Application of the Principle of Invariance to a Distributed Parameter System (A Shell and Tube Heat Exchanger).

Mohammad Reza Karbassian
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in

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ABSTRACT

The invariance control of tubular processes governed by a system of simultaneous partial differential equations was considered. A shell and tube heat exchanger which is used to separate water from a gas mixture coming from a fuel cell was chosen for investigation.

Two different approaches for the design of invariant controllers were considered. One was based upon the transfer functions obtained by Taylor diffusion approximation of the system. A number of modifications in this computational method were investigated. Two different computational schemes were proposed to estimate the new parameters introduced as a result of this modification.

The theoretical frequency response of the system was obtained by a complex domain solution technique. The frequency response of the transfer functions obtained from the Taylor diffusional model was compared to the theoretical frequency response in order to test for their validity. Although the results proved to be satisfactory in the low frequency region, they were not used to design invariant controllers.

A procedure was developed for the design of invariant controllers based upon the determination of the analytical frequency response data of the controllers themselves. The controllers were approximated by a conventional proportional-derivative mode. The effectiveness of the controllers so designed was investigated by comparing the time response of the system to a step change in the incoming disturbance
under the conditions of control and no control. Complete invariance was not achieved as a result of the approximation of the controllers. The results proved to be satisfactory except at initial time response.
CHAPTER I

INTRODUCTION

Systems modeled by distributed parameter equations such as tubular heat exchangers, tubular reactors, etc., constitute a large portion of the types of operations found in chemical processes. In recent years many investigations have been towards the development of a general theory for the control of distributed parameter systems. A similar theory to that of optimal control of lumped parameter systems with quadratic performance criteria has been developed for some classes of linear distributed systems (1, 8, 21, 22, 37). The optimal feedback gains, which are generally a function of time and spatial coordinate, can theoretically be obtained from the solution of a Ricatti type partial differential integral equation. These equations are very complicated and difficult to solve, even for the steady state gain. Implementation requires an infinite number of measurements of all the states along the system, which is not practical. Although a compromise can be made in the number of measurements, the problem of measuring all the states still remains. Another problem, that is not yet answered, is the location of the sensors if a limited number of them are used. Planchard and Shariat (30) have shown that the optimal value of their performance criteria depends on the number of measurements as well as the location of the sensors. Unless the above problems are solved, the applicability of the general theory can be seriously questioned. Some
useful comments toward a practical control theory of distributed systems are given by Athans (1). Lim and Fang (23), through approximation of tubular processes by differential-difference equations, derived a linear feedback control law that minimizes a quadratic performance criteria. Implementation requires measurement of the output only; however, when the terminal time is greater than the residence time of the fluid a time delay element is needed.

In chemical processes, the main objective of control is the regulation of physical or chemical properties of the process output in the face of disturbances entering the system. In practice, properties of the process stream such as chemical composition are frequently not measured. This is due primarily to the difficulty and expense of measuring the properties of the process stream. In conventional control of chemical processes, in order to avoid measuring chemical compositions of the process stream, the secondary variables such as temperature, pressure, level, and flow rate are usually controlled. The basic philosophy underlying the control of secondary variables is that by attempting to insure a constant environment one can hope to have a well regulated process. One way out of this dilemma is the use of invariance controllers.

Unlike the conventional feedback controllers, the invariance controllers do not require measurement of the controlled variable. It is possible to design invariance feedforward as well as feedback controllers that theoretically make the controlled variable invariant in the face of disturbances entering the system.

Invariance theory has been developed in Russia primarily along theoretical lines with little regard for application (28, 29, 34, 35).
Rozonér (28, 29) has shown that the invariance problem is a variational one, and has derived the necessary and sufficient conditions for invariance in linear as well as nonlinear systems by the use of the techniques of the calculus of variation. Vershinin (34) has considered a general nth order system with n forcing functions and has derived, through the relationship between a determinant and its adjoint, the conditions for the invariance of a state in the face of n-1 forcing functions. Also he gives the variation of elements of a system's determinant due to the introduction of a feedback. Vershinin and Kulebakin (35), in a cascade system, studied the question of locations of feedbacks to compensate perturbation and to stabilize the system.

Haskins and Sliepcevich (14) applied the theory to an ideal stirred tank chemical reactor. Because no chemical reaction was taking place the process was reduced to a heat transfer problem. They considered the case of one disturbance and one manipulated variable, and designed three different controllers. The experimental as well as theoretical results, for individual controllers in the face of different types of input disturbance (sine, triangular, etc.), are reported.

To demonstrate the above technique, the approach taken by Haskins and Sliepcevich is extended to a general multi-input, multi-output stationary system. Suppose that the system has n outputs, and r input disturbances represented by column vectors $\mathbf{x}(t)$, and $\mathbf{d}(t)$ respectively. If there exist m manipulated variables represented by column vector $\mathbf{u}(t)$, the mathematical model of the system generally takes the following form:

$$\dot{\mathbf{x}}(t) = A \mathbf{x}(t) + B \mathbf{u}(t) + C \mathbf{d}(t)$$  \hspace{1cm} (1-1)
where \( A, B, \) and \( C \) are matrices of dimension \( n \times n, n \times m, \) and \( n \times r \). Upon Laplace transformation and rearrangement, equation (1-1) becomes

\[
\begin{bmatrix}
(sI - A) & -B \\
-G & -I
\end{bmatrix}
\begin{bmatrix}
x_{\text{nxl}}(s) \\
x_{\text{mxl}}(s)
\end{bmatrix}
= \begin{bmatrix}
x_{\text{nxr}} \\
x_{\text{rxl}}(s)
\end{bmatrix}
\]  
(1-2)

where \( s \) is the Laplacian operator, and \( I \) is a unit matrix. Superscripts specify the dimensions of vectors and matrices. The general control equation can be defined by:

\[
x_{\text{mxl}}(s) = \begin{bmatrix} C_{\text{bx}}(s) \\ C_{\text{fx}}(s) \end{bmatrix} x_{\text{nxl}}(s) + \begin{bmatrix} G_{\text{bx}}(s) \\ G_{\text{fx}}(s) \end{bmatrix} d_{\text{rxl}}(s)
\]  
(1-3)

where \( G_{\text{bx}}(s) \) and \( G_{\text{fx}}(s) \) are the feedback and feedforward control matrices. Combination of equations (1-2) and (1-3) yields

\[
\begin{bmatrix}
(sI - A) & -B \\
-G_{\text{bx}} & -I
\end{bmatrix}
\begin{bmatrix}
x_{\text{nxl}}(s) \\
x_{\text{mxl}}(s)
\end{bmatrix}
= \begin{bmatrix}
x_{\text{nxr}} \\
x_{\text{rxl}}(s)
\end{bmatrix}
\]  
(1-4)

