DYNAMICS AND CONTROL OF DISTRIBUTED PARAMETER SYSTEMS WITH RECYCLES

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TABLE OF CONTENTS

SUMMARY

The objectives of the present study are to understand the dynamics of distributed parameter systems & recycle systems and to control distributed parameter systems with and without recycle. A set of tools were developed in MATLAB along with integrated SIMULINK models to execute the two objectives mentioned above. The developed tools are capable of yielding the dynamic responses of linear and nonlinear tubular reactors (with and without recycle) and heat exchanger systems which are governed by parabolic partial differential equations. Also, tools have been developed which perform the operation of control of such linear distributed systems using modal control theory. A new and novel technique called the modal feedback-feedforward controller has been introduced and found to be successful.

Orthogonal collocation technique is an important method of weighted residuals technique used to obtain the approximate solutions for parabolic partial differential equation. The dimensionalized system is divided into a number of collocation points. Then an approximate solution in the form of a polynomial trial function is used to represent the system. The various polynomial coefficients are obtained by minimizing the error between the true solution and approximate solution. The Orthogonal Collocation technique has been employed extensively in this study.

Modal control theory is a very useful theory in order to analyze the dynamic nature of a system and also design of controllers for such systems. The central theme of modal control is that the transient behavior of a process is governed by the dominant modes associated with the smallest eigenvalues. If it is possible to approximate the high order system by a lower order system (whose slow modes are the same as those of the original system), then attention can be focused on altering the eigenvalues of the slow modes so as to increase the speed of recovery of the process from disturbances. This theory was investigated in detail and implemented on a tubular reactor (with and without recycle) and also on a heat exchanger system.

Lumped parameter systems like the activated sludge process were examined in the early stages, which illustrates some of the weird behavior of recycles. Also a new control strategy called the predictor type recycle compensator was proposed and evaluated on a lot of simulation examples. A new index named "Recycle Effect Index" has been evaluated which measures the effect of recycle using concepts from the minimum variance benchmarking of control loop performance. It also gives guidelines on whether to go for any advanced control strategy such as the use of recycle compensator or not.

NOMENCLATURE

Abbreviation	**Explanation**
BVP	Boundary Value Problem
CSTR	Continuous Stirred Tank Reactor
DCS	Distributed Control Systems
DEE	Differential Equation Editor
DPS	Distributed Parameter System
FOPDT	First Order Plus Dead Time
IMC	Internal Model Control
IVP	Initial Value Problem
MA	Modal Analyzer
MFBC	Modal Feedback Controller
MFFC	Modal Feedforward Controller
MS	Modal Synthesizer
MVC	Minimum Variance Controller
MVFP	Minimum Variance controller based on Forward Path model
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PFR	Plug Flow Reactor
PID	Proportional Integral Derivative
RC	Recycle Compensator
REI	Recycle Effect Index
2D	2 Dimensional
3D	3 Dimensional

LIST OF FIGURES

LIST OF TABLES

LIST OF PUBLICATIONS

1. [G. M. Madhukar and S. Lakshminarayanan], Control of Processes with Recycles using a Predictive Control Structure, 2002, PSE Asia, Taiwan.
2. [S. Lakshminarayanan, K. Onodera and G. M. Madhukar], Recycle Effect Index: A Measure to aid in Control System Design for Recycle Processes, 2003, Industrial and Engineering Chemistry Research, (In Press).
3. [G. M. Madhukar, G. B. Dharmesh, Prabhat Agrawal and S. Lakshminarayanan], Feedback Control of Processes with Recycle: A Control Loop Performance Perspective, submitted to Chemical Engineering Research and Design in November 2003.

CHAPTER 1

INTRODUCTION

The study of distributed parameter systems (DPS) and recycle systems dates back to the late seventies. Since then both these topics have been the focus of attention for many researchers and have continued to receive contributions from academia as well as industry. In the chemical process industry, one frequently encounters complex systems such as tubular reactors, heat exchangers etc. Dynamic mass and energy balance of such systems results in models which are distributed in nature: the system variables vary spatially as well as temporally. These systems are generally described by partial differential equations (PDEs), integral equations or transcendental transfer functions (Ray, 1981). On top of these, material recycles and heat integration complicates the dynamics of such systems. Controller design and tuning are quite challenging for such processes.

In this work the following research objectives were considered:

i. To obtain the dynamics of distributed parameter systems with recycle
ii. Modal control of distributed parameter system with and without recycles.

An introduction to some of the basic concepts related to this field is presented next.

1.1. Lumped Parameter Systems

Lumped parameter systems are those whose behavior is described by ordinary differential equations. For example consider the dye mixing in a perfectly-stirred tank or a continuous stirred tank. The concentration within the tank for a constant flow rate (F) and volume (V) is given by this simple first order ordinary differential equation (ODE):

$$V\frac{dC_1}{dt} = F(C_{in} - C_1) \qquad \textbf{Eqn – 1.1.1}$$

subject to initial condition: $C_1(t = 0) = C_0$, where C_1 is the tank concentration, C_{in} is the inlet concentration. **Eqn - 1.1.1** is an initial value problem (IVP) and can be solved both analytically and numerically easily. Similarly if the ODE is subjected to boundary conditions then it is a boundary value problem (BVP) which is a bit more complicated than Initial value problem (IVP). Extensive research has been carried out on both analytical and numerical solution techniques for both IVP and BVP. One is advised to refer to standard mathematics text books: Kreyszig (1979) for analytical solutions, Numerical Analysis text books like Gerald and Wheatley (1989), Rice and Do (1995) and Ray (2000) for the numerical solutions for such problems.

1.2. Distributed Parameter Systems

Distributed parameter systems are those whose behavior is described by partial differential equations. There are three classes of partial differential equations: elliptic, parabolic and hyperbolic. Any partial differential equation of second order (having two independent variables) can be expressed in the following form,

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu + g = 0 \qquad \textbf{Eqn – 1.1.2}$$

Based on the values of constants a, b and c it is classified as,

Elliptic, if $\left(b^2 - 4ac\right) < 0$, elliptic equations commonly occur in steady-state heat flow, fluid flow, electrical potential distributions etc.

A very well known example is the Laplace equation, $\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)u=0$.

Parabolic, if $\left(b^2 - 4ac\right)=0$, parabolic equations commonly occur in time dependent problems which are very common in chemical engineering like the unsteady state heat flow, mass flow and momentum flow. A very well known parabolic PDE is the equation for one dimensional heat flow in a rod, $k\frac{\partial^2 u}{\partial x^2}=\rho C_P\frac{\partial u}{\partial t}$.

Hyperbolic, if $\left(b^2 - 4ac\right)>0$, hyperbolic equations commonly occur in transport problems, wave mechanics, gas dynamics, supersonic flow etc.

One well known hyperbolic PDE is the wave equation, $\frac{\partial^2 y}{\partial t^2}=\frac{Tg}{w}\frac{\partial^2 y}{\partial x^2}$.

However, to solve **Eqn – 1.1.2** (these DPS model) one requires boundary conditions along with initial conditions, which specify how these model equations, interact with its surroundings. Currently, for simplicity and (definitely for) control purposes, most industrial processes are represented by lumped parameter models even though a large number of these processes are distributed in nature. In this assumption one ignores the spatially varying nature of the DPS and design the controller. The control performance with these controllers suffers from strong interactions and apparent time delays due to the underlying diffusion and convection phenomena inherent in these processes Gay and Ray (1995). Examples such as heat transfer in a sheet forming processes, heat exchangers, tubular reactors and bioreactors are just a few of the many processes in which the dependent variables vary with both time and space.

In chemical engineering, problems which are time-independent or steady state problems are described by elliptic equations. Unsteady state or time-dependent problems are described by parabolic equations. In this thesis we place more emphasis on understanding numerical solution techniques to parabolic partial differential equations and reduction of such systems to low order models for the effective control of such systems. Here is an example of a distributed parameter system (packed tubular reactor) in which mixing of dye takes place. The model equation (parabolic PDE) governing this is, $\frac{\partial C_1}{\partial t} = -\nu \frac{\partial C_1}{\partial z} + D\left[\frac{\partial^2 C_1}{\partial x^2} + \frac{\partial^2 C_1}{\partial y^2} + \frac{\partial^2 C_1}{\partial z^2}\right]$ **Eqn – 1.1.3**

The relevant boundary conditions are: $D\left.\frac{\partial C_1}{\partial z}\right|_{z=0} = \nu(C_1 - C_{in})$ and. $\left.\frac{\partial C_1}{\partial z}\right|_{z=1} = 0$

with initial condition: $C_1(t=0) = C_0$.

The first term of the partial differential equation of the scalar concentration field represents convective-type transport and the second term represents transport by diffusion or dispersion. Note that the flow field (ν) may also be governed by a set of PDEs (e.g. the Navier-Stokes equations). Also there may be one more term ($-K_r * C_1$) added to the above parabolic PDE if we have a first order reaction occurring inside the reactor. Parabolic systems play an important role in the description of the dynamics of a chemical tubular reactor where dispersion phenomena are present; here is an example of linear parabolic PDE,

$$\frac{\partial C(z,\ t)}{\partial t} = D\frac{\partial^2 C(z,\ t)}{\partial z^2} - \nu\frac{\partial C(z,\ t)}{\partial z} - kC(z,\ t)\ , \qquad \textbf{Eqn – 1.14}$$

subject to the Danckwerts boundary conditions[1]:

$$D\frac{\partial C(0,\,t)}{\partial z} = \nu\big(C(0,\,t) - C_{in}\big) \text{ and } \frac{\partial C(L,\ \ t)}{\partial z} = 0\ .$$

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[1] The use of Danckwerts boundary conditions for the modeling of reactors has been justified by many authors. So one may consult [Aris (1999), Pearson (1959)] for further details.

The initial condition: $C(z,0) = C_0(z)$. Here **C** is the reactant concentration, z is the spatial position (m), ν is the superficial fluid velocity (m/s), k is the kinetic constant (1/s), D is the diffusivity, and L is the length of the reactor (m).

Typically parabolic equations modeling tubular reactors with axial dispersion can be viewed as a very general case, which is intermediate between the ideal cases: the continuous stirred tank reactor (CSTR) and the plug-flow reactor (PFR). When the diffusion coefficient is large, the distributed parabolic model tends to the lumped parameter model of a CSTR. Conversely, when it is small, the model tends to the (hyperbolic) plug flow reactor model. This phenomenon has been largely referred to in a number of publications (by using, for example, singular perturbations techniques) like those of Cohen and Poore (1974) and Varma and Aris (1977).

The two extreme cases (CSTR and PFR) rarely occur in practice as there is always some degree of back-mixing in a tubular reactor. It is for this reason that the intermediate axial dispersion model is of great importance, and thus the solution techniques to these parabolic PDEs has been the focus of many researchers. The strong coupling of diffusive, convective and reactive mechanisms is the source of the rich open-loop dynamic behavior exhibited by tubular reactors including multiple steady states, traveling waves, periodic, quasi-periodic and chaotic behavior. The reader may refer to Root and Schmitz (1969, 1970), Georgakis et al. (1977) and the classic paper from Jensen and Ray (1982) for results and references in this field.

Another way of solving linear distributed parameter systems (elliptic and parabolic PDE's) is by means of modal analysis. This technique as described by Ray (1981) reduces the complicated PDE model to an infinite set of ordinary differential equations. Modal analysis is based on the ability to represent the spatially varying input and output of the system as the sum of an infinite series of the system spatial eigenfunctions (eigenmodes) with time dependent coefficients. The dynamic behavior of each coefficient is then obtained as the solution to one of the independent ODE's. A good knowledge of eigenvalues and orthonormal eigenfunctions for the linear operator which describes the distributed system is required as this technique is best suited for self adjoint systems as these orthonormal eigenfunctions are used as basis function for truncated series expansions of the spatially varying inputs and outputs.

The classical modal analysis and control system design technique makes use of the property that the dynamic responses of the spatial eigenmodes coefficients are decoupled. In general, a simple control system design procedure can be used to determine a simple feedback controller for each individual spatial mode. Thus for spatially self adjoint DPS, modal control provides an attractive approach to the control of DPS.

1.3. Recycle Systems

In recent years due to strict environmental regulations and stiff global competition chemical industries are pushing towards design of chemical processes which make heavy use of material and energy recycles. The behavior of plants with material and energy recycles is complicated and can be quite different from the behavior of their constitutive units. Denn and Lavie (1982) showed that the recycle is equivalent to a positive feedback and studied the effect of delay in recycle path. The severe effects of recycles on time constants of a high purity distillation column have been shown by Kapoor et al. (1986). More recently Luyben (1993a, 1993b) has shown how an open loop response can become slow, oscillating and unstable when the gain of the recycle processes changes independent of other parameters. This is verified by the linear systems theory, which says that the recycle structure can affect the location of system poles leading to such responses. Jacobsen (1999) showed that the recycle paths can move both the poles and zeros of the transfer function between the inputs and outputs which are not part of the recycling loop. Morud and Skogestad (1994, 1996) also analyzed the effects of recycles on global plant. Luyben (1994) showed that a steady state phenomenon called the snowball effect occurs for recycle systems specifically for certain control structure configurations.

The standard technique proposed for the control of processes with recycles has been the deployment of a recycle compensator by Taiwo (1986). Scali and Ferrari (1999) illustrated the use of forward path and recycle path models in the design of recycle compensators to alleviate the detrimental effects of recycles on two realistic examples. The identification of models for the forward and recycle paths of the process from plant step response data and open/closed loop time series data has been considered very recently in Lakshminarayanan and Takada (2001) and illustrated using industrial systems by Lakshminarayanan et al. (2001).

1.4. Thesis Scope

Recently, chemical engineers from both academia and industries have started looking keenly at tubular reactors (distributed parameter systems) with recycle, which is a combination of the two fields mentioned above. A series of papers by Berezowski (1990, 1991, 1993, 1995 and 1998) extensively deals with such systems in which the diffusive phenomena are negligible compared to the convective ones and a highly exothermic reaction takes place. Antoniades and Christofides (2000, 2001) dealing with nonlinear feedback control of parabolic partial differential difference equation systems and dynamics and control of tubular reactor with recycle respectively. In this thesis, we give more emphasis on obtaining the dynamics of such tubular reactor (distributed parameter systems) with recycle and also control system design for such systems using modal analysis. An attempt is made towards extending some of the well known concepts in lumped parameter systems with recycle to distributed parameter systems with recycle. We see this as a step towards integrating some of the distributed parameter systems concept with the recycle systems concept.

1.5. Contributions of this Thesis

An approximate recycle compensator has been proposed in this thesis. The new approximate recycle compensation scheme is implemented in a predictive control framework and is based on the lines of the dead time compensator and the inverse response compensator. The simulation case studies show that the scheme is workable. The performance is somewhat inferior compared to that of the ideal recycle compensator; however, the ease of implementation of this scheme may far outweigh its sub-optimal performance and make it a useful alternative for compensating the detrimental effects of the recycle dynamics.

Another novel contribution of this thesis has been the development of Modal feedforward controller for the linear distributed parameter system with and without recycles. The Modal feedforward controller has been developed based on the lines of Modal feedback controller and consists of Modal Synthesizer and Modal Analyzer blocks. A complete set of equations describing these key component blocks has been derived from the fundamentals of Modal analysis theory and is dealt extensively in Chapter 4 of this thesis. The effectiveness of Modal feedforward controller in handling disturbances for such distributed systems (Linear tubular reactor with recycle and linear heat exchanger), in conjunction with Modal feedback controller, has been illustrated in Chapter 5.

In the case of linear tubular reactor with recycle the performance improvement is significant with the deployment of Modal feedforward controller in conjunction with the Modal feedback controller. The movement of the manipulated variable is also less for the combined Modal feedback plus feedforward control strategy. A similar effect can be seen even in case of the linear heat exchanger system. The application of Modal feedforward control on the two examples mentioned above shows the potential applicability of Modal feedforward control strategy for disturbance rejection in distributed parameter systems governed by linear partial differential equations.

1.6. Outline of this Thesis

This thesis is concerned with the discussion of: Dynamics and control of distributed parameter systems and recycle systems in chemical engineering. The organization of this thesis is as follows: Chapter 2 deals with recycles present in the lumped parameter systems. Some of the complicated dynamics exhibited by recycles are illustrated in this using an example of activated sludge process. A new control strategy called the predictor type recycle compensator is proposed (is an approximate recycle compensator in a model predictive framework similar to smith predictor for time delay compensation) and demonstrated to control recycle processes. Lastly an index called recycle effect index is discussed which quantifies the effect of recycles on any process using concepts from the minimum variance benchmarking of control loop performance. An REI value close to 0, means that the effect of the recycle is less and when it is close to 1, the effect of recycles is quite strong. Chapter 3 looks at distributed parameter systems in deeply. Chemical systems like the tubular reactors (both linear and nonlinear) and linear heat exchangers are considered to illustrate the dynamical behavior of such distributed systems. A well known numerical technique called orthogonal collocation has been described in this section, and is used to obtain the dynamics of these distributed parameter systems. The detrimental effect of recycles on a distributed system (tubular reactor) is captured. Chapter 4 illustrates a theory called Modal analysis applicable to linear lumped and distributed systems. Dynamic studies on linear tubular reactors with and without recycles and heat exchangers carried out in the previous chapters and some of the results obtained by collocation technique are cross verified using this technique. Chapter 5 deals with the control studies of these distributed systems using the concept of modal analysis learnt in chapter 4. A novel control strategy called Modal Feedforward control to handle measurable disturbances has been proposed for the tubular reactor with recycle system. Also simple modal feedback control has been designed for both tubular reactor and heat exchanger. Summary and conclusions are drawn at the end of this thesis after chapter 5. An exhaustive literature is provided at the end of the thesis.

CHAPTER 2

DYNAMICS OF LUMPED PARAMETER SYSTEMS WITH RECYCLE

2.1 Introduction

Lumped parameter systems with recycles are very common in chemical process plants. The recycles return valuable material for reprocessing and to recover energy from effluent streams through heat exchange. Such interconnections are termed process integration, are often cited as potential causes of difficulty in plant operations in spite of offering better steady state economy. Therefore it becomes important to understand the effects of recycle on process dynamics. A good literature review has been presented in the introductory chapter (section 1.3) dealing with lumped parameter systems with recycle. Here is a simple and illustrative example showing the effects of recycle on process dynamics.

Consider a reactor (CSTR) with feed-effluent heat exchanger as shown in Figure 2.1.1.

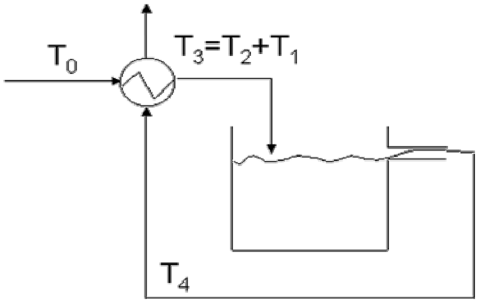


Figure 2.1.1 : A Simple reactor (CSTR) with feed-effluent heat exchanger

The block diagram (Figure 2.1.2) shows the output of the reactor affecting the input to the reactor. This is positive feedback introduced to the plant by the recycle of energy. In order to determine the behavior of integrated plant, the overall input-output transfer function has to be determined.

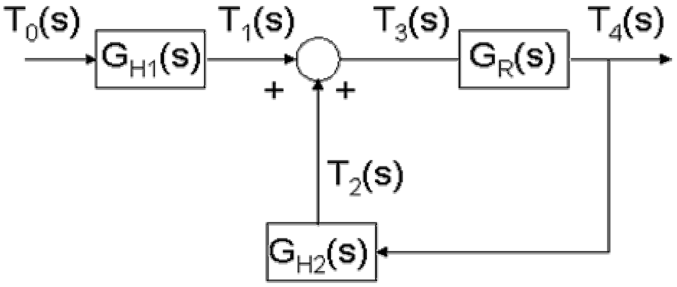


Figure 2.1.2 : Block diagram of reactor-heat exchanger system

The overall transfer function is given by, $\frac{T_4(s)}{T_0(s)} = \frac{G_R(s)G_{H1}(s)}{1 - G_R(s)G_{H2}(s)}$

The presence of recycle has totally changed the system behavior which is apparent from the overall transfer function as compared to the case where the fresh feed is preheated by an "independent" stream at temperature T_4. Now the poles of the overall system are no more same as the poles of individual units. Thus, stability of the system is no more guaranteed, even for cases where the individual units are stable.

To illustrate the effects graphically consider the numerical example from Marlin (1995) (section 5.5 and Figure 5.17), the numerical values for the above block diagram is as follows, $G_R(s) = \frac{3}{10s+1}$, $G_{H1}(s) = 0.4$ and $G_{H2}(s) = 0.3$

With recycle: $\frac{T_4(s)}{T_0(s)} = \frac{12}{100s+1}$,

Without recycle ($G_{H2}(s) = 0$): $\frac{T_4(s)}{T_0(s)} = \frac{1.2}{10s+1}$

The dynamic response for a step change in $T_0(s)$ of 2^0C is shown in Figure 2.1.3.

One can see drastic effect of recycle on steady-state gain and time constant; both increase by a factor of 10 due to recycle. The system is still stable and self-regulatory, because of the parameter values employed in this example, but the recycle has created an inherent positive feedback in the process, which has significantly affected the dynamic response.

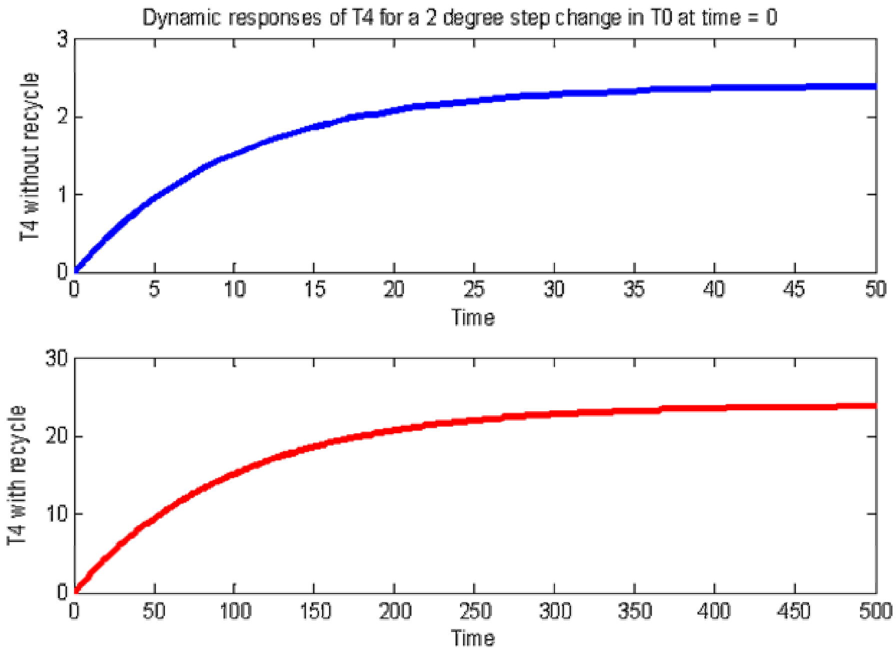


Figure 2.1.3 : Dynamic responses of T_4 with and without recycle

In section 2.2 of this chapter, we consider a biological waste water treatment process (activated sludge process) to illustrate some of the detrimental effects of recycles. This practical system is described by a model of two reactors (CSTR) in series, with a recycle stream from the outlet of the second reactor to the inlet of the first reactor. The topic of discussion of section 2.3 of this chapter is on an advanced automatic control strategy, concept of recycle compensator to eliminate the potentially unfavorable dynamic effects of recycle. The last part of this chapter (section 2.4) gives a brief idea on a benchmark index called the recycle effect index which is a measure of severity of recycle and advises whether one should go for the advanced control strategy described in section 2.3. The index is computed on a scale of [0-1]. If this index is close to one, then one should go for the advance control strategy and when it is close to zero, one would not benefit much from having such an advance control strategy.

2.2 Activated Sludge Process

2.2.1 Introduction

In this section we seek to study the dynamic operation of the biological waste water treatment process by activated sludge. The activated sludge process is a continuous or semi continuous aerobic method for biological waste water treatment. It includes carbonaceous oxidation and nitrification. The process is based on aeration of wastewater with flocculating biological growth, followed by the separation of the treated wastewater from biological growth. Part of this growth is then wasted, and the reminder is returned to the system. This system is analogous to, two reactors in series followed by the separation of the unreacted reactant from products and recycled back to the first reactor.

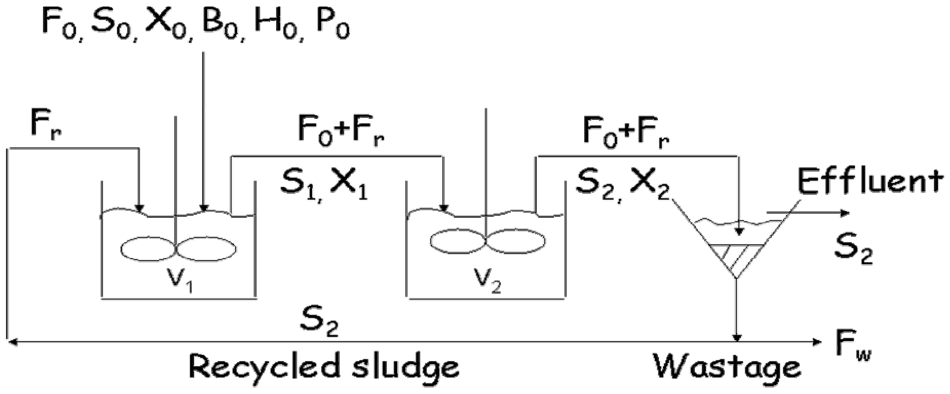


Figure 2.2.1 : Activated sludge plant with two completely mixed reactors in series with recycle

A schematic representation of this process (activated sludge plant with two completely mixed reactors in series with recycle) is shown in Figure 2.2.1. Most chemical processes are designed to operate at a steady-state condition. However, it is well known that for some processes, steady-state operation does not always guarantee best results and at times, unsteady-state operation improves the overall performance.

The average value of the performance of a process operating at unsteady-state is sometimes better and sometimes worse but never the same as the steady state operation. Numerous experimental and theoretical investigations have shown that periodic operation of chemical reactors leads to improved reactor performance by producing more reaction products or a more valuable product distribution than a steady-state reactor operation. For more information on the topic of unsteady state operation of chemical reactors one is recommended to refer the works of Shen and Ray (1998, 2000), Douglas and Rippin (1966), Lee and Bailey (1980) (Lee et al. 1980) and Ray (1995).

The activated sludge waste water treatment process consists of living microorganisms plus organic matter in an oxygen-rich (aerobic) environment. Microorganisms utilize complex organics as a food source to produce more microorganisms that are eventually settled out of the wastewater. The two basic types of microorganisms important to the operation of activated sludge system are the plants and animals. Plants include bacteria, algae and fungi. The bacteria are the most important and are primarily responsible for the removal of organic substances from wastewater. Animals include larger microorganisms, such as protozoa, crustaceans, and rotifers. The animals feed on dispersed bacteria that do not settle well and therefore, help polish the quality of treated effluent. The microorganism population of activated sludge is dynamic in nature. Competition for soluble food occurs among the bacteria, fungi, algae and protozoa. However most of the theoretical considerations of continuous culture systems have dealt with pure cultures of single organisms, although sewage treatment processes contain wide variety of organisms. The theoretical and experimental work of Curds (1971a, 1971b and 1973) has shown that when bacteria and protozoa are grown together in a reactor (as is the situation in the activated sludge process), steady-state conditions do not always exist, instead a series of predator-prey oscillations is observed.

2.2.2 Mathematical Model

Mathematical modeling of a process like the activated sludge process is very important, as it is a useful tool, for optimum design and control studies. The effects of operating variables can be studied far more quickly and inexpensively. Many mathematical models exist for the activated sludge process system, which range from simple to multicomponent to multispecies complex models. The model used in this work is primarily based on the reported work of Curds (1971a, 1971b and 1973) with some modifications as described in Shen and Ray (1998, 2000).

The theory of continuous culture of bacteria growing in a completely mixed reactor vessel was first described by Monod. The model developed relied on the well established fundamental microbiological relationships between the specific growth rate of a bacterium and the concentration of an essential growth substance. The specific growth rate, μ, of an organism is related to the concentrations of its limiting substrate by the Monod equation:

$$\mu = \frac{\mu_m S}{K_S + S} \qquad \textbf{Eqn – 2.2.1}$$

where μ and μ_m are the specific growth rate and maximum specific growth rate of the organism, S is the concentration of the substrate, and K_S is the saturation constant which is numerically equal to the substrate concentration when $\mu = \frac{\mu_m}{2}$. The schematic flow diagram used in the model is shown in figure 2.2.1.

The microbial population in the settling tank concentrates by a factor "b". Some sludge is continuously wasted at a rate F$_W$, the reminder is recycled back into the first reactor at a rate F$_r$. The mathematical model representing the system consists of ten equations, five in each reactor. The mass balance equation in each reactor is given by,

Reactor-1:

$$\frac{dS_1}{dt}=D_1S_0-D_1S_1(1+r)+D_1S_2r-\frac{\mu_{mx}}{Y_X}\left[\frac{S_1}{K_x+S_1}\right]X_1-\frac{\mu_{mb}}{Y_b}\left[\frac{S_1}{K_b+S_1}\right]B_1 \qquad \textbf{Eqn – 2.2.2}$$

$$\frac{dX_1}{dt}=\mu_{mx}\left[\frac{S_1}{K_x+S_1}\right]X_1-D_1X_1(1+r)+D_1rbX_2+D_1X_0 \qquad \textbf{Eqn – 2.2.3}$$

$$\frac{dB_1}{dt}=\mu_{mb}\left[\frac{S_1}{K_b+S_1}\right]B_1-D_1B_1(1+r)+rD_1B_2+D_1B_0-\frac{\mu_{mp}}{Y_P}\left[\frac{B_1}{K_P+B_1}\right]P_1 \qquad \textbf{Eqn – 2.2.4}$$

$$\frac{dP_1}{dt}=\mu_{mp}\left[\frac{B_1}{K_P+B_1}\right]P_1-D_1P_1(1+r)+D_1P_2rb+D_1P_0-\frac{\mu_{mg}}{Y_g}\left[\frac{P_1}{K_P+P_1}\right]G_1 \qquad \textbf{Eqn – 2.2.5}$$

$$\frac{dG_1}{dt}=\mu_{mg}\left[\frac{P_1}{K_P+P_1}\right]G_1-D_1G_1(1+r)+D_1G_2r+D_1G_0 \qquad \textbf{Eqn – 2.2.6}$$

Reactor-2:

$$\frac{dS_2}{dt}=D_2S_1(1+r)-D_2S_2(1+r)-\frac{\mu_{mx}}{Y_X}\left[\frac{S_2}{K_x+S_2}\right]X_2-\frac{\mu_{mb}}{Y_b}\left[\frac{S_2}{K_b+S_2}\right]B_2 \qquad \textbf{Eqn – 2.2.7}$$

$$\frac{dX_2}{dt}=\mu_{mx}\left[\frac{S_2}{K_x+S_2}\right]X_2-D_2X_2(1+r)+D_2X_1(1+r) \qquad \textbf{Eqn – 2.2.8}$$

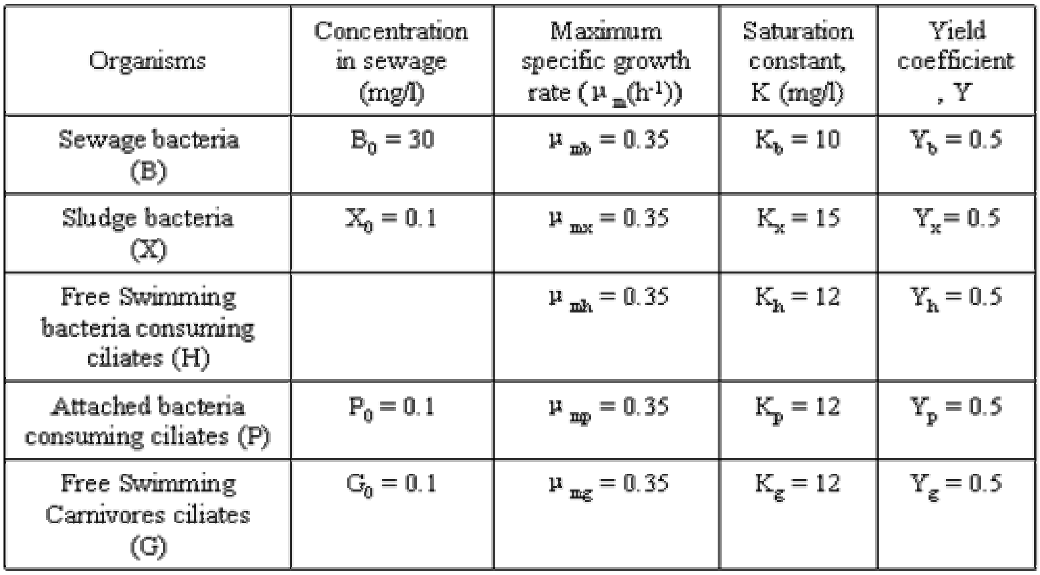
$$\frac{dB_2}{dt}=\mu_{mb}\left[\frac{S_2}{K_b+S_2}\right]B_2-D_2B_2(1+r)+D_2B_1(1+r)-\frac{\mu_{mp}}{Y_P}\left[\frac{B_2}{K_P+B_2}\right]P_2 \qquad \textbf{Eqn – 2.2.9}$$

$$\frac{dP_2}{dt}=\mu_{mp}\left[\frac{B_2}{K_P+B_2}\right]P_2-D_2P_2(1+r)+D_2P_1(1+r)-\frac{\mu_{mg}}{Y_g}\left[\frac{P_1}{K_P+P_1}\right]G_2 \qquad \textbf{Eqn – 2.2.10}$$

$$\frac{dG_2}{dt}=\mu_{mg}\left[\frac{P_2}{K_P+P_2}\right]G_2-D_2G_2(1+r)+D_2G_1(1+r) \qquad \textbf{Eqn – 2.2.11}$$

where C_i is the total concentration of protozoa in the i^{th} reactor. μ_i and Y_i are the specific growth rate and yield constant of the i^{th} species and subscript 'o' indicates the initial concentration of species in the entering sewage.

Table 2.2.1: Kinetic Constants and Feed Concentration Values



Organisms	Concentration in sewage (mg/l)	Maximum specific growth rate (μ_m(h^{-1}))	Saturation constant, K (mg/l)	Yield coefficient , Y
Sewage bacteria (B)	$B_0 = 30$	$\mu_{mb} = 0.35$	$K_b = 10$	$Y_b = 0.5$
Sludge bacteria (X)	$X_0 = 0.1$	$\mu_{mx} = 0.35$	$K_x = 15$	$Y_x = 0.5$
Free Swimming bacteria consuming ciliates (H)		$\mu_{mh} = 0.35$	$K_h = 12$	$Y_h = 0.5$
Attached bacteria consuming ciliates (P)	$P_0 = 0.1$	$\mu_{mp} = 0.35$	$K_p = 12$	$Y_p = 0.5$
Free Swimming Carnivores ciliates (G)	$G_0 = 0.1$	$\mu_{mg} = 0.35$	$K_g = 12$	$Y_g = 0.5$

The kinetic constants and feed concentrations used in computer simulations are given in Table 2.2.1. Source: Shen and Ray (1998).

2.2.3 Solution methodology, results and conclusions

The above set of 10 nonlinear ordinary differential equations was implemented using DEE block of MATLAB/SIMULINK. These equations were embedded into the DEE block in a particular format with a good initial guess of outputs, below is listed some of the steady state guess values for the state variables of first tank and second tank. First tank - $S_{10} = 21.4128$, $X_{10} = 192.796$, $B_{10} = 17.527$, $P_{10} = 16.6385$, $G_{10} = 2.2916$. Second tank - $S_{20} = 1.225$, $X_{20} = 202.0158$, $B_{20} = 7.9514$, $P_{20} = 18.5727$, $G_{20} = 4.0121$. The fresh feed parameter values used in simulation are $S_0 = 260$ mg/lt, $X_0 = 0.1$ mg/lt,

B_0 = 30 mg/lt, P_0 = 0.1 mg/lt and G_0 = 0.1 mg/lt. The other parameter values are D = 0.17 hr^{-1}, D_1 = 0.25 hr^{-1}, $D_2 = (D*D_1)/(D_1-D)$ = 0.53 hr^{-1}, r = 0.35 and b = 1.9. A simulink model was created using this DEE block containing the above set of equations subjected to these parameter values. Various ODE solvers like ODE45, ODE15s, ODE23s etc can be used to simulate this model.

