((x(1)-delta1)./alpha).^2.*...
        (x(2)-delta2)./beta+2.*(x(1)-delta1)./alpha./2+...
        (x(2)-delta2)./beta.*2));
```

B.3 magplot2.m

This MATLAB m-file is used in conjunction with vdpol1.m to create a two dimensional vector field shaded magnitude plot.

The following MATLAB commands were used (at the MATLAB prompt >>) to call it and plot the various graphs :

```
>>m=magplot('vdpoli',[0 1],[270 370],64);
>>shading interp
>>colormap gray
>>surf((0:1/64:1),(270:100/64:370),m);
>>view(2);
```

Here is the MATLAB code:

```
function m=magplot2(vecfun,x_range,y_range,n);

%function [m x y]=magplot2(vecfun,x_range,y_range,n);
%This function will return the magnitude of a 2 dimensional vector field
%over a range specified by x_range, y_range for a function vecfun (of the
%type used for ode23). n is the number of blocks in x and y.

x0=1;
y0=1;

for y1=(y_range(1):(y_range(2)-y_range(1))/n:y_range(2));,
  for x1=(x_range(1):(x_range(2)-x_range(1))/n:x_range(2));,
    a=feval(vecfun,0,[x1 y1]);
    m(x0,y0)=abs(a(1)+j*a(2));
    x0=x0+1;
  end;
  x0=1;
  y0=y0+1;
end;
```

B.4 cstr.m

The matlab function `cstr.m` is the backbone of all of the analysis. It is the implementation of the second order nonlinear model in matlab. If the control engineer makes any errors here they will effect all the results.

```
function xdot = cstrd(t,x);

%constant parameters
```

```
A      =  0.3;
CJ     =  4200;
Cp     =  4200;
U      =  400;
rho    =  1000;
rhoJ   =  1000;
Fe     =  0.0001;
Ve     =  0.15;

%variable parameters: x(3) through x(8)
CAin   =  x(3);          %0.5         [0     ..   1]
F      =  x(4);          %2.8371e-5   [0     ..   1]
FJ     =  x(5);          %0.01        [1e-4  ..   1]
Tin    =  x(6);          %320         [280   .. 360]
TJin   =  x(7);          %320         [300   .. 340]
V      =  x(8);          %0.2         [0.1   .. 0.2]

%chemical reaction parameters
alpha     =  1/2;                     %1/2
beta      =  20;                      %20
gamma     =  4*Fe/Ve;                 %2.667e-3
delta1    =  0.5;                     %0.5
delta2    =  320;                     %320
lambda    =  -2*(beta/alpha)*rho*Cp;  %

%states
CA=x(1); %
T=x(2);  %

%functions
%rate function
f_CA_T=alpha*gamma/2*(-(CA-delta1)./alpha).^2.*(T-delta2)./beta+...
       2.*(CA-delta1)./alpha./2+(T-delta2)./beta.*2);
%f_CA_T=-5e5*exp(-4000./T).*CA+5e8*exp(-8000./T).*(1-CA);
%other functions
AH=2*pi*(pi/A)^0.5*V+2*A;
Te=T-(FJ*rhoJ*CJ*TJin+U*AH*T)/(FJ*rhoJ*CJ+U*AH);

%state e   ons
```

```
dCA=CAin*F/V-CA*F/V-f_CA_T;
dT=Tin*F/V-T*F/V-f_CA_T*lambda/(rho*Cp)-Te*(U*AH)/(rho*Cp*V);

%final conversions

xdot(1)=dCA;
xdot(2)=dT;

xdot(3:8)=[0 0 0 0 0 0]';
```

B.5 mag1.m

This function is very useful as it return the vector field magnitude of a state space model at a particular point. The function passed in must be in the same form as that required for ODE23.

```
function m=mag1(x,vecf,xp);

%m=mag1(x,vecf,xp);
%Special format to work with fmins.

t=0;
m=0;
xdot=feval(vecf,t,[x xp]);

n=length(x);
for k=1:n;,
  m=m+xdot(k)^2;
end;
m=m^0.5;
```

B.6 lin1.m

This function linearizes the given function (again ODE23 format) at a certain point and returns the poles of the system. It uses numerical differentiation to achieve this.

```
function p =lin1(vecf,x,xp);

%p =lin1(vecf,x,xp);
%Returns the poles of a system.
%vecf =  system being analysed (ode23 format)
%x    =  point at which to do the analysis (should be an equilibrium point)
%xp   =  parameter values

t=0;
h=0.001;
tol=0.001;
e=1e6;
y11=1e6;
y21=1e6;
n=1;
maxn=10;

while e>tol,
  x1=[x(1)+h x(2)];
  x2=[x(1)-h x(2)];
  x3=[x(1) x(2)+h];
  x4=[x(1) x(2)-h];
  a1=feval(vecf,t,[x1 xp]);
  a2=feval(vecf,t,[x2 xp]);
  a3=feval(vecf,t,[x3 xp]);
  a4=feval(vecf,t,[x4 xp]);

  y1=(a1-a2)/(2*h);
  y2=(a3-a4)/(2*h);

  e1=abs(y1-y11);
  e2=abs(y2-y21);
  e=e1+e2;

  y11=y1;
  y21=y2;

  n=n+1;
  if n>maxn,
```

```
    e=0;
    disp('maximum number of iterations exceeded - results are unreliable');
  end;
end;

A=[y1(1:2)' y2(1:2)'];
B=[0 1]';
C=[0 1];
D=0;
[z,p,k]=ss2zp(A,B,C,D);
```

B.7 magplot1.m

This function returns the magnitude plot of a vector field.