Suppose that it is desired to have one of the outputs \( x_i(t) \) be invariant in the face of disturbances entering the system. To obtain the controller transfer function, equation (1-4) must be solved for \( x_i(s) \). If Cramer's rule is used, the result is

\[
x_i(s) = \frac{\Delta_i'}{\Delta}
\]  
(1-5)

where \( \Delta \) is a determinant defined by:

\[
\Delta = \text{det}
\begin{bmatrix}
(sI - A) & -B \\
-G_{\text{bx}}(s) & -I
\end{bmatrix}
\]  
(1-6)
and $\Delta'$ is the determinant of the matrix
\[
\begin{pmatrix}
I^{nxn} & A^{nxn} \\
G^{mxn}_b(s) & I^{m xn}
\end{pmatrix}
\]
with its ith column substituted by column vector
\[
\begin{pmatrix}
C^{nxr} \\
G^{mxr}_f(s)
\end{pmatrix}
\]
x(s).

The first invariance condition is that $\Delta'$ must equal zero. The second invariance condition is that determinant $\Delta$ is not equal to zero when all off-diagonal elements in the ith column equal zero. There are infinitely many ways to satisfy the first condition, because all the elements of the matrices $G_b(s)$ and $G_f(s)$ are arbitrary. Once the controller equations are derived the second condition must be checked to see if it has been violated. It should be noted that feedforward controllers (elements of the matrix $G_f(s)$) do not have any effect on the value of the determinant $\Delta$, since these elements do not appear as elements of $\Delta$. For a numerical example the reader is referred to (14).

Stangeland and Foss (32) studied an adiabatic fixed bed tubular reactor where a first order exothermic liquid-liquid reaction was taking place. They locally linearized the nonlinear model about the steady state operating conditions. In the control method that they used, concentration and the temperature disturbances in the feed entering the reactor are detected early in the bed. The concentration disturbances entering the reactor are not measured directly, but are rather inferred from the measurements of temperature at the inlet and some interior point. When temperature disturbances arrive at the interior point, they are compared with the temperature that would appear if a temperature disturbance were only present in the feed. If there
exists any discrepancy between the two, it can be attributed to the effect of a concentration disturbance in the feed. Suppose a temperature disturbance enters the reactor at time t. Then the temperature at the interior point resulting from this disturbance is calculated; this calculated temperature is compared to the measured temperature at a later time equal to the residence time of the fluid to reach that point. The discrepancy is used to determine the concentration disturbance entering the reactor at time t. Contrary to the normal industrial practice of utilizing the flow rate as the manipulated variable, they manipulated either the concentration or temperature by injecting a secondary stream at a point farther downstream from the measurement in order to achieve the control objective. Controllers that they designed are feedforward controllers which make the desired variable (temperature or concentration) invariant at some point downstream.

In order to design the controllers, the analytical transfer functions describing the effect upon temperature and concentration at any downstream point in the reactor in the face of disturbances in the same variables introduced at any point upstream from the point of interest are derived. Because of the complexity of these analytical expressions, the authors approximate them by simpler transfer function models. The derived controller transfer functions are obtained by writing equations that give the response of temperature and concentration at the controlled point (e.g., the output of the reactor) in terms of deviations of the same variables at the injection point. These deviations, that are evaluated through material and energy balance around the injection point, are the effects of input disturbances at the inlet and the injection portion due to the control action. The
former is evaluated by the use of an equation similar to the one used at the control point. The latter is determined by the two controllers and the two temperatures they measure. Finally the temperature at the measuring point is defined in terms of the feed disturbances. To derive the controller equations, the above equations are combined and they are obtained by setting the controlled variable (temperature or concentration) equal to zero at the desired location. The authors use the approximate reactor transfer functions, that are used in obtaining the controller equations, to study the effectiveness of controllers as well as the influence of the injection point on the behavior of the reactor under control. A sample of their work is reported in reference (32).

In this research a double pipe heat exchanger is chosen for investigation. The process stream is a mixture of hydrogen and water coming from a fuel cell, and a countercurrent utility stream. This utility stream is a 60% solution of ethylene glycol and water. The heat exchanger is used to reduce the water content of the process stream to a certain level for recirculation of hydrogen back to fuel cell. The system is modeled by three nonlinear partial differential equations.

The main objective of this research is to design and study the effectiveness of invariance controllers when applied to a particular distributed parameter system. The manipulated variable is the utility flow rate. A technique is presented that enables one to obtain the controller frequency response directly from the linearized, transformed system equations. This technique does not require either the approximation of the system dynamics by simple transfer functions or the derivation of the analytical form of the system transfer functions.
The merits of the controller are studied by digital simulation of the process based on the linearized partial differential equations describing the system.

A parallel study was undertaken to determine the system's transfer functions so that invariant controllers could be designed as in Haskins-Sliepcevich (14). Two techniques were investigated for doing this. The first considers the application of modal analysis to distributed parameter systems and is due to Murry-Lasso (25). The technique requires the expansion of the linear differential operator in terms of its eigenfunctions. It was determined that, for a hyperbolic system, the differential operator does not have eigenvalues (25). A second technique considered the application of a Taylor diffusional model to the system. A transfer function of the system may then be obtained by suitable manipulation as reported by Gould (12). Because the results were not as satisfactory as the case reported by Gould, the original motivation in developing the Taylor model was abandoned and attention was focused on modifying the model with the hope of obtaining more accurate results.