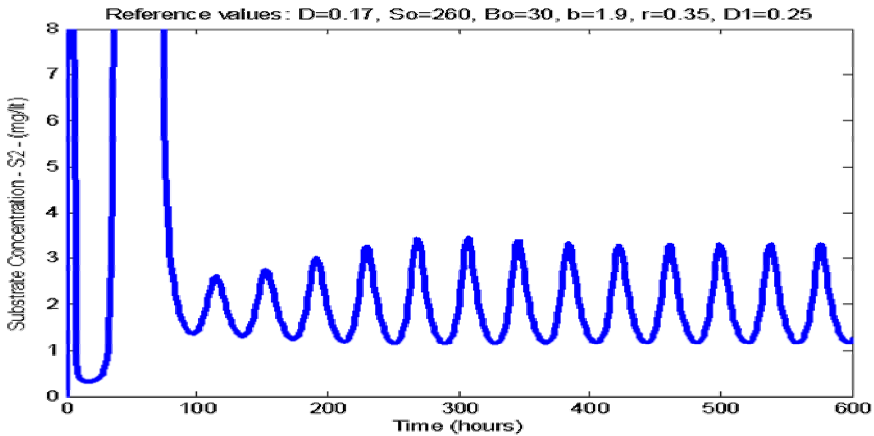


Figure 2.2.2 : Self-sustained natural oscillation (Limit cycles)

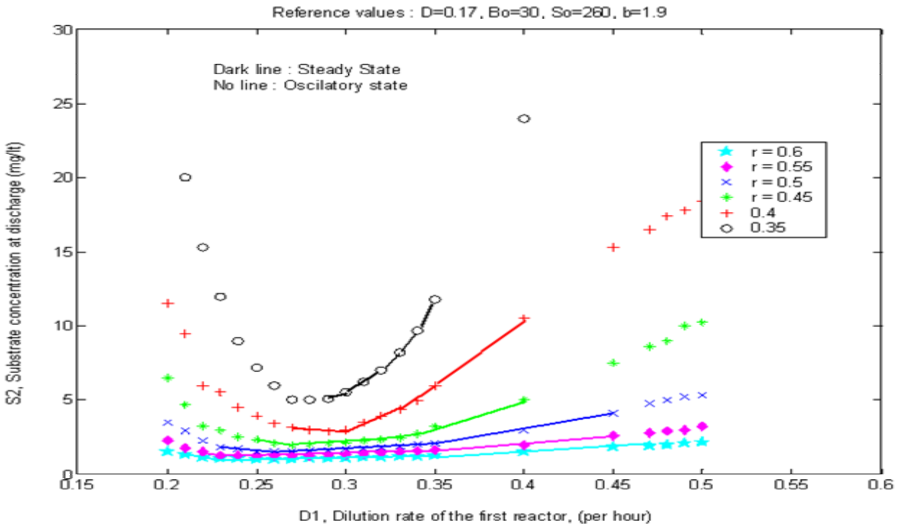


Figure 2.2.3 : Effect of D1 on overall system performance for different recycle ratio (r).

In Figure 2.2.3 we want to see the effect of different recycle ratios and different dilution rates of first reactor, on the substrate concentration S_2. The points which are connected by the dark line are the steady state operating regions or points. The points which are not connected by any line are the points or regions which show oscillatory behavior. The various shapes like diamond, star, plus etc used in the above figure are, to represent the different recycle ratios used in the simulation.

Some of the conclusions that can be drawn from Figure 2.2.3 are, when the dilution rate of the first reactor was kept low (example $D_1 = 0.2$ h^{-1}), while keeping the total dilution rate fixed at 0.17 h^{-1}, it was observed that the reactor system operates under oscillatory state. However, at some intermediate values of D_1 (example $D_1 = 0.25$ h^{-1} for recycle ratio of 0.45) the system changes from oscillatory state to steady state. D_1 was then further increased to a value of about 0.4 h^{-1} for the same recycle ratio, the operation of the system changes again to oscillatory state. The occurrence of the second oscillatory region is because of the recycle of the effluents from the second reactor to the first reactor. It is likely that either the first reactor or the second reactor operates at oscillatory state for a set of process variables when the total dilution rate, D, is kept constant. Then, even though the first reactor operates at steady state for the choice of process parameters, it inherits forced oscillation through recycle of oscillatory-state operation of the second reactor.

From Figure 2.2.3 it is clear that the switch from oscillatory state to steady state to oscillatory state occurs at different values of the dilution rate, D_1, and for different values of the recycle ratio, r. When the fraction recycled is less than about 0.3, the overall system is most of times in oscillatory mode but when fractioned recycled is very much close to zero, the system does show some steady state zone. However the fraction recycles is increased, the overall system does not always operate under oscillatory state. For example, when the fraction recycled is equal to 0.4, no limit cycles exists for D_1 between 0.26 and 0.4 h^{-1}. The study also revealed that, when the first reactor operates under oscillatory state the concentration of the substrate at discharge, is lower than when the second reactor operates under oscillatory state. This is probably because only the fraction of the effluent from the second reactor was recycled to the first reactor. This is apparent from the figure as the difference decreases with the increase of recycle ratio. Figure 2.2.3 further divulges that the concentration of the substrate at discharge from the second reactor decreases with the increase of recycle ratio. Therefore, it is better to operate at a higher recycle ratio although it will increase the operating cost. Similar plots with different values of process parameters (like τ, S_0, X_0, B_0, P_0, H_0, b, etc.) or kinetic parameters (like μ_m, K and Y) can be obtained to determine the regions where oscillatory-state operation occurs and where steady state operation occurs and which one is more advantageous.

From the above discussions it is evident that other parameters (dilution rate, fraction recycled, sewage concentration, and concentration factor) will have same effect on the substrate concentration at the discharge and depending on the parameter values, only steady state or only oscillatory state or both states can exist. In conclusion, oscillations have been reported for systems in all areas of nonlinear dynamics, and the present system is by no means an exception. Therefore, as an engineer, one should be prepared to utilize these situations for economic benefits, or at least should know how to avoid them in practice, by such parametric studies.

2.3 Concept of Recycle Compensator

Material recycles and heat integrations are pretty common in chemical industry. Such features can complicate the dynamics of the processes. Controller design and tuning must be done very carefully. The recycle compensator has been advocated as one possible control strategy to eliminate the detrimental effects of recycles.

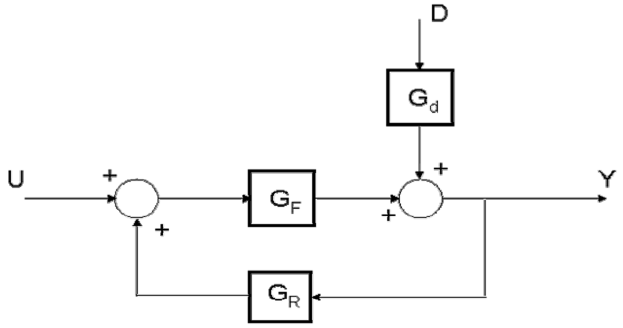


Figure 2.3.1 : The Recycle Process

A block diagram of a process with recycle is shown in Figure 2.3.1. Here G_F represents the forward path dynamics and G_R represents the recycle dynamics. G_d is the disturbance transfer function. Many authors have worked on the dynamics of such systems. A brief literature review was presented in the section 1.3 of chapter 1. The standard technique proposed for the control of processes with recycles has been the deployment of a recycle compensator Taiwo (1986).

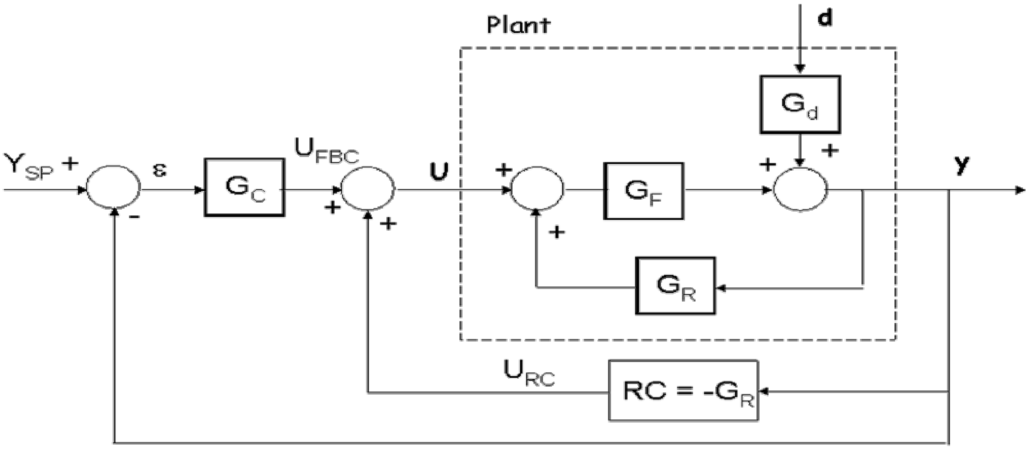


Figure 2.3.2 : Control System with Recycle Compensator

The recycle compensator ("RC" in Figure 2.3.2) can be designed if the recycle path dynamics is known. The feedback controller G_C employed in Figure 2.3.2 can then be designed based only on the forward path model. Scali and Ferrari (1999) have clearly demonstrated the workability of this approach using two realistic examples. Kwok et al. (2001) used a seasonal-model based control strategy for regulating a recycle process. Chodavarapu and Zheng (2001) discuss the issues in the design of controllers for processes with recycles and present some practical guidelines. Emoto and Lakshminarayanan (2002) develop a quantitative measure called recycle effect index that indicates if a recycle compensator is mandatory for satisfactory control of a process with recycle. To date, there has been no reported laboratory or industrial implementation of the recycle compensator. One reason for this could be the difficulties in implementing this strategy on standard industrial DCS systems, as an extra feature containing the recycle compensator has to be created and added to the DCS systems. In order to overcome this difficulty, we propose an approximate recycle compensation scheme that has a predictor structure similar to that of the Smith predictor for time delay compensation (Smith, 1957) or the inverse response compensator of Iinoya and Altpeter (1962). The mathematical expression for the recycle compensator that has the predictor structure will be derived. Then it is simplified to a form that can be implemented on industrial DCS systems. Illustrative examples are provided followed by concluding remarks.

2.3.1 The Predictive Control Structure

A schematic of a predictive control structure is shown in Figure 2.3.3. In the most general sense, G_p represents the true process (assumed to be open loop stable) with the final control element and the sensor, G_d the disturbance transfer function, G_c represents the predictive controller and K the dynamic model of the process. The true process G_P or the "Plant" indicated in Figure 2.3.3 can be decomposed into two components - one a forward path G_F and the other a positive feedback path or the recycle path G_R. We will examine this structure in the context of compensators (such as time delay compensation or the inverse response compensator) where G_C is a PID type feedback controller. In these compensation schemes, the conventional PID controller is employed as the feedback controller G_c. However, this G_c is designed to control a "model" rather than the true process that is devoid of the time delay or the inverse response (as the case may be). This strategy would enable the correct calculation of the manipulated variable to be implemented on the true process. This can provide good control as long as the "model" is perfect. In the absence of a perfect model, the control quality will suffer but zero steady state offset can be accomplished by adherence to easily achieved criteria Marlin (1995).

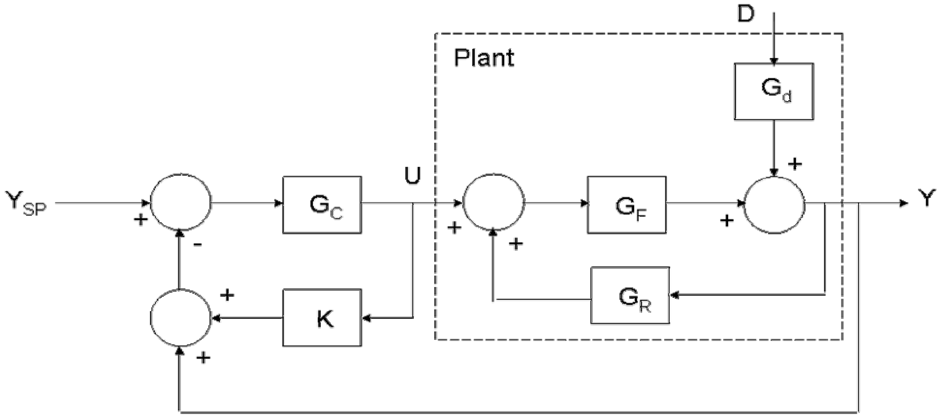


Figure 2.3.3 : The Predictive Control Structure for Approximate Recycle Compensation

Let us assume that the process model G_m (approximation of the true process G_p) can be decomposed into three components G, G_θ and G_{NM}. That is

$$G_m = G G_\theta G_{NM} \qquad \textbf{Eqn – 2.3.1}$$

Where G is free of time delays and non-invertible zeros and is the "desirable" process to control, G_θ comprises of the delay and G_{NM} includes the non-invertible zeros.

The closed loop servo transfer function is given by,

$$y = \frac{G_c\, G_p}{1 + K\, G_c + G_c\, G_p}\, y_{sp} \qquad \textbf{Eqn – 2.3.2}$$

If the model were perfect i.e. $G_p = G_m$ then **Eqn – 2.3.2** becomes,

$$y = \frac{G_c\, G_m}{1 + K\, G_c + G_c\, G_m}\, y_{sp} \qquad \textbf{Eqn – 2.3.3}$$

Now, G_m may contain time delays and non-invertible zeros in which case **Eqn – 2.3.3** can be written as:

$$y = \frac{G_c\, G_m}{1 + K\, G_c + G_c\, G\, G_\theta\, G_{NM}}\, y_{sp} \qquad \textbf{Eqn – 2.3.4}$$

The G_θ and G_{NM} terms prevent more aggressive adjustment of the manipulated variable because they appear in the characteristic equation. We can get rid of such undesirable terms from the characteristic equation by choosing K such that

$$K = G\,(1 - G_\theta\, G_{NM}\,) \qquad \textbf{Eqn – 2.3.5}$$

When this compensator K is implemented as shown in Figure 2.3.3 on the actual process G_p, the closed loop transfer function will be

$$y = \frac{G_c\, G_p}{1 + G\,(1 - G_\theta\, G_{NM}\,)\, G_c + G_c\, G_p}\, y_{sp} \qquad \textbf{Eqn – 2.3.6}$$

$$y = \frac{G_c\, G_p}{1 + G_c\,(G_p - G_m + G)}\, y_{sp} \qquad \textbf{Eqn – 2.3.7}$$

If there is no model plant mismatch (i.e. $G_m = G_p$), then the closed loop servo transfer function reduces to the form,

$$y = \frac{G_c\, G_m}{1 + G\, G_c}\, y_{sp} \qquad \textbf{Eqn – 2.3.8}$$

wherein, we have the characteristic equation free of undesirable dynamics.

Remarks:

- If $\mathrm{G}_{\mathrm{NM}} = 1$ and $\mathrm{G}_\theta = \mathrm{e}^{-\theta s}$, we have a process that is free of any undesirable zero dynamics but contains time delays that need to be compensated for. In this case, the compensator $\mathrm{K} = \mathrm{G}\left(1 - \mathrm{e}^{-\theta s}\right)$ is the well known Smith Predictor for time delay compensation.

- If the process has no delays but only unfavorable zero dynamics (right half plane zeros) i.e. if $\mathrm{G_m = G\,G_{NM}}$, then the compensator $\mathrm{K = G(1 - G_{NM})}$. If $G_m = k_2 \dfrac{-\alpha\, s + 1}{(\tau_1 s + 1)(\tau_2 s + 1)} = G G_{NM}$ with $\alpha < 0$.

  Then we have, $G = k_2 \dfrac{\alpha\, s + 1}{(\tau_1\, s + 1)(\tau_2\, s + 1)}$ and $G_{NM} = \dfrac{-\alpha\, s + 1}{\alpha\, s + 1}$,

  Now the compensator K equals $\dfrac{2\, k_2\, \alpha\; s}{(\tau_1\, s + 1)\,(\tau_2\, s + 1)}$. This is the inverse response compensator proposed by Iinoya and Altpeter.

- Notice that the steady state gain of the compensators for both time delay compensation and inverse response compensation is zero. As long as the controller $\mathrm{G_c}$ contains integral action, this meets the requirements for zero steady-state offset as spelt out in Marlin (1995).

Coming to the central theme of this section (i.e a compensator for recycles), we consider a process with recycle that can be represented by the model as,

$$G_m = \frac{G_F}{1 - G_F\, G_R} = G_F\, \frac{1}{1 - G_F\, G_R} = G\, G^* \qquad \textbf{Eqn – 2.3.9}$$

As seen from **Eqn – 2.3.9**, we consider the forward path model, $\mathrm{G_F}$ to be the desired portion for feedback control and look forward to design the compensator K to handle the undesirable dynamics $\mathrm{G^*}$. Note that G* contains the recycle path dynamics $\mathrm{G_R}$.

The expression for recycle compensator is,

$$K = G_F \left[1 - \frac{1}{1 - G_F\, G_R} \right] = \frac{-\, G_F^2\, G_R}{1 - G_F\, G_R} \qquad \textbf{Eqn – 2.3.10}$$

This expression for the recycle compensator implemented with a predictive control structure is fairly complicated compared to the conventional recycle compensator. We can expand the expression for the recycle compensator given in **Eqn – 2.3.10** as,

$$K = -G_F^2\, G_R(1 + G_F\, G_R + G_F^2\, G_R^2 + \cdots) \qquad \textbf{Eqn – 2.3.11}$$

In **Eqn – 2.3.11**, we may choose to retain only the first term and implement an approximate recycle compensator as,

$$K_A = -G_F^2\, G_R \qquad \textbf{Eqn – 2.3.12}$$

When the recycle compensator is implemented using the predictive structure (i.e. using equations 2.3.11 or 2.3.12), steady state offset will occur either for a step change in set point or the disturbance. As pointed out in Marlin (1995), the condition for zero steady-state offset is that the gain of the feedback predictive controller must be equal to the inverse of the gain of the compensator. If the feedback controller were to include integral action, then one must ensure that the gain of the compensator K be equal to zero. Obviously, the compensator K given by either by equations 2.3.11 or 2.3.12 has a gain different from zero. To ensure zero steady state offset, we must modify our expression for the recycle compensator.

The expression for the complete recycle compensator in the predictive control structure takes the following form

$$K = \frac{-G_F^2\, G_R}{1 - G_F\, G_R} + \frac{K_F^2\, K_R}{1 - K_F\, K_R} \qquad \textbf{Eqn – 2.3.13}$$

The approximate recycle compensator in the predictive control structure is implemented in this form

$$K_A = -G_F^2\, G_R + K_F^2\, K_R \qquad \textbf{Eqn – 2.3.14}$$

Equations 2.3.13 and 2.3.14 are the expressions for the “complete” recycle compensator and approximate recycle compensator implemented using the predictive controller structure.

2.3.2 Examples

Example 1

Consider a system with $G_F = \frac{4.5\, e^{-3s}}{10\, s+1}$ and $G_R = \frac{0.2\, e^{-s}}{s+1}$. We compare three results for this system (see figure 2.3.4). First, we use the overall process model $\frac{G_F}{1 - G_F\, G_R}$ to design a PI feedback controller. Ciancone tuning relations (Marlin, 1995) are employed to design this controller. The response of this controller to a step type disturbance is shown by the dotted line trajectory in Figure 2.3.4. There is a very large deviation from the steady state value and the process takes a significantly long time to recover from the disturbance. A conventional recycle compensator was then employed (schematic shown in Figure 2.3.2). The feedback controller in this case was based on the G_F only. The solid line in Figure 2.3.4 indicates the response of this control strategy to the same disturbance. The performance is seen to be excellent. Thirdly, we implemented the approximate recycle compensator using the predictive control structure as given by **Eqn – 2.3.14** and designed the PI feedback controller based on G_F only (the feedback PI controller used in this scheme is essentially the same employed with the conventional recycle compensation scheme). The performance is seen to be quite acceptable (dashed-dotted line in Figure 2.3.4). The performance of the recycle compensator using the predictive control structure is not as superior as that using the conventional recycle compensator. There is enough accumulated industrial experience in the implementation of dead time compensation and therefore the implementation of recycle compensation is likely to be much easier in industrial DCS systems as compared to the implementation of the conventional recycle compensator.

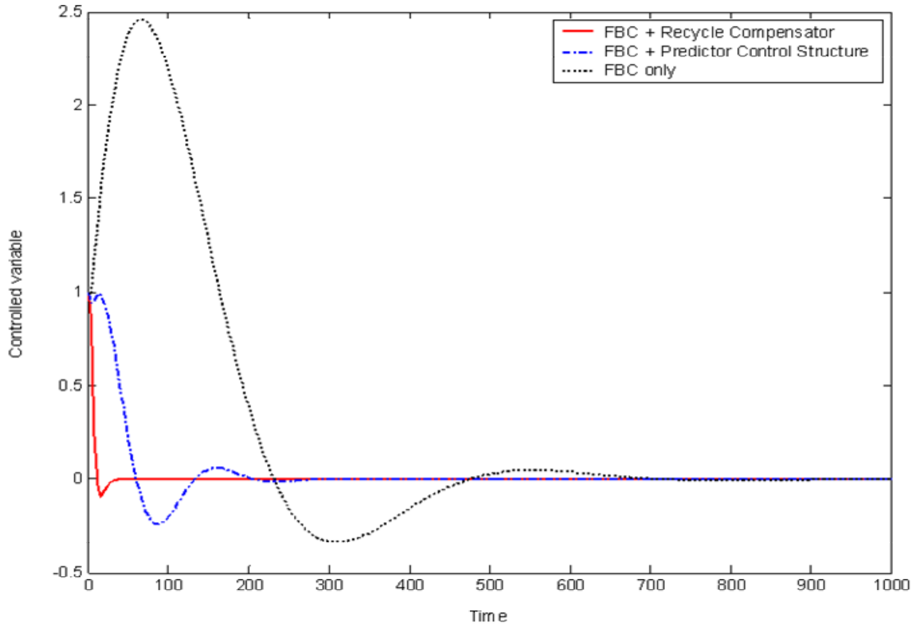


Figure 2.3.4 : Response to a unit step disturbance for example 1

Example 2

The system we consider next consists of two reactors in series with a recycle stream from the outlet of the second reactor to the inlet of the first reactor. The two reactors are assumed well mixed. A more detailed description of the system and the governing equations are provided in Scali and Ferrari (1999). The forward path and the recycle path models for this system are given by: $G_F = \frac{e^{-2.5s}}{2.5s+1}$ and $G_R = \frac{0.9e^{-2.5s}}{5s+1}$.

Four cases were examined,

Case 1: Use of conventional recycle compensation scheme with the feedback controller designed based on forward path model (G_F) only.

Case 2: Only feedback control. The feedback controller is designed using the overall process model.

Case 3: Only feedback control. The feedback controller is designed using the forward path model (G_F) only.

Case 4: Control using approximate recycle compensator in a predictive control structure. The feedback controller is designed based on forward path model (G_F) only.

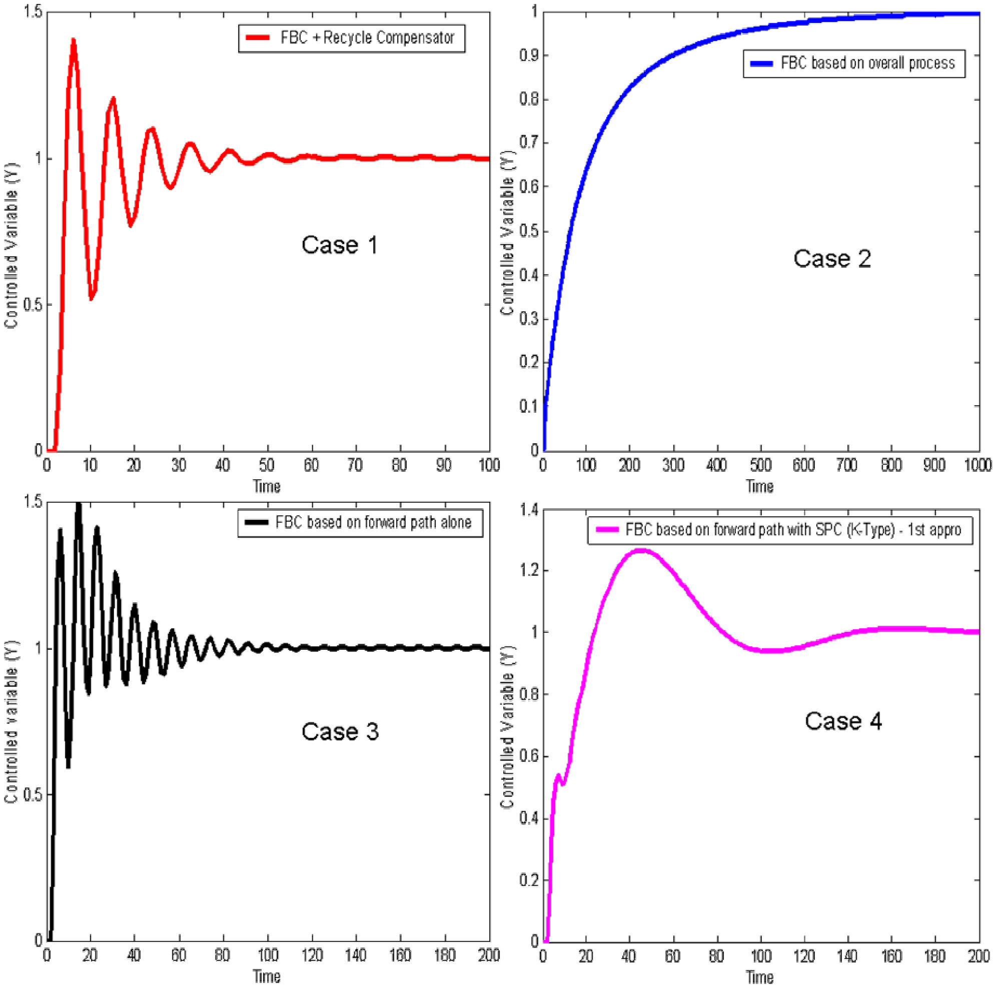


Figure 2.3.5 : Set point tracking for Example 2

The results of the simulations (set point tracking) are provided in Figure 2.3.5. The conventional recycle compensation scheme provides the best performance but is somewhat oscillatory. If the process is controlled by a feedback controller designed based on the overall model the response is very sluggish. When the process is controlled only with a feedback controller designed using forward path model (G_F) only, the performance is very oscillatory. The proposed scheme works well and provides a smooth approach to the new target value.

Example 3

Here, the forward path dynamics and recycle dynamics are given by $G_F = \frac{e^{-10s}}{10s+1}$ and $G_R = \frac{0.75e^{-28s}}{s+1}$ respectively. In contrast to Example 1, the recycle path has a larger time delay compared to the forward path. Four control strategies similar to that examined in Example 2 were considered. The results for the above case are summarized in Figures 2.3.6 and 2.3.7. In Figure 2.3.6, the set point tracking capability of the four different control schemes are provided. It is seen that the conventional recycle compensation works well followed by the predictive structure based approximate recycle compensation.

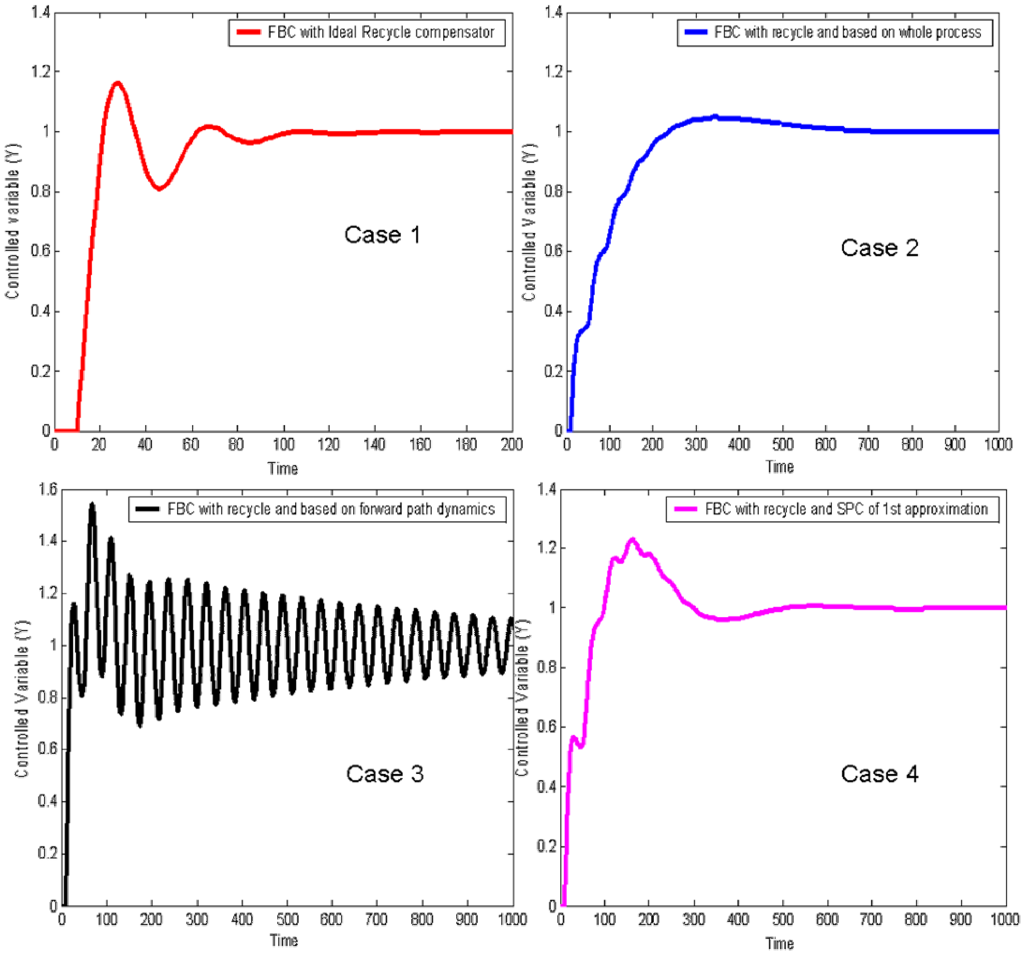


Figure 2.3.6 : Set point tracking for Example 3

This pattern is also seen with the disturbance rejection properties of the four schemes depicted in Figure 2.3.7. It is very obvious that if the feedback controller design ignores the presence of the recycle path dynamics, the performance can become quite oscillatory. This example again demonstrates that the approximate recycle compensator in a predictive framework can provide adequate regulation of a process with recycle.

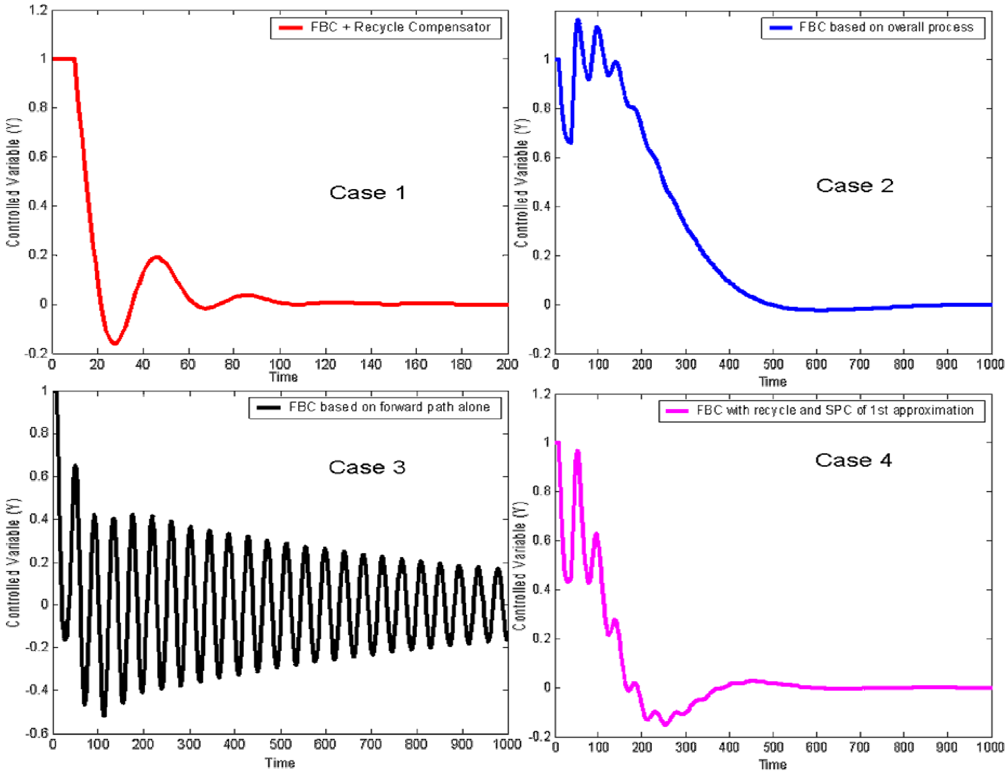


Figure 2.3.7 : Disturbance Rejection for Example 3

2.3.3 Remarks

Section 2.3 of this thesis has proposed and evaluated a recycle compensation scheme along the lines of the dead time compensator and the inverse response compensator. This new approximate recycle compensation scheme is implemented in a predictive control framework. The simulation case studies show that the scheme is workable. In comparison to the traditional recycle compensation scheme this method provides somewhat inferior performance. However, the ease of implementation of this scheme may far outweigh its sub-optimal performance and make it a useful alternative for compensating the detrimental effects of the recycle dynamics.

2.4 Recycle Effect Index

Consider a process with recycle for which the forward path and the recycle path models are available. Now the control engineer must quantify the strength of recycle and then decide if an advanced control structure such as the recycle compensator is necessary. If the recycle compensator is deemed important, then it can be implemented and a feedback controller can be designed for the compensated plant (i.e. forward path only). If the recycle is insignificant, then we may remove any consideration of it (the recycle path dynamics) in the design of the feedback controller. For such a recycle system considered above, we proposed a measure of the effect of the recycle using concepts from the minimum variance benchmarking of control loop performance. This measure termed as the *"recycle effect index"* (REI) can help decide about the control structure necessary for the process in question. The theoretical expressions for REI are outlined below and its practical applications are dealt in detail in Lakshminarayanan et al. (2003).

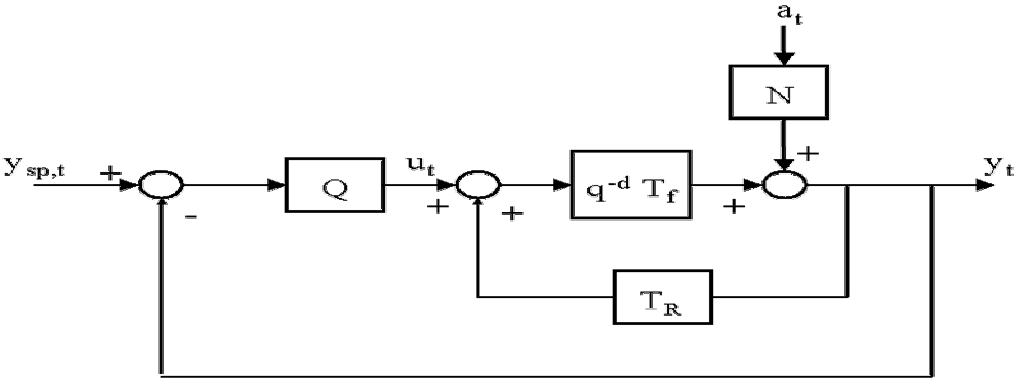


Figure 2.4.1 : Feedback Control System for the Process with Recycle

Consider the plant (under feedback control) shown in the Figure 2.4.1. When the set point is constant (zero in terms of deviation variables), we can derive the relationship

$$y_t = \frac{N}{1+q^{-d}T_f(Q-T_R)}a_t \qquad \textbf{Eqn – 2.4.1}$$

N can be expanded as $N = \Psi + q^{-d}\Omega$ **Eqn – 2.4.2**

Substituting this in the **Eqn – 2.4.1**, we get

$$y_t = \frac{\Psi + q^{-d}\Omega}{1+q^{-d}T_f(Q-T_R)}a_t = \frac{\Psi(1+q^{-d}T_f(Q-T_R)) + q^{-d}(\Omega - \Psi T_f(Q-T_R))}{1+q^{-d}T_f(Q-T_R)}a_t$$

$$= \Psi a_t + \frac{q^{-d}(\Omega - \Psi T_f Q + \Psi T_f T_R)}{1+q^{-d}T_f(Q-T_R)}a_t$$

Eqn – 2.4.3

The first part Ψa_t denotes the controller invariant term that is independent of the control law Q. The second part is dependent on the controller and can be manipulated by a proper choice of the controller Q.