```
function m=magplot1(vecfun,x_range,y_range,n,xp);

%m=magplot1(vecfun,x_range,y_range,n,xp);
%This function will return the magnitude of a 2 dimensional vector field
%over a range specified by x_range, y_range for a function vecfun (of the
%type used for ode23). n is the number of blocks in x and y.
%xp is a vector of the parameters passed to the vector field function.

x0=1;
y0=1;

for y1=(y_range(1):(y_range(2)-y_range(1))/n:y_range(2)),
  for x1=(x_range(1):(x_range(2)-x_range(1))/n:x_range(2)),
    a=feval(vecfun,0,[x1 y1 xp]);
    m(x0,y0)=abs(a(1)+j*a(2));
    x0=x0+1;
  end;
  x0=1;
  y0=y0+1;
end;
```

B.8 magplot2.m

This function returns a number of vector field magnitude data sets for a parameter range.

```
function M =magplot2(vecfun,x_range,y_range,n,xp,p,m,f);

%M=magplot2(vecfun,x_range,y_range,n,xp,p,m,f);
%The range is specified by x_range, y_range for a function vecfun (of the
%type used for ode23). n is the number of blocks in x and y.
%xp is a vector of the parameters passed to the vector field function.
%This function is similar to magplot1 except it produces f plots linearly
%spaced over the parameter range given by p. xp specifies the set of
%parameters. m is the index of the parameter which is being varied in xp.
%It stores the data and an information header at the beginning:
%[x_range y_range n p1 m [reshaped data....] ]

k=1;
for p1=(p(1):(p(2)-p(1))/(f-1):p(2));,
  xp(m)=p1;
  m1=magplot1(vecfun,x_range,y_range,n,xp);
  s1=size(m1);
  M(:,k)=[x_range y_range n p1 m reshape(m1,s1(1)*s1(2),1)']';
  k=k+1;
  calculated=k-1
end;
```

B.9 magplot3.m

This function lets you pick off a starting point for analysis using the mouse for a certain parameter value.

```
function [start,p1]=magplot3(M,p);

%[start pout]=magplot3(M,p);
%Displays data from magplot2
%M=data
```

```
%p=parameter value
%start is a starting point for numerical analysis chosen using the mouse
%pout is the actual parameter value at which the analysis will be perfromed

s=size(M);
pmin=M(6,1);
pmax=M(6,s(2));
disp(sprintf('Parameter range : [%f %f]',pmin,pmax));
k=min(find(M(6,:)>p))-1;
if p<=pmax & p>=pmin,
  x_range=M(1:2,k);
  y_range=M(3:4,k);
  n=M(5,k);
  p1=M(6,k);
  m=M(7,k);
  m1=reshape(M(8:s(1),k),n+1,n+1);
  clip=max(max(m1))/10;
  I=find(m1>clip);
  mc=m1;
  for z=1:length(I);,mc(I(z))=clip;,end;
  figure;
  surf((x_range(1):(x_range(2)-x_range(1))/n:x_range(2)),...
       (y_range(1):(y_range(2)-y_range(1))/n:y_range(2)),mc);
  shading flat
  colormap(jet);
  view(2);
  colorbar;
  title(sprintf('parameter%i = %f',m,p1));
  disp('Select numerical analysis start point...');
  start=ginput(1);
  close;
else
  disp('Parameter out of range.');
  start=[-1 -1];
end;
```

B.10 equil.m

This is the heart of the analysis alogrythm. This function searches for an equilibrium point, given starting point and a function (of ODE23 form). If no equilibrium point is found, the result [0 280] is returned. Obviously for higher order models, this would have to be fixed.

```
function [x,poles] = equil(vecf,xp,p,m,start);

%[x,poles] = equil(vecf,xp,p,m,start);
%vecf =  system being analysed (ode23 format)
%xp   =  parameter values
%p    =  new parameter value
%m    =  new parameter index (in xp)
%start=  starting point for numerical analysis

%Calculate equilibrium point

tol         =  1e-5;     %Tolerance for equilibrium point checking
OPTIONS(1)  =  0;        %Display intermediate steps (1=yes)
OPTIONS(2)  =  1e-8;     %termination tolerance for x
OPTIONS(3)  =  1e-8;     %termination tolerance for f
OPTIONS(14) =  10000;    %maximum number of iterations

xp(m)=p;
x=fmins('mag1',start,OPTIONS,[],vecf,xp);

%Calculate the poles of the system

poles=lin1(vecf,x,xp)';

%Check for equilibrium

if mag1(x,vecf,xp)>tol,
  x=[0 280];
  poles=[0 0];
end;
```

B.11 findequi2.m

This function solves for a whole parameter range of equilibrium points and poles using continuation methods. This is a very important function.

```
function [x,pol,parm]=findequi2(M,p,xp,start,f);

%findequi(M,p,xp,start);
%Searches forward and backward for an f number of equililibrium points.
%M     = data
%p     = parameter value
%xp    = parameters
%start = equilibrium start point
%f     = number of frames to use in the analysis

s=size(M);
pmin=M(6,1);
pmax=M(6,s(2));
disp(sprintf('Parameter range : [%f %f]',pmin,pmax));
k=min(find(M(6,:)>p))-1;
if p<=pmax & p>=pmin,
  x_range=M(1:2,k);
  y_range=M(3:4,k);
  n=M(5,k);
  p1=M(6,k);
  m=M(7,k);
  disp('Solving forward...')
  w=0;
  st1=start;
  for z=p:(pmax-pmin)/f:pmax,
    disp(sprintf('parameter = %f',z));
    w=w+1;
    [xf(w,1:2) polf(w,1:2)]=equi1('cstr',xp,z,m,st1);
    parmf(w)=z;
    if xf(w,1)~=0, st1=xf(w,1:2);,end;
  end;
  disp('Solving backwards...');
  w=0;
```