In Chapter II the mathematical model of the system, which consists of three nonlinear partial differential equations, is derived. Local linearization of the system equations are carried out around the steady state operating conditions. The techniques for the solution of steady state as well as unsteady state equations are presented. Chapter III deals with development of the Taylor diffusion model. The technique to obtain the frequency response data of the system, which is used as a comparison base to validate the Taylor model, is also given.
In Chapter IV the invariance controllers are designed and their merits are investigated by digital simulation of the linearized system's partial differential equations. In Chapter V the results of the investigation are discussed.
CHAPTER II

HEAT EXCHANGER MATHEMATICAL MODEL

A. Introduction

At the outset of any control system design problem, the first step is to establish a mathematical model of the process. Having established the model, which is hopefully a good representation of the actual process, one not only obtains a clear picture of the physical system itself by studying the behavior of the model implied by mathematics, but also the problem of control system design often becomes a much easier task if one has a thorough understanding of the uncontrolled process. The type of equations comprising the model depends upon the particular system under investigation. These equations are normally nonlinear, and the application of the well developed linear theory requires linearization of the model. Additionally, investigation of either controlled or uncontrolled process necessitates some mathematical techniques for the solution of the related equations.

In this chapter the mathematical model of the system is developed first. The model consists of a set of nonlinear partial differential equations. These equations are then locally linearized about the steady state. The linearized set have some coefficients that are spatially dependent, and their evaluation requires the steady state solution of the model. Then the numerical technique for the solution of steady state equations is discussed. Finally, the solution method
for partial differential equations is presented.

B. Mathematical Model of the System

The system chosen for investigation is a double pipe heat exchanger. The process stream is a mixture of hydrogen and water coming from a fuel cell. This gas mixture, which is normally saturated with water, flows through the shell. The cooling media is 60% ethylene glycol in water and flows countercurrently through the tube. The total pressure, at which the system operates, is one atmosphere. In order to recycle the hydrogen back to the fuel cell, the partial pressure of water should be reduced to a certain level. The heat exchanger is used to accomplish this purpose.

It was mentioned in Chapter I that a parallel study was undertaken to consider the application of a Taylor diffusional model to the system. Rosenbrock (27), and Gould (12) suggest that the model gives a reasonable approximation of the dynamic behavior of heat exchangers if the number of transfer units are greater than two. These criteria are defined in the next chapter in the Taylor diffusion model section. The dimension of the heat exchanger, the gas and the coolant flow rates were chosen so as to satisfy these criteria rather than the original specification of the system. The physical properties of the gas, the coolant, and the correlations used to evaluate the heat and mass transfer coefficients were taken from (2). The physical properties, flow rates, and the dimension of the heat exchanger are given in Table 1. The correlations used to evaluate the heat and mass transfer coefficients are:
For laminar flow

\[
\frac{h D_i}{k} = 1.86 \left( \frac{D_i G_i}{\mu} \right)^{1/3} \left( \frac{C P}{k} \right)^{1/3} \left( \frac{D_i L}{\mu_w} \right)^{0.14}
\]  

(2-1)

For turbulent flow

\[
\frac{h D_i}{k} = 0.023 \left( \frac{D_i G_i}{\mu} \right)^{0.8} \left( \frac{C P}{k} \right)^{1/3} \left( \frac{\mu}{\mu_w} \right)^{0.14}
\]  

(2-2)

where 

- \( h \) = heat transfer coefficient Btu/hr. ft\(^2\) °F
- \( D_i \) = diameter or equivalence diameter ft
- \( k \) = thermal conductivity of the fluid Btu/hr. ft °F
- \( G_i \) = mass velocity lbs/hr. ft\(^2\)
- \( C_P \) = specific heat of the fluid Btu/lbs. °F
- \( \mu \) = viscosity of the fluid lbs/hr. ft
- \( \mu_w \) = viscosity at the wall temperature lbs/hr. ft
- \( L \) = length of heat exchanger ft

The mass transfer coefficient may be related to the heat transfer coefficient through the J-factor analogy as follows:

\[
\frac{h_g}{k^* C_{P_m}} = \left( \frac{S_c}{P_r} \right)^{2/3}
\]  

(2-3)

where

- \( h_g \) = gas side heat transfer coefficients Btu/hr. ft\(^2\) °F
- \( S_c \) = Schmit modulus, dimensionless
- \( P_{r} \) = Prandtl modulus, dimensionless
- \( P \) = total pressure atm.
- \( C_{P_m} \) = gas specific heat Btu/lb mole °F
- \( k^* \) = mass transfer coefficient lb moles/hr. ft\(^2\) atm.
<table>
<thead>
<tr>
<th>Property</th>
<th>Shell Side</th>
<th>Tube Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inside diameter inches</td>
<td>0.606</td>
<td>0.37</td>
</tr>
<tr>
<td>Outside diameter inches</td>
<td>3/4</td>
<td>1/2</td>
</tr>
<tr>
<td>Flow cross sectional area ft²</td>
<td>$0.64 \times 10^{-3}$</td>
<td>$0.746 \times 10^{-3}$</td>
</tr>
<tr>
<td>Flow rates lbs/hr.</td>
<td>3.2</td>
<td>20.16</td>
</tr>
<tr>
<td>Average density lbs/ft³</td>
<td>0.084</td>
<td>53.</td>
</tr>
<tr>
<td>Average velocity ft/min.</td>
<td>993.0</td>
<td>8.46</td>
</tr>
<tr>
<td>Conductivity coefficients Btu/hr. ft °F</td>
<td>0.113</td>
<td>0.242</td>
</tr>
<tr>
<td>Specific heat Btu/lb °F</td>
<td>2.11</td>
<td>0.766</td>
</tr>
<tr>
<td>Viscosity lbs/ft hr.</td>
<td>0.022</td>
<td>6.84</td>
</tr>
</tbody>
</table>

Heat of evaporation of water $\lambda = 1024$ Btu/lbs
Inlet coolant temperature = 74.9°F
Inlet gas temperature = 131°F
Inlet partial pressure of water = 0.15532 atm.
Length of heat exchanger $L = 40$ ft
Total pressure of the system = 1 atm.
Assuming ideal gas behavior, equation (2-3) may be written
\[
\frac{h_g}{k_C P} = \frac{k_{RT}}{C_{Pm} g} \cdot \left( \frac{RT}{PD_g} \right)^{2/3}
\]  
(2-4)

where \( k_g \) = thermal conductivity of the gas, Btu/hr. ft °F

\( R = \) gas constant, atm. ft\(^3\)/lb mole (degree Rankin)

\( T = \) gas temperature, °R

\( D_g = \) binary diffusivity of water vapor with hydrogen, ft\(^2\)/hr.