If Q is designed as: $Q = T_R + \frac{\Omega}{\Psi T_f}$ **Eqn – 2.4.4**

the second term becomes identically zero and the lower bound on the output error variance can be achieved. Q is then the MVC for the overall (forward path + recycle path) process. When the MVC is designed based on the forward path model alone (by neglecting the recycle transfer function T_R) as: $Q = \frac{\Omega}{\Psi T_f}$ **Eqn – 2.4.5**

the expression for y_t becomes:

$$y_{t,MVFP} = \Psi a_t + \frac{q^{-d}\Psi T_f T_R}{(1+q^{-d}\frac{\Omega}{\Psi} - q^{-d}T_f T_R)}a_t \qquad \textbf{Eqn – 2.4.6}$$

(the subscript MVFP denotes that this output can be expected when we have a Minimum Variance controller based on the Forward Path only acting on a process with recycle). When T_R is zero, we will have the minimum variance performance as expected.

$$y_{t,MV} = \Psi a_t = \psi_0 a_t + \psi_1 a_{t-1} + \cdots + \psi_{d-1} a_{t-d+1} \qquad \textbf{Eqn – 2.4.7}$$

This gives $\sigma^2_{MV,NRC} = (\psi_0^2 + \psi_1^2 + \cdots + \psi_{d-1}^2)\, \sigma_a^2$.

The second term in the expression for $y_{t,MVFP}$ may be denoted as:

$$e_t = \left[\frac{\Psi T_f T_R}{(1 + q^{-d} \dfrac{\Omega}{\Psi} - q^{-d} T_f T_R)} \right] a_{t-d} = \left[\xi_0 + \xi_1 q^{-1} + \xi_2 q^{-2} + \cdots\cdots \right] a_{t-d} \qquad \textbf{Eqn – 2.4.8}$$

This implies that $\sigma_e^2 = [\xi_0^2 + \xi_1^2 + \xi_2^2 + \cdots\cdots]\, \sigma_a^2$.

Based on the expression for $y_{t,MVFP}$ we can write

$$\sigma^2_{MV,RC} = \sigma^2_{MV,NRC} + [\xi_0^2 + \xi_1^2 + \xi_2^2 + \cdots]\sigma_a^2 = [\psi_0^2 + \cdots + \psi_{d-1}^2 + \xi_0^2 + \xi_1^2 + \cdots]\sigma_a^2$$

Eqn – 2.4.9

where $\sigma^2_{MV,RC}$ is the minimum achievable output variance when a MVC is designed and implemented (by ignoring the recycle path in the process) on a process with recycle. Obviously, $\sigma^2_{MV,RC}$ is greater than or equal to $\sigma^2_{MV,NRC}$ which is the minimum output variance achievable for a process without recycle.

We are now ready to define the recycle effect index (ϕ) as:

$$\phi = 1 - \frac{\sigma^2_{MV,NRC}}{\sigma^2_{MV,RC}} = \frac{\xi_0^2 + \xi_1^2 + \xi_2^2 + \cdots\cdots}{\psi_0^2 + \psi_1^2 + \cdots + \psi_{d-1}^2 + \xi_0^2 + \xi_1^2 + \xi_2^2 + \cdots} \qquad \textbf{Eqn – 2.4.10}$$

The recycle effect index ϕ, therefore captures the inflation in variance that is caused by the recycle path element(s) if a MVC is designed and implemented based on the forward path dynamics alone. Note that the computation of ϕ requires knowledge of the forward path model, recycle path model and the disturbance model N. Also, since the value of ϕ depends on many factors, it would help if some simple-to-use guidelines were provided. When recycle effect index is close to 0, it means that the effect of the recycle is less and when it is close to 1 it implies that the effect of recycle is quite strong. The challenge is to determine the conditions under which the recycle effect index is under a certain threshold value (say $\phi < 0.25$) so that we may go about designing a MVC based on the forward path dynamics alone and not bother about advanced control structures such as the recycle compensator. One can refer to Madhukar et al. (2003) which provide such information via extensive simulations.

2.5 Conclusions

A new approximate recycle compensator in the lines of model predictive frame work was proposed and evaluated. The results show that the scheme is workable. In comparison to the ideal recycle compensation scheme this method provides somewhat inferior performance. However, the ease of implementation of this scheme may far outweigh its sub-optimal performance and make it a useful alternative for compensating the detrimental effects of recycles. One of the key conclusions emerging from the studies of REI (Recycle Effect Index) is that the PI controllers are capable of yielding high control performance in the presence of stationary disturbances over a wide range of parameters (gain, time constant and time delay) for the forward and recycle paths. However, the PI controller settings might depend both on the characteristics of both the forward and recycle paths. Correlations between optimal PI controller settings and the characteristics of the forward and recycle path models need to be developed for this scenario. If the disturbances are non-stationary, the PI controllers are not capable of providing high control performance even for low K_F K_R values and large ${}^{\tau_R}\!/_{\tau_F}$ values and PI feedback plus recycle compensator control strategy is likely to be of limited use.

CHAPTER 3

DYNAMICS OF DISTRIBUTED PARAMETER SYSTEMS WITH & WITHOUT RECYCLE

3.1 Introduction

The tubular reactor is a good example of a distributed parameter system. The control of tubular reactors, with or without catalytic beds is complicated due to non availability of online measurements of the controlled variables and the distributed nature of the problem. Further complexities are anticipated when there is either heat integration or material recycles. The primary goal of the control of tubular reactor is the regulation of the outlet concentration at optimum levels, while at the same time attention is paid to the maintenance of a safe operation, by requiring that the temperature in the reactor does not exceed some prespecified maximum value. The outlet concentration cannot be easily measured online, so it must be inferred from the available temperature measurements. Fluctuations in the inlet flow or concentration, coolant temperature, measurement noise and changes in the model parameters, such as kinetic constants (catalyst activity) and transport coefficients are some of the possible disturbances for the tubular reactor system.

From numerical simulation point of view, before one proceeds with the control studies of tubular reactors, there should be a good set of tools to provide the dynamic responses of such systems for any change in the inputs. So this chapter of the thesis is devoted to the description of the tools that have been developed in this regard. Firstly, a set of MATLAB codes have been developed - these yield both the temperature and concentration profiles inside the tubular reactors for any given set of input conditions. Next, this is extended to tubular reactors with recycle where an integration of SIMULINK models with the MATLAB codes has been used. This set of programs help in studying the effect of recycles.

3.2 Mathematical model of a Nonlinear Tubular reactor

The tubular reactor to be investigated is a homogeneous, non-adiabatic reactor in which a first order, irreversible, exothermic reaction occurs. The model of the reactor given by equations 3.2.1 to 3.2.5, represents either an empty reactor or a catalytic reactor assuming a pseudohomogeneous model with phenomenological reaction rates and transport properties. The reactant A enters the reactor with an initial concentration of C_{io} and an initial temperature of T_{io}. Axial diffusion of heat and mass are considered and radial gradients are neglected. Heat is extracted from the system through the wall by means of a coolant medium. Assuming the reactor wall temperature to be T_W, the equations governing the dynamic behavior of such reactors are,

$$\frac{\partial \overline{C}}{\partial t'} = D\frac{\partial^2 \overline{C}}{\partial z'^2} - v\frac{\partial \overline{C}}{\partial z'} - \overline{C}k\,exp\left(-\frac{E}{R\overline{T}}\right) \qquad \textbf{Eqn – 3.2.1}$$

$$\frac{\partial \overline{T}}{\partial t'} = \frac{k}{\rho C_P}\frac{\partial^2 \overline{T}}{\partial z'^2} - v\frac{\partial \overline{T}}{\partial z'} + \frac{-\Delta H}{\rho C_P}\overline{C}k\,exp\left(-\frac{E}{R\overline{T}}\right) + \frac{2h}{R\rho C_P}\left(\overline{T}_W - \overline{T}\right) \qquad \textbf{Eqn – 3.2.2}$$

valid for $0<z'<L$ and $t'>0$, with the boundary conditions,

$$-D\frac{\partial \overline{C}}{\partial z'} = v(\overline{C}_i - \overline{C}),\ z' = 0, t' \geq 0 \qquad \textbf{Eqn – 3.2.3}$$

$$-\frac{k}{\rho C_P}\frac{\partial \overline{T}}{\partial z'} = v(\overline{T}_i - \overline{T}),\ z' = 0, t' \geq 0 \qquad \textbf{Eqn – 3.2.4}$$

$$\frac{\partial \overline{C}}{\partial z^{|}} = 0, \frac{\partial \overline{T}}{\partial z^{|}} = 0, z^{|} = L, t^{|} \geq 0 \qquad \textbf{Eqn – 3.2.5}$$

The above set of equations has been considered by many researchers in the past. A more detailed analysis on the modeling aspect can be obtained from either of the following references: Alvarez et al. (1981), Georgakis et al. (1977), Varma and Amundson, (1972, 1973), McGowin and Perlmutter (1971) and Hlavacek and Hofmann (1970). To put the system in the dimensionless form, define the following dimensionless variables: $C = \frac{\overline{C}}{C_{ref}}, T = \frac{\overline{T}}{T_{ref}}, z = \frac{z^{|}}{L}, t = \frac{t^{|}D}{L^2}$

where C_{ref} and T_{ref} are reference values for concentration and temperature. Also, define the dimensionless parameters as follows:

$$Pe_m = \frac{Lv}{D}, Pe_h = \frac{Lv\rho C_P}{k}, \delta = \frac{E}{RT_{ref}}, \beta = \frac{-\Delta HC_{ref}}{\rho C_P T_{ref}}$$

$$\alpha = \frac{L^2 C_{ref}\ exp\left(\delta\left[1 - 1/T_{ref}\right]\right)}{DC_{ref}}, \gamma = \frac{2hL^2}{\rho C_P DR}$$

Eqns 3.2.1 - 3.2.5 can now be rewritten as follows:

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial z^2} - Pe_m \frac{\partial C}{\partial z} - \alpha C\, exp[\delta(1 - 1/T)] \qquad \textbf{Eqn – 3.2.6}$$

$$\frac{\partial T}{\partial t} = \frac{1}{Le}\frac{\partial^2 T}{\partial z^2} - Pe_h \frac{\partial T}{\partial z} + \alpha\beta C\, exp[\delta(1 - 1/T)] + \gamma(T_W - T) \qquad \textbf{Eqn – 3.2.7}$$

valid for 0<z<1 and t>0, with the boundary conditions,

$$\frac{\partial C}{\partial z} = Pe_m(C - C_i), z = 0, t \geq 0 \qquad \textbf{Eqn – 3.2.8}$$

$$\frac{\partial T}{\partial z} = Pe_h(T - T_i), z = 0, t \geq 0 \qquad \textbf{Eqn – 3.2.9}$$

$$\frac{\partial C}{\partial z} = 0, \frac{\partial T}{\partial z} = 0, z = 1, t \geq 0 \qquad \textbf{Eqn – 3.2.10}$$

The following set of parameter values were used in the simulations. These values are reported in Alvarez et al. (1981).

$$Le = 1, Pe_m = Pe_h = 5, \alpha = 0.875, \beta = 0.5, \delta = 25, T_W = 1, T_i = 1.05, C_i = 0.85, \gamma = 13$$

3.3 Numerical Solution Technique

The analytical solution of equations 3.2.6 to 3.2.10 is impossible. The equations must be solved numerically by discretization to obtain the approximate solution. The method of finite differences has been used extensively in the past, but it usually requires a large number of discretization points and results in a correspondingly large set of ordinary differential equations. On the other hand, the collocation technique approximates the solution by a polynomial trial function, and the resulting system often has a considerably smaller number of ordinary differential equations. This method has been modified and improved in recent years and successfully used in the solution of many chemical engineering problems (Finlayson, 1972). The orthogonal collocation technique is a special case of the method of weighted residuals and thus closely related to quadrature formulas. The essentials of the method as applied to the problem of interest have been outlined below.

The first and the foremost step of a collocation technique, is to choose the number of grid points or the collocation points (X_K). If these are chosen to be the roots of orthogonal jacobi polynomial of Nth degree then it is called orthogonal collocation. Any other orthogonal polynomial function can be used but the jacobi polynomials are popular and accurate. The choice of collocation points is very crucial and cannot be arbitrary. To reap the benefits of collocation technique fully, the collocation points has to chosen "optimally" or atleast "judiciously". Most of the finite domains can be expressed over the set [0, 1] and the orthogonality property can also be satisfied on this domain. Hence consider the jacobi polynomials on this domain.

The jacobi polynomial of degree N has the power series representation,

$$J_N^{(\alpha,\beta)}(x) = \sum_{i=0}^{N} (-1)^{N-i} \gamma_{N,i} x^i \qquad \textbf{Eqn – 3.3.1}$$

with $\gamma_{N,0} = 1$. Here, $\gamma_{N,i}$ are constant coefficients, and α and β are parameters characterizing the polynomials. $J_N^{(\alpha,\beta)}(x)$ is the polynomial orthogonal to the weighting function $x^{\beta}(1-x^{\alpha})$. The term $(-1)^{N-i}$ is introduced to ensure the coefficients γ are always positive. Utilizing the orthogonality property of the Jacobi polynomials we have,

$$\int_0^1 J_j^{(\alpha,\beta)}(x) J_N^{(\alpha,\beta)}(x) \left[x^{\beta}(1-x^{\alpha})\right] dx = 0 \qquad \textbf{Eqn – 3.3.2}$$

for j = 0, 1, 2… (N-1). Solving these N linear equations (equations 3.3.2) for N unknowns the following explicit solution is obtained for γ (Villadsen, 1970).

$$\gamma_{N,i} = \frac{N!}{i!(N-i)!} \frac{\Gamma(N+i+\alpha+\beta+1)\Gamma(\beta+1)}{\Gamma(N+\alpha+\beta+1)\Gamma(i+\beta+1)} \qquad \textbf{Eqn – 3.3.3}$$

The above equation provides the explicit solution but for the purpose of computation it is easier to evaluate the coefficients using the following recurrence formula,

$$\frac{\gamma_{N,i}}{\gamma_{N,i-1}} = \frac{N-i+1}{i} \cdot \frac{N+i+\alpha+\beta}{i+\beta} \qquad \textbf{Eqn – 3.3.4}$$

starting with $\gamma_{N,0} = 1$. Using the formula obtained above for the coefficients, we can evaluate the jacobi polynomial, with specified or known α and β. Once the jacobi polynomials are known then the roots of this polynomial equation $J_N(x) = 0$ are the collocation points within the domain from 0 to 1. A simple MATLAB function named, (getcollocationpoints1) was developed to obtain the collocation points between [0, 1] for any given values of α, β and N.

The jacobi polynomials are very useful in finding the collocation points. Now, for a given set of data points (x_1, y_1), (x_2, y_2). . . (x_N, y_N) and (x_{N+1},y_{N+1}), an interpolating polynomial passing through all the N+1 points is an N^{th} degree polynomial. Such an interpolating polynomial is expressed as

$$y_N(x) = \sum_{i=1}^{N+1} y_i l_i(x) \qquad \textbf{Eqn – 3.3.5}$$

where $y_N(x)$ is the N^{th} degree polynomial, y_i is the value of i at the point x_i, and $l_i(x)$ is called the lagrange interpolating polynomial. The building blocks for the interpolating polynomial are given as,

$$l_i(x) = \prod_{\substack{j=1 \\ j \neq i}}^{N+1} \frac{(x - x_j)}{(x_i - x_j)} \qquad \textbf{Eqn – 3.3.6}$$

The jacobi and lagrange polynomials developed helps one to proceed with the development of orthogonal collocation method. The lagrange polynomial obtained above is continuous and can be differentiated as well as integrated. The first and second derivatives of the lagrange interpolation polynomial are given by

$$\frac{dy_N(x)}{dx} = \sum_{i=1}^{N+1} y_i \frac{dl_i(x)}{dx} \qquad \textbf{Eqn - 3.3.7}$$

$$\frac{d^2 y_N(x)}{dx^2} = \sum_{i=1}^{N+1} y_i \frac{d^2 l_i(x)}{dx^2} \qquad \textbf{Eqn – 3.3.8}$$

In particular, if one is interested in obtaining the first and second derivatives at the interpolation points, one can substitute x = x_i. In a compact vector notation we have,

$$y_N^{|} = \left[\frac{dy_N(x_1)}{dx}, \frac{dy_N(x_2)}{dx}, \ldots, \frac{dy_N(x_N)}{dx}, \frac{dy_N(x_{N+1})}{dx} \right]^T \qquad \textbf{Eqn – 3.3.9}$$

$$y_N^{||} = \left[\frac{d^2 y_N(x_1)}{dx^2}, \frac{d^2 y_N(x_2)}{dx^2}, \ldots, \frac{d^2 y_N(x_N)}{dx^2}, \frac{d^2 y_N(x_{N+1})}{dx^2} \right]^T \quad \textbf{Eqn – 3.3.10}$$

The function vector is defined as values of y at the N+1 collocation points as $y = [\, y_1, y_2, y_3, \ldots., y_N, y_{N+1} \,]^T$. With these definitions of vectors y and its derivative vectors, equations 3.3.9 and 3.3.10 can now be written as

$y^{|} = A \bullet y$ and $y^{||} = B \bullet y$ where A and B matrices are defined as

$$A = \left\{ a_{ij} = \frac{dl_j(x_i)}{dx} ; i, j = 1,2,3,\ldots, N, N+1 \right\}$$

$$B = \left\{ b_{ij} = \frac{d^2 l_j(x_i)}{dx^2} ; i, j = 1,2,3,\ldots, N, N+1 \right\}$$

The matrices A and B are $(\mathrm{N}+1)\times(\mathrm{N}+1)$ square matrices. Once the N+1 interpolation points are obtained as described previously, all the lagrange building blocks are completely known and thus A and B matrices are also known. For computational purposes, a_{ij} and b_{ij} are calculated from

$$a_{ij} = \frac{dl_j(x_i)}{dx} = \begin{cases} \dfrac{1}{2} \dfrac{p_{N+1}^{(2)}(x_i)}{p_{N+1}^{(1)}(x_i)} ; j = i \\ \dfrac{1}{(x_i - x_j)} \dfrac{p_{N+1}^{(1)}(x_i)}{p_{N+1}^{(1)}(x_j)} ; i \neq j \end{cases} \quad \textbf{Eqn – 3.3.11}$$

$$b_{ij} = \frac{d^2 l_j(x_i)}{dx^2} = \begin{cases} \dfrac{1}{3} \dfrac{p_{N+1}^{(3)}(x_i)}{p_{N+1}^{(1)}(x_i)} ; j = i \\ 2a_{ij} \left[a_{ii} - \dfrac{1}{(x_i - x_j)} \right] ; i \neq j \end{cases} \quad \textbf{Eqn – 3.3.12}$$

where the $p_{N+1}^{(1)}$, $p_{N+1}^{(2)}$ and $p_{N+1}^{(3)}$ are calculated from the following recurrence formula

$$\mathrm{p}_0(\mathrm{x}) = 1,\ \mathrm{p}_\mathrm{j}(\mathrm{x}) = (\mathrm{x} - \mathrm{x}_\mathrm{j})\mathrm{p}_{\mathrm{j-1}}(\mathrm{x});\ p_j^{(1)}(x) = (x - x_j) p_{j-1}^{(1)}(x) + p_{j-1}(x);$$

$$p_j^{(2)}(x) = (x - x_j) p_{j-1}^{(2)}(x) + 2 p_{j-1}^{(1)}(x);\ p_j^{(3)}(x) = (x - x_j) p_{j-1}^{(3)}(x) + 3 p_{j-1}^{(2)}(x);$$

for j = 1, 2,...., N+1. With $p_0^{(1)}(x) = p_0^{(2)}(x) = p_0^{(3)}(x) = 0$

With the availability of both "A" and "B" matrices, the first and second derivatives can be substituted as $\left[\frac{dy}{dx}\right]_i = \sum_{j=1}^{N+1} A_{ij} y_j$ and $\left[\frac{d^2 y}{dx^2}\right]_i = \sum_{j=1}^{N+1} B_{ij} y_j$ where y_j is the unknown value of y at the interpolation point x_j. Now that the N+1 interpolation points are chosen, the matrices A and B are completely known. Extending this technique to the system considered in section 3.2 (tubular reactor), we have both temperature and concentration as the unknown values at the collocation points. So substitute $\left[\frac{dC}{dz}\right]_i = \sum_{j=1}^{N+2} A_{i,j} C^j$ and $\left[\frac{d^2 C}{dz^2}\right]_i = \sum_{j=1}^{N+2} B_{i,j} C^j$ for the unknown concentrations C^j and $\left[\frac{dT}{dz}\right]_i = \sum_{j=1}^{N+2} A_{i,j} T^j$ and $\left[\frac{d^2 T}{dz^2}\right]_i = \sum_{j=1}^{N+2} B_{i,j} T^j$ for the unknown temperatures T^j in both the boundary conditions as well as in the partial differential equations 3.2.6 to 3.2.10.

From the boundary conditions we get the boundary points in terms of other internal collocation points. For example we have

temperature (T^1) at $z = 0$ as: $$T^1 = \frac{\left[\dfrac{Pe_h * T_i + \sum_{j=2}^{N+1} A_{1,j} T^j}{Pe_h - A_{1,1}} - \dfrac{\left[A_{1,N+2} \sum_{j=2}^{N+1} A_{N+2,j} T^j\right]}{\left[Pe_h - A_{1,1}\right] A_{N+2,N+2}}\right]}{\left[1 + \dfrac{A_{1,N+2} A_{N+2,1}}{A_{N+2,N+2}\left[Pe_h - A_{1,1}\right]}\right]}$$

concentration (C^1) at $z = 0$ as: $$C^1 = \frac{\left[\dfrac{\left[Pe_m * C_i + \sum_{j=2}^{N+2} A_{1,j} C^j\right]}{\left[Pe_m - A_{1,1}\right]} - \dfrac{\left[A_{1,N+2} \sum_{j=2}^{N+1} A_{N+2,j} C^j\right]}{\left[Pe_m - A_{1,1}\right] A_{N+2,N+2}}\right]}{\left[1 + \dfrac{A_{1,N+2} A_{N+2,1}}{A_{N+2,N+2}\left[Pe_m - A_{1,1}\right]}\right]}.$$

The temperature (T^{N+2}) and concentration (C^{N+2}) at $z = 1$ are given by:

$$T^{N+2} = \frac{-\left[\dfrac{Pe_h * T_i * A_{N+2,1}}{A_{N+2,N+2}\left[Pe_h - A_{1,1}\right]} + \dfrac{A_{N+2,1}\sum\limits_{j=2}^{N+1} A_{1,j}T^j}{A_{N+2,N+2}\left[Pe_h - A_{1,1}\right]} + \dfrac{\sum\limits_{j=2}^{N+1} A_{N+2,j}T^j}{A_{N+2,N+2}}\right]}{\left[\left[1 + \dfrac{A_{1,N+2}A_{N+2,1}}{A_{N+2,N+2}\left[Pe_h - A_{1,1}\right]}\right]\right]}$$ and

$$C^{N+2} = \frac{-\left[\dfrac{Pe_m * C_i * A_{N+2,1}}{A_{N+2,N+2}\left[Pe_m - A_{1,1}\right]} + \dfrac{A_{N+2,1}\sum\limits_{j=2}^{N+1} A_{1,j}C^j}{A_{N+2,N+2}\left[Pe_m - A_{1,1}\right]} + \dfrac{\sum\limits_{j=2}^{N+1} A_{N+2,j}C^j}{A_{N+2,N+2}}\right]}{\left[\left[1 + \dfrac{A_{1,N+2}A_{N+2,1}}{A_{N+2,N+2}\left[Pe_m - A_{1,1}\right]}\right]\right]}$$

Similarly, from the partial differential equations, we have:

$$\left[\frac{dC}{dt}\right]_i = \sum_{j=1}^{N+2} B_{i,j}C^j - Pe_m \sum_{j=1}^{N+2} A_{i,j}C^j - \alpha C^i \, exp[\, \delta(1 - 1/T^i)]$$

$$\left[\frac{dT}{dt}\right]_i = \frac{1}{Le}\sum_{j=1}^{N+2} B_{i,j}T^j - Pe_h \sum_{j=1}^{N+2} A_{i,j}T^j + \alpha\beta C^i \, exp[\delta(1 - 1/T^i)] + \gamma(T_W - T^i)$$

for i = 2 to N+1. As the boundary points z = 0 and z = 1 are already known to be in terms of internal grid points. The above N ordinary differential equations in N unknowns is a set of coupled nonlinear ordinary differential equation system which can be solved in MATLAB using ODE solvers if one can have a good initial guess to these set of equations. At steady state the above equations reduces to this form:

$$\sum_{j=1}^{N+2} B_{i,j}C^j - Pe_m \sum_{j=1}^{N+2} A_{i,j}C^j - \alpha C^i \, exp[\, \delta(1 - 1/T^i)] = 0$$

$$\frac{1}{Le}\sum_{j=1}^{N+2} B_{i,j}T^j - Pe_h \sum_{j=1}^{N+2} A_{i,j}T^j + \alpha\beta C^i \, exp[\, \delta(1 - 1/T^i)] + \gamma(T_W - T^i) = 0$$

These equations represent a set of coupled nonlinear algebraic equations which can be solved by the well known technique of Newton Raphson method. Once the solution to these equations are obtained, this solution can be used as a good initial guess for solving the coupled nonlinear ordinary differential equations by MATLAB ODE solvers which makes use of the well known Runge-Kutta method. A series of MATLAB codes (main program along with many functions) were developed which upon execution would give the dynamic response of such a distributed parameter system. Furthermore, the above set of equations approximates accurately the distributed model (3.2.6 to 3.2.10) when N (number of collocation points) is large enough. The accuracy increases with increasing N, but so does the computational effort. Therefore, the family of orthogonal polynomials and the value of N should be properly chosen (a good N value is 40 but 20 is also acceptable) so that the computational effort is minimized while the accuracy remains very good.

3.4 Results and Discussions

Let us consider the steady state and dynamic behavior of the reactor resulting when the above mentioned parameter values of Alvarez et al. (1981) are used.

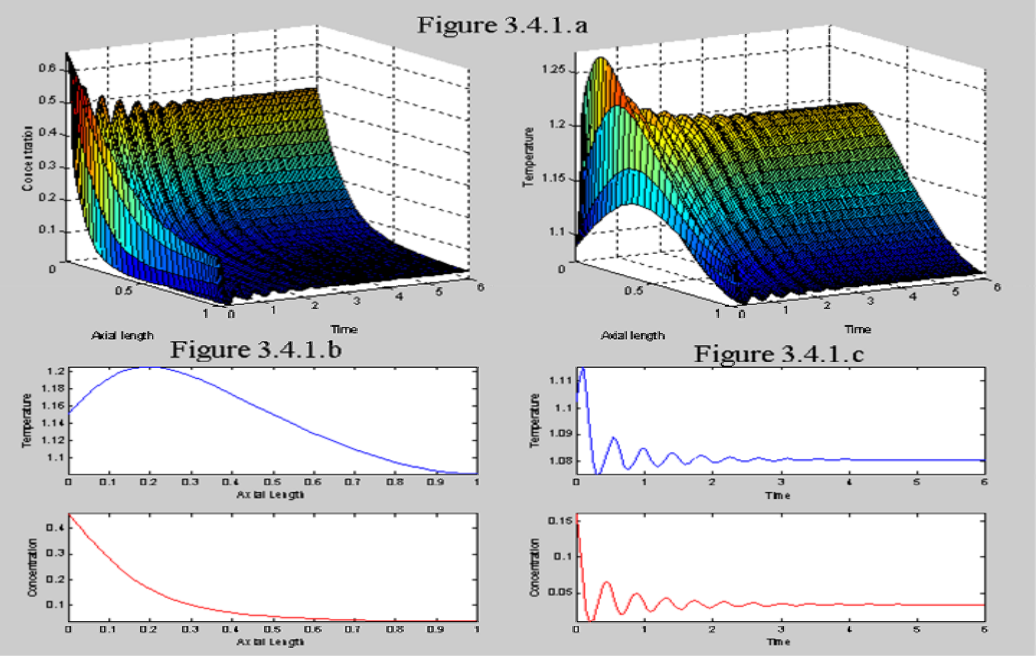


Figure 3.4.1: Dynamic and Steady State Temperature and Concentration Profiles

Figure 3.4.1 represents some of these results. The top 3D plots (Figure 3.4.1.a) describe the concentration and temperature profiles inside the reactor at various times. The bottom two plots indicate the steady state profiles. The left (Figure 3.4.1.b) shows the temperature and concentration profile along the length of the reactor at fixed time, and the right (Figure 3.4.1.c) shows profile at different times at fixed axial length.

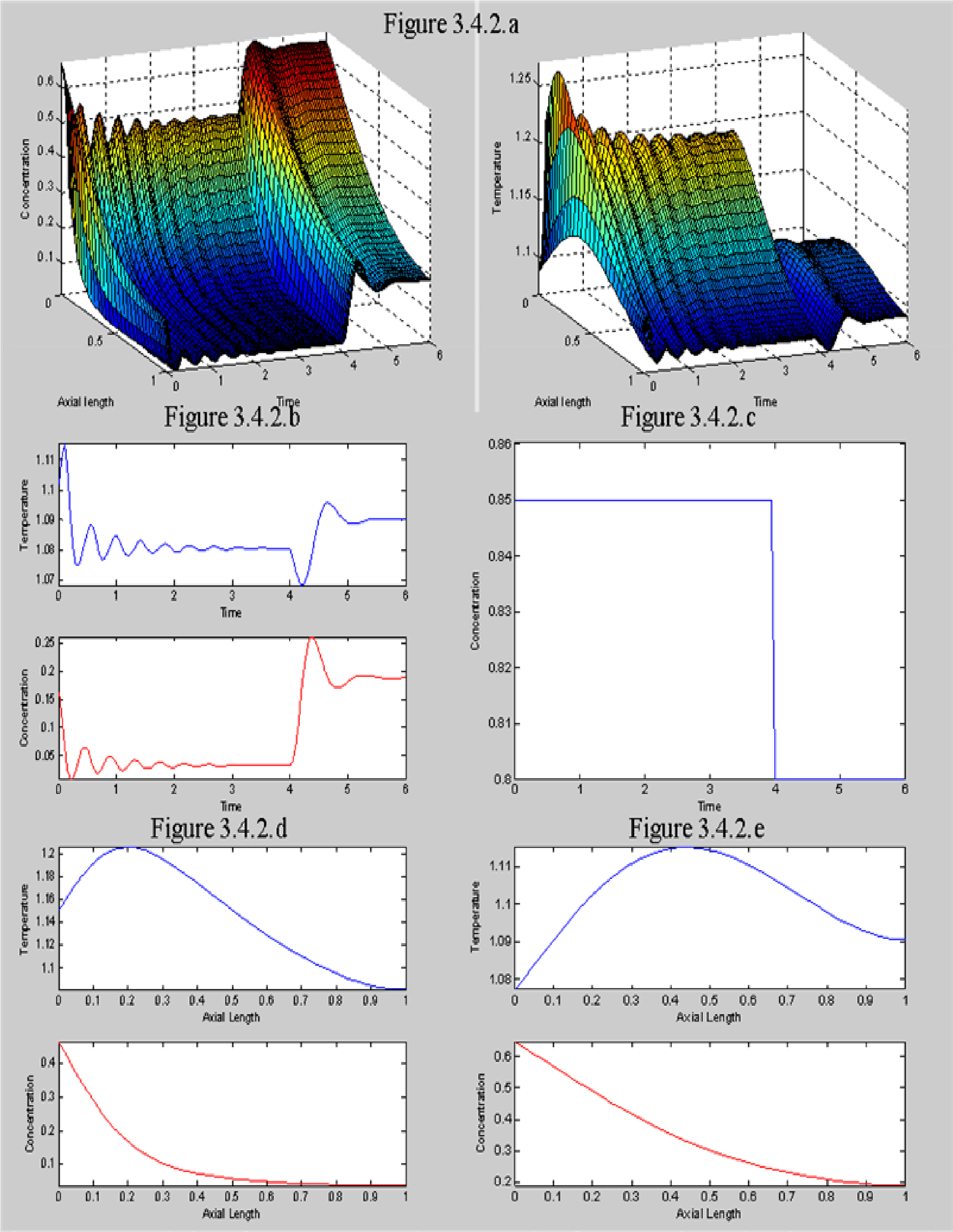


Figure 3.4.2: Variation of Temperature and Concentration for a step change in Inlet Concentration

Figure 3.4.2 depicts the variation of temperature and concentration inside the reactor for a step change in inlet concentration introduced at time t = 4. This figure consists of six subplots; the top two 3D plots (Figure 3.4.2.a) indicate the dynamic profiles of temperature and concentration. The middle plot consists of a left plot and right plot. The left plot (Figure 3.4.2.b) shows the temperature and concentration at the exit of the reactor at different times. The right plot (Figure 3.4.2.c) shows the variation of inlet concentration with time. The bottom plots (Figure 3.4.2.d and Figure 3.4.2.e) show the steady state temperature and concentration profiles before and after the step change in inlet concentration at times equal to 3.5 and 5.5 time units respectively.

Consider that during the operation of the reactor the parameter α (the domain parameter associated with the kinetics rate constant) is decreased suddenly from the initial value of 0.875 to the new value of 0.8. It should be noted that for catalytic tubular reactors, the parameter alpha (α) reflects the catalyst activity during the operation of the reactor. The new temperature and concentration profiles are shown in Figure 3.4.3. It shows the variation of temperature and concentration inside the reactor for a step change in catalyst activity. This figure consists of six subplots; the top two 3D plots (Figures 3.4.3.a) indicate the dynamic profiles of temperature and concentration at different lengths in the reactor. The middle part consists of a left plot and right plot. The left plot (Figure 3.4.3.b) shows the temperature and concentration at the exit of the reactor at different times. The right plot (Figure 3.4.3.c) shows the variation of catalyst activity with time. The bottom plots (Figure 3.4.3.d and Figure 3.4.3.e) show the steady state temperature and concentration profiles before and after the step change in catalyst activity. If we notice this figure carefully, then we find that due to the change in catalyst activity the temperature along the reactor is reduced, the conversion decreases and the hotspot moves towards the middle of the reactor. This study would help one to understand the dynamics inside the reactor and maintain the operating conditions accordingly.

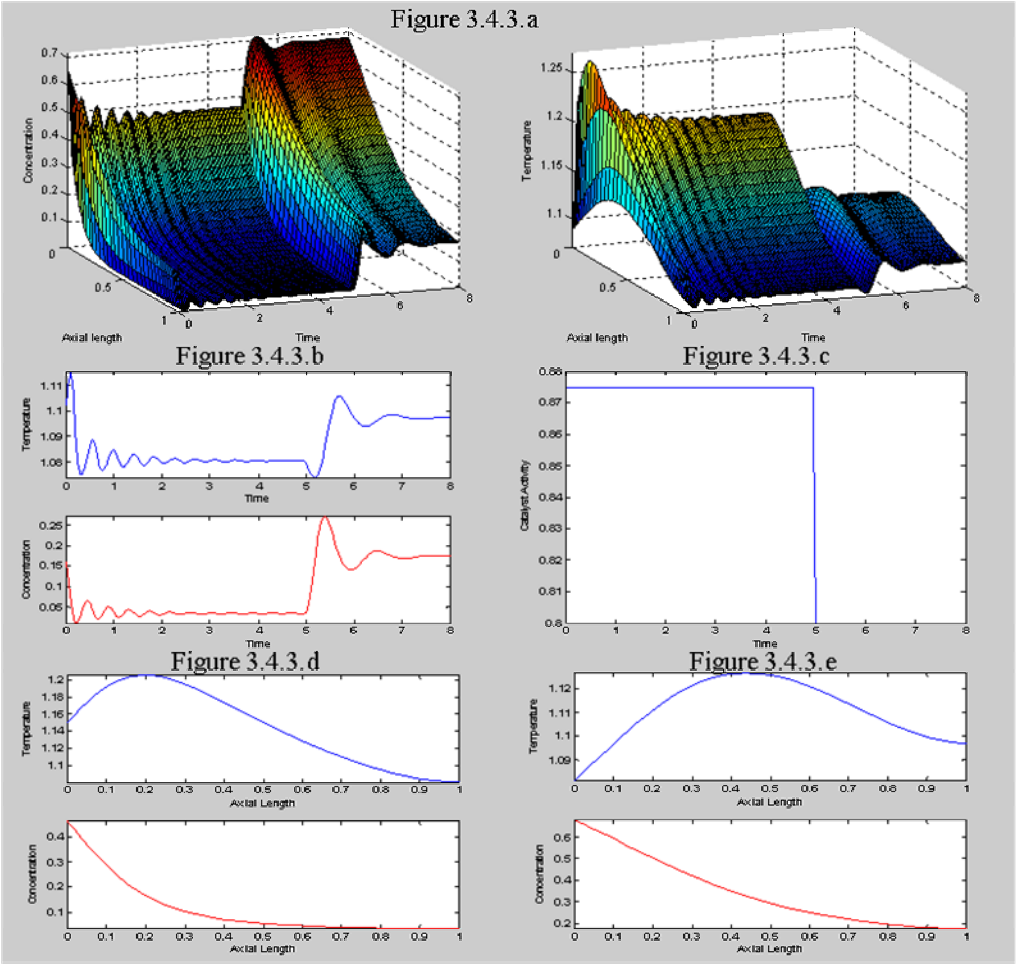


Figure 3.4.3.a

Figure 3.4.3.b

Figure 3.4.3.c

Figure 3.4.3.d

Figure 3.4.3.e

Figure 3.4.3 : Variation of Temperature and Concentration for a step change in catalyst activity

3.5 Mathematical model of a Nonlinear Tubular reactor with recycle

Tubular reactor with recycle is an exemplar of distributed parameter systems with recycle. The control of such systems is complex due to complicated dynamics exhibited not only due to distributed nature of the problem but also due to positive feedback acting on the system (recycles). The primary goal of the control studies is the regulation of the outlet concentration at optimum levels, while at the same time attention is paid to the maintenance of a safe operation, by requiring that the temperature in the reactor do not exceed some prespecified maximum value. As stated in the previous section, one should have a good dynamic profile generator before venturing into control studies. So in this section we integrated some of the earlier developed MATLAB codes with SIMULINK models to yield the temperature and concentration profiles inside the tubular reactors for a given set of input conditions and at different recycle ratios and recycle dynamics.