```
  st1=start;
  for z=p:-(pmax-pmin)/f:pmin,
    disp(sprintf('parameter = %f',z));
    w=w+1;
    [xb(w,1:2) polb(w,1:2)]=equi1('cstr',xp,z,m,st1);
   parmb(w)=z;
    if xb(w,1)~=0, st1=xb(w,1:2);,end;
  end;
  for z=1:length(xb);,
    x(z,1:2)=xb(length(xb)-z+1,1:2);
    pol(z,1:2)=polb(length(xb)-z+1,1:2);
    parm(z)=parmb(length(xb)-z+1);
  ,end;
  for z=length(xb):(length(xb)+length(xf)-1);,
    x(z,1:2)=xf(z-length(xb)+1,1:2);
    pol(z,1:2)=polf(z-length(xb)+1,1:2);
    parm(z)=parmf(z-length(xb)+1);
  ,end;
else
  disp('Parameter out of range.');
  x=[];
  pol=[];
end;
```

B.12 bigsim.m

This function simulates the whole of the example system. Takes a long time to finish working.

```
load data1 %data created using equi2.m
[x1,po1,pa1]=findequi2(M1,0.5,xp,[0.5 320],80);
[x2,po2,pa2]=findequi2(M2,0.0001,xp,[0.5 320],80);
[x3,po3,pa3]=findequi2(M3,0.0001,xp,[0.5 320],80);
[x4,po4,pa4]=findequi2(M4,315,xp,[0.5 320],80);
[x5,po5,pa5]=findequi2(M5,315,xp,[0.5 320],80);
[x6,po6,pa6]=findequi2(M6,0.15,xp,[0.5 320],80);
save data2 x1 po1 pa1 x2 po2 pa2 x3 po3 pa3 x4 po4 pa4 x5 po5 pa5 x6 po6 pa6
```

B.13 cstr_p.mat

This is a mat file used for the standard parameters (and ranges) when doing simulations. Here is an example of the variables and what they might contain for the CSTR.

```
>> xp

xp =

    0.5000    0.0000    0.0000  320.0000  310.0000    0.1500

>> xp_r

xp_r =

         0    1.0000
    0.0001    0.0002
         0    0.0005
  310.0000  330.0000
  300.0000  320.0000
    0.1000    0.2000
```

B.14 magmovie.m

Makes a "movie" of the magnitude data created by `magplot2.m` for an entire parameter range.

```
M0 = moviein(f);
s=size(M);
for k=1:s(2)
  x_range=M(1:2,k);
  y_range=M(3:4,k);
  n=M(5,k);
  p1=M(6,k);
  m=M(7,k);
  m1=reshape(M(8:s(1),k),n+1,n+1);
```