Using an equation (3) to estimate the binary diffusion of water vapor with hydrogen, the following result is obtained:
\[
\left( \frac{RT}{PD_g} \right)^{2/3} = \frac{5200}{T^{0.89}}
\]  
(2-5)

Combination of equations (2-4) and (2-5) results in
\[
\frac{h_g}{k_C P} = \frac{k_g}{C_{Pm} g} \cdot \left( \frac{5200}{T^{0.89}} \right)
\]  
(2-6)

Assuming no resistance to the transfer of heat through the wall, the overall heat transfer coefficient on the basis of outside tube area will be
\[
\frac{1}{uA_o} = \frac{1}{h_{g o}} + \frac{1}{h_{c i}}
\]  
(2-7)

where \( A_o = \) outside tube area, ft\(^2\)/ft

\( A_i = \) inside tube area, ft\(^2\)/ft

\( h_g, h_c = \) shell side, and tube side heat transfer coefficients

\( u = \) overall heat transfer coefficients
The data in Table 1, equations (2-1), (2-6), and (2-7) are used to evaluate the overall heat transfer coefficients, and mass transfer coefficient. In evaluating the mass transfer coefficient \( k^* \) by the use of equation (2-6), the average temperature is taken to be 100°F and \( C_{pm} \) equal to 7.0.

Their values, after conversion of time unit from hour to minute, are:

\[
U = 0.1383, \text{ Btu/min. ft}^2 \text{ °F} \\
\frac{k^*}{g} = 0.02667, \text{ lb moles/min. ft}^2 \text{ atm.}
\]

The following assumptions are made in developing the mathematical model of the system:

1) Perfect mixing in radial direction
2) Zero axial mixing that is associated with plug flow
3) No axial or radial diffusion
4) The gas obeys the ideal gas law
5) Constant gas mass flow rate; in other words, the rate of loss of water as a result of mass transfer is negligible compared to the total mass flow rate. Also it is assumed that the gas density is constant.

To develop the model, the first general principle that is needed is that of conservation. This means that if a closed volume is considered, the net flow of mass, energy, or momentum into the volume must equal the rate of increase of mass, energy, or momentum within the volume. It can be stated as:

\[
\text{Inflow - outflow = Accumulation}
\]

The other principles that are needed depend upon the nature of the
process and they are referred to as particular law. For the system under investigation these are:

1) Newton's cooling law and its counterpart in mass transfer

2) Ideal gas law

3) Vapor-liquid equilibrium relationship of water as a function of temperature.

Referring to Figure 2-1, the conservation of energy and mass of water is applied to the elements of volume in the tube and shell side.

![Figure 2-1. Heat Exchanger](image)

Conservation of energy applied to the tube side

\[
A_c C_c c_p C_c T_c \bigg|_{z+\Delta z} + U S \Delta z (T_g - T_c) - A_c C_c c_p C_c T_c \bigg|_z = \frac{3}{\delta t} (A_c \Delta z c_p C_c T_c) \quad (2-8)
\]
Conservation of energy applied to the shell side

\[ A V g C g p g T g |_{z} ^{z+\Delta z} + U S \Delta z (T_{c} - T_{g}) + 18 K^{*} S \Delta z \lambda (P_{g} - P_{\lambda}) - A V g p C p g T p g |_{z+\Delta z} \]

\[ = \frac{\partial}{\partial t} (A g \Delta z p C g p g T p g) \quad (2-9) \]

Conservation of mass of water applied to the shell side element

\[ A V g \rho g m \bigg|_{z} ^{z+\Delta z} + 18 K^{*} S \Delta z (P_{\lambda} - P_{g}) - A V g \rho g m \bigg|_{z+\Delta z} = \frac{\partial}{\partial t} (A g \Delta z \rho g m) \quad (2-10) \]

where
- \( A_{C} \) = inside tube cross sectional area, \( ft^{2} \)
- \( A_{g} \) = shell side cross sectional area, \( ft^{2} \)
- \( C_{pc} \) = coolant specific heat, Btu/lbs. °F
- \( C_{pg} \) = gas specific heat, Btu/lbs. °F
- \( K^{*}_{g} \) = mass transfer coefficient, lb mole/ft² atm. min.
- \( m \) = mass fraction of water in the gas at every point
- \( P_{g} \) = partial pressure of water in the gas, atm.
- \( P_{\lambda} \) = vapor pressure of water, atm., evaluated at the wall temperature which is taken equal to average between the coolant and the gas temperature
- \( S \) = outside tube perimeter, ft
- \( T_{c} \) = coolant temperature, °F
- \( T_{g} \) = gas temperature, °F
- \( U \) = overall heat transfer coefficient, Btu/min. ft² °F
- \( V_{c} \) = coolant velocity, ft/min.
- \( V_{g} \) = gas average velocity, ft/min.
- \( \rho_{c} \) = coolant density, lbs./ft³
- \( \rho_{g} \) = average gas density, lbs./ft³
- \( \lambda \) = heat of evaporation of water, Btu/lbs.
Using the ideal gas law, and considering that the total pressure is one atmosphere, it can be shown that

\[ P_g = \frac{m}{9-8m} \]  
(2-11)

Multiplying both sides of equation (2-10) by \( \lambda \) to meet the requirement for the development of the Taylor model, substituting for \( P_g \) in equations (2-9) and (2-10) by using equation (2-11), dividing by \( \Delta z \) and taking the limit as \( \Delta z \rightarrow 0 \) results in

\[
H_1 \frac{\partial}{\partial t} T_c = H_1 V_c \frac{\partial}{\partial z} T_c + k_1 (T_c - T) \]

\[
H_2 \frac{\partial}{\partial t} T_g = -H_2 V_g \frac{\partial}{\partial z} T_g + k_1 (T_c - T_g) + k_2 \left( \frac{m}{9-8m} - P_\lambda \right) \]

\[
H_3 \frac{\partial}{\partial t} m = -H_3 V_g \frac{\partial}{\partial z} m + k_2 (P_\lambda - \frac{m}{9-8m}) \]  
(2-12)

where

\[
H_1 = A_c \rho C_p C_c \]

\[
H_2 = A_g \rho C_g \]

\[
H_3 = A_g \rho \lambda \]

\[
k_1 = 18K^s \lambda \]

\[
k_2 = 18K^s \lambda \]

The following correlation (17) is used to evaluate \( P_\lambda \) at the wall temperature along the heat exchanger

\[
\log_{10} \frac{P_c}{P_\lambda} = \frac{x}{1 + \frac{a' + b'x + c'x^2}{1 + d'x}} \]  
(2-14)
where \( P_c = 218.167 \) atm. (critical pressure of water)
\[ P^* = 218.167 \text{ atm. (critical pressure of water)} \]

\( P^* = \) vapor pressure of water atm. at temperature \( T \)

\( T = \) temperature at which \( P^* \) is evaluated degree Kelvin

\[ x = 647.27 - T \]

\[ a' = 3.2437814 \quad b' = 5.86826 \times 10^{-3} \]

\[ c' = 1.1702379 \times 10^{-8} \quad d' = 2.1878462 \times 10^{-3} \]

The wall temperature is assumed to be equal to \( \frac{T_c + T_g}{2} \). The above correlation is valid in the temperature range of 10°C to 150°C.