The mathematical model chosen is similar to that of earlier with minor modifications:

$$\frac{\partial \overline{C}}{\partial t^{|}} = D\frac{\partial^2 \overline{C}}{\partial z^{|2}} - v\frac{\partial \overline{C}}{\partial z^{|}} - \overline{C}k\,exp\left(-\frac{E}{R\overline{T}}\right) \qquad \textbf{Eqn – 3.5.1}$$

$$\frac{\partial \overline{T}}{\partial t^{|}} = \frac{k}{\rho C_P}\frac{\partial^2 \overline{T}}{\partial z^{|2}} - v\frac{\partial \overline{T}}{\partial z^{|}} + \frac{-\Delta H}{\rho C_P}\overline{C}k\,exp\left(-\frac{E}{R\overline{T}}\right) + \frac{hA_S}{\rho C_P}\left(\overline{T}_W - \overline{T}\right) \qquad \textbf{Eqn – 3.5.2}$$

valid for $0 < z^{|} < L$ and $t^{|} > 0$, with the boundary conditions,

$$\frac{\partial \overline{C}}{\partial z^{|}} = \frac{v}{D}\left(\overline{C} - \overline{C}_i^*\right), z^{|} = 0, t^{|} \geq 0 \qquad \textbf{Eqn – 3.5.3}$$

$$\frac{\partial \overline{T}}{\partial z^{|}} = \frac{v\rho C_P}{k}(\overline{T} - \overline{T}_i^*), z^{|} = 0, t^{|} \geq 0 \qquad \textbf{Eqn – 3.5.4}$$

where $\overline{C}_i^* = (1-r)*\overline{C}_i + r*\overline{C}_r$ and $\overline{T}_i^* = (1-r)*\overline{T}_i + r*\overline{T}_r$

in which $\overline{C}_r$ and $\overline{T}_r$ are the concentration and temperature values obtained after the reactor exit stream passes through the recycle path and enters the mixer. The variable r is the recycle ratio. $\frac{\partial \overline{C}}{\partial z^{|}} = 0, \frac{\partial \overline{T}}{\partial z^{|}} = 0, z^{|} = L, t^{|} \geq 0$ **Eqn – 3.5.5**

The above set of equations has been considered early by Antoniades and Christofides (2001). Dimensionalize the above equations using these dimensionless variables:

$$C = \frac{\overline{C} - C_{ref}}{C_{ref}}, T = \frac{\overline{T} - T_{ref}}{T_{ref}}, C_i = \frac{\overline{C}_i - C_{ref}}{C_{ref}}, T_i = \frac{\overline{T}_i - T_{ref}}{T_{ref}}, C_r = \frac{\overline{C}_r - C_{ref}}{C_{ref}},$$

$$T_r = \frac{\overline{T}_r - T_{ref}}{T_{ref}}, T_W = \frac{\overline{T}_W - T_{ref}}{T_{ref}}, z = \frac{z^{|}}{L}, t = \frac{t^{|} v}{L}, Pe_h = \frac{\rho C_P v L}{k}, Pe_m = \frac{vL}{D}$$

$$Le = \frac{k}{\rho C_P D}, \beta_T = \frac{h A_s L}{\rho C_P v}, \gamma = \frac{E}{R T_{ref}}, B_T = \frac{-(\Delta H) C_{ref}}{\rho C_P T_{ref}}, B_c = \frac{k\, exp\left(- E / R T_{ref}\right) L}{v}$$

where C_{ref} and T_{ref} are reference values for concentration and temperature.

Eqns 3.5.1 - 3.5.5 can be rewritten as follows:

$$\frac{\partial C}{\partial t} = \frac{1}{Pe_m} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - B_C\, exp\left(\frac{\gamma T}{1 + T} \right)(1 + C) \qquad \textbf{Eqn – 3.5.6}$$

$$\frac{\partial T}{\partial t} = \frac{1}{Le * Pe_h} \frac{\partial^2 T}{\partial z^2} - \frac{\partial T}{\partial z} + B_T B_C\, exp\left(\frac{\gamma T}{1 + T} \right)(1 + C) + \beta_T (T_W - T) \qquad \textbf{Eqn – 3.5.7}$$

valid for $0 < z < 1$ and $t > 0$, with the boundary conditions,

$$\frac{\partial C}{\partial z} = Pe_m (C - C_i^*), z = 0, t \geq 0 \qquad \textbf{Eqn – 3.5.8}$$

$$\frac{\partial T}{\partial z} = Pe_h (T - T_i^*), z = 0, t \geq 0 \qquad \textbf{Eqn – 3.5.9}$$

$$\frac{\partial C}{\partial z} = 0, \frac{\partial T}{\partial z} = 0, z = 1, t \geq 0 \qquad \textbf{Eqn – 3.5.10}$$

where Le is Lewis Number, Pe is Peclet Number, $C_i^* = (1 - r) * C_i + r * C_r$ and $T_i^* = (1 - r) * T_i + r * T_r$ in which C_r and T_r are the concentration and temperature values obtained after the reactor exit stream passes through the recycle path element and enters the mixer. The variable r denotes the recycle ratio. The following parameter values (Antoniades and Christofides, 2001) are used to characterize the steady state of this system: $Le = 1, Pe_m = Pe_h = 7, B_C = 0.1, \beta_T = 2$

$B_T = 2.5, T_W = -0.0048, T_i = 0.036, C_i = -0.001, \gamma = 10$

3.6 Solution Methodology, Results and Discussions

SIMULINK models integrated with MATLAB codes (written earlier to perform the operation of orthogonal collocation) were used to solve this problem. A sample SIMULINK model is shown below (Figure 3.6.1):

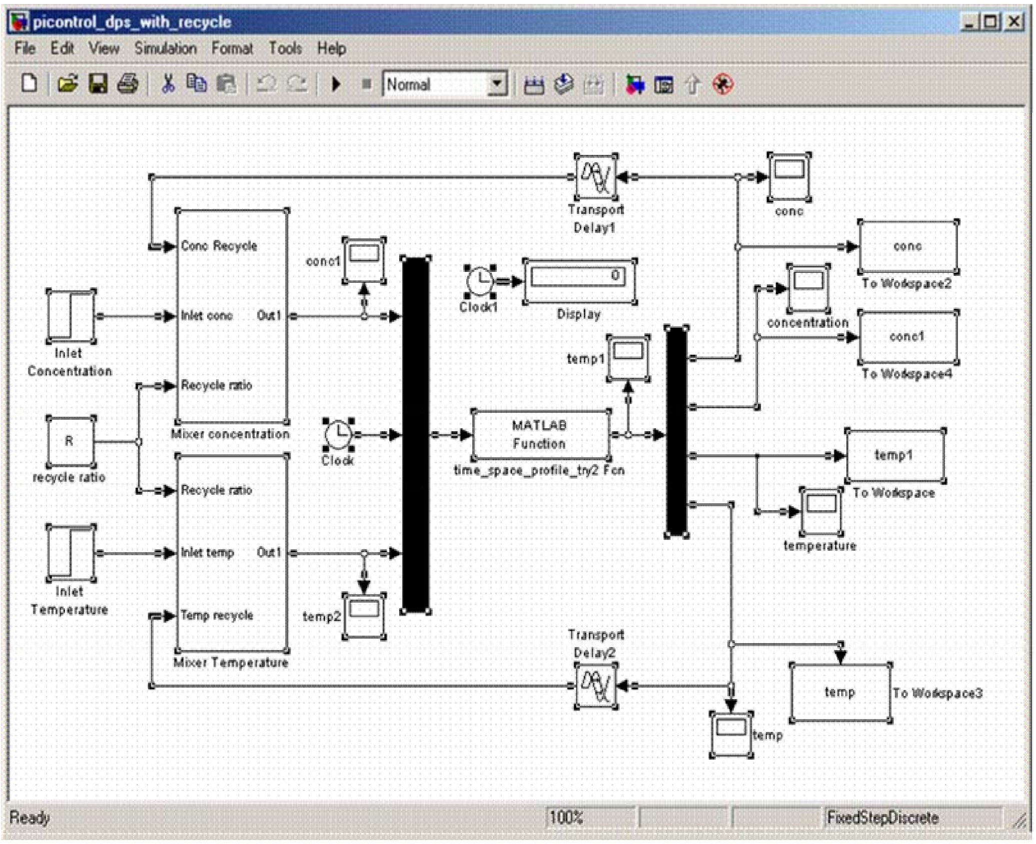


Figure 3.6.1: SIMULINK model consisting of Tubular reactor with FOPDT recycle dynamics

Figure 3.6.1 represents a SIMULINK block diagram of a tubular reactor with recycle. The block named "Tubular Reactor" is a MATLAB function which uses an earlier coded mfile to obtain the dynamic temperature and concentration profiles. The inputs to this system are inlet temperature, inlet concentration, simulation time and Peclet number. The outputs from this program are the exit concentration and exit temperature of the reactor, the concentration and temperature at a particular length in the reactor (in this case it is at a dimensionless distance of 0.5 in the reactor).

A FOPDT (first order plus dead time) recycle dynamics is introduced into the system by passing the outputs from the tubular reactor (both temperature and concentration) through FOPDT transfer function block and sending it to the mixer. Inside the mixer both the fresh stream and the recycle stream are mixed in a proper mass balance ratio and sent into the reactor, depending upon the choice of "r" (recycle ratio) value chosen by the user. Below is the graph (Figure 3.6.2) showing the effect of recycle ratio on the behavior of the tubular reactor with recycle.

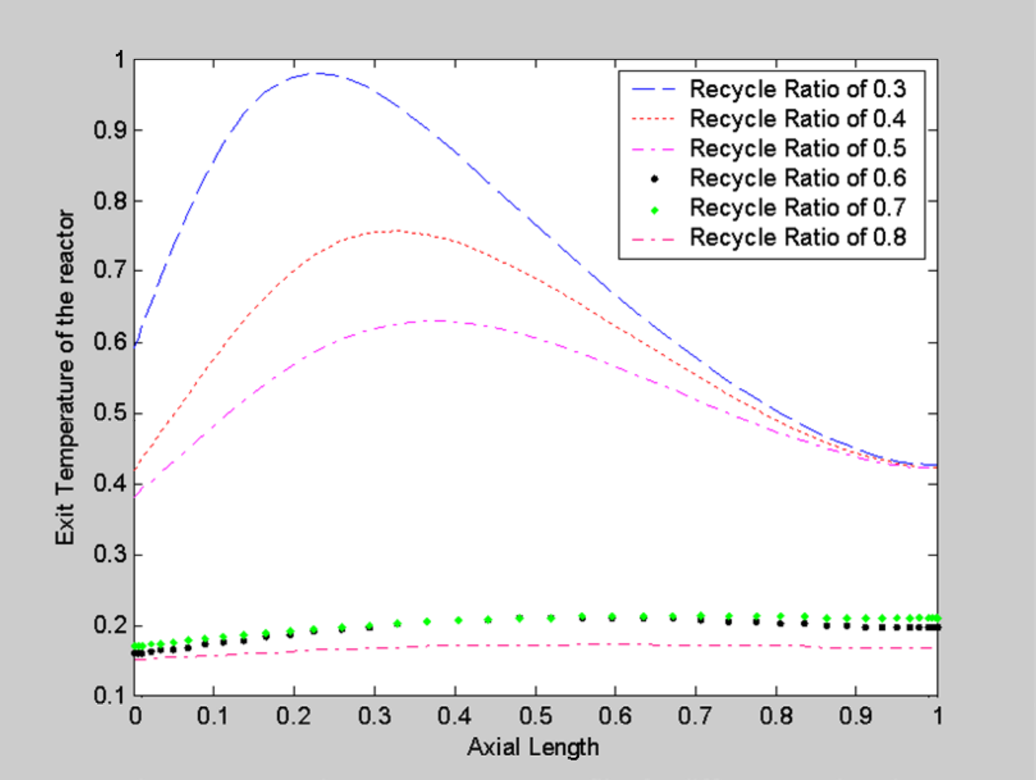


Figure 3.6.2: Steady State Temperature profiles for different recycle ratios

Our study is focused on the effect of recycle on the open-loop dynamics and on the behavior of the closed-loop system. For the open-loop system, we have (r = 0). This system possesses a unique globally asymptotically stable spatially non-uniform steady state, this has been verified numerically through extensive simulations of the open-loop system for different initial conditions. Figure 3.6.2 (solid line) shows the steady state profile of exit temperature, without any recycle. One can observe that the hotspots occur close to the entrance of the reactor. Subsequently recycles of different magnitude were introduced into the system; the flow rate of the fresh feed to the system is reduced depending upon the recycle flow rate so that the total flow rate remains constant. Figure 3.6.2 shows the steady state profile of exit temperature for various recycle ratios, (r = 0.3 – dashed line, r = 0.4 – dotted line, r = 0.5 – dashed-dotted line, r = 0.6 - ◊, r = 0.7 - ● and r = 0.8 - ►). As the recycle ratio increases, the amount of the fresh feed entering the reactor decreases and thus the temperature of the hotspot inside the reactor decreases and the location of the hotspots moves towards the centre of the reactor. But one drawback of introducing recycles is that the stable steady state of the open-loop process gets closer to the instability limit. In particular, when the recycle ratio is equal to 0.39, the spatially non-uniform steady state becomes unstable and a globally asymptotically stable periodic (limit cycle) spatially non-uniform state appears.

Figure 3.6.3 shows limit cycle behavior in the reactor. It consists of 2 sub plots, one Figure 3.6.3.a showing the limit cycle behavior at a distance of 0.4 inside the reactor and the other Figure 3.6.3.b showing the limit cycle behavior at the exit of the reactor.

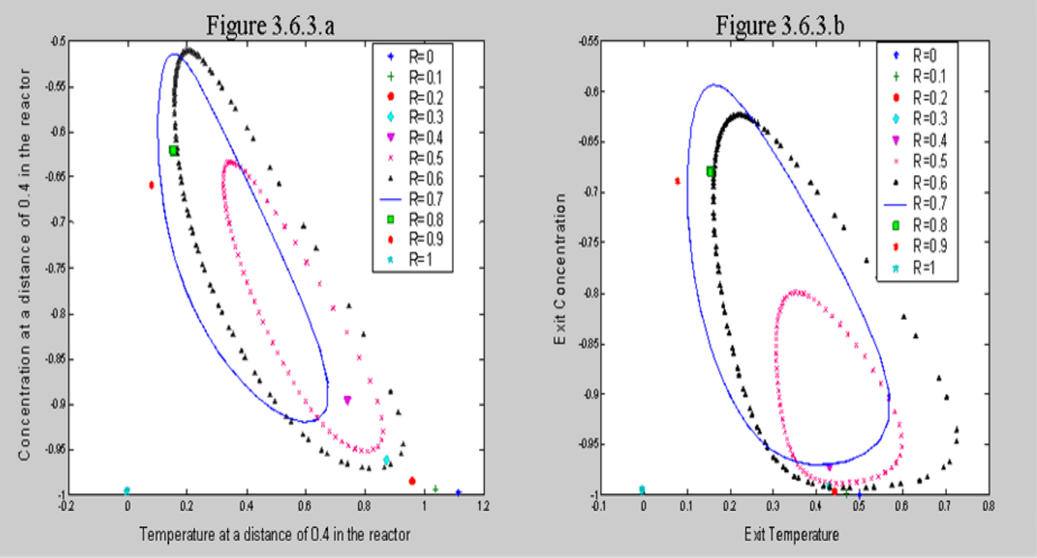


Figure 3.6.3.a

Figure 3.6.3.b

Figure 3.6.3: Limit cycles in the reactor for R=0-1 in steps of 0.1, Td=0.1, N=40

From the Figure 3.6.3.a and Figure 3.6.3.b it is very clear that, when recycle ratio is greater than 0.4 and less than 0.8 the reactor moves to the periodic spatially non-uniform steady state or exhibits limit cycle behavior.

3.7 Mathematical model of a Linear Tubular reactor

In this section, we consider an isothermal tubular reactor with one reactant and simple linear reaction kinetics. This example will be used in future sections to show the potential application of modal decomposition on distributed parameter system leading to lumped parameter models usable for controller design. A Modal feedforward / feedback controller is designed in the new modal space for this system to handle measured disturbances anticipated in the inlet concentration by manipulating the recycle ratio. This is discussed in the last section of this thesis.

The linear parabolic partial differential equation representing a reaction with a single reactant C_A occurring in a tubular reactor with axial dispersion and first order kinetics is:

$$\frac{\partial C_A\left(z^{\prime},t^{\prime}\right)}{\partial t^{\prime}} = -\nu \frac{\partial C_A\left(z^{\prime},t^{\prime}\right)}{\partial z^{\prime}} + D_r \frac{\partial^2 C_A\left(z^{\prime},t^{\prime}\right)}{\partial z^{\prime 2}} - k_r C_A\left(z^{\prime},t^{\prime}\right) \qquad \textbf{Eqn – 3.7.1}$$

with initial condition: $C_A\left(z^{\prime},0\right) = C_{A1}(z^{\prime})$, where $\mathbf{C_A}$ is the reactant concentration inside the tubular reactor, $\mathbf{z}^{\prime}$ - spatial position (m), $\mathbf{t}^{\prime}$ **-** time scale (s), $\boldsymbol{\nu}$ **-** superficial axial fluid velocity (m/s), $\mathbf{k_r}$ - kinetic rate constant (1/s), $\mathbf{D_r}$ – diffusivity and **L** - length of the reactor (m). This partial differential equation is subjected to the following Danckwerts boundary conditions:

$$D_r \frac{\partial C_A\left(0,t^{\prime}\right)}{\partial z^{\prime}} = \upsilon\left(C_A\left(0,t^{\prime}\right) - C_{A,in}\left(t^{\prime}\right)\right) \text{ and } \frac{\partial C_A\left(L,t^{\prime}\right)}{\partial z^{\prime}} = 0 \qquad \textbf{Eqn – 3.7.2}$$

The above set of equations has been considered by Brown (2001).

The above systems of equations are made dimensionless using the following definitions: $z = \frac{z^{|}}{L}, t = \frac{t^{|}\upsilon}{L}, x = \frac{C_A}{C_{A0}}, x_{in} = \frac{C_{A,in}}{C_{A0}}, Pe = \frac{\upsilon L}{D_r} = 1, B = \frac{k_r L}{\upsilon} = 1.14$

where **C_{A0}** is some reference reactant concentration. The new sets of equations are,

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) \qquad \textbf{Eqn – 3.7.3}$$

with initial condition: $x(z,0) = x_1(z)$, where **x** is the reactant concentration inside the tubular reactor. The boundary conditions becomes,

$$\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x_{in}(t)\right) \text{ and } \frac{\partial x(1,t)}{\partial z} = 0 \qquad \textbf{Eqn – 3.7.4}$$

The parameter values for Pe and B given above (used by Brown, 2001) were used to establish the steady state for this system.

3.8 Solution Methodology, Results and Discussion

The orthogonal collocation technique was used to obtain the solution for the above problem. Firstly, the collocation points are chosen to be the roots of the orthogonal jacobi polynomials as described in section 3.3. Now obtain the A and B matrices such that they satisfy $A = \left\{ a_{ij} = \frac{dl_j(x_i)}{dx}; i, j = 1,2,..., N, N+1 \right\}$ and $B = \left\{ b_{ij} = \frac{d^2 l_j(x_i)}{dx^2}; i, j = 1,2,..., N, N+1 \right\}$. With the availability of both "A" and "B" matrices the first and second derivatives can be substituted as $\left[\frac{dy}{dx}\right]_i = \sum_{j=1}^{N+1} A_{ij} y_j$ and $\left[\frac{d^2 y}{dx^2}\right]_i = \sum_{j=1}^{N+1} B_{ij} y_j$ where y_j is the unknown value of y at the interpolation point x_j. Now that the N+1 interpolation points are chosen, the matrices

A and B are completely known. With the unknown concentration value at the collocation points, substitute $\left[\frac{dx}{dz}\right]_i = \sum_{j=1}^{N+2} A_{i,j}x^j$ and $\left[\frac{d^2x}{dz^2}\right]_i = \sum_{j=1}^{N+2} B_{i,j}x^j$ for the unknown concentrations x^j in both the boundary conditions, as well as in the partial differential equations 3.7.3 to 3.7.4. From the boundary conditions, we get the boundary points in terms of other internal collocation points.

For example, the concentration (x^1) at $z = 0$ is given by:

$$x^1 = \frac{\left[\frac{\left[Pe * x_i + \sum_{j=2}^{N+2} A_{1,j}x^j\right]}{\left[Pe - A_{1,1}\right]} - \frac{\left[A_{1,N+2}\sum_{j=2}^{N+1} A_{N+2,j}x^j\right]}{\left[Pe - A_{1,1}\right]A_{N+2,N+2}}\right]}{\left[1 + \frac{A_{1,N+2}A_{N+2,1}}{A_{N+2,N+2}\left[Pe - A_{1,1}\right]}\right]}.$$

The concentration (x^{N+2}) at $z = 1$ is given by:

$$x^{N+2} = \frac{-\left[\frac{Pe * x_i * A_{N+2,1}}{A_{N+2,N+2}\left[Pe - A_{1,1}\right]} + \frac{A_{N+2,1}\sum_{j=2}^{N+1} A_{1,j}x^j}{A_{N+2,N+2}\left[Pe - A_{1,1}\right]} + \frac{\sum_{j=2}^{N+1} A_{N+2,j}x^j}{A_{N+2,N+2}}\right]}{\left[\left[1 + \frac{A_{1,N+2}A_{N+2,1}}{A_{N+2,N+2}\left[Pe - A_{1,1}\right]}\right]\right]}$$

Similarly from the partial differential equation we have:

$$\left[\frac{dx}{dt}\right]_i = \frac{1}{Pe}\sum_{j=1}^{N+2} B_{i,j}x^j - \sum_{j=1}^{N+2} A_{i,j}x^j - Bx^i \qquad \text{for}\left(i = 2,\ldots, N+1\right).$$

As the boundary points z = 0 and z = 1 are already known to be in terms of internal grid points. The above N ordinary differential equations in N unknowns is a set of coupled nonlinear ordinary differential equations which can be solved in MATLAB using any of the ODE solvers, if one has a good initial guess to these set of equations. A good initial guess can be obtained by considering the steady state conditions of the above ordinary differential equations.

At steady state, the above equation reduces to this form:

$$\frac{1}{Pe}\sum_{j=1}^{N+2} B_{i,j}C^{j} - \sum_{j=1}^{N+2} A_{i,j}C^{j} - BC^{i} = 0\,.$$

These equations represent a set of coupled linear algebraic equations which can be solved very easily. Once the solution to these equations are obtained then this solution can be used as initial guess for solving the coupled linear ordinary differential equations using MATLAB ODE solvers (which implements the well known Runge-Kutta methods). MATLAB codes (main program with many sub functions) were developed which upon execution would give the dynamic response of the reactor.

Furthermore, the above set of equations approximates accurately the distributed model (3.7.3 to 3.7.4) when N (the number of collocation points) becomes large enough. The accuracy increases with increasing N, but so does the computational effort. So the family of orthogonal polynomials and the value of N should be properly chosen in a manner that the computational effort is minimized while the accuracy remains very good. In this work, N=40 provides high level of accuracy, but a value of 20 also works well. Figure 3.8.1.a shows the 3D unforced concentration profile in a tubular reactor.

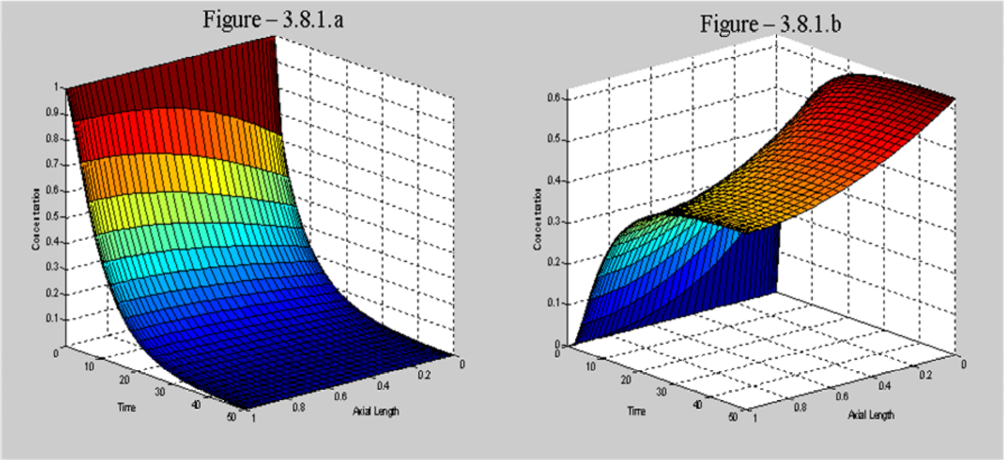


Figure 3.8.1: Unforced and Forced Concentration Profiles for a Linear Tubular reactor by Orthogonal Collocation

In this case we have the initial guess for the concentration variable to be equal to one throughout the length of the reactor and the inlet concentration to the reactor is assumed to be zero. Similarly Figure 3.8.1.b shows the 3D forced concentration profile inside the reactor. Here the initial guess is equal to zero and the inlet concentration is assumed to be equal to one.

3.9 Linear Tubular reactor with recycle

The modeling of the tubular reactor with recycle is quite similar to what we saw earlier but with a slight change in the boundary condition. The governing equation remains same (**Eqn – 3.7.3** is equal to **Eqn – 3.9.1**) but the boundary conditions change as follows: $\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x^*_{in}(t)\right)$ and $\frac{\partial x(1,t)}{\partial z} = 0$ **Eqn – 3.9.2**

where $x^*_{in}(t) = (1-R) * x_{in}(t) + R * x_r(t)$ and $\mathbf{x_r}$ is the reactant concentration in the recycle loop (at the entrance point of the reactor), $\mathbf{x_{in}}$ is the fresh feed inlet concentration entering the reactor and **R** is the recycle ratio.

A similar solution methodology mentioned in the earlier sections (about orthogonal collocation) is used to obtain the results for this case also. SIMULINK models integrated with MATLAB codes as hinted earlier were developed. The parameter values used are also the same as used in the previous section as mentioned by Brown (2001). Firstly, the steady state equations (which are a set of algebraic equations) are solved and then later this solution is used as an initial guess to solve the system of ODE's by using any of the MATLAB ODE solvers like ODE45, ODE15s, ODE23s etc which makes use of Runge-Kutta method to provide the numerical solution.

Figure 3.9.1 shows the forced concentration profile for linear tubular reactor with recycle. One can see the characteristic kinks produced by the recycle. A simple first order dynamics was considered for the recycle with a dead time of significant magnitude (approximately 10% of the total simulation time) and a recycle ratio value of 0.2 was used to simulate the process results of which are shown in Figure 3.9.1.

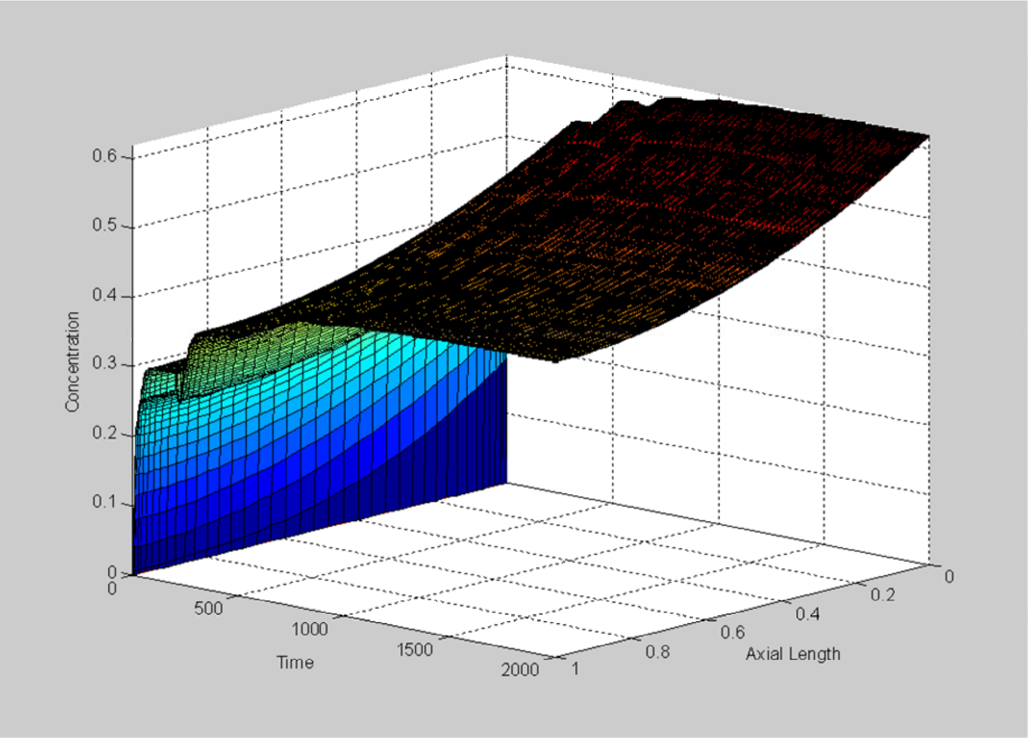


Figure 3.9.1: Forced concentration profile for a linear tubular reactor with recycle by orthogonal collocation

3.10 Mathematical model of a Linear Heat exchanger

Here we consider a simple linear tubular heat exchanger with single-pass on both shell side and tube side. The liquid stream enters the tube of the heat exchanger and is heated by convection from the inner wall. Heat is supplied to the tube by means of condensing steam in the jacket. Some of the assumptions made in deriving the mathematical model (Hahn et al., 1971) are, System parameters are constant and uniform with respect to time. Axial heat diffusion and mixing are significant for the tube side stream. Steam temperature is a function of time only and heat capacity of the tube is finite. Tube-side temperature and velocity are constant with respect to radial distance. Axial heat conduction in the tube is negligible. Outer shell effects are neglected. Based on these assumptions, an energy balance over a differential section of the tube side of the exchanger yields:

$$\frac{\partial T_l}{\partial \tau} = D\frac{\partial^2 T_l}{\partial l^2} - \upsilon\frac{\partial T_l}{\partial l} + \frac{h_{wl}P_l}{C_{pl}\rho_l A_l}\left(T_w - T_l\right) \qquad \textbf{Eqn – 3.10.1}$$

Taking an energy balance over a differential section of wall gives:

$$\frac{\partial T_w}{\partial \tau} = \frac{h_{ws}P_s}{C_{pw}\rho_w A_w}\left(T_s - T_w\right) + \frac{h_{wl}P_l}{C_{pw}\rho_w A_w}\left(T_l - T_w\right) \qquad \textbf{Eqn – 3.10.2}$$

subject to following boundary conditions:

$$\frac{\partial T_l(0,\tau)}{\partial l} = \frac{\upsilon}{D}\left(T_l(0,\tau) - T_l^f(\tau)\right)\text{and}\frac{\partial T_l(L,\tau)}{\partial l} = 0 \qquad \textbf{Eqn – 3.10.3}$$

The above equations are dimensionalized by introducing these parameters,

Mean residence time: $\tau_r = L/\upsilon$ sec, Axial Peclet Number: $\beta = \upsilon L/D$, Dimensionless time: $t = \tau/\tau_r$, Dimensionless axial distance: $x = l/L$, Dimensionless liquid temperature: $u_1 = T_l/T_r$, Dimensionless wall temperature: $u_2 = T_w/T_r$, Dimensionless steam temperature: $\theta = T_s/T_r$, The other parameters are:

$$\frac{1}{\tau_1} = \frac{h_{wl}P_l}{C_{pl}\rho_l A_l}sec^{-1}, \frac{1}{\tau_{21}} = \frac{h_{wl}P_l}{C_{pw}\rho_w A_w}sec^{-1}, \frac{1}{\tau_{22}} = \frac{h_{ws}P_s}{C_{pw}\rho_w A_w}sec^{-1}.$$

Hence the system of equations with boundary conditions is:

$$\frac{\partial u_1}{\partial t} = \frac{1}{\beta}\frac{\partial^2 u_1}{\partial x^2} - \frac{\partial u_1}{\partial x} + \frac{\tau_r}{\tau_1}\left(u_2 - u_1\right) \qquad \textbf{Eqn – 3.10.4}$$

$$\frac{\partial u_2}{\partial t} = \frac{\tau_r}{\tau_{22}}\left(\theta - u_2\right) + \frac{\tau_r}{\tau_{21}}\left(u_1 - u_2\right) \qquad \textbf{Eqn – 3.10.5}$$

subjected to: $$\frac{\partial u_1(0,t)}{\partial x} = \beta\left(u_1(0,t) - u_1^f(t)\right) \ \& \ \frac{\partial u_1(1,t)}{\partial x} = 0 \qquad \textbf{Eqn – 3.10.6}$$

The numerical values used in this study are as follows:

$\beta = 1, \tau_r = 3\,sec, \tau_1 = 3.69\,sec, \tau_{21} = 2.65\,sec, \tau_{22} = 1.05\,sec, u_1^f = 0.53, \theta = 0.795$.

We now apply the orthogonal collocation technique to the above system by substituting the first and the second derivative as follows:

$$\left[\frac{du_1}{dx}\right]_i = \sum_{j=1}^{N+1} A_{ij} u_1^j \ , \ \left[\frac{d^2 u_1}{dx^2}\right]_i = \sum_{j=1}^{N+1} B_{ij} u_1^j$$

With these substitutions the equations 3.10.4 and 3.10.5 change as follows:

$$\frac{du_1^i}{dt} = \frac{1}{\beta}\sum_{j=1}^{N+2} B_{ij} u_1^j - \sum_{j=1}^{N+2} A_{ij} u_1^j + \frac{\tau_r}{\tau_1}\left(u_2^i - u_1^i\right) \qquad \textbf{Eqn – 3.10.6}$$

$$\frac{du_2^i}{dt} = \frac{\tau_r}{\tau_{22}}\left(\theta - u_2^i\right) + \frac{\tau_r}{\tau_{21}}\left(u_1^i - u_2^i\right) \qquad \textbf{Eqn – 3.10.7}$$

$$u_1^1 = \frac{\left[\dfrac{\beta * u_1^i + \sum_{j=2}^{N+1} A_{1,j} u_1^j}{\beta - A_{1,1}} - \dfrac{\left[A_{1,N+2}\sum_{j=2}^{N+1} A_{N+2,j} u_1^j\right]}{\left[Pe_h - A_{1,1}\right] A_{N+2,N+2}}\right]}{\left[1 + \dfrac{A_{1,N+2} A_{N+2,1}}{A_{N+2,N+2}\left[\beta - A_{1,1}\right]}\right]} \qquad \textbf{Eqn – 3.10.8}$$

$$u_1^{N+2} = \frac{-\left[\dfrac{\beta * u_1^i * A_{N+2,1}}{A_{N+2,N+2}\left[\beta - A_{1,1}\right]} + \dfrac{A_{N+2,1}\sum_{j=2}^{N+1} A_{1,j} u_1^j}{A_{N+2,N+2}\left[\beta - A_{1,1}\right]} + \dfrac{\sum_{j=2}^{N+1} A_{N+2,j} u_1^j}{A_{N+2,N+2}}\right]}{\left[1 + \dfrac{A_{1,N+2} A_{N+2,1}}{A_{N+2,N+2}\left[\beta - A_{1,1}\right]}\right]} \qquad \textbf{Eqn – 3.10.9}$$

The above system of equations with these boundary conditions are first solved for the steady state solution and later used as the initial guess for the dynamic solution.