```
  clip=max(max(m1))/10;
  I=find(m1>clip);
  mc=m1;
  for z=1:length(I);,mc(I(z))=clip;,end;
  surf((x_range(1):(x_range(2)-x_range(1))/n:x_range(2)),...
       (y_range(1):(y_range(2)-y_range(1))/n:y_range(2)),mc);
  shading flat
  colormap(jet);
  view(2);
  title(sprintf('parameter = %f',m,pi));
  M0(:,k) = getframe;
end
```

Appendix C

CSTR Parameter Relationships

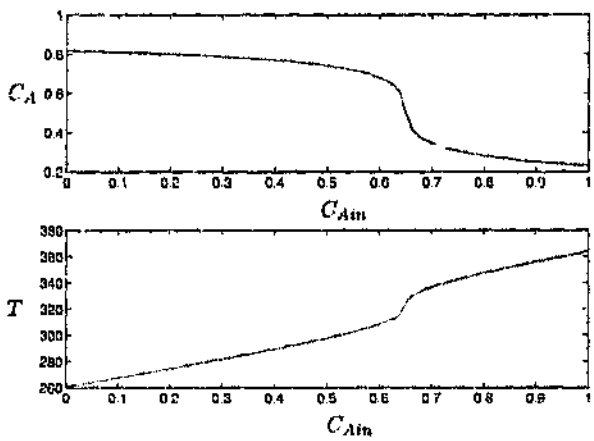


Figure C.1: Changes in equilibrium point versus C_{Ain}

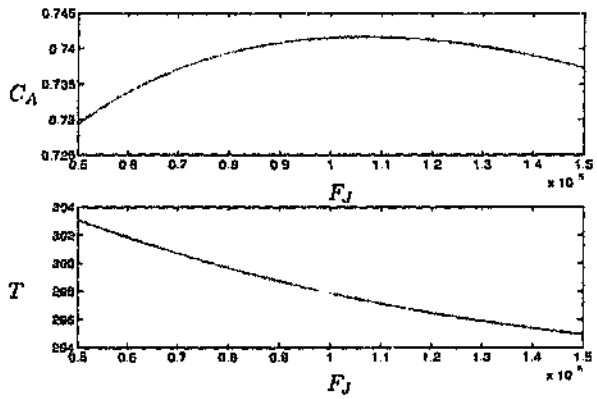


Figure C.2: Changes in equilibrium point versus F_{in}

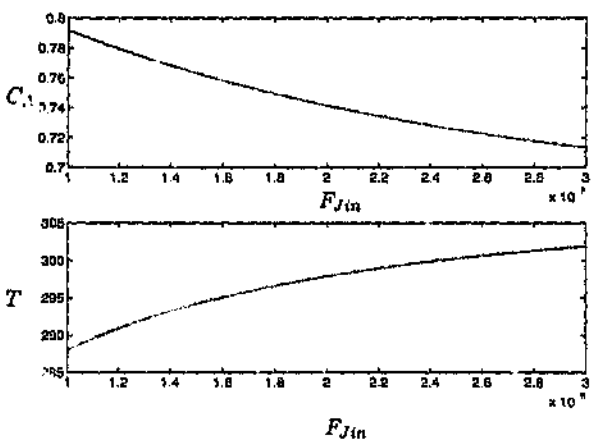


Figure C.3: Changes in equilibrium point versus F_{Jin}

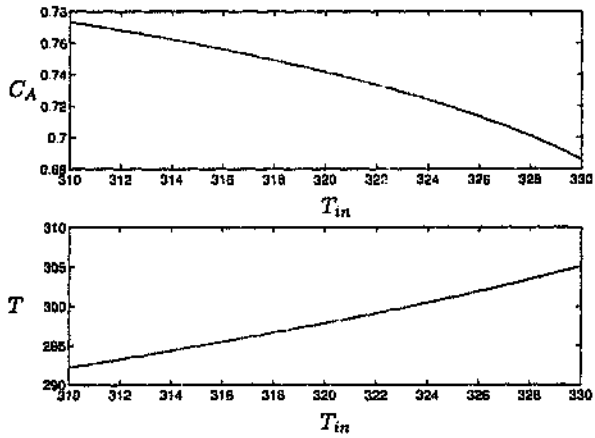


Figure C.4: Changes in equilibrium point versus T_{in}

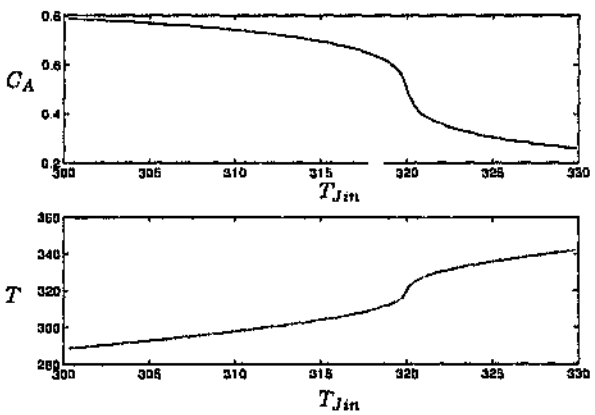


Figure C.5: Changes in equilibrium point versus T_{Jin}

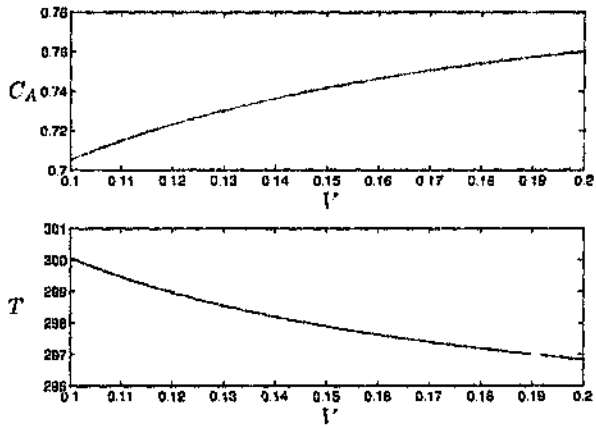


Figure C.6: Changes in equilibrium point versus V

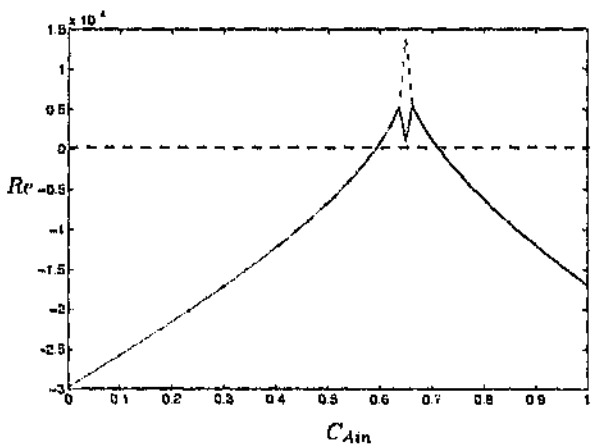


Figure C.7: Changes in stability versus C_{Ain}

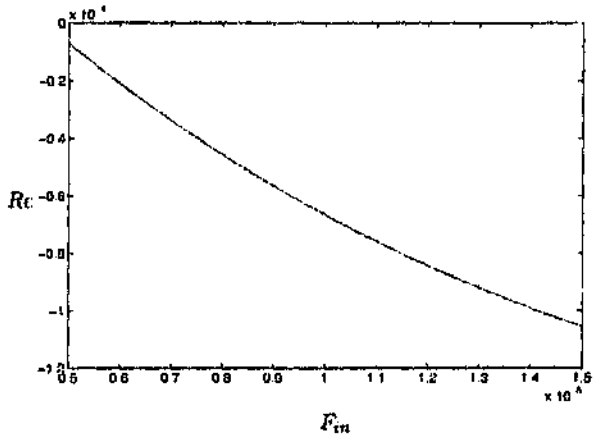


Figure C.8: Changes in stability versus F_{in}

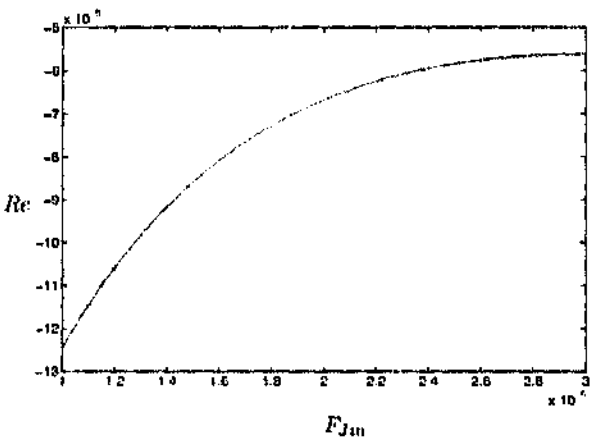


Figure C.9: Changes in stability versus F_{Jin}

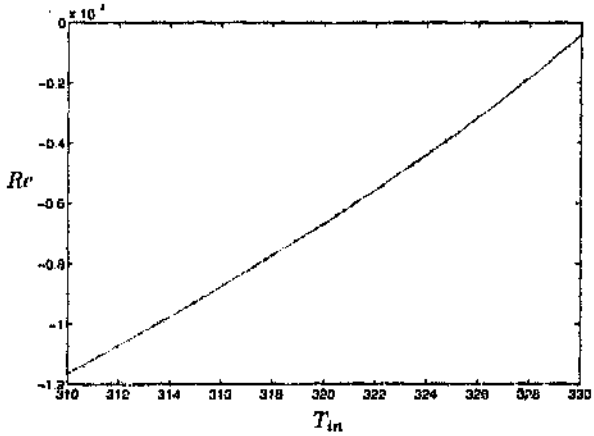


Figure C.10: Changes in stability versus T_{in}

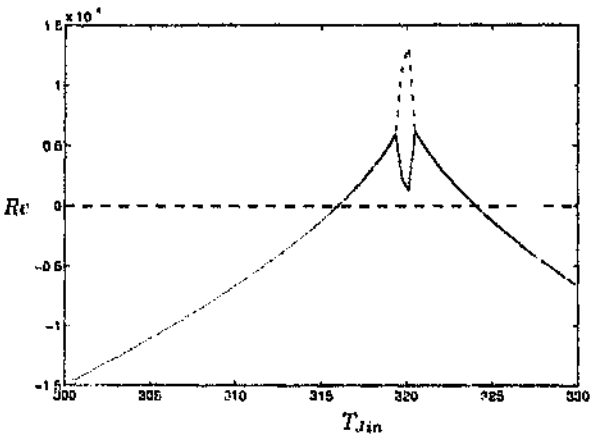


Figure C.11: Changes in stability versus T_{Jin}

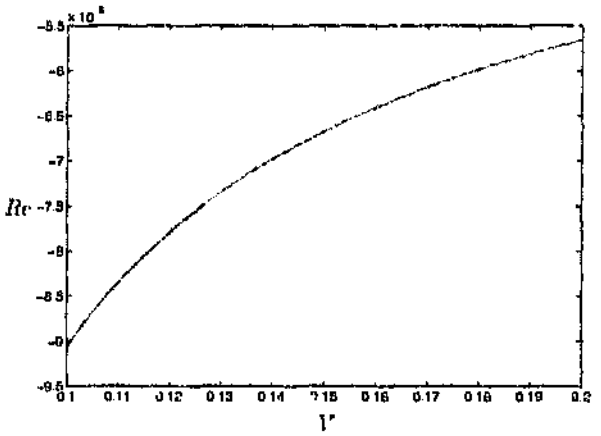


Figure C.12: Changes in stability versus V

Appendix D

Derivation of Unit Models

D.1 Tank

D.1.1 Energy Balance on the Tank

$$\left\{\begin{array}{l} \textit{Internal Energy IN+} \\ \textit{Internal Energy} \\ \textit{GENERATED} \end{array}\right\} = \left\{\begin{array}{l} \textit{Internal Energy OUT+} \\ \textit{Internal Energy} \\ \textit{ACCUMULATED} \end{array}\right\} \quad \text{(D.1)}$$

$$\left\{\begin{array}{l} \textit{Internal Energy IN} \\ \textit{by flow in time } \Delta t \end{array}\right\} = \{F_{in}C_v(T_{in} - T_b)\rho\Delta t\} \quad \text{(D.2)}$$

$$\left\{\begin{array}{l} \textit{Internal Energy IN} \\ \textit{by heat exchange in} \\ \textit{time } \Delta t \end{array}\right\} = UA_H(T_S - T)\Delta t \quad \text{(D.3)}$$

$$\textit{Internal Energy GENERATED} = 0 \quad \text{(D.4)}$$

$$\left\{\begin{array}{l} \textit{Internal Energy OUT} \\ \textit{by flow in time } \Delta t \end{array}\right\} = F_{out}C_v\rho(T - T_b)\Delta t \quad \text{(D.5)}$$

$$\textit{Internal Energy in tank} = \rho V C_v(T - T_b) \quad \text{(D.6)}$$

therefore

$$\left\{\begin{array}{l} \textit{ACCUMULATION} \\ \textit{in time } \Delta t \end{array}\right\} = \left\{\begin{array}{l} (\rho V C_v(T - T_b))|_{t+\Delta t} - \\ (\rho V C_v(T - T_b))|_t \end{array}\right\}$$

$$= \rho C_v\left((VT)|_{t+\Delta t} - (VT)|_t\right) \quad \text{(D.7)}$$

substituting