The system of equations (2-12) forms a set of nonlinear partial differential equations that coupled with equation (2-14) constitute the mathematical model of the system.

C. Linearization of the System Equations

Control theory is far more advanced for linear systems than it is for nonlinear systems. The most attractive features of the linear systems are the availability of the well developed transform techniques, and the validity of the principle of superposition.

Linearization is normally based on the truncated Taylor series expansion of the nonlinear terms about the steady state operating conditions. As long as small excursions occur about the steady state, the nonlinear terms may be replaced by linear approximations. To achieve faithful modeling, representations of nonlinear effects should be retained in determination of the steady state about which the linearization is made. Investigation of the merits of this type modeling has been the subject of several experimental and computational studies and has been found to represent accurately the dynamic effects observed (4, 30, 31).
In carrying out the linearization of the model (equations (2-12)), it is convenient to define the following variables

\[ T_c(z,t) = \overline{T}_c(z) + \delta T_c(z,t) \]

\[ T_g(z,t) = \overline{T}_g(z) + \delta T_g(z,t) \]

\[ m(z,t) = \overline{m}(z) + \delta m(z,t) \]

\[ v_c(t) = \overline{v}_c + \delta v_c(t) \]

\[ v_g(t) = \overline{v}_g + \delta v_g(t) \]

Here the variables on the left hand side are called total variables. Each equals the sum of two terms, the first one being the steady part and independent of time, and the second term being the deviation from the steady state. To linearize the system equations (2-12), the non-linear terms are expended in a Taylor series. If the terms with order greater than one are neglected, the result will be as follows:

\[ v_c(t) \frac{\partial}{\partial z} T_c(z,t) = \overline{v}_c \frac{\partial}{\partial z} \overline{T}_c(z) + \left( \frac{\partial}{\partial z} \overline{T}_c(z) \right) \delta v_c(t) + \overline{v}_c \frac{\partial}{\partial z} \delta T_c(z,t) \]

\[ v_g(t) \frac{\partial}{\partial z} T_g(z,t) = \overline{v}_g \frac{\partial}{\partial z} \overline{T}_g(z) + \left( \frac{\partial}{\partial z} \overline{T}_g(z) \right) \delta v_g(t) + \overline{v}_g \frac{\partial}{\partial z} \delta T_g(z,t) \]

\[ v_g(t) \frac{\partial}{\partial z} m(z,t) = \overline{v}_g \frac{\partial}{\partial z} \overline{m}(z) + \left( \frac{\partial}{\partial z} \overline{m}(z) \right) \delta v_g(t) + \overline{v}_g \frac{\partial}{\partial z} \delta m(z,t) \]

\[ \frac{m(z,t)}{9-8m(z)} = \frac{\overline{m}(z)}{9-8m(z)} + \frac{9}{(9-8m(z))^2} \delta m(z,t) \]

\[ F_{\lambda} \left( \frac{T_c(z,t) + T_g(z,t)}{2} \right) = \overline{F}_{\lambda} \left( \frac{T_c(z) + T_g(z)}{2} \right) \]

\[ + \frac{\partial}{\partial T_c} \left( \frac{T_c(z,t) + T_g(z,t)}{2} \right) \left( \delta T_c(z,t) + \delta T_g(z,t) \right) \]

(2-16)
Up to now each dependent variable had its independent variables as its arguments inside parentheses. From now on the parentheses and the independent variables will be dropped unless doing so causes confusion. The nomenclature will be as is defined by equations (2-15) without the arguments. The variables with the bar stand for steady state, variables without the bar represent the total variables, and variables with \( \delta \) indicate incremental variables.

If the total variables \( T_C, T_g, \) and \( m \), as they are defined by equations (2-15), and the nonlinear terms using equations (2-16) are substituted in the system of equations (2-12); the result is

\[
H_1 \frac{\partial}{\partial t} \delta T_C = H_1 \left[ \frac{\bar{v}}{c} \frac{\partial}{\partial z} \bar{T}_C + \left( \frac{\partial}{\partial z} \bar{T}_C \right) \delta v_C + \frac{\bar{v}}{c} \frac{\partial}{\partial z} \delta T_C \right] \\
+ k_1 \left[ (\bar{T}_g - \bar{T}_C) + (\delta T_g - \delta T_C) \right]
\]

\[
H_2 \frac{\partial}{\partial t} \delta T_g = - H_2 \left[ \frac{\bar{v}}{g} \frac{\partial}{\partial z} \bar{T}_g + \left( \frac{\partial}{\partial z} \bar{T}_g \right) \delta v_g + \frac{\bar{v}}{g} \frac{\partial}{\partial z} \delta T_g \right] \\
+ k_1 \left[ (\bar{T}_C - \bar{T}_g) + (\delta T_C - \delta T_g) \right]
\]

\[
+ k_2 \left[ \left( \frac{\bar{m}}{(9-8\bar{m})} - \bar{P}_\lambda \right) + \frac{9}{(9-8\bar{m})^2} \delta m - \left( \frac{\partial P}{\partial T} \right) \right] \left( \delta T_C + \delta T_g \right)
\]

\[
H_3 \frac{\partial}{\partial t} \delta m = - H_3 \left[ \frac{\bar{v}}{g} \frac{\partial}{\partial z} \bar{m} + \left( \frac{\partial}{\partial z} \bar{m} \right) \delta v_g + \frac{\bar{v}}{g} \frac{\partial}{\partial z} \delta m \right] \\
+ k_2 \left[ \left( \bar{P}_\lambda - \frac{\bar{m}}{(9-8\bar{m})} \right) - \frac{9}{(9-8\bar{m})^2} \delta m + \left( \frac{\partial P}{\partial T} \right) \right] \left( \delta T_C + \delta T_g \right)
\]