3.11 Results and Discussions

The Figure 3.11.1.a and 3.11.1.b consist of dynamic profiles for tube side fluid temperature and wall side fluid temperature.

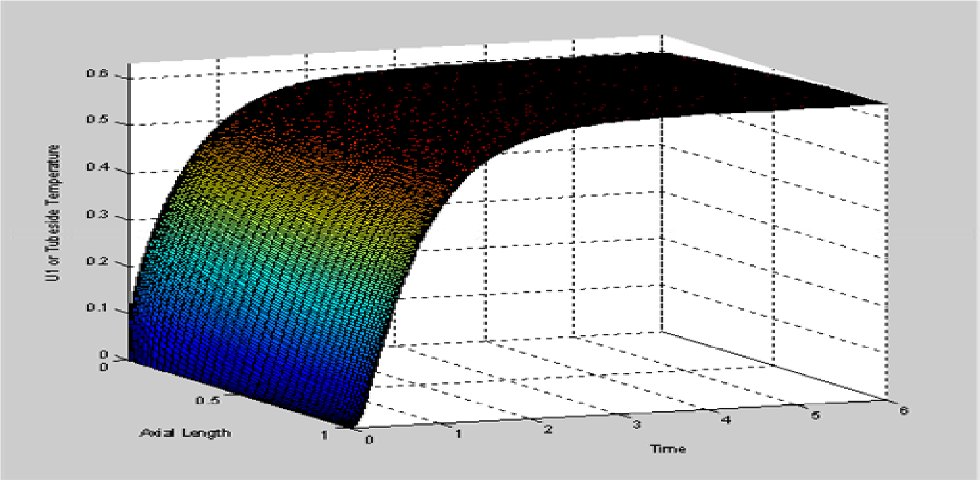


Figure 3.11.1.a : Dynamic profiles for tube side temperature

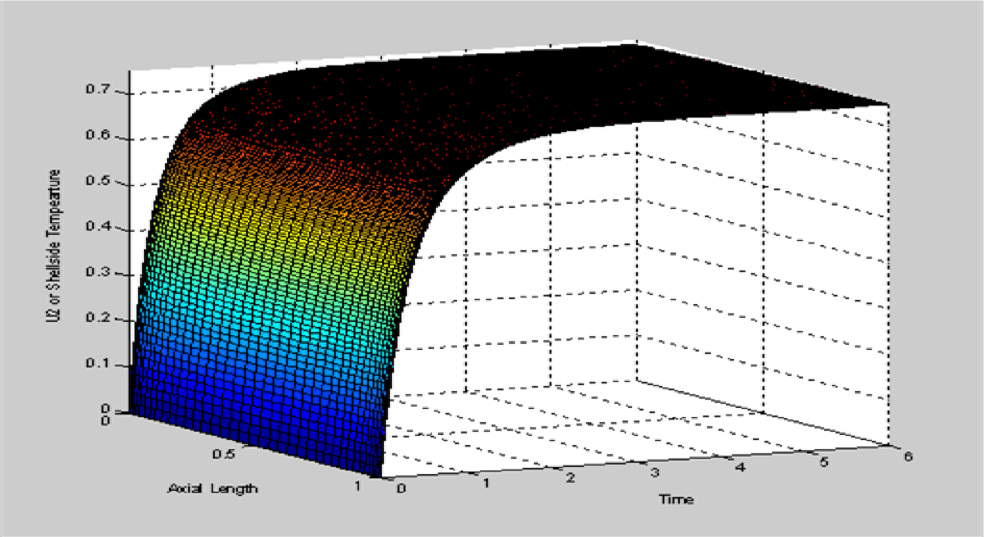


Figure 3.11.1.b : Dynamic profiles for shell side temperature

The Figure 3.11.1.c and 3.11.1.d show the steady state tube side temperature and wall side temperature along the length of the reactor. Figure 3.11.2 shows the exit temperature profiles of the tube side fluid at different times and at different (β - Peclet number) values. It emphasizes on the effect of Axial Peclet number on the exit tube side fluid temperature.

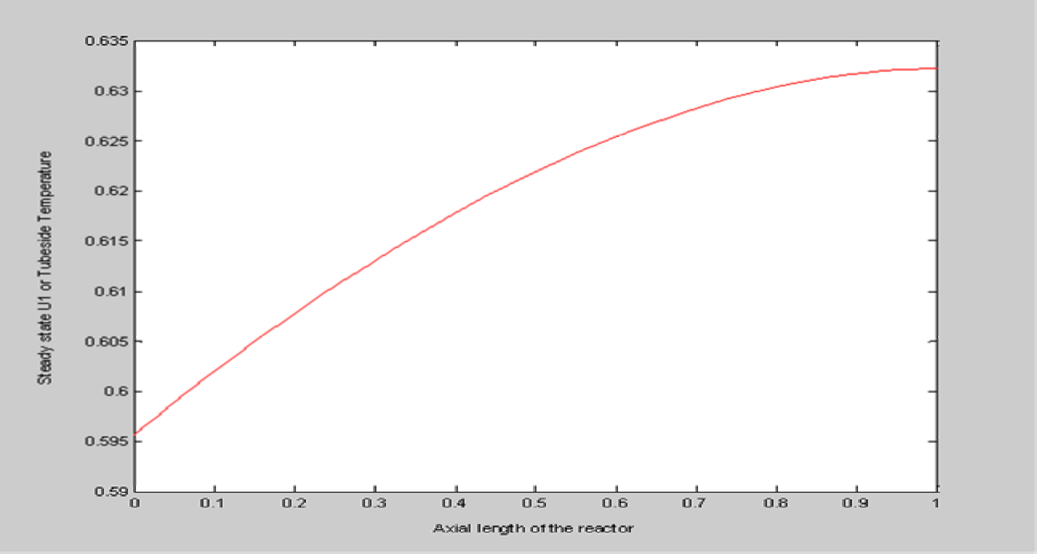


Figure 3.11.1.c : Steady state tube side temperature

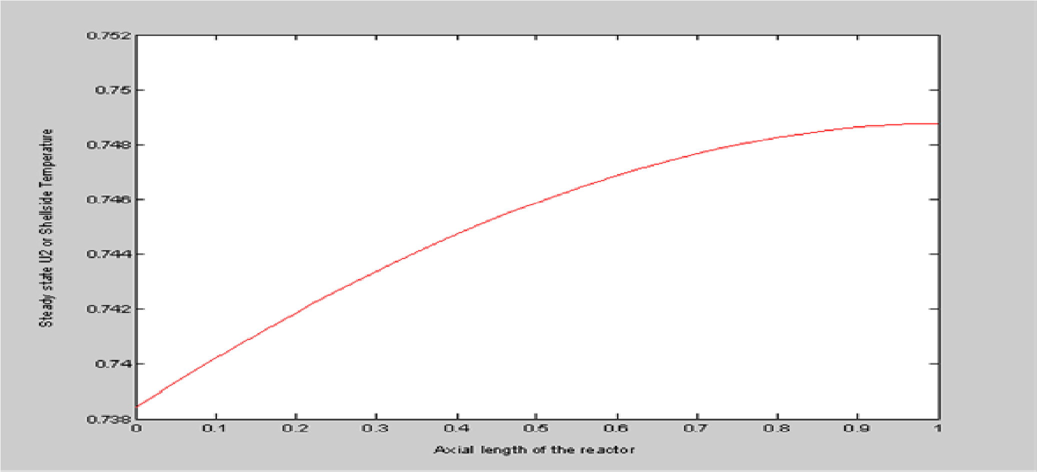


Figure 3.11.1.d: Steady state shell side temperature

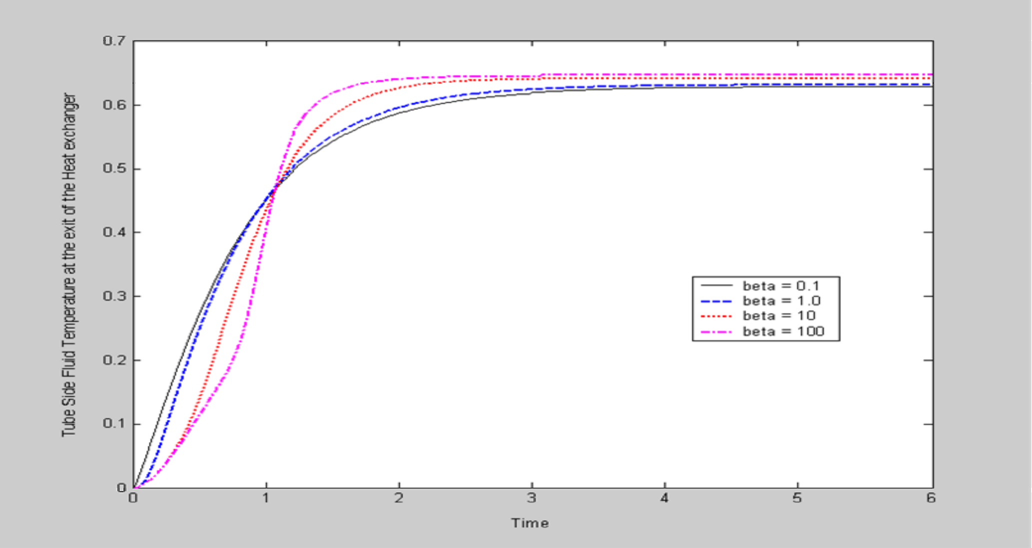


Figure 3.11.2: Variation of exit tube side fluid temperature with time for different beta values

One can observe that the exit tube side fluid temperature reaches steady state quickly as the Peclet number value increases. At low Peclet numbers the exit tube side fluid temperature exhibit a sluggish response.

3.12 Conclusion and future directions

In addition to the tubular reactors whose dynamics was studied here, study was also done on other examples of tubular reactors considered by Hlavacek and Hofmann (1970) and McGowin and Perlmutter (1970). Most of the results quoted by these researchers in their paper were replicated using some of the tools developed as part of this research. The illustration of the orthogonal collocation technique (in section 3.2), one of the weighted residuals techniques, on the linear and nonlinear tubular reactor, can also be extended to other physical systems like the heat exchangers which are described by parabolic partial differential equations as shown in sections 3.10 and 3.11. Thus, the orthogonal collocation technique provides best approximate solution to most of the physical systems considered and its accuracy is comparable to Galerkin method (another weighted residuals technique) and also finite difference approximation. This is evident by some of the accurate results obtained using a minimal set of collocation points. The orthogonal collocation was chosen to deal with the above problems due to its expediency in handling parabolic partial differential equations and also for the ease in programming. Because of this attribute, collocation method has found wide applications in chemical engineering and other branches of engineering. The future direction would be to use this technique to simulate the dynamic responses of these physical systems for changes in different input variables and this would help us to study various control strategies developed for these systems.

CHAPTER 4

MODAL ANALYSIS OF DISTRIBUTED PARAMETER SYSTEMS

4.1 Introduction

This chapter is concerned with the exposition of a novel approach to the dynamic analysis and design of control systems for very complex processes. This method not only serves as controller tuning guidelines but also can serve as a systematic guide for selecting the control system structure or configuration. The approach is based on the idea that the dynamic behavior of a system can be represented by the motion of a point in an n-dimensional space (state space) which leads to a mathematical model in the form of n first-order differential equations. The ideas presented in this chapter are largely due to Rosenbrock (1962), with extensions to distributed parameter systems by Murray-Lasso (1965) and Gould and Murray-Lasso (1966). The central theme here is that the transient behavior of a process is governed by the dominant modes associated with the smallest eigenvalues. If it is possible to approximate the high order system by a lower order system whose slow modes are the same as those of the original system, then attention can be focused on altering the eigenvalues of the slow modes so as to increase the speed of recovery of the process from disturbances. It is essential to be aware of the fact that various disturbances excite the modes differently so that a scheme which is based on a lower-order model may be inappropriate if a disturbance injects most of its "energy” in a fast mode which has been neglected. However, implicit in Rosenbrock's approach is the possibility of altering each eigenvalue separately so that the resulting control system can be viewed as being non-interacting in the sense that manipulation of one mode may not alter any other mode. Thus it may be possible, with enough measurements and controls (manipulations), to speed up the recovery from any expected disturbance. There are obvious limitations to this, since all the states cannot be measured in practice and controls cannot be applied to all states. This will limit the extent to which the speed of response of a mode can be increased. The problem of representing a linear distributed parameter system in terms of its modes is examined here and consideration is given to the limitations imposed by being able to make only finite discrete measurements and to manipulate only a finite number of modes.

4.2 Modal analysis of Lumped parameter systems

One of the approaches to multivariable controller design is to use Modal Feedback Control. This technique makes use of the linear nature of the system model to design a control scheme which allows one to specify the closed-loop eigenvalues of the system. To illustrate this, let us consider the modal control of a simple CSTR in which irreversible first order reactions $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ takes place. The rates of the reactions are given by $r_1 = k_1 C_A$ and $r_2 = k_2 C_B$ where k_1 and k_2 are constants. The modeling equations take the form,

$$V \frac{dC_A}{dt} = F\left(C_{Af} - C_A\right) - V\left(k_1 C_A\right) \text{ with } C_A(t=0) = C_{A0} \qquad \textbf{Eqn – 4.2.1}$$

$$V \frac{dC_B}{dt} = F\left(C_{Bf} - C_B\right) + V\left(k_1 C_A - k_2 C_B\right) \text{ with } C_B(t=0) = C_{B0} \qquad \textbf{Eqn – 4.2.2}$$

Now it is desired to control C_A and C_B as close as possible to a desired set point C_{Ad} and C_{Bd} by adjusting C_{Af} and C_{Bf} (the feed concentrations of A and B).

Let us now define some of the dimensionless constants,

$$Da_1 = \frac{k_1 V}{F}, Da_2 = \frac{k_2 V}{F}, t = \frac{t^{|} F}{V}, x_1 = \frac{C_A}{C_{A,ref}}, x_2 = \frac{C_B}{C_{B,ref}}, u_1 = \frac{C_A}{C_{A,ref}}, u_2 = \frac{C_A}{C_{A,ref}}$$

where $C_{A,ref}$ and $C_{B,ref}$ are arbitrary reference concentrations of A and B respectively. In this instance, the modeling equations take the form,

$$\frac{dx_1}{dt} = -(1 + Da_1)x_1 + u_1 \text{ with } x_1(t = 0) = x_{10} \qquad \textbf{Eqn – 4.2.3}$$

$$\frac{dx_2}{dt} = Da_1 x_1 - (1 + Da_2)x_2 + u_2 \text{ with } x_2(t = 0) = x_{20} \qquad \textbf{Eqn – 4.2.4}$$

Thus one wishes to control the reactor outlet concentration x_1, x_2 by adjusting the feed concentrations u_1 and u_2. Putting the system into linear state variable matrix form i.e.

$\dot{x} = Ax + Bu$ we have, $\quad A = \begin{bmatrix} -(1 + Da_1) & 0 \\ Da_1 & -(1 + Da_2) \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Let us suppose that both x_1 and x_2 are available as outputs, so any output of the form $y = Cx$ is possible. Now if we apply a simple single-loop proportional feedback control on the states (where we assume the set points to be zero) we have,

$U_1 = -k_{11}x_1$ and $U_2 = -k_{22}x_2$. Then the system equations are

$$\frac{dx_1}{dt} = -(1 + Da_1 + k_{11})x_1 \text{ and } \frac{dx_2}{dt} = Da_1 x_1 - (1 + Da_2 + k_{22})x_2 .$$

Even though k_{11} may be used to control x_1, there is a strong influence of x_1 on the state x_2. Let us now apply modal control to the problem. We begin by determining the eigenvalues and eigenvectors of the state matrix **A**. Thus we have the eigenvalues of **A** matrix as $\quad \lambda_1 = -(1 + Da_1)$ and $\lambda_2 = -(1 + Da_2)$.

From standard matrix algebra, we have their right and left eigenvectors as

$$r_1 = \begin{bmatrix} Da_1 - Da_2 \\ -Da_1 \end{bmatrix} \text{ and } r_2 = \begin{bmatrix} 0 \\ Da_1 \end{bmatrix} \; l_1 = \begin{bmatrix} Da_1 \\ 0 \end{bmatrix} \text{ and } l_2 = \begin{bmatrix} Da_1 \\ Da_1 - Da_2 \end{bmatrix}.$$

Now because each eigenvector is uniquely determined only up to a multiplicative constant, one can divide the r$_1$ and r$_2$ by $Da_1(Da_1 - Da_2)$ to make the matrix of right and left-hand eigenvectors orthonormal. Thus finally we have,

$$R = \begin{bmatrix} \dfrac{1}{Da_1} & 0 \\ \dfrac{-1}{Da_1 - Da_2} & \dfrac{1}{Da_1 - Da_2} \end{bmatrix} \text{and } L = \begin{bmatrix} Da_1 & 0 \\ Da_1 & Da_1 - Da_2 \end{bmatrix}$$

and one may verify that **LR = I**. Now if we let **C = L** and choose G$_C$ to be a diagonal proportional controller of the form $K = G_C = \begin{bmatrix} k_{11} & 0 \\ 0 & k_{22} \end{bmatrix}$ then we have $y_1 = Da_1 x_1$ and $y_2 = Da_1 x_1 + (Da_1 - Da_2) x_2$ and the feedback control law becomes $u = -RKLx$ where

$$RKL = \begin{bmatrix} k_{11} & 0 \\ \dfrac{Da_1(k_{22} - k_{11})}{Da_1 - Da_2} & k_{22} \end{bmatrix}.$$

Therefore we have the system as, $\dfrac{dx_1}{dt} = -(1 + Da_1 + k_{11})x_1$ **Eqn – 4.2.5**

$$\frac{dx_2}{dt} = Da_1\left(1 + \frac{k_{11} - k_{22}}{Da_1 - Da_2}\right)x_1 - (1 + Da_2 + k_{22})x_2 \qquad \textbf{Eqn – 4.2.6}$$

The outputs are then given by: $\dfrac{dy_1}{dt} = -(1 + Da_1 + k_{11})y_1$ **Eqn – 4.2.7**

$$\frac{dy_2}{dt} = -(1 + Da_2 + k_{22})y_2 \qquad \textbf{Eqn – 4.2.8}$$

shows no interaction. Now if one considers, the features of modal feedback control for this problem we have the outputs to be controlled independently without any interaction, and this is an advantage if a meaningful set point could be devised. Another advantage of the controller matrix is that if k_{11} and k_{22} are chosen so that

$$k_{22} - k_{11} = Da_1 - Da_2$$

then the equations for the states (**Eqn – 4.3.5** and **Eqn – 4.3.6**) do not show any interactions. This is not a general property of modal control, but is due to the particular structure of this example problem. Because the matrix A should be known and all the states must be accessible, modal control design in the transformed domain is a little artificial. However, one may obviously use it if one desires. For a more complex example of modal control of lumped parameter systems, the reader is advised to refer to Davison and Goldberg (1969) or Davison and Chadha (1972).

4.3 Modal analysis of a distributed parameter system - Linear Tubular reactor

A convenient way and useful form of analysis of second order partial differential equations is through modal decomposition. This form of analysis is possible when the equation is of this form:

$$\frac{\partial x}{\partial t} = Ax + Bu \qquad \textbf{Eqn - 4.3.1}$$

where

$$Ax(z,t) = A_2(z)\frac{\partial^2 x}{\partial z^2} + A_1(z)\frac{\partial x}{\partial z} + A_0(z)x \qquad \textbf{Eqn – 4.3.2}$$

is a spatial operator in one dimension and which has a real, discrete spectrum of eigenvalues. This leads to a second order parabolic set of PDE's. It is possible to extend this to two and higher space dimensions also. A wider discussion on this can be found in Ray (1981). Perhaps the best means of discussing the modal reduction of distributed parameter systems is by considering some example problems. We begin by studying the control of exit concentration of a Tubular reactor in which a simple first order reaction occurs and the reactor is assumed to be isothermal in nature so that the nonlinearities introduced from the rate of equation term do not enter the system.

A tubular reactor is depicted in Figure 4.3.1

Figure 4.3.1 : Tubular Reactor for Convection-Diffusion-Reaction Systems

Often these reactors are fed at the inlet boundary (z = 0) with a certain reactant concentration (X_r) in order to obtain a desired outlet product concentration at (z = L). As a result, the input ($X_{r,in}$) appears in the boundary condition of the model. The first step in rendering the model amenable to modal decomposition is to make the boundary conditions homogenous. The method of separation of variables is used, and the spatial ODE is solved using some of the well known mathematical tools relating to eigenvalues and eigenvectors.

4.3.1 Mathematical Model of a linear Tubular reactor

The linear parabolic partial differential equation representing a reaction involving a single reactant A occurring in a tubular reactor with axial dispersion and first order kinetics is:

$$\frac{\partial C_A(z',t')}{\partial t'} = -\nu \frac{\partial C_A(z',t')}{\partial z'} + D_r \frac{\partial^2 C_A(z',t')}{\partial z'^2} - k_r C_A(z',t') \quad \textbf{Eqn – 4.3.1.1}$$

with initial condition: $C_A(z',0) = C_{A1}(z')$, where $\mathbf{C_A}$ is the reactant concentration inside the tubular reactor, $\mathbf{z'}$ - spatial position (m), $\mathbf{t'}$ - time scale (s), ν - superficial axial fluid velocity (m/s), $\mathbf{k_r}$ - kinetic rate constant (1/s), $\mathbf{D_r}$ – diffusivity and **L** -

length of the reactor (m). This partial differential equation is subject to the following Danckwerts boundary conditions:

$$D_r \frac{\partial C_A(0,t')}{\partial z'} = \upsilon\left(C_A(0,t') - C_{A,in}(t')\right) \text{ and } \frac{\partial C_A(L,t')}{\partial z'} = 0 \quad \textbf{Eqn – 4.3.1.2}$$

The above set of equations has been considered by Brown (2001). To convert the above equation system to a dimensionless form, we define

$$z = \frac{z'}{L}, t = \frac{t'\upsilon}{L}, x = \frac{C_A}{C_{A0}}, x_{in} = \frac{C_{A,in}}{C_{A0}}, Pe = \frac{\upsilon L}{D_r} = 1, B = \frac{k_r L}{\upsilon} = 1.14$$

where **C_{A0}** is some reference reactant concentration. The new sets of equations are,

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) \qquad \textbf{Eqn – 4.3.1.3}$$

with initial condition: $x(z,0) = x_1(z)$, where **x** is the reactant concentration inside the tubular reactor. The boundary conditions also changes as follows,

$$\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x_{in}(t)\right) \text{ and } \frac{\partial x(1,t)}{\partial z} = 0 \qquad \textbf{Eqn – 4.3.1.4}$$

The above system of equation is not homogeneous; hence make the system homogeneous by shifting the non homogeneous part of the boundary condition into the partial differential equation using a Dirac delta function.

With the above modification, the system becomes

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) + \delta(z)x_{in}(t) \quad \textbf{Eqn – 4.3.1.5}$$

with initial condition: $x(z,0) = x_1(z)$, where **x** is concentration of reactant inside the tubular reactor. The boundary conditions also changes as follows,

$$\frac{\partial x(0,t)}{\partial z} = Pe * x(0,t) \text{and} \frac{\partial x(1,t)}{\partial z} = 0 \qquad \textbf{Eqn – 4.3.1.6}$$

Now the above system **Eqn – 4.3.1.5** and **Eqn – 4.3.1.6** is amenable to modal decomposition or variable separable method.

Let us assume the solution to be of the form: $x(z,t)=\sum_{n=1}^{\infty}a_n(t)\phi_n(z)$, Similarly the inlet concentration can also be expanded as: $\delta(z)x_{in}(t)=\sum_{n=1}^{\infty}c_n(t)\phi_n(z)$.

Introducing these approximate solutions into **Eqn – 4.3.1.5** we have **Eqn – 4.3.1.7**,

$$\frac{\phi_n(z)da_n(t)}{dt}=-a_n(t)\frac{d\phi_n(z)}{dz}+\frac{a_n(t)}{Pe}\frac{d^2\phi_n(z)}{dz^2}-a_n(t)\phi_n(z)B+c_n(t)\phi_n(z)$$

Dividing **Eqn – 4.3.1.7** by $a_n(t)\phi_n(z)$ yields an ODE which can be divided into a left side which depends solely on "t" and a right side that is a function of "z" alone. For this equality to hold for all (z,t), both sides must be equal to constant ($-\lambda_n$), resulting in

$$\frac{1}{a_n(t)}\left[\frac{da_n(t)}{dt}-c_n(t)\right]=\frac{1}{\phi_n(z)}\left[-\frac{d\phi_n(z)}{dz}+\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2}-B\phi_n(z)\right]=-\lambda_n \qquad \textbf{Eqn – 4.3.18}$$

Now **Eqn – 4.3.1.8** can be separated into the following ODE's:

$$\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2}-\frac{d\phi_n(z)}{dz}+(\lambda_n-B)\phi_n(z)=0 \qquad \textbf{Eqn – 4.3.1.9}$$

$$\frac{da_n(t)}{dt}+\lambda_n a_n(t)=c_n(t) \qquad \textbf{Eqn – 4.3.1.10}$$

The boundary condition is as follows, $\frac{d\phi_n(0)}{dz}=Pe*\phi_n(0)$ and $\frac{d\phi_n(1)}{dz}=0$

The above system is the familiar eigenvalue problem. The solution to **Eqn – 4.3.1.9** subject to the above boundary conditions is obtained by putting it into Sturm-Liouville form. A detailed analysis can be obtained from Ray (1981).

The solution $\phi_n(z)$ is of the form: $\phi_n(z)=B_n\,exp\left(\frac{Pe*z}{2}\right)\left[cos(\alpha_n z)+\frac{Pe}{2\alpha_n}sin(\alpha_n z)\right]$,

where $\boldsymbol{\alpha_n}$ is obtained by solving $tan(\alpha_n)=\frac{\alpha_n Pe}{\alpha_n^2-\frac{Pe^2}{4}}$,

λ_n is given by, $\lambda_n = \dfrac{\alpha_n^2}{Pe} + \dfrac{Pe}{4} + B$ and

B_n is given by, $B_n = \left[\int_0^1 \left(cos(\alpha_n z) + \dfrac{Pe}{2\alpha_n} sin(\alpha_n z) \right)^2 dz \right]^{-1/2}$

Along with $\mathbf{B_n}$, $a_n(t)$'s and $c_n(t)$'s also satisfy the orthonormal property and are obtained as follows, $c_n(t) = \int_0^1 \delta(z) x_{in}(t) \phi_n(z) exp(-Pe * z) dz = x_{in}(t) * \phi_n(0)$.

$$a_n(t=0) = a_{n0} = \int_0^1 x(z,0) \phi_n(z) exp(-Pe * z) dz$$

Once the c_n's are obtained, **Eqn – 4.3.1.10** can be used either for obtaining dynamic responses of the system or for control studies on the system.

4.3.2 Results and Discussions

The dynamic response to the system can be studied in two phases,

1. Unforced solution 2. Forced solution.

In the unforced solution case we have, $x_{in}(t = 0) = 0$, hence $c_n = 0$ and $x(z,0) = 1$ and in the forced solution case we have, $x_{in}(t = 0) = 1$, and $x(z,0) = 0$ hence we have $a_{n0} = 0$. The unforced and the forced solution to the above problem can be clearly understood by studying Figure 4.3.2 consisting of four sub plots. The top sub plots represent the plots for the unforced solution and the bottom two sub plots represent the forced solution of the tubular reactor. This figure basically shows the effect of number of modes on the solution, four simulations were done. First simulation shows the unforced solution ($x_{in}(t = 0) = 0$, hence $c_n = 0$) from a nonzero initial condition $x(z,0) = 1$, with only five modes (n = 5).

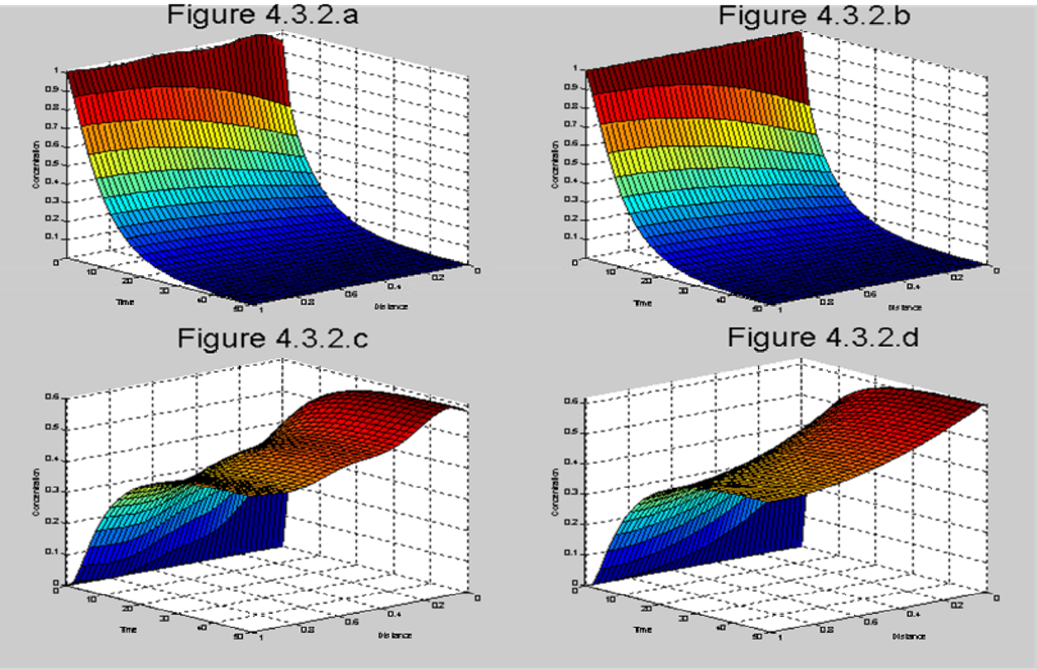


Figure 4.3.2.a
Figure 4.3.2.b
Figure 4.3.2.c
Figure 4.3.2.d

Figure 4.3.2 : Unforced and Forced solution of the Tubular Reactor

The temporal ODE given by **Eqn – 4.3.1.10** is solved using the initial condition calculated by $a_n(t=0)=a_{n0}=\int_0^1 x(z,0)\phi_n(z)exp(-Pe*z)dz$.

Therefore the solution to **Eqn – 4.3.1.10** is given by $a_n(t)=a_{n0}*exp(-\lambda_n t)$. The eigenvalues corresponding to the first five modes are as follows,

$$\lambda_n = [2.312, \quad 13.162, \quad 42.84, \quad 92.204, \quad 161.3 \quad].$$

The other vectors are given by $B_n = [0.92139,\ 1.3446,\ 1.3934,\ 1.4046,\ 1.4087\ ]$.

$$a_{n0} = [0.85327,\ 0.083182,\ 0.023981,\ 0.010981,\ 0.0062439\ ].$$

$$\alpha_n = [0.96019, \quad 3.431, \quad 6.4382, \quad 9.5296, \quad 12.645 \quad].$$

One can see from figure 4.3.2.a that initially there are small oscillations in the solution (across the reactor in 'z'), but then the solution progresses smoothly from its initial value of x(z,0) = 1 down to zero. Figure 4.3.2.b shows the same unforced solution obtained by considering more number of modes (n = 25). The difference in unforced solution obtained by these two different number of modes is negligible over the entire time span. The forced solution is found by using the same procedure as in the unforced case, but we begin with an initial condition of x(z,0) = 0 and an input $x_{in}(t = 0) = 1$. Therefore $c_n(t)$ is calculated by,

$$c_n(t) = \int_0^1 \delta(z) x_{in}(t) \phi_n(z) exp(-Pe * z) dz = x_{in}(t) * \phi_n(0) \,.$$

Figure 4.3.2.c shows the response when five modes were considered and Figure 4.3.2.d shows the response when twenty five modes were considered. If only five modes are used, the forced solution shows signs of the sin and cosine oscillations from using too few modes; this is evident in Figure 4.3.2.c. From the above discussion one can conclude that it is possible to capture the behavior of the system with a small number of modes, and thus may be able to represent the infinite dimensional system as a low dimensional lumped parameter system and use conventional control methods. The original distributed system, **Eqn – 4.3.1.1,** has now been decomposed into a set of n ODE's characterized by the system's eigenfunctions, Φ_n and its eigenvalues λ_n. If the infinite dimensional system can be represented by finite dimensional approximation, then it is possible to apply conventional control techniques in this new modal space.

4.4 Modal analysis of a distributed parameter system - Linear Heat Exchanger

Here we consider the linear tubular heat exchanger with axial diffusion. A simple single-pass shell and tube heat changer is considered. The main objective would be to control the tube-side outlet temperature at a desired value, in-spite of disturbances and changes in set points. The load disturbances are assumed to be fluctuations in the feed temperature and the manipulated variable is taken to be the steam temperature in the shell, which is a function of time only.

A simple schematic depicting the heat exchanger is shown above in Figure 4.4.1,

Figure 4.4.1: Simple Single-Pass Shell and Tube Heat Exchanger

4.4.1 Mathematical model of a linear heat exchanger

A simple linear tubular heat exchanger with single-pass on both shell side and tube side is considered. The liquid stream enters the tube of the heat exchanger and is heated by convection from the inner wall. Heat is supplied to the tube by means of condensing steam in the jacket. Some of the assumptions made in deriving the mathematical model (Hahn et al., 1971) are stated in section 3.10.

Based on the assumptions made in section 3.10 and an energy balance over a differential section of the tube side of the exchanger yields:

$$\frac{\partial T_l}{\partial \tau} = D\frac{\partial^2 T_l}{\partial l^2} - \upsilon\frac{\partial T_l}{\partial l} + \frac{h_{wl}P_l}{C_{pl}\rho_l A_l}\left(T_w - T_l\right) \qquad \textbf{Eqn – 4.4.1.1}$$

Taking an energy balance over a differential section of wall gives:

$$\frac{\partial T_w}{\partial \tau} = \frac{h_{ws}P_s}{C_{pw}\rho_w A_w}\left(T_s - T_w\right) + \frac{h_{wl}P_l}{C_{pw}\rho_w A_w}\left(T_l - T_w\right) \qquad \textbf{Eqn – 4.4.1.2}$$

subject to following boundary conditions:

$$\frac{\partial T_l(0,\tau)}{\partial l} = \frac{\upsilon}{D}\left(T_l(0,\tau) - T_l^f(\tau)\right) \text{and} \frac{\partial T_l(L,\tau)}{\partial l} = 0 \qquad \textbf{Eqn – 4.4.1.3}$$

The above equations are dimensionalized by introducing the following parameters, Mean residence time: $\tau_r = L/\upsilon$ sec, Axial Peclet Number: $\beta = \upsilon L/D$, Dimensionless time: $t = \tau/\tau_r$, Dimensionless axial distance: $x = l/L$, Dimensionless liquid temperature: $u_1 = T_l/T_r$, Dimensionless wall temperature: $u_2 = T_w/T_r$, Dimensionless steam temperature: $\theta = T_s/T_r$, The other parameters are:

$$\frac{1}{\tau_1} = \frac{h_{wl}P_l}{C_{pl}\rho_l A_l} sec^{-1}, \frac{1}{\tau_{21}} = \frac{h_{wl}P_l}{C_{pw}\rho_w A_w} sec^{-1}, \frac{1}{\tau_{22}} = \frac{h_{ws}P_s}{C_{pw}\rho_w A_w} sec^{-1}.$$

Hence the system of equations with boundary conditions is:

$$\frac{\partial u_1}{\partial t} = \frac{1}{\beta}\frac{\partial^2 u_1}{\partial x^2} - \frac{\partial u_1}{\partial x} + \frac{\tau_r}{\tau_1}(u_2 - u_1) \qquad \textbf{Eqn – 4.4.1.4}$$

$$\frac{\partial u_2}{\partial t} = \frac{\tau_r}{\tau_{22}}(\theta - u_2) + \frac{\tau_r}{\tau_{21}}(u_1 - u_2) \qquad \textbf{Eqn – 4.4.1.5}$$

subject to:

$$\frac{\partial u_1(0,t)}{\partial x} = \beta\left(u_1(0,t) - u_1^f(t)\right) \ \& \ \frac{\partial u_1(1,t)}{\partial x} = 0 \qquad \textbf{Eqn – 4.4.1.6}$$

where u_1^f is the inlet fluid temperature and θ is the steam temperature. The numerical values used in this study are as follows: $\beta = 1, \tau_r = 3\,sec, \tau_1 = 3.69\,sec, \tau_{21} = 2.65\,sec$ $\tau_{22} = 1.05\ sec,\ u_1^f = 0.53, \theta = 0.795, \frac{\tau_r}{\tau_1} = 0.813, \frac{\tau_r}{\tau_{21}} = 1.1321, \frac{\tau_r}{\tau_{22}} = 2.8571$.