$$\left\{\begin{array}{l} \rho F_{in}C_v(T_{in} - T_b)\Delta t + \\ UA_H(T_S - T)\Delta t \end{array}\right\} = \left\{\begin{array}{l} F_{out}C_v\rho(T - T_b)\Delta t + \\ \rho C_v\left((VT)|_{t+\Delta t} - (VT)|_t\right) \end{array}\right\} \quad \text{(D.8)}$$

taking limits

$$\frac{d(VT)}{dt} = F_{in}(T_{in} - T_b) - F_{out}(T - T_b) - \frac{UA_H}{\rho C_v}(T - T_S) \quad \text{(D.9)}$$

Setting $T_b = 0$ and assuming that $C_v = C_p$

$$\frac{d(VT)}{dt} = F_{in}T_{in} - F_{out}T - \frac{UA_H}{\rho C_p}(T - T_S) \quad \text{(D.10)}$$

D.2 CSTR

D.2.1 Mass Balance on the Reactor

$$\left\{ \begin{array}{l} moles\ \mathrm{A}\ IN+ \\ moles\ \mathrm{A} \\ GENERATED \end{array} \right\} = \left\{ \begin{array}{l} moles\ \mathrm{A}\ OUT+ \\ moles\ \mathrm{A}\ ACCUMULATED \end{array} \right\} \quad \text{(D.11)}$$

$$\left\{ \begin{array}{l} moles\ \mathrm{A}\ IN \\ in\ time\ \Delta t \end{array} \right\} = F_{in}C_{Ain}\Delta t \quad \text{(D.12)}$$

$$\left\{ \begin{array}{l} moles\ \mathrm{A}\ out \\ in\ time\ \Delta t \end{array} \right\} = F_{out}C_A \quad \text{(D.13)}$$

$$\left\{ \begin{array}{l} moles\ \mathrm{A} \\ GENERATED \\ in\ time\ \Delta t \end{array} \right\} = r_A V \Delta t \quad \text{(D.14)}$$

$$moles\ \mathrm{A}\ in\ tank = VC_A \quad \text{(D.15)}$$

$$\text{(D.16)}$$

therefore

$$\left\{ \begin{array}{l} moles\ \mathrm{A}\ accumulated \\ in\ time\ \Delta t \end{array} \right\} = (VC_A)|_{t+\Delta t} - (VC_A)|_t \quad \text{(D.17)}$$

therefore

$$F_{in}C_{Ain}\Delta t + r_A V \Delta t = F_{out}C_A\Delta t + (VC_A)|_{+\Delta t} - (VC_A)|_t \quad \text{(D.18)}$$

taking limits

$$\frac{d(VC_A)}{dt} = F_{in}C_{Ain} - F_{out}C_A + r_A V \quad \text{(D.19)}$$

$$\text{but } r_A = -f(C_A, T)$$

therefore

$$\frac{d(VC_A)}{dt} = F_{in}C_{Ain} - F_{out}C_A - Vf(C_A, T) \quad \text{(D.20)}$$

D.2.2 Energy Balance on the Reactor

Assume C_v constant with T

T_b is the basis temp ·ture

ρ is constant

$$\left\{\begin{array}{l} Internal\ Energy\ IN+ \\ Internal\ Energy \\ GENERATED \end{array}\right\} = \left\{\begin{array}{l} Internal\ Energy\ OUT+ \\ Internal\ Energy \\ ACCUMULATED \end{array}\right\} \quad \text{(D.21)}$$

$$\left\{\begin{array}{l} Internal\ Energy\ IN \\ by\ flow\ in\ time\ \Delta t \end{array}\right\} = F_{in}C_v(T_{in} - T_b)\rho\Delta t \quad \text{(D.22)}$$

$$\left\{\begin{array}{l} Internal\ Energy\ IN \\ by\ heat\ exchange\ in \\ time\ \Delta t \end{array}\right\} = UA_H(T_J - T)\Delta t \quad \text{(D.23)}$$

$$\left\{\begin{array}{l} Internal\ Energy \\ GENERATED \\ by\ reaction\ in\ time\ \Delta t \end{array}\right\} = r_A V\lambda\Delta t$$

$$= -f(C_A, T)V\lambda\Delta t \quad \text{(D.24)}$$

$$\left\{\begin{array}{l} Internal\ Energy\ OUT \\ by\ flow\ in\ time\ \Delta t \end{array}\right\} = F_{out}C_v\rho(T - T_b)\Delta t \quad \text{(D.25)}$$

$$Internal\ Energy\ in\ tank = \rho VC_v(T - T_b) \quad \text{(D.26)}$$

therefore