(2-17)
The problem is now separated into two different parts. One is the steady state portion of the solution, and the other is the transient portion of the solution. As the system approaches steady state, the incremental variables tend to go to zero. To obtain the steady state part, it is sufficient to set the incremental variables equal to zero. Doing so, the result is

\[ H_1 V_c \frac{3}{\partial z} T_c + k_1 (T_g - T_c) = 0 \]

\[ H_2 V_g \frac{3}{\partial z} T_g - k_1 (T_g - T_c) - k_2 \left( \frac{m}{9-8m} - \frac{P_1}{P_2} \right) = 0 \] (2-18)

\[ H_3 V_g \frac{3}{\partial z} m - k_2 \left( \frac{P_1}{9-8m} - \frac{m}{9-8m} \right) = 0 \]

To obtain the transient part of the problem, each equation in the system of equations (2-18) is subtracted from the corresponding one in equations (2-17). The result is

\[ H_1 \frac{3}{\partial t} \delta T_c = H_1 V_c \frac{3}{\partial z} \delta T_c + k_1 (\delta T_g - \delta T_c) + H_1 \left( \frac{3}{\partial z} T_c \right) \delta V_c \]

\[ H_2 \frac{3}{\partial t} \delta T_g = -H_2 V_g \frac{3}{\partial z} \delta T_g + k_1 (\delta T_c - \delta T_g) \]

\[ + k_2 \left[ \frac{9}{(9-8m)^2} \delta m - \left( \frac{3}{\partial T_c} \right) \left( \delta T_c + \delta T_g \right) \right] - H_2 \left( \frac{3}{\partial z} T_g \right) \delta V_g \]

\[ H_3 \frac{3}{\partial t} \delta m = -H_3 V_g \frac{3}{\partial z} \delta m + k_2 \left[ \left( \frac{3}{\partial T_c} \right) \left( \delta T_c + \delta T_g \right) - \frac{9}{(9-8m)^2} \delta m \right] \]

\[ - H_3 \left( \frac{3}{\partial z} m \right) \delta V_g \] (2-19)
D. Solution of the System Equations

Solution of the nonlinear partial differential equations (2-12) requires the steady state solution of the system equations as the starting point. The solution of the incremental partial differential equations (2-19) also requires the steady state solution to evaluate the spatially dependent coefficients. Additionally, the Taylor diffusion model, and the complex domain solution of the transformed incremental equations which gives the frequency response of the system (both discussed in the next chapter), require the steady state solution to evaluate the spatially dependent coefficients of equations (2-19). Therefore the procedure to solve the steady state equation is given next. Then the method of solution of the partial differential equations is presented.

1. Steady State Solution

Steady state equations (2-18) are normalized first by making the following transformation:

\[ y = \frac{Z}{L} \]

where \( L \) is the length of the heat exchanger. Using the chain rule gives

\[ \frac{\partial (\cdot)}{\partial Z} = \frac{1}{L} \frac{\partial (\cdot)}{\partial y} \quad (2-20) \]

Combination of equation (2-20) with equations (2-18) results in the following:


\[
\frac{dT_c}{dy} = - \frac{k_1 L}{H_1 V_c} (\bar{T}_c - \bar{T}_q)
\]

\[
\frac{dT_q}{dy} = - \frac{k_1 L}{H_2 V_q} (\bar{T}_q - \bar{T}_c) + \frac{k_2 L}{H_2 V_g} \left( \frac{\bar{m}}{9-8m} - \bar{P}_\lambda \right)
\]

\[
\frac{dm}{dy} = - \frac{k_2 L}{H_3 V_g} \left( \frac{\bar{m}}{9-8m} - \bar{P}_\lambda \right)
\]

Equation (2-21)

\(\bar{P}_\lambda\) is evaluated at the wall temperature assumed to be equal to \(\frac{T_c + T_q}{2}\) by the use of equation (2-14). The boundary conditions in normalized form (Table 1) are:

\[\bar{T}_q (y=0) = 131^\circ F\]

\[\bar{m}(y=0) = 0.62334\]

\[\bar{T}_c (y=1) = 74.9^\circ F\]

Here use has been made of equation (2-11) to evaluate \(m(y=0)\) from the partial pressure of water at the inlet. The parameters of the system are evaluated by the use of equations (2-13), the data given in Table 1, and the mass and overall heat transfer coefficients which were already evaluated. These parameters are given in the following table:

**Table 2.--PARAMETERS OF THE SYSTEM**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H_1)</td>
<td>(0.303 \times 10^{-1} \text{ Btu/ft } ^\circ F)</td>
</tr>
<tr>
<td>(k_2)</td>
<td>(64.32 \text{ Btu/min. ft atm.})</td>
</tr>
<tr>
<td>(H_2)</td>
<td>(0.1135 \times 10^{-3} \text{ Btu/ft } ^\circ F)</td>
</tr>
<tr>
<td>(V_c)</td>
<td>(8.46 \text{ ft/min.})</td>
</tr>
<tr>
<td>(H_3)</td>
<td>(0.552 \times 10^{-1} \text{ Btu/ft})</td>
</tr>
<tr>
<td>(V_g)</td>
<td>(993.0 \text{ ft/min.})</td>
</tr>
<tr>
<td>(k_1)</td>
<td>(0.1812 \times 10^{-1} \text{ Btu/min. ft } ^\circ F)</td>
</tr>
</tbody>
</table>
The steady state equations (2-21) coupled with equations (2-14) and with the associated boundary conditions fall into a general class of problems that are called split boundary value, as opposed to initial value problems. The technique to solve the system of equations (2-21) is called the shooting method in contrast to the finite difference technique. In the finite difference method, the derivative terms are approximated by a finite difference analog. This results in a set of linear algebraic equations if the original system is linear, and non-linear algebraic equations otherwise. The system of simultaneous equations can be solved iteratively. When the system equations are non-linear, the question of uniqueness must be addressed and the generation of any solution may be very difficult.

The shooting method reduces the problem to an iterative solution of initial value problem. The general procedure is to choose the boundary that has the most specified conditions as the initial point and assume any other conditions that are missing. The initial value problem is then solved. Until the computed solution agrees with the specified boundary conditions, the assumed initial conditions are adjusted and the solution is repeated to the point where the assumed initial conditions yield, within a specified tolerance, a solution that agrees with the specified boundary conditions.