The above system of equation is not homogeneous; hence we make the system homogeneous by shifting the non homogeneous part of the boundary condition into the partial differential equation using the Dirac delta function.

With the above modification, the system becomes:

$$\frac{\partial u_1}{\partial t} = \frac{1}{\beta}\frac{\partial^2 u_1}{\partial x^2} - \frac{\partial u_1}{\partial x} + \frac{\tau_r}{\tau_1}(u_2 - u_1) + \delta(x)u_1^f(t) \qquad \textbf{Eqn – 4.4.1.7}$$

$$\frac{\partial u_2}{\partial t} = \frac{\tau_r}{\tau_{22}}(\theta - u_2) + \frac{\tau_r}{\tau_{21}}(u_1 - u_2) \qquad \textbf{Eqn – 4.4.1.8}$$

subject to: $$\frac{\partial u_1(0,t)}{\partial x} = \beta u_1(0,t) \ \& \ \frac{\partial u_1(1,t)}{\partial x} = 0 \qquad \textbf{Eqn – 4.4.1.9}$$

Now the above system **Eqn – 4.4.1.7, Eqn – 4.4.1.8** and **Eqn – 4.4.1.9** is amenable to modal decomposition or variable separable method.

Let us assume the solution to be of the form:

$$u_1(x,t) = \sum_{n=1}^{\infty} a_n(t)\phi_n(x) \text{ and } u_2(x,t) = \sum_{n=1}^{\infty} b_n(t)\phi_n(x)$$

Similarly the inlet temperature and steam temperature can also be expanded as:

$$\delta(x)u_1^f(t) = \sum_{n=1}^{\infty} c_n(t)\phi_n(x) \text{ and } \theta(t) = \sum_{n=1}^{\infty} d_n(t)\phi_n(x)$$

Introducing these approximate solutions into **Eqn – 4.4.1.7, Eqn – 4.4.1.8** and in the boundary conditions **Eqn – 4.4.1.9** we have **Eqn – 4.4.1.10, Eqn – 4.4.1.11** and the boundary conditions **Eqn – 4.4.1.12** respectively.

$$\frac{\phi_n(x)da_n(t)}{dt} = -a_n(t)\frac{d\phi_n(x)}{dx} + \frac{a_n(t)}{\beta}\frac{d^2\phi_n(x)}{dx^2} + 0.813[b_n(t) - a_n(t)]\phi_n(x) + c_n(t)\phi_n(x)$$

Eqn – 4.4.1.10

$$\frac{\phi_n(x)db_n}{dt} = \frac{\tau_r}{\tau_{22}}(d_n(t) - b_n(t))\phi_n(x) + \frac{\tau_r}{\tau_{21}}(a_n(t) - b_n(t))\phi_n(x) \qquad \textbf{Eqn – 4.4.1.11}$$

$$\frac{d\phi_n(0)}{dx} = \beta * \phi_n(0) \text{and} \frac{d\phi_n(1)}{dx} = 0 \qquad \textbf{Eqn – 4.4.1.12}$$

Dividing **Eqn – 4.4.1.10** by $a_n(t)\phi_n(x)$ yields an ODE which can be divided into a left side which depends solely on "t" and a right side that is a function of "x" alone. For this equality to hold for all x and t, both sides must be equal to constant ($-\lambda_n$), resulting in:

$$\frac{1}{a_n(t)}\left[\frac{da_n(t)}{dt} - c_n(t) - 0.813b_n(t)\right] = -\lambda_n \qquad \textbf{Eqn – 4.4.1.13}$$

and $$\frac{1}{\phi_n(x)}\left[-\frac{d\phi_n(x)}{dx} + \frac{1}{\beta}\frac{d^2\phi_n(x)}{dx^2} - 0.813\phi_n(x)\right] = -\lambda_n \qquad \textbf{Eqn – 4.4.1.14}$$

The above ODE's can be simplified:

$$\frac{1}{\beta}\frac{d^2\phi_n(x)}{dx^2}-\frac{d\phi_n(x)}{dx}+(\lambda_n-B)\phi_n(x)=0 \qquad \textbf{Eqn – 4.4.1.15}$$

$$\frac{da_n(t)}{dt}+\lambda_n a_n(t)=c_n(t)+0.813b_n(t) \qquad \textbf{Eqn – 4.4.1.16}$$

The boundary condition remains the same as above (**Eqn – 4.4.1.12**).

Dividing **Eqn – 4.4.1.11** by $\phi_n(x)$ yields an ODE which can be written as,

$$\frac{db_n(t)}{dt}=\frac{\tau_r}{\tau_{22}}(d_n(t)-b_n(t))+\frac{\tau_r}{\tau_{21}}(a_n(t)-b_n(t)) \qquad \textbf{Eqn – 4.4.1.17}$$

Eqn – 4.4.1.15 subject to boundary condition **Eqn – 4.4.1.12**, has following solution:

$$\phi_n(x)=B_n\,exp\left(\frac{\beta * x}{2}\right)\left[cos(\alpha_n x)+\frac{\beta}{2\alpha_n}sin(\alpha_n x)\right],$$

where $\boldsymbol{\alpha_n}$ is obtained by solving $\quad tan(\alpha_n)=\dfrac{\alpha_n\beta}{\alpha_n^2-\dfrac{\beta^2}{4}},$

$\boldsymbol{\lambda_n}$ is given by $\quad \lambda_n=\dfrac{\alpha_n^2}{\beta}+\dfrac{\beta}{4}+0.813$ and

$\mathbf{B_n}$ is given by $\quad B_n=\left[\displaystyle\int_0^1\left(cos(\alpha_n x)+\frac{\beta}{2\alpha_n}sin(\alpha_n x)\right)^2 dx\right]^{-1/2}$

Along with $\mathbf{B_n}$, $d_n(t)$'s and $c_n(t)$'s also satisfy the orthonormal property and are obtained as follows,

$$c_n(t)=\int_0^1 \delta(x)u_1^f(t)\phi_n(x)exp(-\beta * x)dx = u_1^f(t)*\phi_n(0).$$

$$d_n(t)=\theta(t)\int_0^1 \phi_n(x)exp(-\beta * x)dx\ .$$

On simplification this yields,

$$d_n(t) = \theta(t)B_n \int_0^1 exp\left(\frac{-\beta * x}{2}\right)\left[cos(\alpha_n x) + \frac{\beta}{2\alpha_n} sin(\alpha_n x)\right]dx$$

With the availability of $c_n(t)$ and $d_n(t)$ one can solve both equations **Eqn – 4.4.1.16** and **Eqn – 4.4.1.17** simultaneously either analytically or numerically. Here numerical solution was obtained by solving these equations simultaneously using stiff ODE solvers in MATLAB like ODE15s. If one uses other ODE solvers like ODE45 or ODE23s etc the simulation time taken is very long and meaningful results are not guaranteed. Once we obtain $a_n(t)$ and $b_n(t)$ then using the relationships

$$u_1(x,t) = \sum_{n=1}^{\infty} a_n(t)\phi_n(x) \text{ and } u_2(x,t) = \sum_{n=1}^{\infty} b_n(t)\phi_n(x)$$

one can obtain the dimensionless tube side fluid temperature (u_1) and the dimensionless shell side fluid temperature (u_2). Now one can reconvert the dimensionless temperatures to the original temperatures with the help of the dimensionalizing variables. Thus, modal analysis yields both the dynamic solution as well as helps one to perform other control studies.

4.4.2 Results and Discussions

Simple computer programs were developed to perform the operation of modal decomposition. The earlier suggested parameter values were used and some of these results are presented below. These results can be compared with the orthogonal collocation results presented in the section (3.11). Figure 4.4.2 shows the dynamic and steady state temperature profiles of shell side fluid and tube side fluid in the linear heat exchanger. The top two 3D plots (Figure 4.4.2.a and Figure 4.4.2.b) consist of dynamic profiles for tube side fluid temperature and wall side fluid temperature. The bottom two plots (Figure 4.4.2.c and Figure 4.4.2.d) show the steady state wall side and tube side temperature along the length of the reactor. The bottom two plots showing the steady state profiles consist of 3 distinctive curves.

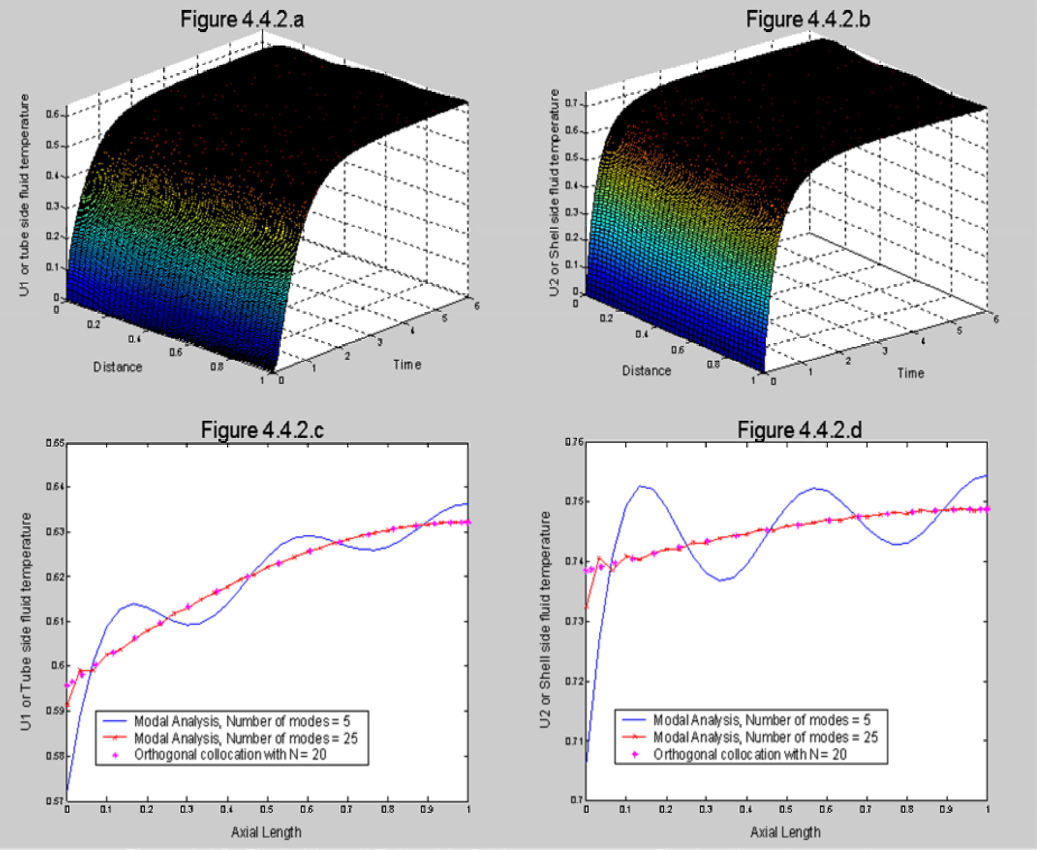


Figure 4.4.2: Shell side and Tube side fluid temperature profiles in a linear heat exchanger

The one which is solid-line shows oscillations and is obtained when five modes were used to approximate the distributed parameter system. This sort of approximation is quite useful when one proceeds for control studies in which one is limited to have a as few sensors as possible. The curve which is (*) is the one obtained from orthogonal collocation described in the earlier chapter (refer sections 3.10 and 3.11). The curve with dashes and 'x' is the one obtained by modal analysis using more number of modes (N = 25). One can observe that as the number of modes are increased the accuracy of the solution increases significantly and at infinite number of modes one can have an exact solution of the system. With even 25 - number of modes the modal analysis solution is in close agreement with the orthogonal collocation results obtained with 20 collocation points. Except at the initial part of the reactor the solutions are in very good agreement at all other points in the reactor.

4.5 Modal analysis of a linear tubular reactor with recycle

Consider an isothermal linear tubular reactor with recycle shown in Figure 4.5.1, in which an irreversible first order reaction of the form $A \rightarrow B$ takes place. The outlet from the tubular reactor is fed to a separator where the unreacted species **A** is separated from product **B**. Here the separator is assumed to be of negligible dynamics and hence removed from the picture. The unreacted species **A** is then fed back to the tubular reactor through a recycle loop, which has a simple first order dynamics. It is assumed that there is negligible time delay in the recycle path and the mixing in the mixer (represented by the summation block in Figure 4.5.1) is instantaneous.

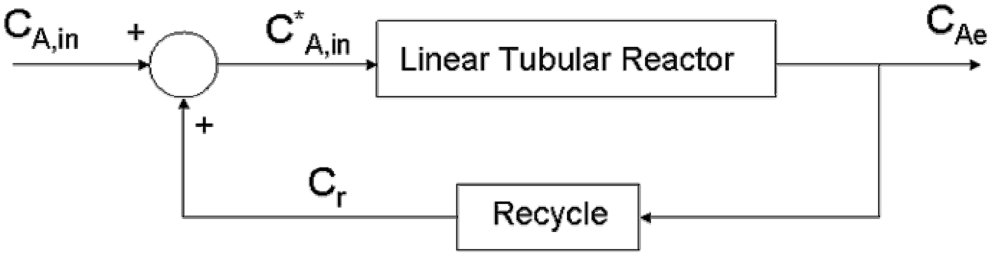


Figure 4.5.1 : An Isothermal Tubular Reactor with Recycle

A linear parabolic second order partial differential equation describes the tubular reactor dynamics and a simple first order ordinary differential equation describes the recycle path dynamics. Assume that the density, mass diffusivity, reaction rate constant and axial fluid velocity are constant. Also, we assume that there is negligible reaction taking place in the recycle loop and there is instantaneous mixing of the fresh feed and recycle feed at the reactor inlet. The model can now be written as

$$\frac{\partial C_A(z',t')}{\partial t'} = -\nu \frac{\partial C_A(z',t')}{\partial z'} + D_r \frac{\partial^2 C_A(z',t')}{\partial z'^2} - k_r C_A(z',t') \qquad \textbf{Eqn – 4.5.1}$$

$$T_R \frac{\partial C_r(t')}{\partial t'} + C_r(t') = K_R C_{Ae}(z',t') \qquad \textbf{Eqn – 4.5.2}$$

with initial condition: $C_A(z',0)=C_{A1}(z')$, where **C_A** is the reactant concentration inside the tubular reactor and $C_r(t'=0)=C_{Ae}$, where **C_r** is the reactant concentration in the recycle loop. **z'** - spatial position (m), **t' -** time scale (s), **ν -** superficial axial fluid velocity (m/s), **k_r** - kinetic rate constant (1/s), **D_r** - diffusivity, **L** - length of the reactor (m), **T_R** – recycle path time constant (s) and **K_R** - gain in the recycle path.

These partial differential equations are subject to the following Danckwerts boundary conditions: $D_r \frac{\partial C_A(0,t')}{\partial z'} = \upsilon\left(C_A(0,t') - C^*_{A,in}(t')\right)$ and $\frac{\partial C_A(L,t')}{\partial z'} = 0$ **Eqn – 4.5.3**

where $C^*_{A,in}(t') = (1-R)*C_{A,in}(t') + R*C_r(t')$, is obtained from taking a material balance on the mixer present at the entrance of the tubular reactor. Here **$C_{A,in}$** is the fresh feed reactant concentration, **C_r** is the reactant concentration coming from the recycle loop and **R** is the recycle ratio.

The above equations are to be made dimensionless, so put

$$z=\frac{z'}{L}, t=\frac{t'\upsilon}{L}, x=\frac{C_A}{C_{A0}}, x^*_{in}=\frac{C^*_{A,in}}{C_{A0}}, x^*_r=\frac{C_r}{C_{A0}}, x_1=\frac{C_{A1}}{C_{A0}}, Pe=\frac{\upsilon L}{D_r}=1, B=\frac{k_r L}{\upsilon}=1.14$$

where **C_{A0}** is some reference reactant concentration. The new sets of equations are:

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) \qquad \textbf{Eqn – 4.5.4}$$

$$\tau_R \frac{\partial x_r(t)}{\partial t} + x_r(t) = K_R x(1,t) \qquad \textbf{Eqn – 4.5.5}$$

where **x** is the reactant concentration inside the tubular reactor, **x_r** is the reactant concentration in the recycle loop, with initial condition: $x(z,0)=x_1(z)$, $x_r(t=0)=x(1,t)$

The boundary conditions also change as follows,

$$\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x_{in}^{*}(t)\right) \text{and} \frac{\partial x(1,t)}{\partial z} = 0 \qquad \textbf{Eqn – 4.5.6}$$

where $x_{in}^{*}(t) = (1-R) * x_{in}(t) + R * x_r(t)$

The above system of equation is not homogeneous; hence make the system homogeneous by shifting the non homogeneous part of the boundary condition into the partial differential equation using a Dirac delta function. With the above modification, the system becomes

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) + \delta(z)x_{in}^{*}(t) \qquad \textbf{Eqn – 4.5.7}$$

where $x_{in}^{*}(t) = (1-R) * x_{in}(t) + R * x_r(t)$

$$\tau_R \frac{\partial x_r(t)}{\partial t} + x_r(t) = K_R x(1,t) \qquad \textbf{Eqn – 4.5.8}$$

with initial condition:

$x(z,0) = x_1(z)$, **x** is the reactant concentration inside the tubular reactor.

$x_r(t=0) = x(1,t)$, $\mathbf{x_r}$ is the reactant concentration in the recycle loop.

The boundary conditions also changes as follows,

$$\frac{\partial x(0,t)}{\partial z} = x(0,t) * Pe \text{ and } \frac{\partial x(1,t)}{\partial z} = 0 \qquad \textbf{Eqn – 4.5.9}$$

Now two kinds of study can be carried out,

1. Fix the recycle ratio and obtain the dynamic response of the system by varying the inlet concentration.
2. Keep inlet concentration fixed and obtain the dynamic response of the system by varying the recycle ratio.

Case 1:

Now apply modal decomposition technique to solve item 1, considered above:

Let us assume the solution to x(z,t) as $x(z,t) = \sum_{n=1}^{\infty} a_n(t)\phi_n(z)$.

Similarly the inlet concentration and recycle concentration can also be expanded as

$$\delta(z)x_{in}(t) = \sum_{n=1}^{\infty} b_n(t)\phi_n(z) \text{ and } \delta(z)x_r(t) = \sum_{n=1}^{\infty} c_n(t)\phi_n(z).$$

Therefore **Eqn – 4.5.7** changes to the following form

$$\frac{\phi_n(z)da_n(t)}{dt} = -a_n(t)\frac{d\phi_n(z)}{dz} + \frac{a_n(t)}{Pe}\frac{d^2\phi_n(z)}{dz^2} - Ba_n(t)\phi_n(z) + (1-R)b_n(t)\phi_n(z) + Rc_n(t)\phi_n(z)$$

Eqn – 4.5.10

Dividing **Eqn – 4.5.10** by a$_n$(t)ϕ$_n$(z) yields an ODE which can be separated into a left side which depends solely on "t" and right side that is a function of "z" alone. For this equality to hold for all (z,t), both sides must be equal to constant (-λ$_n$), resulting in

$$\frac{1}{a_n(t)}\left[\frac{da_n(t)}{dt} - Rc_n(t) - (1-R)b_n(t)\right] = \frac{1}{\phi_n(z)}\left[-\frac{d\phi_n(z)}{dz} + \frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2} - B\phi_n(z)\right] = -\lambda_n \quad \textbf{Eqn – 4.5.11}$$

Now **Eqn – 4.5.11** can be separated into the following ODE's:

$$\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2} - \frac{d\phi_n(z)}{dz} + (\lambda_n - B)\phi_n(z) = 0 \qquad \textbf{Eqn – 4.5.12}$$

$$\frac{da_n(t)}{dt} + \lambda_n a_n(t) = Rc_n(t) + (1-R)b_n(t) \qquad \textbf{Eqn – 4.5.13}$$

The boundary condition is as follows, $\frac{d\phi_n(0)}{dz} = Pe * \phi_n(0)$ and $\frac{d\phi_n(1)}{dz} = 0$.

Eqn – 4.5.12 subject to the above boundary condition has following solution:

$$\phi_n(z) = B_n \exp\left(\frac{Pe * z}{2}\right)\left[\cos(\alpha_n z) + \frac{Pe}{2\alpha_n}\sin(\alpha_n z)\right],$$

where **α$_n$** is obtained by solving $\tan(\alpha_n) = \frac{\alpha_n Pe}{\alpha_n^2 - \frac{Pe^2}{4}}$,

$\lambda_{\mathbf{n}}$ is given by $$\lambda_n = \frac{\alpha_n^2}{Pe} + \frac{Pe}{4} + B$$

$\mathbf{B_n}$ is given by $$B_n = \left[\int_0^1 \left(cos(\alpha_n z) + \frac{Pe}{2\alpha_n} sin(\alpha_n z) \right)^2 dz \right]^{-1/2}$$

Along with B_n, $a_n(t)$'s and $c_n(t)$'s also satisfy the orthonormal property and are obtained as follows,

$$b_n(t) = \int_0^1 \delta(z) x_{in}(t) \phi_n(z) exp(-Pe * z) dz = x_{in}(t) * \phi_n(0)$$

$$c_n(t) = \int_0^1 \delta(z) x_r(t) \phi_n(z) exp(-Pe * z) dz = x_r(t) * \phi_n(0)$$

For the forced solution to the above problem we have, $x_{in}(t = 0) = 1$ and $x(z,0) = 0$ hence we have $a_{n0} = 0$. Similarly **Eqn – 4.5.8** changes to the following form,

$$\frac{\tau_R dc_n(t)}{dt} + c_n(t) = K_R B_n \sum_{m=1}^{\infty} a_m(t) \phi_m(1) \qquad \textbf{Eqn – 4.5.14}$$

Once the Φ are known then one should solve **Eqn – 4.5.13** and **Eqn – 4.5.14** simultaneously as they are coupled equations and other parameters like R and $b_n(t)$ are known. This can be done by arranging **Eqn – 4.5.13** and **Eqn – 4.5.14** together in state space form: $\frac{dY}{dt} = AY + BU$ where $Y = [a_1, a_2 ..., a_n, c_1, c_2 ..., c_n]$ and $U = [b_1, b_2 ..., b_n]$.

Assuming that four modes (n = 4) are sufficient to approximate the system we have the A and B matrices as:

$$A = \begin{bmatrix} -\lambda_1 & 0 & 0 & 0 & R & 0 & 0 & 0 \\ 0 & -\lambda_2 & 0 & 0 & 0 & R & 0 & 0 \\ 0 & 0 & -\lambda_3 & 0 & 0 & 0 & R & 0 \\ 0 & 0 & 0 & -\lambda_4 & 0 & 0 & 0 & R \\ A_{51} & A_{52} & A_{53} & A_{54} & \frac{-1}{\tau_R} & 0 & 0 & 0 \\ A_{61} & A_{62} & A_{63} & A_{64} & 0 & \frac{-1}{\tau_R} & 0 & 0 \\ A_{71} & A_{72} & A_{73} & A_{74} & 0 & 0 & \frac{-1}{\tau_R} & 0 \\ A_{81} & A_{82} & A_{83} & A_{84} & 0 & 0 & 0 & \frac{-1}{\tau_R} \end{bmatrix}$$

$$B = \begin{bmatrix} (1-R) & 0 & 0 & 0 \\ 0 & (1-R) & 0 & 0 \\ 0 & 0 & (1-R) & 0 \\ 0 & 0 & 0 & (1-R) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

where $A_{pq} = \dfrac{K_R B_q \phi_{p-n}(q)}{\tau_R}$. p stands for the row number and q represents the column number. p can take values ranging from n+1 to 2n and q can take values from 1 to n. Now the above state space system can be easily solved by any of the MATLAB ODE solvers like the ODE45, ODE15s and ODE23s etc. Once the solution for Y is obtained one can decompose it into $a_n(t)$ and $c_n(t)$ parts. After obtaining $a_n(t)$ and $c_n(t)$, the dynamics x(z,t) can be obtained using the relationship $x(z,t) = \sum_{n=1}^{4} a_n(t)\phi_n(z)$.

<u>Case 2:</u>

Apply modal decomposition technique to this item 2 mentioned above. Let us assume the solution to be $x(z,t) = \sum_{n=1}^{\infty} a_n(t)\phi_n(z)$,

Similarly the recycle ratio and recycle concentration can also be expanded as

$$\delta(z)(1 - R(t)) = \sum_{n=1}^{\infty} b_n(t)\phi_n(z) \text{ and } \delta(z)x_r(t) = \sum_{n=1}^{\infty} c_n(t)\phi_n(z).$$

Therefore the **Eqn – 4.5.7** changes to:

$$\frac{\phi_n(z)da_n(t)}{dt} = -a_n(t)\frac{d\phi_n(z)}{dz} + \frac{a_n(t)}{Pe}\frac{d^2\phi_n(z)}{dz^2} - Ba_n(t)\phi_n(z) + x_{in}(t)b_n(t)\phi_n(z) + Rc_n(t)\phi_n(z)$$

Eqn – 4.5.15

Dividing **Eqn – 4.5.15** by $a_n(t)\phi_n(z)$ yields an ODE which can be separated into a left side which depends solely on "t" and right side that is a function of "z" alone. For this equality to hold for all (z,t), both sides must be equal to constant ($-\lambda_n$), resulting in

$$\frac{1}{a_n(t)}\left[\frac{da_n(t)}{dt}-Rc_n(t)-x_{in}b_n(t)\right]=\frac{1}{\phi_n(z)}\left[-\frac{d\phi_n(z)}{dz}+\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2}-B\phi_n(z)\right]=-\lambda_n \qquad \textbf{Eqn -- 4.5.16}$$

Now **Eqn – 4.5.16** can be separated into the following ODE's:

$$\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2}-\frac{d\phi_n(z)}{dz}+(\lambda_n-B)\phi_n(z)=0 \qquad \textbf{Eqn -- 4.5.17}$$

$$\frac{da_n(t)}{dt}+\lambda_n a_n(t)=Rc_n(t)+x_{in}b_n(t) \qquad \textbf{Eqn -- 4.5.18}$$

The boundary condition is as follows, $\frac{d\phi_n(0)}{dz}=Pe*\phi_n(0)$ and $\frac{d\phi_n(1)}{dz}=0$.

Eqn – 4.5.12 subject to the above boundary condition has following solution:

$$\phi_n(z)=B_n\, exp\left(\frac{Pe*z}{2}\right)\left[cos(\alpha_n z)+\frac{Pe}{2\alpha_n}sin(\alpha_n z)\right],$$

where $\boldsymbol{\alpha_n}$ is obtained by solving $\quad tan(\alpha_n)=\dfrac{\alpha_n Pe}{\alpha_n^2-\dfrac{Pe^2}{4}}$,

$\boldsymbol{\lambda_n}$ is given by $\quad \lambda_n=\dfrac{\alpha_n^2}{Pe}+\dfrac{Pe}{4}+B$

and $\mathbf{B_n}$ is given by $\quad B_n=\left[\int_0^1\left(cos(\alpha_n z)+\dfrac{Pe}{2\alpha_n}sin(\alpha_n z)\right)^2 dz\right]^{-1/2}$

Along with $\mathbf{B_n}$**,** $a_n(t)$'s and $c_n(t)$'s also satisfies the orthonormal property and are obtained as follows, $b_n(t)=\int_0^1\delta(z)(1-R(t))\phi_n(z)exp(-Pe*z)dz=(1-R(t))*\phi_n(0)$

$$c_n(t)=\int_0^1\delta(z)x_r(t)\phi_n(z)exp(-Pe*z)dz=x_r(t)*\phi_n(0)$$

For the forced solution to the above problem we have, $x_{in}(t = 0) = 1$, and $x(z,0) = 0$ hence we have $a_{n0} = 0$. Similarly **Eqn – 4.5.8** changes to the following form,

$$\frac{\tau_R dc_n(t)}{dt} + c_n(t) = K_R B_n \sum_{m=1}^{\infty} a_m(t)\phi_m(1) \qquad \textbf{Eqn – 4.5.19}$$

Once the Φ_n are known then one should solve **Eqn – 4.5.18** and **Eqn – 4.5.19** simultaneously as they are coupled equations and other parameters like R and $b_n(t)$ are known. This can be done by arranging **Eqn – 4.5.18** and **Eqn – 4.5.19** together in state space form $$\frac{dY}{dt} = AY + BU$$

where $$Y = [a_1, a_2 \ldots a_{n-1}, a_n, c_1, c_2 \ldots c_{n-1}, c_n]$$

and $$U = [b_1, b_2 \ldots\ldots b_{n-1}, b_n].$$

Assuming that four modes (n = 4) are sufficient to approximate the system we have A and B matrices as:

$$A = \begin{bmatrix} -\lambda_1 & 0 & 0 & 0 & R & 0 & 0 & 0 \\ 0 & -\lambda_2 & 0 & 0 & 0 & R & 0 & 0 \\ 0 & 0 & -\lambda_3 & 0 & 0 & 0 & R & 0 \\ 0 & 0 & 0 & -\lambda_4 & 0 & 0 & 0 & R \\ A_{51} & A_{52} & A_{53} & A_{54} & \frac{-1}{\tau_R} & 0 & 0 & 0 \\ A_{61} & A_{62} & A_{63} & A_{64} & 0 & \frac{-1}{\tau_R} & 0 & 0 \\ A_{71} & A_{72} & A_{73} & A_{74} & 0 & 0 & \frac{-1}{\tau_R} & 0 \\ A_{81} & A_{82} & A_{83} & A_{84} & 0 & 0 & 0 & \frac{-1}{\tau_R} \end{bmatrix}$$

$$B = \begin{bmatrix} x_{in} & 0 & 0 & 0 \\ 0 & x_{in} & 0 & 0 \\ 0 & 0 & x_{in} & 0 \\ 0 & 0 & 0 & x_{in} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

where $A_{pq} = \frac{K_R B_q \phi_{p-n}(q)}{\tau_R}$. p stands for the row number and q represents the column number. p can take values ranging from n+1 to 2n and q can take values from 1 to n. Now the above state space system can be easily solved by any of the MATLAB ODE solvers like the ODE45, ODE15s and ODE23s etc. Once the solution for Y is obtained one can decompose it into $a_n(t)$ and $c_n(t)$ parts. After obtaining $a_n(t)$ and $c_n(t)$ then one can obtain the dynamics x(z,t) completely by $x(z,t) = \sum_{n=1}^{4} a_n(t)\phi_n(z)$.

4.6 Results and discussions on modal analysis of DPS with recycles

The most interesting feature is that even though the modal analysis of DPS with recycle was carried out by two ways both end up giving the same result. This helps us to analyze the process behavior for both recycle ratio and inlet concentration as manipulated variables. Consequently, in the next chapter an extensive study is carried out in which a modal feedforward controller is designed to handle disturbances anticipated in the inlet concentration by manipulating the recycle ratio. The result for the tubular reactor with recycle is presented in the Figure 4.6.1. It consists of four subplots. Figure 4.6.1.a, Figure 4.6.1.b and Figure 4.6.1.c show the 3D dynamic profiles and Figure 4.6.1.d shows the steady state profiles. Figure 4.6.1.a is obtained by the above illustrated modal analysis theory (section 4.5 - both case 1 and case 2) and using five number of modes. Figure 4.6.1.b is also obtained by modal analysis theory only but using twenty five number of modes. Figure 4.6.1.c is obtained from orthogonal collocation technique (section 3.9) with twenty collocation points. Figure 4.6.1.d shows a comparison of modal analysis and orthogonal collocation in terms of steady state concentration profiles along the length of the reactor.

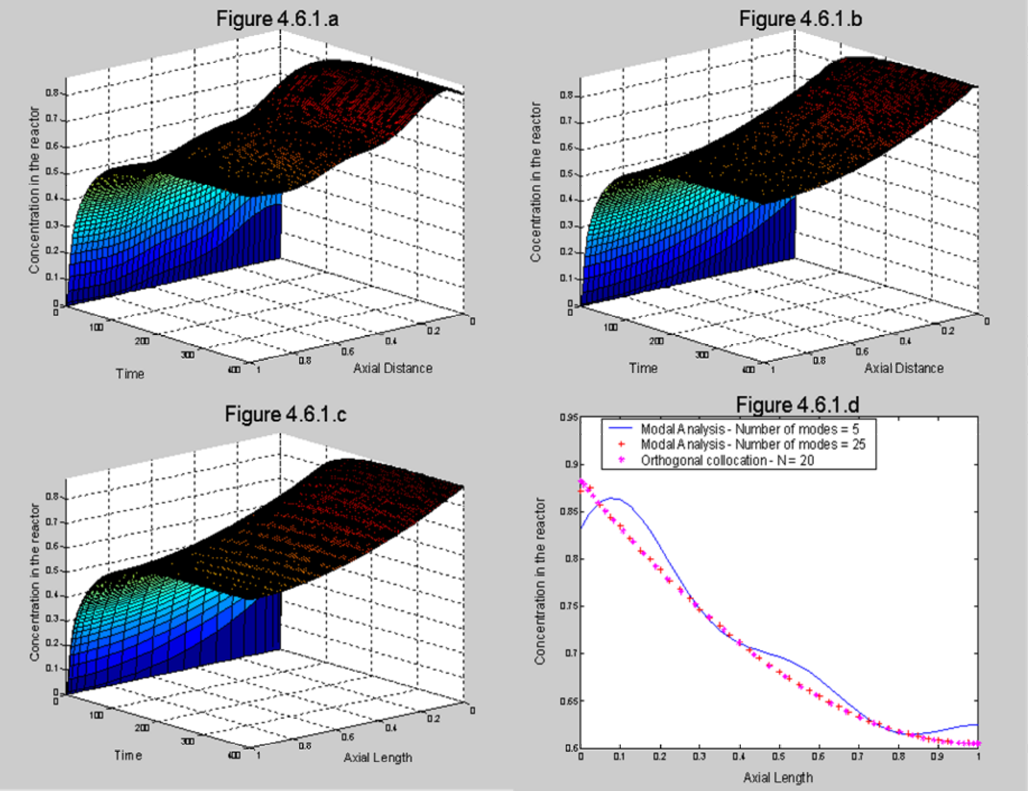


Figure 4.6.1: Dynamic and steady state Concentration profiles in a Tubular reactor with recycle (R) = 0.2

Three important things to be observed are:

1. The time taken to reach the steady state in case of tubular reactor with recycle is significantly (eight times) higher than tubular reactor without recycle.
2. The exit concentration value has increased from 0.6 (approx) to 0.8 (approx).
3. Both the orthogonal collocation (N = 20) and modal analysis with 25 modes give same results and are in perfect match as seen in Figure 4.6.1.d.

4.7 Conclusions

A very attractive technique (Modal Analysis) was investigated in this section for treating PDEs which have a real, discrete spectrum of eigenvalues and can be made self-adjoint. This technique is a natural reduction method and works well with only a few modes for the different physical systems, as illustrated by the simulation results.

CHAPTER 5

MODAL CONTROL OF DISTRIBUTED PARAMETER SYSTEMS

5.1 Introduction

A very valuable use of modal decomposition is in the design of control systems. Such applications have been discussed by Ajinkya et al. (1975), Gilles (1973), Wang (1972), Gould (1969) and Gould and Murray-Lasso (1966). Let us consider the control structure in Figure 5.1.1, where we assume the outputs to be the state variable itself. The control "u" is applied to the plant, yielding state x(z,t).