$$\left\{\begin{array}{l} ACCUMULATION \\ in\ time\ \Delta t \end{array}\right\} = \left\{\begin{array}{l} (\rho VC_v(T - T_b))|_{t+\Delta t} - \\ (\rho VC_v(T - T_b))|_t \end{array}\right\}$$

$$= \rho C_v\left((VT)|_{t+\Delta t} - (VT)|_t\right) \quad \text{(D.27)}$$

substituting

$$\left\{\begin{array}{l} \rho F_{in}C_v(T_{in} - T_b)\Delta t+ \\ UA_H(T_J - T)\Delta t+ \\ f(C_A, T)V\lambda\Delta t \end{array}\right\} = \left\{\begin{array}{l} F_{out}C_v\rho(T - T_b)\Delta t+ \\ \rho C_v\left((VT)|_{t+\Delta t} - (VT)|_t\right) \end{array}\right\} \quad \text{(D.28)}$$

taking limits

$$\frac{d(VT)}{dt} = F_{in}(T_{in} - T_b) - F_{out}(T - T_b) - \frac{f(C_A, T)V\lambda}{\rho C_v} - \frac{UA_H}{\rho C_v}(T - T_J) \quad \text{(D.29)}$$

Setting $T_b = 0$ and assuming that $C_v = C_p$

$$\frac{d(VT)}{dt} = F_{in}T_{in} - F_{out}T - \frac{f(C_A, T)V\lambda}{\rho C_p} - \frac{UA_H}{\rho C_p}(T - T_J) \quad \text{(D.30)}$$

D.2.3 Energy Balance on the Jacket

$$\left\{ \begin{array}{l} Internal\ Energy\ IN+ \\ GENERATED \end{array} \right\} = \left\{ \begin{array}{l} OUT+ \\ ACCUMULATED \end{array} \right\} \quad (D.31)$$

$$\left\{ \begin{array}{l} Internal\ Energy\ IN \\ by\ flow\ in\ time\ \Delta t \end{array} \right\} = F_J \rho_J C_{v_J} (T_{Jin} - T_b) \Delta t \quad (D.32)$$

$$Internal\ Energy\ GENERATED = 0 \quad (D.33)$$

$$\left\{ \begin{array}{l} Internal\ Energy\ OUT \\ by\ heat\ exchange \\ in\ time\ \Delta t \end{array} \right\} = U A_H (T_J - T) \Delta t \quad (D.34)$$

$$Internal\ Energy\ in\ Jacket = \rho_J V_J C_{v_J} (T_J - T) \quad (D.35)$$

therefore

$$ACCUMULATION = \rho_J V_J C_{v_J} (T_J|_{t+\Delta t} - T_J|_t) \quad (D.36)$$

therefore (note $T_b = 0$)

$$\begin{aligned} F_J \rho_J C_{v_J} T_{Jin} \Delta t &= F_J \rho_J C_{v_J} T_J \Delta t + U A_H (T_J - T) \Delta t + \\ &\quad \rho_J V_J C_{v_J} (T_J|_{t+\Delta t} - T_J|_t) \end{aligned} \quad (D.37)$$

Taking Limits (Assume $C_{v_J} = C_{p_J} = C_J$)

$$\frac{dT_J}{dt} = \frac{F_J}{V_J}(T_{Jin} - T_J) + \frac{U A_H}{V_J \rho_J C_J}(T - T_J) \quad (D.38)$$

D.3 Pipe and Pump with a Control Valve

D.3.1 Flow Rate in the Pipe

The flow rate in the pipe is determined by the interaction of two characteristics :

1. The pressure developed by the pump versus flow rate.
2. The pressure drop through the system versus flow rate.

When the pressure developed by the pump is equal to the pressure required by the system (in equilibrium) then the flow rate will be set and remain constant. Figure D.1 shows the two characteristic curves and the effect of changing the system parameters. Note that P_0 is the minimum pressure required to overcome the effect

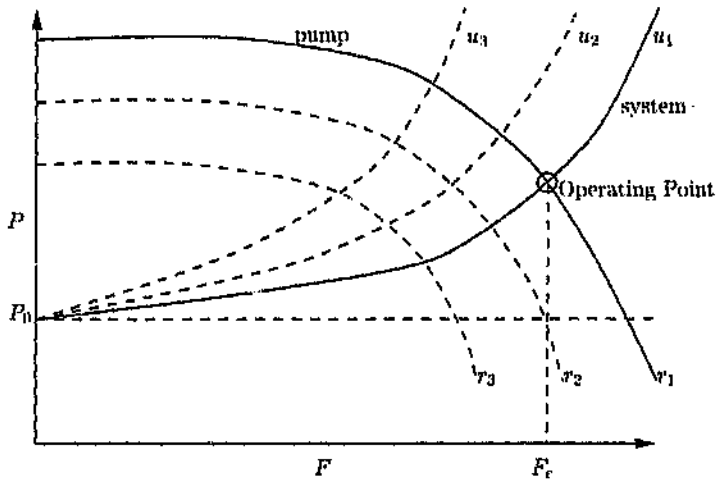


Figure D.1: Characteristic Curves for the Pipe and Pump

of input and output pressures as well as the effects of changes in height. Also note that $u_1 > u_2 > u_3$ and $r_1 > r_2 > r_3$.