The algorithm to adjust the assumed initial conditions that results in a sequence of ever-improving solution is not a universal one. The choice among different techniques, from a simple root finding procedure to the more sophisticated optimization routines, depends on the degree of nonlinearity of the system and the number of missing boundary conditions at the chosen initial point. There are no known algorithms
which guarantee a successful solution of any arbitrary boundary value problem.

The method chosen in this study consisted of Gill's modification of the fourth order Runge-Kutta and Regula-Falsi algorithm to adjust the assumed initial condition (6). Any time the solution with the assumed initial condition \(T_c(y=0)\) is carried out, an error term given by

\[
E = (T_c(y=1))_{\text{specified}} - (T_c(y=1))_{\text{computed}}
\]  

is evaluated. The absolute value of this term is compared with the tolerance \(10^{-6}\) to see if the assumed initial condition has yielded the solution that agrees with the specified boundary condition \(T_c(y=1)\). The procedure is summarized in Figure 2-2.

2. Solution of Partial Differential Equations

Incremental partial differential equations are normalized first, by combining equation (2-20) with the system of equations (2-19). The result is

\[
H_1 \frac{\partial}{\partial t} \delta T_c = \frac{H_1 V}{L} \frac{\partial}{\partial y} \delta T_c + k_1 (\delta T_g - \delta T_c) + \frac{H_1}{L} \left( \frac{\partial}{\partial y} \frac{\partial}{\partial T} \right) \delta V_c
\]

\[
H_2 \frac{\partial}{\partial t} \delta T_g = -\frac{H_2 V}{L} \frac{\partial}{\partial y} \delta T_g + k_1 (\delta T_c - \delta T_g)
\]

\[
+ k_2 \left[ \frac{9}{(9-8m)^2} \delta m - \frac{\partial P_c}{\partial T_c} \delta T_c + \delta T_g \right] - \frac{H_2}{L} \left( \frac{\partial}{\partial y} \frac{\partial}{\partial y} \right) \delta V_g
\]

\[
H_3 \frac{\partial}{\partial t} \delta m = -\frac{H_3 V}{L} \frac{\partial}{\partial y} \delta m + k_2 \left[ \frac{\partial P_c}{\partial T_c} \delta T_c + \delta T_g \right] - \frac{9}{(9-8m)^2} \delta m
\]

\[
- \frac{H_3}{L} \left( \frac{\partial}{\partial y} \frac{\partial}{\partial m} \right) \delta V_g
\]  

(2-23)
Figure 2-2. Flow diagram to solve steady state equation
The spatially dependent coefficients of equations (2-23) are called sensitivity coefficients. These are represented as follows:

\[
S_1(y) = \frac{1}{L} \left( \frac{\partial}{\partial y} \frac{T_c}{T_g} \right) \\
S_2(y) = \frac{9}{(9-8m)^2} \\
S_3(y) = \frac{\partial P_\lambda}{\partial T_c} \\
S_4(y) = \frac{1}{L} \left( \frac{\partial}{\partial y} \frac{T_c}{T_g} \right) \\
S_5(y) = \frac{1}{L} \left( \frac{\partial}{\partial y} \bar{m} \right)
\]

(2-24)

Once the steady state solution, which was discussed previously, is obtained, the sensitivity coefficients can be calculated. Figures 2-3 through 2-7 are plots of these coefficients versus the normalized spatial coordinate \( y \).

There are two general procedures to solve a system of partial differential equations of this type. These are:

1) Approximation of the system of partial differential equations by a set of differential difference equations. This is done by substituting either the time or space derivatives by a finite difference analog. When this is done, it is often referred to as a lumped approximation. Gould (12) discusses in detail the lumped approximation and shows an equivalent electrical circuit for a counter flow process with two dependent variables. He also treats the case where the diffusional term is present and derives the necessary number of base points, in terms of the parameter of the system, to have a reasonable approximation of the system.
Figure 2-3
SENSITIVITY COEFFICIENT VERSUS DIMENSIONLESS DISTANCE

Figure 2-4
SENSITIVITY COEFFICIENT VERSUS DIMENSIONLESS DISTANCE

Figure 2-5
SENSITIVITY COEFFICIENT VERSUS DIMENSIONLESS DISTANCE

Figure 2-6

DIMENSIONLESS DISTANCE
2) Finite difference formulations that must often reduce the system of equations to a set of simultaneous algebraic equations. The solution is obtained by simple algebraic operations. This is suitable for digital computer solution in contrast to differential difference equations which are amenable to hybrid solution.

The technique chosen for simulation of the system under investigation was the finite difference formulation. Suppose \( V(y, t) \) is the dependent variable which is a function of time and space \( y \). Time \( t \) increases without limit, while the space domain \( y \) varies between zero and one. This is always possible by normalizing the spatial coordinate as has already been done.

Contrary to the continuous algorithm where the dependent variable \( V(y, t) \) is defined over the whole range of the time and the space domain, in the discrete algorithm \( V(y, t) \) is defined only at discrete points. It is convenient to choose a notation for discrete to show the correspondence between the dependent variable \( V \) and the independent variables \( y \) and \( t \). The continuous variable \( y \) is defined at a finite number of points spaced equally with the increment \( \Delta y \). The variable \( t \) is defined as the space domain \( y \), but there is no limit to the number of integral points, and the time interval \( \Delta t \), between two successive time integrals, is not necessarily constant. It is a common practice to increase \( \Delta t \) as the solution progresses. In Figure 2-8, the grid points (represented by circles), where the dependent variable is to be determined, are shown for two successive time levels.
The space index is \(i\), and that of time is \(n\). These indexes take on integral values at the grid points. With this nomenclature, the value of the dependent variable \(V\) at the grid point \(i\), and time level \(t_n\) can be represented by \(V_{i,n}\). The value of \(y\) at this point is \(1 \times Ay\), and \(t_n = \frac{\sum_{j=1}^{n} (\Delta t)_j}{n}\). Note that \(\Delta t\) might have different values for different values of the index \(j\).