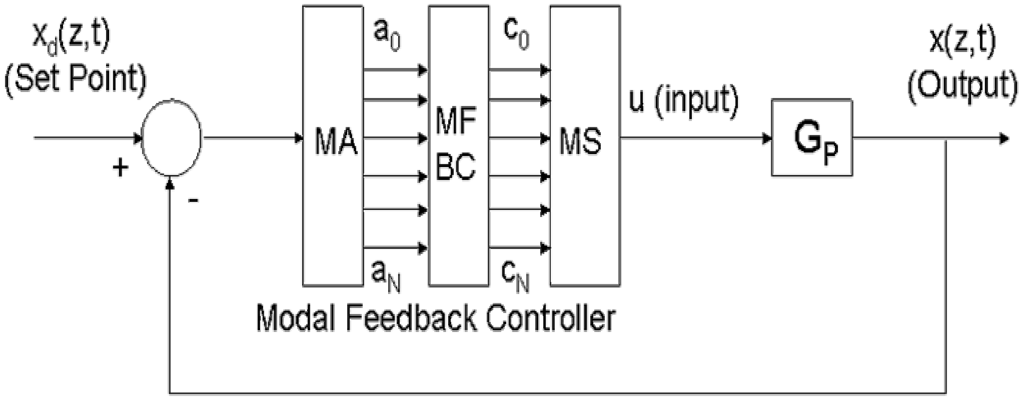


Figure 5.1.1: A distributed parameter modal control scheme

The state x(z,t) and the desired state x_d(z,t) are fed to the Modal Analyzer (MA) given

by: $$a_n(t) = \int_0^1 \left[x_d(z,t) - x(z,t)\right]\phi_n(z)\exp(-Pe * z)dz \quad \textbf{Eqn – 5.1.1}$$

The resulting coefficients (a_n(t)) are the error signal $a_n = x_d - x$ for n = 0, 1, 2 …. N, are fed to the N+1 variable lumped parameter feedback controller (MFBC). The outputs of this are the controller coefficients c_n(t).

These are then fed to a Modal Synthesizer (MS) which is governed by:

$$c_n(t) = \int_0^1 \delta(z) x_{in}(t) \phi_n(z) exp(-Pe * z) dz = x_{in}(t) * \phi_n(0) \quad \textbf{Eqn – 5.1.2}$$

This produces the control signal u(t) which is fed to the plant. Notice that the multivariable controller for this linear problem now consists of N+1 single-loop controllers. This is because there are no interactions in the modal formulation for linear problems, i.e the coefficient $c_n(t)$ only influences coefficient a_n. In principle, this control scheme requires that the complete state x(z,t) must be specified as an output. In practice, of course, this is impossible. However, one can provide this information in several ways.

1. One can measure $x(z_i,t)$, i = 1, 2, ….L, at a large number of points and simply smooth these data to get x(z,t).
2. One can measure $x(z_i,t)$, at only a few points (possibly one or two) and use a state estimator to provide estimates of x(z,t).
3. One can also use the matrix scheme suggested by Gould (1969).

The best way to understand modal control studies is through examples. So in this chapter we present two illustrative examples - a tubular reactor with recycle and a heat exchanger. Modal control will be demonstrated on these systems.

5.2 Modal control of a linear tubular reactor with recycle

Consider an isothermal linear tubular reactor with recycle shown in Figure 5.2.1, in which an irreversible first order reaction of the form $A \rightarrow B$ takes place. The outlet from the tubular reactor is fed to a separator where the unreacted species **A** is separated from product **B**. Here the separator is assumed to be of negligible dynamics and hence removed from the picture. The unreacted species **A** is then fed back to the tubular reactor through a recycle loop, which has a simple first order dynamics. It is assumed that there is negligible time delay in the recycle path and the mixing in the mixer (represented by the summation block in Figure 5.2.1) is instantaneous.

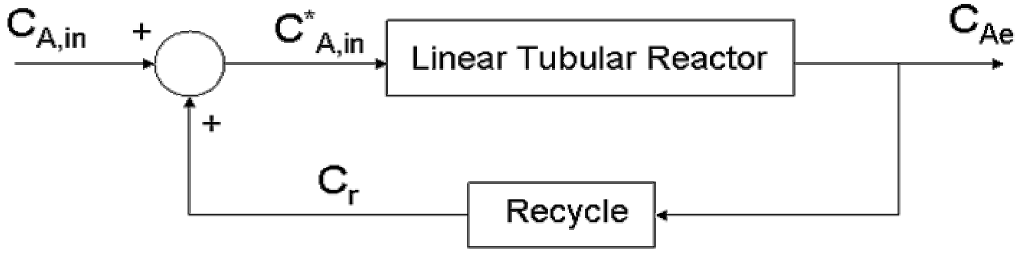


Figure 5.2.1: An Isothermal Tubular Reactor with Recycle

A linear parabolic second order partial differential equation describes the tubular reactor dynamics and a simple first order ordinary differential equation describes the recycle path dynamics. Assume that the density, mass diffusivity, reaction rate constant and axial fluid velocity are constant. Also, we assume that there is negligible reaction taking place in the recycle loop and there is instantaneous mixing of the fresh feed and recycle feed at the reactor inlet. The model can now be written as

$$\frac{\partial C_A(z',t')}{\partial t'} = -v\frac{\partial C_A(z',t')}{\partial z'} + D_r\frac{\partial^2 C_A(z',t')}{\partial z'^2} - k_r C_A(z',t') \qquad \textbf{Eqn – 5.2.1}$$

$$T_R\frac{\partial C_r(t')}{\partial t'} + C_r(t') = K_R C_A(L,t') \qquad \textbf{Eqn – 5.2.2}$$

with initial condition: $C_A(z',0)=C_{A1}(z')$, where $\mathbf{C_A}$ is the reactant concentration inside the tubular reactor and $C_r(t'=0)=C_{Ae}$, where $\mathbf{C_r}$ is the reactant concentration in the recycle loop. $\mathbf{z'}$ - spatial position (m), $\mathbf{t'}$ - time scale (s), ν - superficial axial fluid velocity (m/s), $\mathbf{k_r}$ - kinetic rate constant (1/s), $\mathbf{D_r}$ - diffusivity, **L** - length of the reactor (m), $\mathbf{T_R}$ – recycle path time constant (s) and $\mathbf{K_R}$ - gain in the recycle path.

These partial differential equations are subject to the following Danckwerts boundary conditions:

$$D_r \frac{\partial C_A(0,t')}{\partial z'} = \upsilon\left(C_A(0,t') - C^*_{A,in}(t')\right) \text{ and } \frac{\partial C_A(L,t')}{\partial z'} = 0 \qquad \textbf{Eqn – 5.2.3}$$

where $C^*_{A,in}(t') = (1-R) * C_{A,in}(t') + R * C_r(t')$, is obtained from taking a material balance on the mixer present at the entrance of the tubular reactor. Here $\mathbf{C_{A,in}}$ is the fresh feed reactant concentration, $\mathbf{C_r}$ is the reactant concentration coming from the recycle loop and **R** is the recycle ratio.

The above equations are to be made dimensionless, so put

$$z = \frac{z'}{L}, t = \frac{t'\upsilon}{L}, x = \frac{C_A}{C_{A0}}, x^*_{in} = \frac{C^*_{A,in}}{C_{A0}}, x^*_r = \frac{C_r}{C_{A0}}, x_1 = \frac{C_{A1}}{C_{A0}}, Pe = \frac{\upsilon L}{D_r}, B = \frac{k_r L}{\upsilon}$$

where $\mathbf{C_{A0}}$ is some reference reactant concentration. The new sets of equations are:

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) \qquad \textbf{Eqn – 5.2.4}$$

$$\tau_R \frac{\partial x_r(t)}{\partial t} + x_r(t) = K_R x(1,t) \qquad \textbf{Eqn – 5.2.5}$$

with initial condition:

$x(z,0) = x_1(z)$, where **x** is the reactant concentration inside the tubular reactor.

$x_r(t=0) = x(1,t)$, where $\mathbf{x_r}$ is the reactant concentration in the recycle loop.

The boundary conditions also change as follows,

$$\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x^*_{in}(t)\right) \text{ and } \frac{\partial x(1,t)}{\partial z} = 0 \qquad \textbf{Eqn – 5.2.6}$$

where $x^*_{in}(t) = (1-R) * x_{in}(t) + R * x_r(t)$.

Due to the presence of recycle, the dynamic response of the system is complicated in nature. Controller design and tuning for such processes has to be done very carefully. One control strategy of handling processes with recycle is to design a recycle compensator to nullify the detrimental effects of recycle. A block diagram of a recycle process with a recycle compensator is shown in Figure 5.2.2 in the context of the tubular reactor. For more information on recycle compensator theory and design, the reader is advised to refer Taiwo (1984, 1986), Scali and Ferrari (1999) to understand the effects of recycle stream on the controllability of integrated plants and direct compensation of recycles to improve the control performance in such plants.

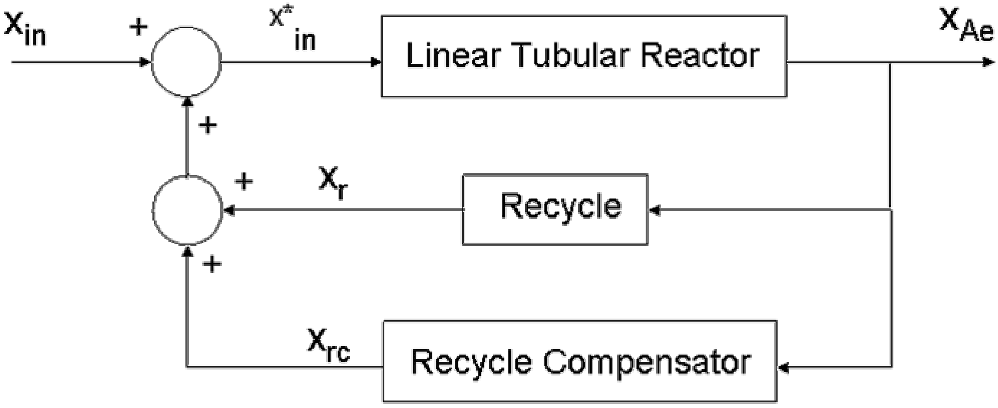


Figure 5.2.2 : An Isothermal Tubular Reactor with Recycle and Recycle compensator

The design of recycle compensator is possible with the knowledge of the recycle path model (G_r). Once recycle path model is available then the recycle compensator is simply $(G_{RC} = -G_r)$ .With the addition of recycle compensator to the above complicated tubular reactor with recycle system the model equations changes to the following form,

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^2 x(z,t)}{\partial z^2} - Bx(z,t) \qquad \textbf{Eqn – 5.2.7}$$

$$\tau_R \frac{\partial x_r(t)}{\partial t} + x_r(t) = K_R x(1,t) \qquad \textbf{Eqn – 5.2.8}$$

$$\tau_R \frac{\partial x_{rc}(t)}{\partial t} + x_{rc}(t) = K_R x(1,t) \qquad \textbf{Eqn – 5.2.9}$$

where **x** is the reactant concentration inside the tubular reactor, $\mathbf{x_r}$ is the reactant concentration in the recycle loop, $\mathbf{x_{rc}}$ is the reactant concentration signal from the recycle compensator. With initial condition: $x(z,0) = x_1(z)$, $x_r(t=0) = x(1,t)$, $x_{rc}(t=0) = -x(1,t)$. The boundary conditions also changes as follows,

$$\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x_{in}^{*}(t)\right) \text{ and } \frac{\partial x(1,t)}{\partial z} = 0$$ **Eqn – 5.2.10**

where $x_{in}^{*}(t) = (1-R) * x_{in}(t) + R * x_{r}(t) + R * x_{rc}(t)$

Since $G_{RC}(s) = -G_{R}(s)$, we have $\mathrm{x_{rc}} = -\mathrm{x_{r}}$ Therefore **Eqn – 5.2.9** and **Eqn – 5.2.10** cancel out one another leaving **Eqn – 5.2.8** to be solved.

In the boundary condition, $x_{in}^{*} = (1-R) * x_{in}$ as the other two terms cancel out.

Therefore the final set of equations is,

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^{2} x(z,t)}{\partial z^{2}} - Bx(z,t)$$ **Eqn – 5.2.11**

with initial condition: $x(z,0) = x_{1}(z)$, where **x** is the reactant concentration inside the tubular reactor. The boundary conditions also changes as follows,

$$\frac{\partial x(0,t)}{\partial z} = Pe\left(x(0,t) - x_{in}^{*}(t)\right) \text{ and } \frac{\partial x(1,t)}{\partial z} = 0$$ **Eqn – 5.2.12**

where $x_{in}^{*}(t) = (1-R) * x_{in}(t)$

The above system of equation is not homogeneous; hence make the system homogeneous by shifting the non homogeneous part of the boundary condition into the partial differential equation using a Dirac delta function. With the above modification, the system becomes

$$\frac{\partial x(z,t)}{\partial t} = -\frac{\partial x(z,t)}{\partial z} + \frac{1}{Pe}\frac{\partial^{2} x(z,t)}{\partial z^{2}} - Bx(z,t) + \delta(z) x_{in}^{*}(t)$$ **Eqn – 5.2.13**

where $x_{in}^{*}(t) = (1-R) * x_{in}(t)$, with initial condition: $x(z,0) = x_{1}(z)$, where **x** is concentration of reactant inside the tubular reactor. The boundary conditions also changes as follows, $\frac{\partial x(0,t)}{\partial z} = Pe * x(0,t)$ and $\frac{\partial x(1,t)}{\partial z} = 0$ **Eqn – 5.2.14**

Consider the last term in **Eqn – 5.2.13** $\delta(z) x_{in}^{*}(t) = \delta(z)[(1 - R(t)) * x_{in}(t)]$

where R and x_{in} are both functions of time. Then the system becomes nonlinear as it involves the product of $(1 - \mathrm{R})$ and x_{in} which has to be linearized around a steady state operating point before application of modal analysis.

Linearize $F(R,x_{in}) = (1 - R(t)) * x_{in}(t)$, using Taylor series expansion.

$$F(R,x_{in}) = F(R_s,x_{ins}) + \left.\frac{\partial F}{\partial R}\right|_{\substack{R=R_s \\ X_{in}=X_{ins}}} (R - R_s) + \left.\frac{\partial F}{\partial x_{in}}\right|_{\substack{R=R_s \\ X_{in}=X_{ins}}} (x_{in} - x_{ins}) \quad \textbf{Eqn - 5.2.15}$$

$$F(R,x_{in}) = F(R_s,x_{ins}) + (-x_{ins})(R - R_s) + (1 - R_s)(x_{in} - x_{ins}) \quad \textbf{Eqn – 5.2.16}$$

Now considering the steady state condition of **Eqn – 5.2.13** we have,

$$-\frac{dx_s(z,t)}{dz} + \frac{1}{Pe}\frac{d^2x_s(z,t)}{dz^2} - Bx_s(z,t) + \delta(z)x_{ins}^*(t) = 0 \quad \textbf{Eqn – 5.2.17}$$

Substitute **Eqn – 5.2.16** into **Eqn – 5.2.13** and subtract **Eqn – 5.2.17** from this and put $\hat{x} = x - x_s, \hat{R} = R - R_s \;\&\; \hat{x}_{in} = x_{in} - x_{ins}$, where x_s, R_s & x_{ins} are steady state values of reactant concentration, recycle ratio and inlet concentration. Finally we have,

$$\frac{\partial(\hat{x})}{\partial t} = -\frac{\partial(\hat{x})}{\partial z} + \frac{1}{Pe}\frac{\partial^2(\hat{x})}{\partial z^2} - B(\hat{x}) + \delta(z)[(-x_{ins})(\hat{R}) + (1 - R_s)(\hat{x}_{in})] \quad \textbf{Eqn – 5.2.18}$$

with initial condition: $\hat{x}(z,0) = x_1(z)$, where $\hat{x}$ is concentration of reactant inside the tubular reactor. The boundary conditions are,

$$\frac{\partial\hat{x}(0,t)}{\partial z} = Pe * \hat{x}(0,t) \text{ and } \frac{\partial\hat{x}(1,t)}{\partial z} = 0 \quad \textbf{Eqn – 5.2.19}$$

Now the above system **Eqn – 5.2.18** & **Eqn – 5.2.19** is amenable to modal decomposition or variable separable method. Suppressing the (^) notation, let us assume the solution to x(z,t) as $x(z,t) = \sum_{n=1}^{\infty} a_n(t)\phi_n(z)$.

Similarly the inlet concentration and recycle ratio can also be expanded as

$$\delta(z)R(t)=\sum_{n=1}^{\infty}b_n(t)\phi_n(z) \text{ and } \delta(z)x_{in}(t)=\sum_{n=1}^{\infty}c_n(t)\phi_n(z).$$

Introducing these approximate solutions into **Eqn – 5.2.18** we have,

$$\frac{\phi_n(z)da_n(t)}{dt}=$$
$$-a_n(t)\frac{d\phi_n(z)}{dz}+\frac{a_n(t)}{Pe}\frac{d^2\phi_n(z)}{dz^2}-Ba_n(t)\phi_n(z)-x_{ins}b_n(t)\phi_n(z)+(1-R_s)c_n(t)\phi_n(z)$$

Eqn – 5.2.20

Dividing **Eqn – 5.2.20** by $a_n(t)\phi_n(z)$ yields an ODE which can be divided into a left side which depends solely on "t" and right side that is a function of "z" alone. For this equality to hold for all (z,t), both sides must be equal to constant ($-\lambda_n$), resulting in:

$$\frac{1}{a_n(t)}\left[\frac{da_n(t)}{dt}+x_{ins}b_n(t)-(1-R_s)c_n(t)\right]=\frac{1}{\phi_n(z)}\left[-\frac{d\phi_n(z)}{dz}+\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2}-B\phi_n(z)\right]=-\lambda_n$$

Eqn – 5.2.21

Now **Eqn – 5.2.21** can be separated into the following ODE's:

$$\frac{1}{Pe}\frac{d^2\phi_n(z)}{dz^2}-\frac{d\phi_n(z)}{dz}+(\lambda_n-B)\phi_n(z)=0$$ **Eqn – 5.2.22**

$$\frac{da_n(t)}{dt}+\lambda_n a_n(t)=(1-R_s)c_n(t)-x_{ins}b_n(t)$$ **Eqn – 5.2.23**

The boundary condition is as follows, $\frac{d\phi_n(0)}{dz}=Pe*\phi_n(0)$ and $\frac{d\phi_n(1)}{dz}=0$

The above system formulates the eigenvalue problem. The solution to **Eqn – 5.2.22** subject to the above boundary conditions is obtained by putting it into Sturm-Liouville form. A detailed analysis can be obtained from Ray (1981).

The solution $\phi_n(z)$ is of this form: $\phi_n(z)=B_n\, exp\left(\frac{Pe*z}{2}\right)\left[cos(\alpha_n z)+\frac{Pe}{2\alpha_n}sin(\alpha_n z)\right]$

where α_n is obtained by solving $tan(\alpha_n) = \dfrac{\alpha_n Pe}{\alpha_n^2 - \dfrac{Pe^2}{4}}$

λ_n is given by, $\lambda_n = \dfrac{\alpha_n^2}{Pe} + \dfrac{Pe}{4} + B$

B_n is given by, $B_n = \left[\int_0^1 \left(cos(\alpha_n z) + \dfrac{Pe}{2\alpha_n} sin(\alpha_n z) \right)^2 dz \right]^{-1/2}$

Along with B_n, $b_n(t)$'s and $c_n(t)$'s also satisfy the orthonormal property and are obtained as follows,

$$b_n(t) = \int_0^1 \delta(z) R(t) \phi_n(z) \exp(-Pe * z) dz = R(t) * \phi_n(0)$$

$$c_n(t) = \int_0^1 \delta(z) x_{in}(t) \phi_n(z) exp(-Pe * z) dz = x_{in}(t) * \phi_n(0).$$

Once b_n's and c_ns are obtained, **Eqn – 5.2.23** can be used either for obtaining dynamic responses of the system or for control studies. R_s and x_{ins} are the steady state values. Laplace transforms of **Eqn – 5.2.23** yields,

$$(s + \lambda_n) a_n(s) = (1 - R_s) c_n(s) - x_{ins} b_n(s) \quad \textbf{Eqn – 5.2.24}$$

On simplifying **Eqn – 5.2.24**, $a_n(s) = \dfrac{1 - R_s}{s + \lambda_n} c_n(s) - \dfrac{x_{ins}}{s + \lambda_n} b_n(s)$.

Upon careful observation of the above equation we see that the output a_n's (Plant output – x(z,t)) is affected by c_n's (recycle ratio - R) and b_n's (inlet concentration - x_{in}). As we anticipate a measured disturbance in the inlet concentration ($x_{in}(t)$) affecting the plant, a feedforward controller can now be designed using recycle ratio (R(t)) as manipulated variable. Figure 5.2.3 exemplifies the modal representation of a tubular reactor with recycle and a recycle compensator.

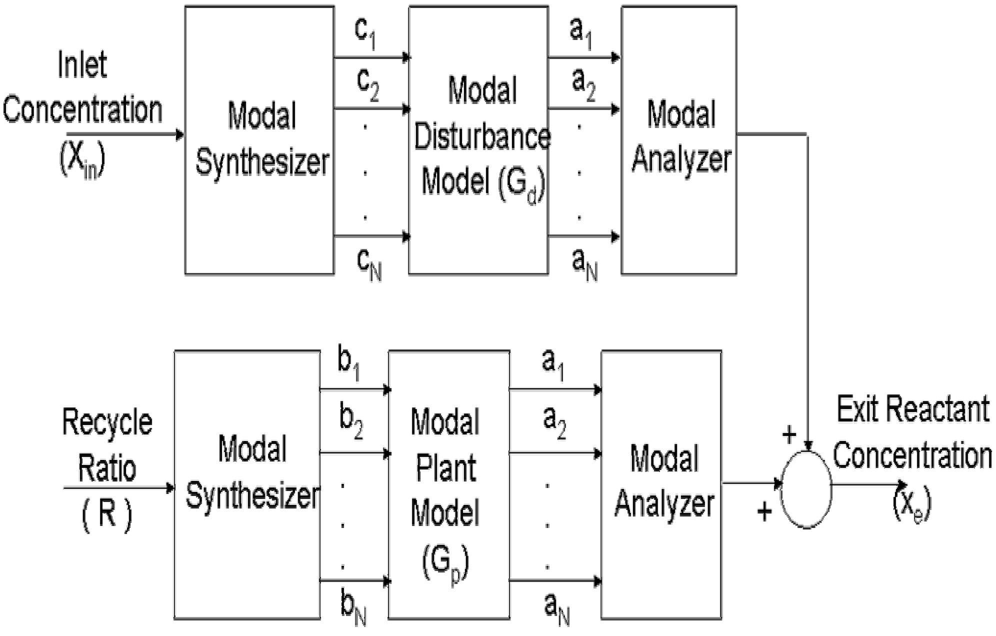


Figure 5.2.3: Modal representation of the Plant with Disturbance

Hence the modal process model is, $G_p(s) = \frac{a_n(s)}{b_n(s)} = \frac{-x_{ins}}{s+\lambda_n}$ **Eqn – 5.2.25**

and the modal disturbance model is, $G_d(s) = \frac{a_n(s)}{c_n(s)} = \frac{1-R_s}{s+\lambda_n}$ **Eqn – 5.2.26**

With the knowledge of G_p and G_d one can design feedforward controller as

$$MFFC = \frac{-G_d(s)}{G_p(s)} = \frac{-(1-R_s)}{-x_{ins}} = \frac{1-R_s}{x_{ins}} \qquad \textbf{Eqn – 5.2.27}$$

To handle load disturbances that cannot be measured or anticipated, feedforward control is always combined with feedback control in practical applications. For designing a feedback controller one should have the process model (G_p). Since (G_p) in this case is a simple first order without any time delays the feedback control design is very simple. The Ciancone PID tuning correlations provided by Marlin (1995) is employed here. The final block diagram illustrating the above control strategy (modal feedforward and modal feedback control of a tubular reactor with recycle and a recycle compensator) is shown in Figure 5.2.4,

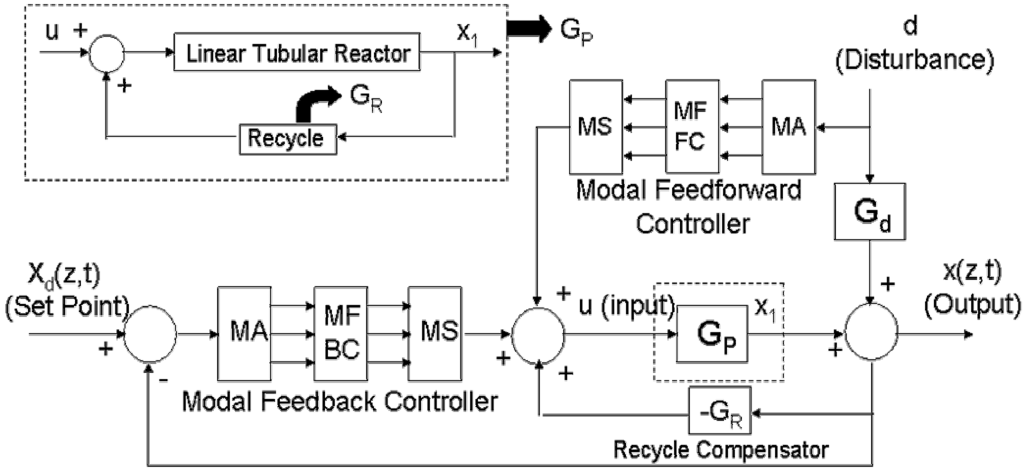


Figure 5.2.4: Feedback and Feedforward Modal Control of Distributed parameter systems with recycle and Recycle Compensator

5.3 Results and Discussions

The modal control of tubular reactor with recycle was also carried out in two ways,

1. Control the tubular reactor with recycle system using inlet concentration as manipulated variable with constant recycle ratio.
2. Control the tubular reactor with recycle system using recycle ratio as manipulated variable assuming disturbances in inlet concentration.

The above control studies carried out are similar to the two ways of modal analysis of tubular reactor with recycle discussed earlier in section 4.5 of chapter 4.

A very important question which arises in some of these control studies mentioned above is how, one should provide the set points (with an intention to control reactor concentrations at different points in the reactor) for this system having only one manipulated variable. From degrees of freedom analysis, one finds that this is impossible as one cannot control concentrations at different points in the reactor using only one manipulated variable. After a careful study, it was found that for a particular value of inlet concentration (manipulated variable) there is always a fixed concentration profile i.e. a fixed set of concentration values at different points in the reactor (controlled variable). Now this control problem satisfies the degrees of freedom rule as we are trying to control a single profile using inlet concentration and this profile of concentration is referred in the following sections as "set point profile". From the modal analysis studies carried out in section 4.5, on tubular reactor with recycles, we find that four to five modes are sufficient to describe its dynamic response. Hence we chose five measurement locations inside the tubular reactor randomly and attempt to control the concentrations at these five locations. So the set points at these five locations inside the reactor represent the "set point profile" mentioned above. As this set point profile is very unique to a particular value of inlet concentration, one can define a particular set point profile only from the previous knowledge of the dynamics of the tubular reactor. If an arbitrary set point profile is given, the controller will try to get as "close" as possible to it (in a least square sense).

The case 1 control strategy mentioned above was carried out by designing a modal feedback controller to maintain the reactor concentrations of the system at specified values (set point profile) using inlet concentration as the manipulated variable. Figures 5.3.1, 5.3.2 and 5.3.3 show some of the results pertaining to this control study. In Figure 5.3.1 we show the dynamic variation of concentrations at different locations in the reactor. This study was carried out in the absence of recycle compensator. The next figure, (Figure 5.3.2) also shows the dynamic variation of concentrations but this study was carried out in the presence of recycle compensator. The last figure, (Figure 5.3.3) compares the variation of the manipulated variable (inlet concentration) in the presence and absence of recycle compensator.

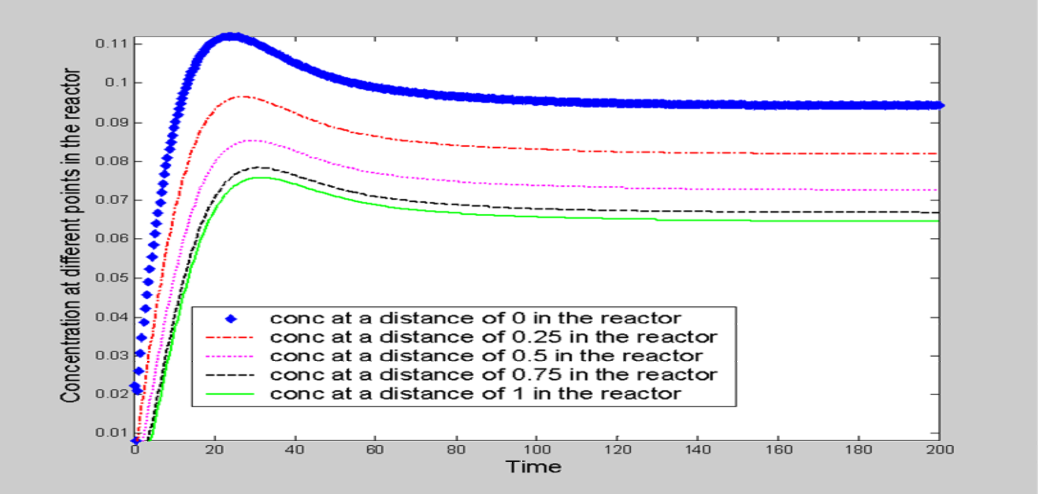


Figure 5.3.1 : Set point tracking of reactor conc by manipulating inlet conc without recycle compensator

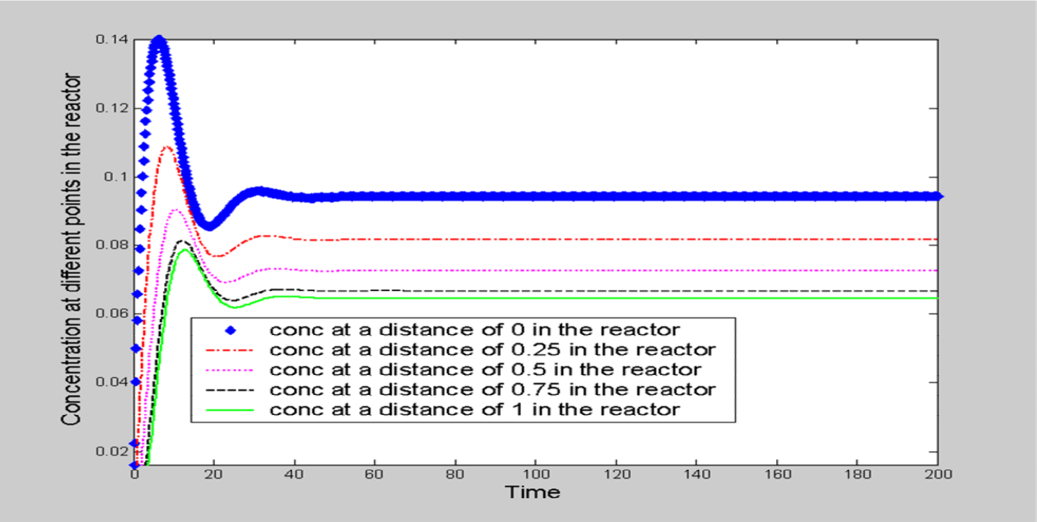


Figure 5.3.2 : Set point tracking of reactor conc by manipulating inlet conc with recycle compensator

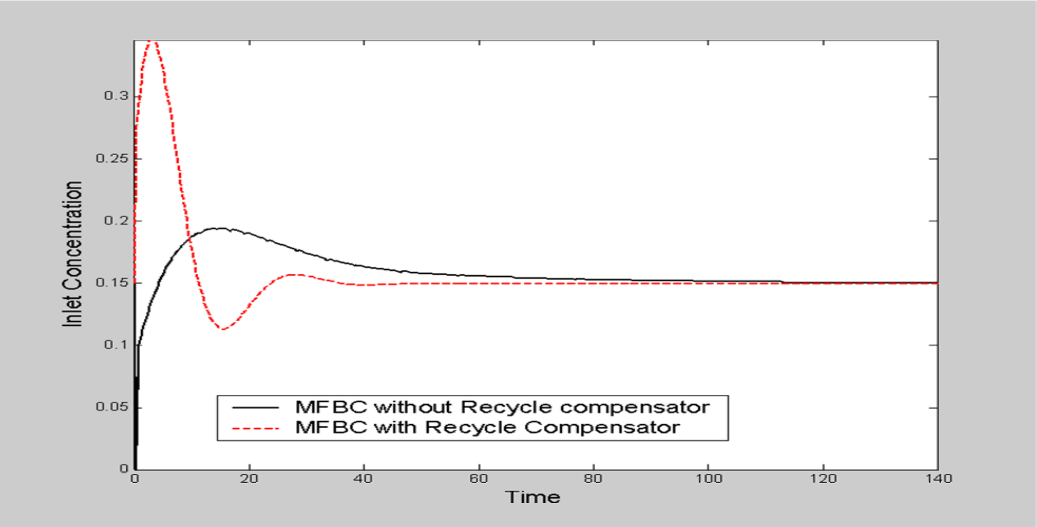


Figure 5.3.3 : Plot of manipulated variable (Inlet conc final value - 0.15) vs. time

We proposed a novel strategy (case 2 control strategy) to handle disturbances anticipated in the inlet concentration by designing a modal feedforward controller which manipulates the recycle ratio. The recycle ratio is no more a constant but a function of time. This makes the system nonlinear and hence should be linearized around a steady state before applying modal analysis theory. The above principle is explained in detail in section 5.2 with complete derivation (equations 5.2.1 to 5.2.27) and the block diagram representing this control strategy (Figure 5.2.4).

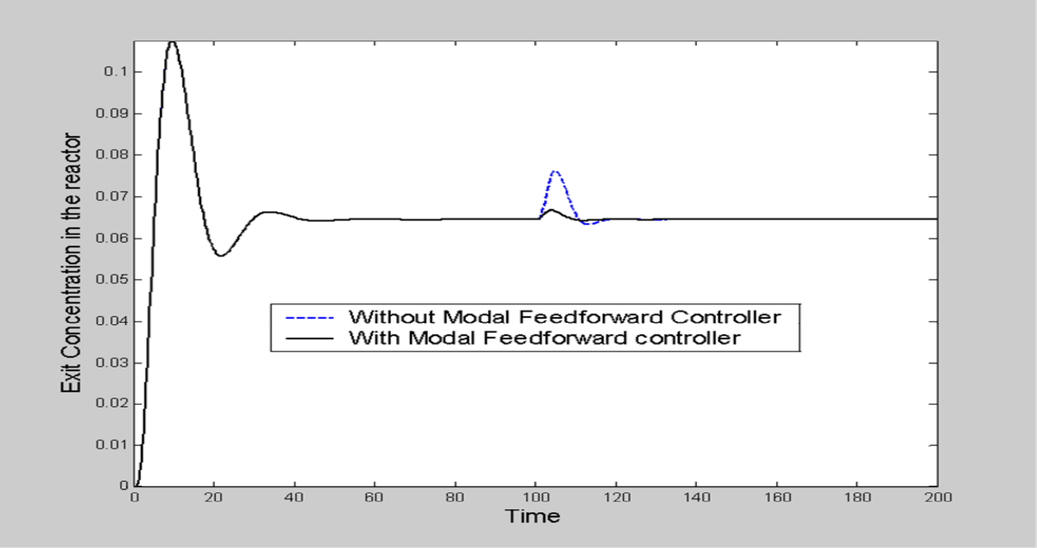


Figure 5.3.4 : Disturbance rejection in exit reactor concentration by manipulating recycle ratio (final value - 0.90625)

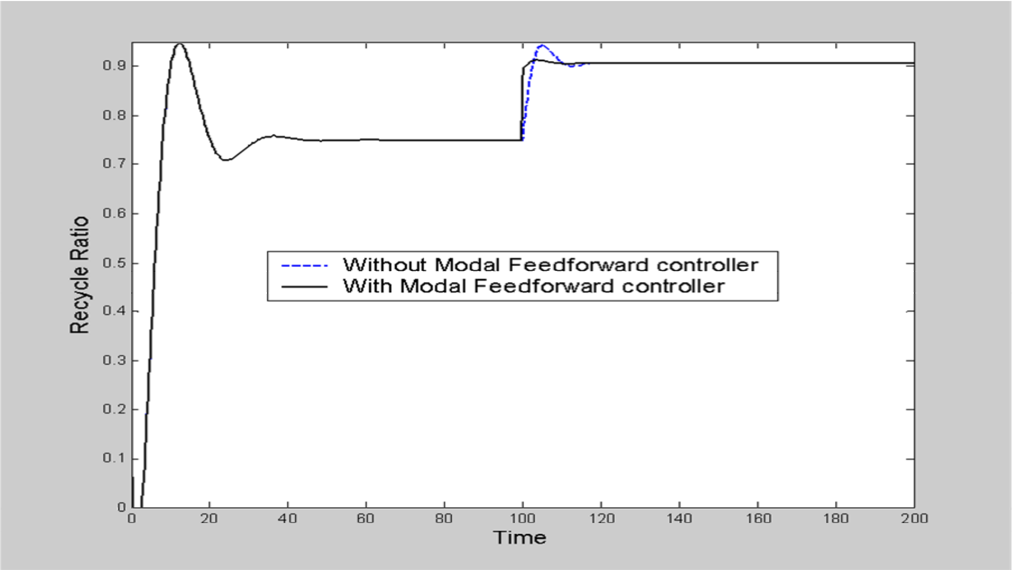


Figure 5.3.5 : Plot of manipulated variable (recycle ratio final value - 0.90625) vs. time

Figure 5.3.4 shows the results obtained by simulating the block diagram (Figure 5.2.4) in MATLAB. It shows the response of exit concentration subjected to a disturbance in inlet concentration at 100 time units. For the first 100 time units the simulation was run for a particular set point profile until the steady state was reached. This figure has two lines one dashed line and the other solid line. During the initial phase both the lines overlap on one another. The dashed line shows the response without modal feedforward controller (only modal feedback controller and recycle compensator). The solid line is the one which includes modal feedforward controller along with modal feedback controller and recycle compensator. The response of the system with modal feedforward controller (solid line) is obviously better than the response of the system without modal feedforward controller (dashed line).