If the dynamics of the pump motor and rotor are assumed to be much faster than the rate of change of the flow, then the rotor dynamics can be assumed to be instantaneous and hence be ignored. The two characteristic surfaces which describe the system and the pump ($P_p(F,r)$ and $P_s(F,u)$) can be obtained from data sheets and by using the techniques employed in fluid dynamics [25].

Using the characteristic surfaces and assuming that the only important dynamic besides those of the control valve is the acceleration of the liquid in the pipe, equation D.39 results.

$$\frac{dF}{dt} = \frac{A}{\rho L}\left[P_p(F,r) - P_p(F,u)\right] \tag{D.39}$$

D.3.2 Energy Balance on the Pipe

$$\left\{\begin{array}{l} Internal\ Energy\ IN+ \\ Internal\ Energy \\ GENERATED \end{array}\right\} = \left\{\begin{array}{l} Internal\ Energy\ OUT+ \\ Internal\ Energy \\ ACCUMULATED \end{array}\right\} \tag{D.40}$$

$$\left\{ \begin{array}{l} Internal\ Energy\ IN \\ by\ flow\ in\ time\ \Delta t \end{array} \right\} = \{F_{in}C_v(T_{in} - T_b)\rho\Delta t\} \quad (D.41)$$

$$\left\{ \begin{array}{l} Internal\ Energy\ IN \\ by\ heat\ exchange\ in \\ time\ \Delta t \end{array} \right\} = UA_H(T_S - T)\Delta t \quad (D.42)$$

$$Internal\ Energy\ GENERATED = 0 \quad (D.43)$$

$$\left\{ \begin{array}{l} Internal\ Energy\ OUT \\ by\ flow\ in\ time\ \Delta t \end{array} \right\} = F_{out}C_v\rho(T - T_b)\Delta t \quad (D.44)$$

$$Internal\ Energy\ in\ tank = \rho VC_v(T - T_b) \quad (D.45)$$

therefore

$$\left\{ \begin{array}{l} ACCUMULATION \\ in\ time\ \Delta t \end{array} \right\} = \left\{ \begin{array}{l} (\rho VC_v(T - T_b))|_{t+\Delta t} - \\ (\rho VC_v(T - T_b))|_t \end{array} \right\}$$

$$= \rho C_v \left((VT)|_{t+\Delta t} - (VT)|_t \right) \quad (D.46)$$

substituting

$$\left\{ \begin{array}{l} \rho F_{in}C_v(T_{in} - T_b)\Delta t + \\ UA_H(T_S - T)\Delta t \end{array} \right\} = \left\{ \begin{array}{l} F_{out}C_v\rho(T - T_b)\Delta t + \\ \rho C_v \left((VT)|_{t+\Delta t} - (VT)|_t \right) \end{array} \right\} \quad (D.47)$$

taking limits

$$\frac{d(VT)}{dt} = F_{in}(T_{in} - T_b) - F_{out}(T - T_b) - \frac{UA_H}{\rho C_v}(T - T_S) \quad (D.48)$$

Setting $T_b = 0$ and assuming that $C_v = C_p$
Let $T_1 = T$

$$\frac{d(T)}{dt} = \frac{F}{V}(T_{in} - T_1) - \frac{UA_H}{\rho C_p}(T_1 - T_S) \quad (D.49)$$

The transport delay is $\tau = \frac{LA}{F}$, hence

$$T_2(t) = T_1(t - \tau) \quad (D.50)$$

D.3.3 Control Valve Dynamics

The control valve has been modelled to take into account first order dynamics. These dynamics are given by the first order differential equation D.51 (τ_v is the first order time constant).

$$\frac{du}{dt} = \frac{1}{\tau_v}(v - u) \quad (D.51)$$

References

[1] Isidori A. *Nonlinear Control Systems.* Springer, 1995.

[2] Wigdorowitz B. Application of linearization analysis to aircraft dynamics. *Journal of Guidance, Control, and Dynamics*, 15, May-June 1992.