The next figure, (Figure 5.3.5) shows the comparative study of the movement of the manipulated variable for the case of system without modal feedforward controller (dashed line) and with feedforward controller (solid line). For the first 100 time units the simulation was run for a particular set point profile until the steady state was reached. During the initial phase both the lines overlap on one another. One can observe a very smooth movement in the case of solid line compared to the dashed line. Thus one will be able to achieve the desired set point profiles even in presence of disturbances with a combination of modal feedforward/feedback and recycle compensator control strategy.

5.4 Modal control of a linear heat exchanger

A linear tubular single-pass shell and tube heat exchanger with axial diffusion is considered. The main objective would be to control the tube-side outlet temperature at a desired value, in-spite of disturbances and changes in set points. The load disturbances are assumed to be fluctuations in the feed temperature and the manipulated variable is taken to be the steam temperature in the shell, which is a function of time only. The liquid stream enters the tube of the heat exchanger and is heated by convection from the inner wall. Heat is supplied to the tube by means of condensing steam in the jacket. Some of the assumptions made in deriving the mathematical model (Hahn et al., 1971) are stated in section 3.10. Based on these assumptions and an energy balance over a differential section of the tube side of the exchanger yields:

$$\frac{\partial T_l}{\partial \tau} = D\frac{\partial^2 T_l}{\partial l^2} - \upsilon\frac{\partial T_l}{\partial l} + \frac{h_{wl}P_l}{C_{pl}\rho_l A_l}\left(T_w - T_l\right) \qquad \textbf{Eqn – 5.4.1}$$

Taking an energy balance over a differential section of wall gives:

$$\frac{\partial T_w}{\partial \tau} = \frac{h_{ws}P_s}{C_{pw}\rho_w A_w}\left(T_s - T_w\right) + \frac{h_{wl}P_l}{C_{pw}\rho_w A_w}\left(T_l - T_w\right) \qquad \textbf{Eqn – 5.4.2}$$

subject to following boundary conditions:

$$\frac{\partial T_l(0,\tau)}{\partial l} = \frac{\upsilon}{D}\left(T_l(0,\tau) - T_l^f(\tau)\right) \text{ and } \frac{\partial T_l(L,\tau)}{\partial l} = 0 \qquad \textbf{Eqn – 5.4.3}$$

The above equations are dimensionalized by introducing these parameters,

Mean residence time: $\tau_r = L/\upsilon$ sec, Axial Peclet Number: $\beta = \upsilon L/D$, Dimensionless time: $t = \tau/\tau_r$, Dimensionless axial distance: $x = l/L$, Dimensionless liquid temperature: $u_1 = T_l/T_r$, Dimensionless wall temperature: $u_2 = T_w/T_r$, Dimensionless steam temperature: $\theta = T_s/T_r$, The other parameters are:

$$\frac{1}{\tau_1} = \frac{h_{wl}P_l}{C_{pl}\rho_l A_l} sec^{-1}, \frac{1}{\tau_{21}} = \frac{h_{wl}P_l}{C_{pw}\rho_w A_w} sec^{-1}, \frac{1}{\tau_{22}} = \frac{h_{ws}P_s}{C_{pw}\rho_w A_w} sec^{-1}.$$

Hence the system of equations with boundary conditions is:

$$\frac{\partial u_1}{\partial t} = \frac{1}{\beta}\frac{\partial^2 u_1}{\partial x^2} - \frac{\partial u_1}{\partial x} + \frac{\tau_r}{\tau_1}\left(u_2 - u_1\right) \qquad \textbf{Eqn – 5.4.4}$$

$$\frac{\partial u_2}{\partial t}=\frac{\tau_r}{\tau_{22}}(\theta-u_2)+\frac{\tau_r}{\tau_{21}}(u_1-u_2)$$ **Eqn – 5.4.5**

subject to: $$\frac{\partial u_1(0,t)}{\partial x}=\beta\left(u_1(0,t)-u_1^f(t)\right) \text{ and } \frac{\partial u_1(1,t)}{\partial x}=0$$ **Eqn – 5.4.6**

where u_1^f is the inlet fluid temperature and θ is the steam temperature. The numerical values used in this study are as follows $\beta=1,\tau_r=3\,sec,\tau_1=3.69\,sec,\tau_{21}=2.65\,sec$ $\tau_{22}=1.05\,sec,\ u_1^f=0.53,\theta=0.795,\frac{\tau_r}{\tau_1}=0.813,\frac{\tau_r}{\tau_{21}}=1.1321,\frac{\tau_r}{\tau_{22}}=2.8571$.

The above system of equation is not homogeneous; hence make the system homogeneous by shifting the non homogeneous part of the boundary condition into the partial differential equation using a Dirac delta function.

With the above modification the system becomes,

$$\frac{\partial u_1}{\partial t}=\frac{1}{\beta}\frac{\partial^2 u_1}{\partial x^2}-\frac{\partial u_1}{\partial x}+\frac{\tau_r}{\tau_1}(u_2-u_1)+\delta(x)u_1^f(t)$$ **Eqn – 5.4.7**

$$\frac{\partial u_2}{\partial t}=\frac{\tau_r}{\tau_{22}}(\theta-u_2)+\frac{\tau_r}{\tau_{21}}(u_1-u_2)$$ **Eqn – 5.4.8**

subject to: $$\frac{\partial u_1(0,t)}{\partial x}=\beta(u_1(0,t))\text{and}\frac{\partial u_1(1,t)}{\partial x}=0$$ **Eqn – 5.4.9**

Now the above system **Eqn – 5.4.7**, **Eqn – 5.4.8** and **Eqn – 5.4.9** is amenable to modal decomposition or variable separable method.

Let us assume the solution to be of this form:

$$u_1(x,t)=\sum_{n=1}^{\infty}a_n(t)\phi_n(x) \text{ and } u_2(x,t)=\sum_{n=1}^{\infty}b_n(t)\phi_n(x)$$

Similarly the inlet temperature and steam temperature can also be expanded as:

$$\delta(x)u_1^f(t)=\sum_{n=1}^{\infty}c_n(t)\phi_n(x) \text{ and } \theta(t)=\sum_{n=1}^{\infty}d_n(t)\phi_n(x)$$

Introducing these approximate solutions into **Eqn – 5.4.7**, **Eqn – 5.4.8** and in the boundary conditions **Eqn – 5.4.9** we have,

$$\frac{\phi_n(x)da_n(t)}{dt} = -a_n(t)\frac{d\phi_n(x)}{dx} + \frac{a_n(t)}{\beta}\frac{d^2\phi_n(x)}{dx^2} + 0.813[b_n(t) - a_n(t)]\phi_n(x) + c_n(t)\phi_n(x)$$

Eqn – 5.4.10

$$\frac{\phi_n(x)db_n}{dt} = \frac{\tau_r}{\tau_{22}}(d_n(t) - b_n(t))\phi_n(x) + \frac{\tau_r}{\tau_{21}}(a_n(t) - b_n(t))\phi_n(x)$$ **Eqn – 5.4.11**

$$\frac{d\phi_n(0)}{dx} = \beta * \phi_n(0) \text{ and } \frac{d\phi_n(1)}{dx} = 0$$ **Eqn – 5.4.12**

Dividing **Eqn – 5.4.10** by $a_n(t)\phi_n(x)$ yields an ODE which can be divided into a left side which depends solely on "t" and a right side that is a function of "x" alone. For this equality to hold for all x and t, both sides must be equal to constant ($-\lambda_n$), resulting in:

$$\frac{1}{a_n(t)}\left[\frac{da_n(t)}{dt} - c_n(t) - 0.813b_n(t)\right] = -\lambda_n$$ **Eqn – 5.4.13**

and

$$\frac{1}{\phi_n(x)}\left[-\frac{d\phi_n(x)}{dx} + \frac{1}{\beta}\frac{d^2\phi_n(x)}{dx^2} - 0.813\phi_n(x)\right] = -\lambda_n$$ **Eqn – 5.4.14**

The above ODE's can be simplified:

$$\frac{1}{\beta}\frac{d^2\phi_n(x)}{dx^2} - \frac{d\phi_n(x)}{dx} + (\lambda_n - B)\phi_n(x) = 0$$ **Eqn – 5.4.15**

$$\frac{da_n(t)}{dt} + \lambda_n a_n(t) = c_n(t) + 0.813b_n(t)$$ **Eqn – 5.4.16**

The boundary condition remains the same as above (**Eqn – 5.4.12**).

Dividing **Eqn – 5.4.11** by $\phi_n(x)$ yields an ODE which can be written as,

$$\frac{db_n(t)}{dt} = \frac{\tau_r}{\tau_{22}}(d_n(t) - b_n(t)) + \frac{\tau_r}{\tau_{21}}(a_n(t) - b_n(t))$$ **Eqn – 5.4.17**

Eqn – 5.4.15 subjected to boundary condition **Eqn – 5.4.12**, has following solution:

$$\phi_n(x) = B_n\, exp\left(\frac{\beta * x}{2}\right)\left[cos(\alpha_n x) + \frac{\beta}{2\alpha_n} sin(\alpha_n x)\right],$$

where α_n is obtained by solving $tan(\alpha_n) = \dfrac{\alpha_n \beta}{\alpha_n^2 - \dfrac{\beta^2}{4}}$,

λ_n is given by $\lambda_n = \dfrac{\alpha_n^2}{\beta} + \dfrac{\beta}{4} + 0.813$

B_n is given by $B_n = \left[\displaystyle\int_0^1 \left(cos(\alpha_n x) + \frac{\beta}{2\alpha_n} sin(\alpha_n x)\right)^2 dx\right]^{-1/2}$

Along with B_n, $d_n(t)$'s and $c_n(t)$'s also satisfy the orthonormal property and are obtained as follows,

$$c_n(t) = \int_0^1 \delta(x) u_1^f(t) \phi_n(x) exp(-\beta * x) dx = u_1^f(t) * \phi_n(0).$$

$$d_n(t) = \theta(t) \int_0^1 \phi_n(x) exp(-\beta * x) dx$$

On simplification this yields,

$$d_n(t) = \theta(t) B_n \int_0^1 exp\left(\frac{-\beta * x}{2}\right)\left[cos(\alpha_n x) + \frac{\beta}{2\alpha_n} sin(\alpha_n x)\right] dx$$

Once the $\phi_n{}'s$, c_n's and d_n's are obtained then take Laplace transforms of **Eqn – 5.4.16** and **Eqn – 5.4.17** which results in following equations,

$$(s + \lambda_n) a_n(s) = c_n(s) + 0.813 b_n(s) \qquad \textbf{Eqn – 5.4.18}$$

$$\left(s + \left(\frac{\tau_r}{\tau_{22}} + \frac{\tau_r}{\tau_{21}}\right)\right) b_n(s) = \frac{\tau_r}{\tau_{22}} d_n(s) + \frac{\tau_r}{\tau_{21}} a_n(s) \qquad \textbf{Eqn – 5.4.19}$$

$$(s + 3.9892) b_n(s) = 2.8571 d_n(s) + 1.1321 a_n(s) \qquad \textbf{Eqn – 5.4.20}$$

Eliminating $b_n(s)$ from both **Eqn – 5.4.20** and **Eqn – 5.4.18** we have,

$$a_n(s)=\frac{2.8571*0.813*d_n(s)+(s+3.9892)*c_n(s)}{s^2+(3.9892+\lambda_n)s+(3.9892*\lambda_n-0.9204)}$$ **Eqn – 5.4.21**

From **Eqn – 5.4.21** we can say that $\frac{a_n(s)}{d_n(s)}$ represents the process transfer function and that $\frac{a_n(s)}{c_n(s)}$ represents the disturbance transfer function in the modal space.

Hence we can say the second order process transfer function as,

$$G_P=\frac{a_n(s)}{d_n(s)}=\frac{2.8571*0.813}{s^2+(3.9892+\lambda_n)s+(3.9892*\lambda_n-0.9204)}$$ **Eqn – 5.4.22**

and the second order disturbance transfer function as,

$$G_d=\frac{a_n(s)}{c_n(s)}=\frac{(s+3.9892)}{s^2+(3.9892+\lambda_n)s+(3.9892*\lambda_n-0.9204)}$$ **Eqn – 5.4.23**

These second order transfer functions can be considered as a set of reduced order lumped parameter models for the distributed parameter system.

From **Eqn – 5.4.22** we can say that the second order parameters of the process are:

The time constant for the second order system is, $\tau=\frac{1}{\sqrt{(3.9892*\lambda_n-0.9204)}}$.

The damping coefficient for the systems is, $\zeta=\frac{(3.9892+\lambda_n)}{2*\sqrt{(3.9892*\lambda_n-0.9204)}}$

The gain of the system is, $K_P=\frac{2.8571*0.813}{(3.9892*\lambda_n-0.9204)}$

Now for this set of lumped parameter system models a corresponding set of controller can be designed as these are non interacting multiloop systems.

IMC-PID tunings were calculated for the above system as indicated in Chien et al. (1990). The PI tunings were only considered and is given below,

$$K_C=\frac{2\zeta\tau}{\tau_{CL}K_P}=\frac{3.9892+\lambda_n}{\tau_{CL}*2.8571*0.813}\text{ and }\tau_I=2\zeta\tau=\frac{3.9892+\lambda_n}{3.9892*\lambda_n-0.9204}$$

Hence a simple feedback controller can be designed in the new modal space. Since we have both the process model (G_P) and the disturbance model (G_d) one can easily tackle any measured or anticipated disturbances appearing in the inlet temperature of the reactor and can be easily rejected from the system if a feedforward controller is designed so that it manipulates the steam temperature accordingly.

A simple feedforward controller is given by,

$$MFFC = \frac{-G_d}{G_P} = \frac{s+3.9892}{-2.8571*0.813} = -1.7173(0.2507*s+1) \quad \textbf{Eqn – 5.4.24}$$

Since the above structure is not realizable, a lead-lag transfer function was considered as follows,

$$MFFC1 = \frac{-1.7173*(0.2507*s+1)}{(\beta*0.2507*s+1)} \quad \textbf{Eqn – 5.4.25}$$

A suitable value of β generally ranges from 0.1 to 1 and for most of the simulation purposes in our study a β value of 0.9 was used. Hence we have the feedforward controller as $MFFC1 = \frac{-1.7173*(0.2507*s+1)}{(0.9*0.2507*s+1)} = \frac{-1.7173*(0.2507*s+1)}{0.2256*s+1}$

It was found that in most of the simulations this value of β gave pretty good results as can be verified by the figures shown in the results and discussions section below.

5.5 Results and Discussions

The performance of modal feedback controller for the heat exchanger system will be evaluated first and then the importance of modal feedforward controller in the presence of disturbance is illustrated. Figure 5.5.1 shows the 3D set point tracking of the temperature in the heat exchanger. The simulation was run for a particular set point profile initially (for 0 to 15 time units) until the steady state is reached and then the system was subjected to a change in set point profile. One can see from Figure

5.5.1 that the system is brought to the desired set point profile within 5 time units. Hence the performance of modal feedback controller for the set point tracking is quite good. Figure 5.5.2 shows the disturbance rejection of temperature in the heat exchanger using a modal feedback controller. The disturbance considered here is in the inlet temperature of the reactor (magnitude of 0.2 dimensionless units).

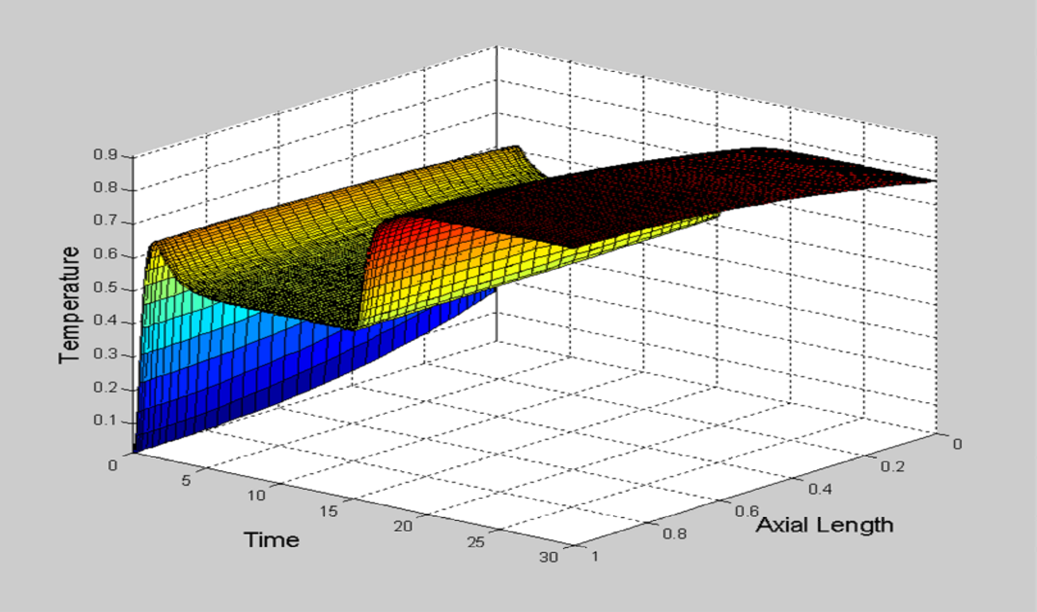


Figure 5.5.1 : Set point tracking of temperature in a linear heat exchanger using a modal feedback controller (MFBC)

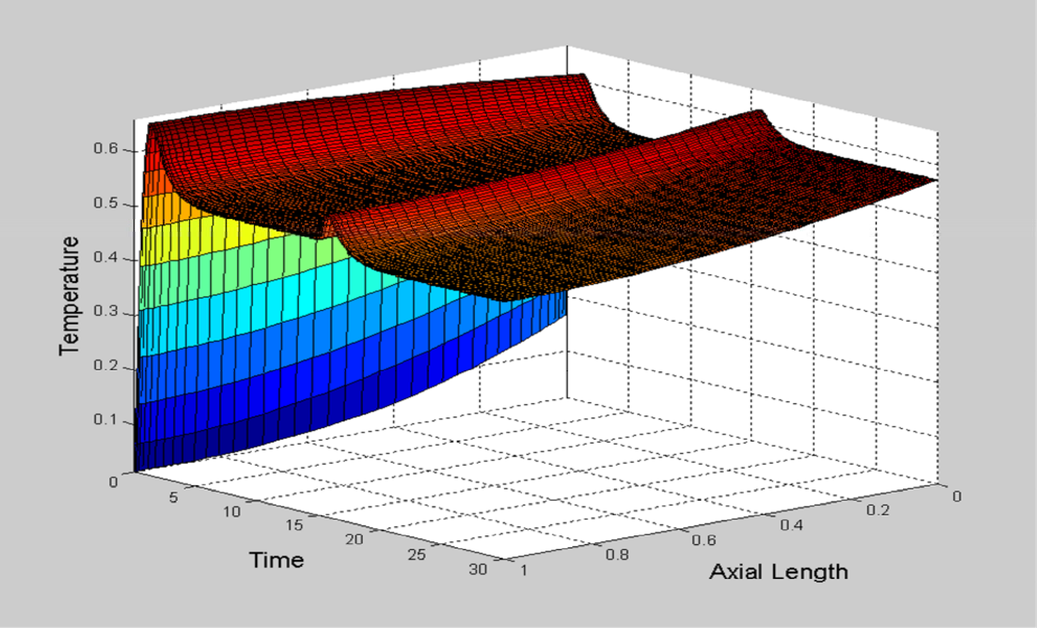


Figure 5.5.2 : Disturbance rejection of temperature in a linear heat exchanger using a modal feedback controller (MFBC)

One can observe from the figure (Figure 5.5.2) that the system is not brought back to the original set point profile even after a long time and an offset is observed. This is one of the interesting results, observed during the simulation. Such a result is possible because, in the presence of disturbance, there might not be a suitable value of manipulated variable (steam temperature) which can bring the system to the initial set point profile. Chakravarti and Ray (1999) have also observed this phenomenon in their studies on boundary control of a tubular reactor. Assuming the disturbance in inlet temperature to be measurable, a novel strategy was designed to handle such disturbances namely modal feedforward controller in combination with modal feedback controller. The problem of offset continued its presence even in this case but the response was better with less overshoot and settling time as seen in Figure 5.5.3 in comparison with Figure 5.5.2. Note that the modal feedforward/feedback controller can still operate with only one manipulated variable and therefore cannot remove the offset.

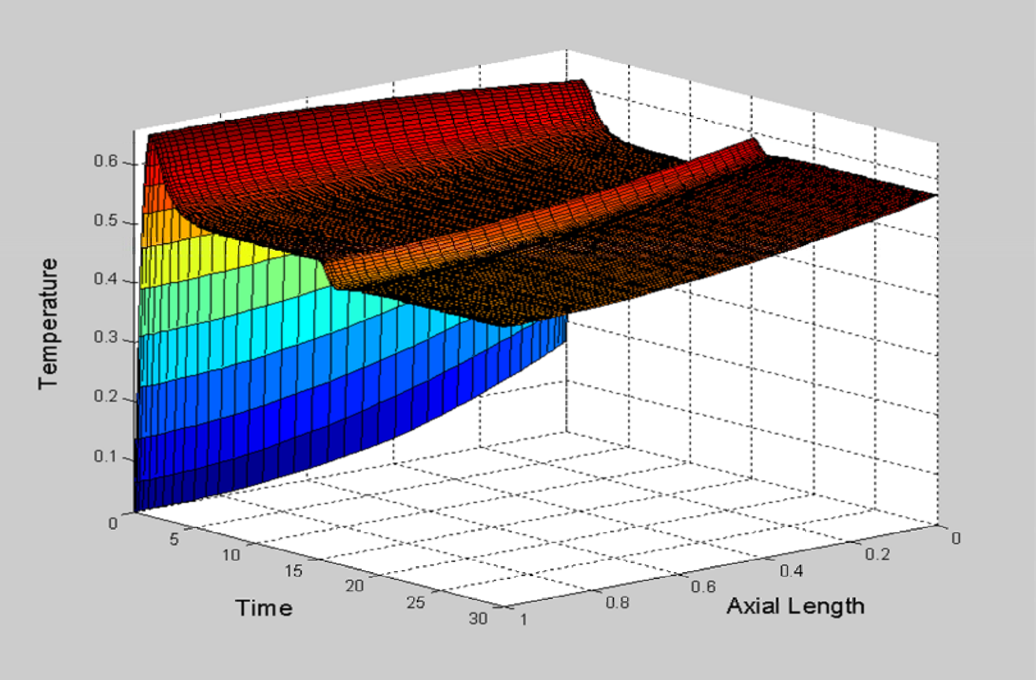


Figure 5.5.3 : Disturbance rejection of temperature in a linear heat exchanger using modal feedforward and feedback controllers (MFBC & MFFC)

One would have a better understanding of the results shown above by 3D graphs, if the same result is split into many 2D plots. Figures 5.5.4 and 5.5.5 show a comparison of results in the absence and presence of modal feedforward controller.

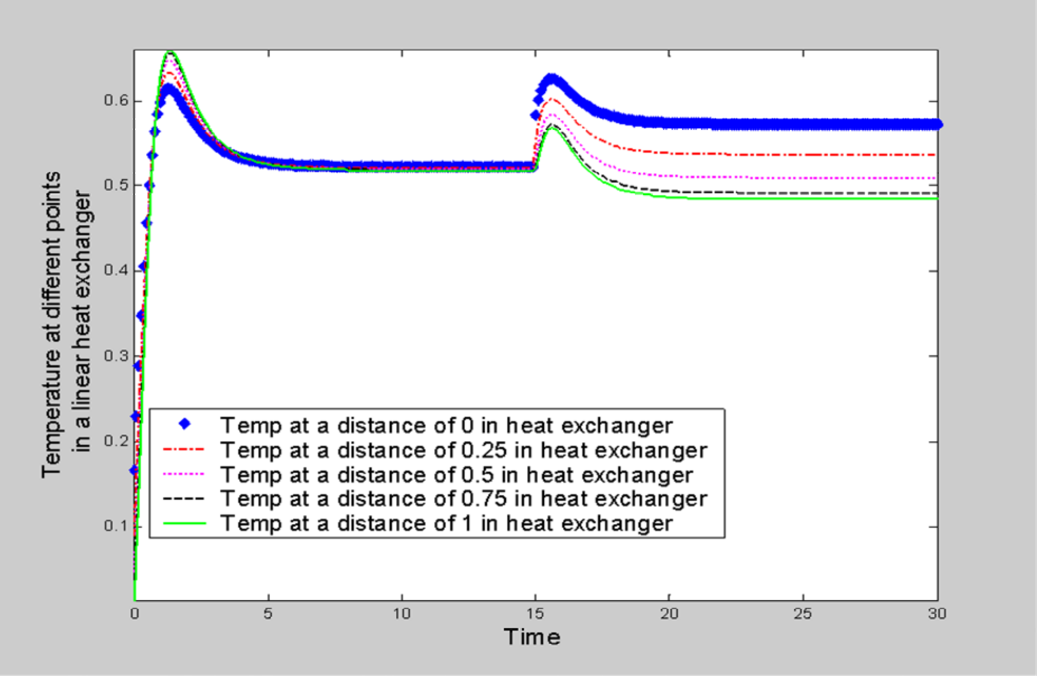


Figure 5.5.4 : 2D plot of disturbance rejection of temperature in a linear heat exchanger using MFBC

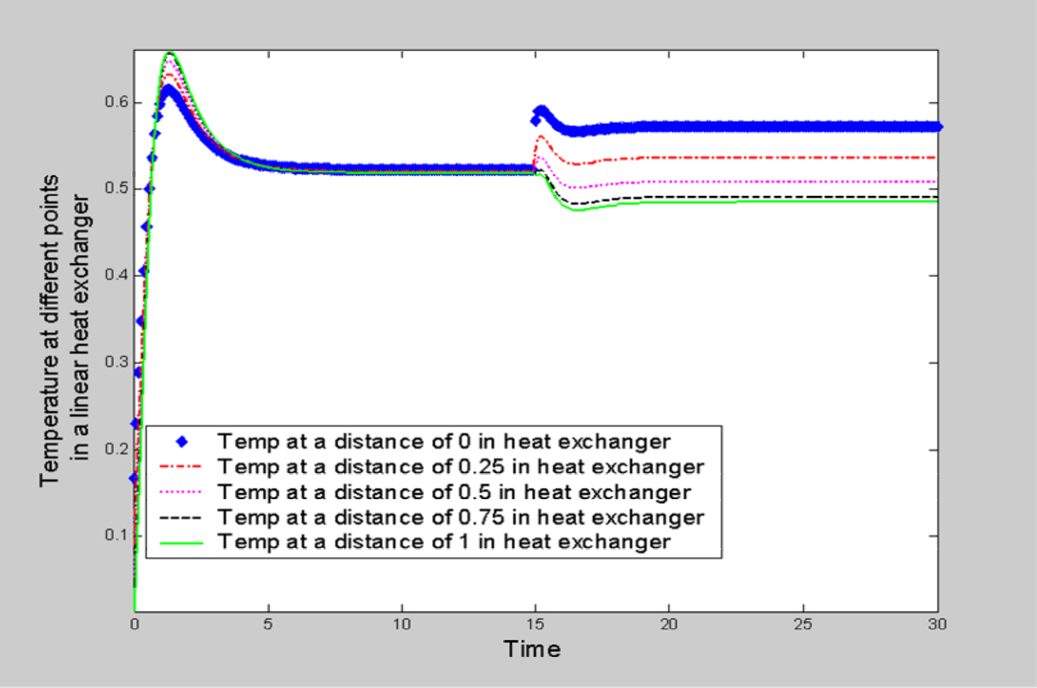


Figure 5.5.5 : 2D plot of disturbance rejection of temperature in a linear heat exchanger using MFBC and MFFC

If one observes the Figures 5.5.4 and 5.5.5 carefully we can find that before the disturbance hits the process (0–15 time units) the temperature is found to have a positive slope (i.e. temperature increases along the length of the reactor). After the disturbance hits the process (15-30 time units) the temperature is found to have negative slope (i.e. temperature decreases along the length of the reactor). Similar observations can be inferred from the 3D Figures 5.5.2 and 5.5.3. This complicates the system and makes it more difficult to control.

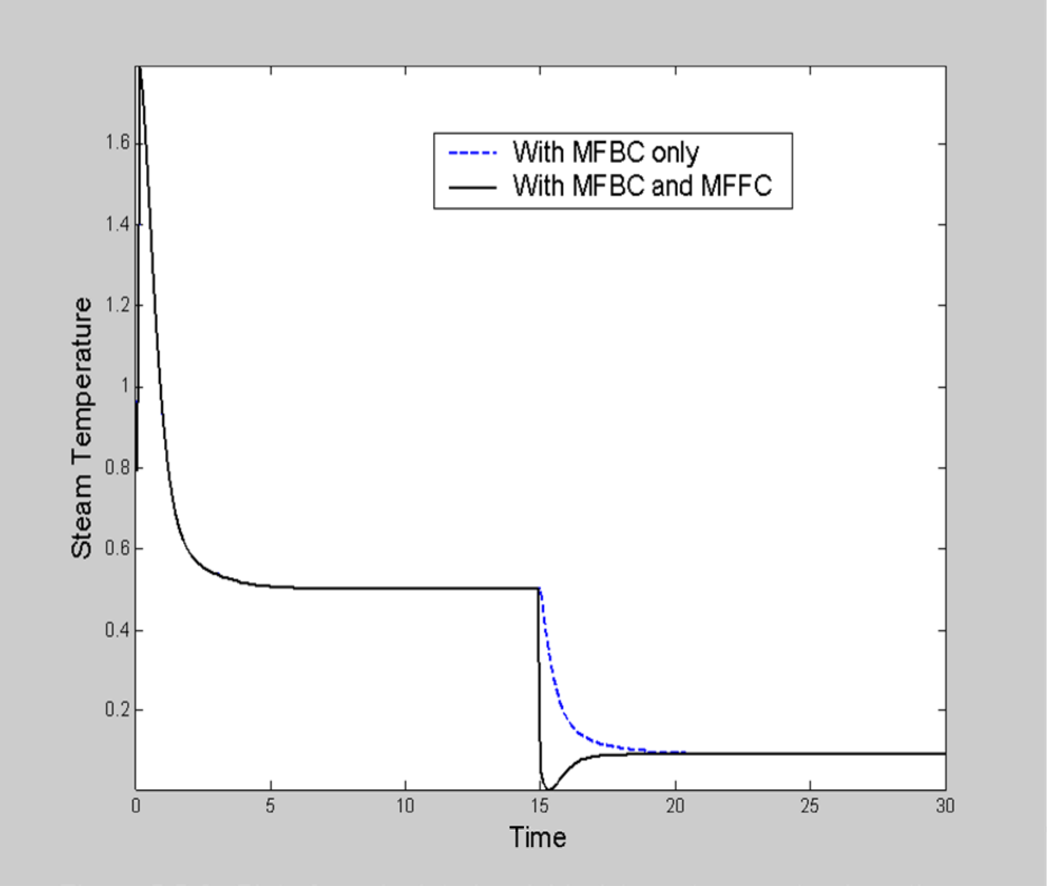


Figure 5.5.6 : Plot of manipulated variable (steam temperature) vs. time with MFBC and with and without MFFC

Figure 5.5.6 shows how the variable (steam temperature) was manipulated to compensate for the disturbance. The dashed line is for the case when only a modal feedback controller was used and the solid line is for the case in which both the modal feedback and modal feedforward controller are used. The solid line shows a little over shoot but reaches the steady state value of the variable much more quickly (faster settling time). Thus one has to manipulate steam temperature in the lines of solid line to have less variation in the temperature of heat exchanger.

5.6 Conclusions

An important contribution of this chapter is in the development and implementation of a modal feedforward control strategy to complement the modal feedback control strategy. While the modal feedback control is well established in the literature, (to the best of our knowledge) there has been no reported application of the modal feedforward control strategy. The application of modal control on the two examples of tubular reactor and heat exchanger show its potential applicability for such systems described by a linear partial differential equation. This strategy can also be applied to nonlinear distributed parameter systems by linearizing them around a steady state value and this would be of much practical use as many of the industrial reactors are described by nonlinear distributed parameter models. Further direction for research in this area would be to evaluate some of these eigenfunctions for such systems, either from routine plant data or experimental plant data, and some of the control strategies illustrated here can be tested based on these empirical eigenfunctions.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

In this research two broad goals were considered,

i. To obtain the dynamics of distributed parameter systems with recycle
ii. Modal control of distributed parameter system with and without recycles.

The first objective involved development of tools which provide the dynamic responses for a distributed parameter system. A set of codes were compiled in MATLAB to do this job. Then the recycles were introduced into the distributed parameter system which complicated the dynamics and this was done by integrating the earlier developed MATLAB codes with SIMULINK models. Once the tools were available parametric studies were carried out on this system.

The second objective was met by understanding the modal decomposition of a distributed parameter system through two exciting examples (tubular reactor and heat exchanger systems). Further the modal control theory was also extended to tubular reactors with recycles. While fulfilling the second objective we proposed a novel control strategy called the modal feedforward controller and showed its workability on the tubular reactor with recycle and heat exchanger examples. A manuscript pertaining to this study is in progress.

Apart from the work on distributed parameter systems, the initial phase of research involved studies on the lumped parameter systems. An activated sludge process was carefully studied and some of the weird effects of recycle on such systems were seen through simulations. A predictor type recycle compensator was proposed later, in order to handle the detrimental effects of recycle. An index called the recycle effect index was developed utilizing the concepts of minimum variance to quantify the effect of recycles and also advice upon the implementation of advanced control strategy like the recycle compensator for such cases. Each of this study has been explained in detail, in their corresponding manuscripts listed in the list of publications and also a brief idea has been given in chapter 2 of this thesis. Personally I felt the project was very challenging and involved learning of various solution methodologies for solving such systems and good programming skills. As the area is new, a lot of contribution is anticipated in near future.

6.2 Recommendations

A good basic knowledge on distributed parameter systems can be obtained from a list of references Alvarez et al. (1981), Antoniades and Christofides (2001), Georgakis et al. (1972) and Rice and Do (1995). These literatures give a wonderful insight into the solution methodologies like the orthogonal collocation technique, finite differences and Galerkin technique. Upon usage of orthogonal collocation to solve some of these problems, an advice in this regard would be is to try to simulate the results with different initial guesses as these are nonlinear problems and convergence is not guaranteed always. Orthogonal collocation technique is programmable friendly and a set of tools can be easily generated, to handle such complicated distributed systems. If one is interested in the basics of Modal Analysis then one can refer to Ray (1981), a more advanced approach can be had from Ajinkya et al. (1975), Gilles (1973), Gould and Murray-Lasso (1966) and Gould (1969).

A systematic procedure for performing the modal decomposition has also been provided in chapter 4 of this thesis. Modal control theory is regaining its popularity and many advanced control strategies are emerging in this area. One such novel strategy is the implementation of modal feedforward controller to complement already existing modal feedback controller to handle measured disturbances. The usefulness of this strategy has been shown on two illustrative examples (tubular reactor with recycle and heat exchanger). Many exciting advanced control strategies like, the model predictive control in modal space, are being investigated recently. Another up-coming thing in the field of distributed parameter system is evaluation of eigenfunctions for such distributed systems, either from routine plant data or experimental plant data, and application of some of the control strategies illustrated here on these empirical eigenfunctions.

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