[3] Wigdorowitz B and Petrick M. Modelling concepts arising from an investigation into a chaotic system. *Mathematical and Computational Modelling*, 15, 1991.

Luss D. Steady-state multiplicity features of chemically reacting systems. *Chemical Engineering Education*, 20, Winter 1986.

[5] Adomaitis R A et al. Bifurcation behaviour of an autothermal packed bed tubular reactor. *Chemical Engineering Science*, 43, 1988.

[6] Agrawal P et al. Theoretical investigations of dynamic behaviour of isothermal continuous stirred tank biological reactors. *Chemical Engineering Science*, 37, 1982.

[7] Bartusiak R D et al. Nonlinear feedforward/feedback control structures designed by reference system synthesis. *Chemical Engineering Science*, 44, 1989.

[8] Chang H et al. Bifurcation characteristics of nonlinear systems under conventional pid control. *Chemical Engineering Science*, 39, 1984.

[9] Giona M et al. Bifurcation analysis and stability of a controlled CSTR. *Computers and Chemical Engineering*, 18, 1994.

[10] Harold M P et al. Use of bifurcation map for kinetic parameter estimation. *Industrial Engineering Chemistry Research*, 26, October 1987.

[11] Inamdar S R et al. Dynamics of reacting systems in the presence of time delay. *Chemical Engineering Science*, 46, 1991.

[12] Menle A et al. On the dynamics of the circulation loop reactor - numerical methods and analysis. *Chemical Engineering Science*, 50, 1994.

[13] Pinsky M A et al. Analysis and control of bifurcation phenomena in aircraft flight. *Journal of Guidance, Control and Dynamics*, 17, May 1994.

[14] Razon L et al. Multiplicities and instabilities in chemically reacting systems — a review. *Chemical Engineering Science*, 42, 1987.

[15] Seborg E et al. *Process Dynamics and Control.* John Wiley & Sons. 1989.

[16] Guckenheimer J and Holmes P. *Nonlinear Oscillations, Dynamical Systems and Bifurcation of Vector Fields.* Springer-Verlag, 1985.

[17] Thompson JMT and Stewart HB. *Nonlinear Dynamics and Chaos.* John Wiley and Sons, 1986.

[18] Huseyin K. *Multiple Parameter Stability Theory and its Applications.* Clarendon Press Oxford, 1986.

[19] Luyben W L. *Process Modeling, Simulation, and Control for Chemical Engineers.* McGraw-Hill International Book Company, 1974.

[20] Denn M M. *Process Modeling.* Longman Scientific & Technical, 1986.

[21] Koper M T M. Some simple bifurcation sets of an extended van der pol model and their relation to chemical oscillators. *Journal of Chemical Physics*, 102, April 1995.

[22] Kubicek M and Marek M. *Computational Methods in Bifurcation Theory and Dissipative Structures.* Springer-Verlag, 1983.

[23] Petrick M. *Nonlinear Analysis Techniques -- MSc Project Report.* University of the Witwatersrand, Johannesburg, 1990.

[24] Rasband S N. *Chaotic Dynamics of Nonlinear Systems.* John Wiley & Sons, 1990.

[25] Daily J W and Harleman D R F. *Fluid Dynamics.* Addison-Wesley, 1966.

[26] Guttinger W. *Structura Stability in Physics.* Springer, 1979.