To derive the finite difference equations for a system of partial differential equations, the derivatives and the variables (dependent or independent) should be somehow expressed in terms of discrete variables. A number of finite difference analogs are available (6, 36), but one which has proven very successful for a number of problems is the centered difference equations. These analogs are centered in both space and time with respect to the grid points at which the values of the dependent variables are to be determined. The cross point in Figure 2-8 represents the location about which the finite difference analog is written. The coordinate of this point is \((y_{i-\frac{1}{2}}, t_{n+\frac{1}{2}})\). The space and time derivatives are approximated by:
In order to derive the centered difference equations for a hyperbolic system, the derivatives are substituted by equations (2-25), the dependent variables at the cross point are substituted by the average taken over the four grid points surrounding the cross point. If there exist any coefficients that are functions of independent variables \( y \) and \( t \), they should also be evaluated at the cross point. Although the resulting finite difference equations are explicit for a linear initial value problem, it is not so for a split boundary problem. Combination of equations (2-23) and (2-24) results in

\[
\begin{align*}
H_1 \frac{\partial}{\partial t} \delta T_c &= \frac{H_1 \overline{V}_c}{L} \frac{\partial}{\partial y} \delta T_c + \frac{H_1 \overline{V}_c}{L} k_1 (\delta T_g - \delta T_c) + S_1(y) \delta V_c \\
H_2 \frac{\partial}{\partial t} \delta T_g &= -\frac{H_2 \overline{V}_g}{L} \frac{\partial}{\partial y} \delta T_g + \frac{H_2 \overline{V}_g}{L} k_1 (\delta T_c - \delta T_g) + k_2 [S_2(y) \delta m] \\
&\quad - S_3(y)(\delta T_c + \delta T_g)] - S_4(y) \delta V_g \\
H_3 \frac{\partial}{\partial t} \delta m &= -\frac{H_3 \overline{V}_g}{L} \frac{\partial}{\partial y} \delta m + k_2 [S_3(y)(\delta T_c + \delta T_g) - S_2(y) \delta m] \\
&\quad - S_5(y) \delta V_g
\end{align*}
\]

The centered difference equations for the system of equations (2-26) are given in Appendix A. The shooting technique was used to solve the set of implicit simultaneous algebraic equations. The Newton-Raphson technique was used to adjust the assumed missing boundary condition at initial point \((i=1)\).
The boundary conditions associated with equations (2-26) depend entirely on the way the steady state is defined. Two distinct types of boundary condition can be defined:

1) The steady state part of total variables in equations (2-15) are initial steady states. It is apparent from equations (2-15) that the initial distribution of incremental variables \( \delta T_C(y,0), \delta T_g(y,0), \) and \( \delta m(y,0) \) are zero. Suppose at the time \( t=0 \), a step change occurs in one of the input variables, e.g., \( \delta T_g(0,0)=1 \), then:

\[
\begin{align*}
\delta T_C(y,0) &= \delta T_g(y,0) = \delta m(y,0) = 0 & 0 \leq y \leq 1 \\
\delta T_g(0,t) &= 1 \\
\delta m(0,t) &= 0 \\
\delta T_C(1,t) &= 0 
\end{align*}
\]

This type of boundary condition is used in the numerical solution of the partial differential equations in equation (2-26). It should be noted that the sensitivity coefficient can be assumed to be independent of the way the steady states are defined, since small excursions are considered.

2) The steady state part of the total variables in equations (2-15) are final steady states. In this case the initial distribution of the incremental variable is not zero. Suppose that it is desired to investigate the behavior of the system to a step change of the inlet gas temperature. Two approaches can be taken to obtain the initial incremental distribution. One approach is on the basis of the linearized
model, and the other one is on the basis of nonlinear model.

If the former approach is chosen, the time derivatives in equations (2-26) are set equal to zero. The resulting differential equations are solved. The boundary conditions are as follows:

\[
\begin{align*}
\delta T_g \bigg|_{y=0} &= -1 \\
\delta m \bigg|_{y=0} &= 0 \\
\delta T_c \bigg|_{y=1} &= 0
\end{align*}
\]

If the latter approach is chosen, the nonlinear steady state equations (2-21) are solved for two sets of boundary conditions. These are

- Set No. 1
  - \( \overline{T}_g (y=0) = 131°F \)
  - \( \overline{m}(y=0) = 0.62334 \)
  - \( \overline{T}_c (y=1) = 74.9°F \)

- Set No. 2
  - \( \overline{T}_g (y=0) = 130°F \)
  - \( \overline{m}(y=0) = 0.62334 \)
  - \( \overline{T}_c (y=1) = 74.9°F \)

Representing the solutions from each set of boundary conditions accordingly, the initial distribution is obtained as follows:

\[
\begin{align*}
\delta T_c (y,0_+) &= \left[ \overline{T}_c (y) \right]_2 - \left[ \overline{T}_c (y) \right]_1 \\
\delta T_g (y,0_+) &= \left[ \overline{T}_g (y) \right]_2 - \left[ \overline{T}_g (y) \right]_1 \\
\delta m(y,0_+) &= \left[ \overline{m}(y) \right]_2 - \left[ \overline{m}(y) \right]_1
\end{align*}
\]
These initial incremental distributions are used as the starting point of the solution of partial differential equations (2-26) subject to the following boundary conditions.

\[ \delta T_C(1,t) = 0 \]
\[ \delta T_g(0,t) = 0 \]
\[ \delta m(0,t) = 0 \]

These types of boundary conditions are used to develop the Taylor diffusional model in the next chapter.
CHAPTER III

IDENTIFICATION

A. Introduction

It was discussed in Chapter I that the main objective of control in chemical processes is the regulation of the process output in the face of disturbances entering the system. If one is concerned with the use of conventional control system design procedures such as frequency-domain design methods, the knowledge of transfer functions relating the output (controlled variable) to load disturbances and manipulated variables is essential. Once these transfer functions are obtained, the problem of designing controllers is straightforward (12, 13, 26).

One of the earliest techniques of obtaining frequency response data is direct sinusoidal process testing (7, 33). The technique is experimental in concept and it is still occasionally used on a laboratory scale (31). The limitation of the technique is discussed by Hougen and Walsh (16). Some facts concerning the obtaining of experimental frequency response data are discussed by Murrill (26). Most limitations of direct sinusoidal process testing were overcome by pulse testing and the Fourier analysis method that has been extensively investigated by Hougen et al. (9, 10, 15, 16).

Parallel to these experimental deterministic techniques is the stochastic model building technique through time series analysis (5).
The basic tools for identification of the transfer function model are autocorrelation, partial autocorrelation functions of the input and output, and the cross correlation function between input and output. The technique has been successfully applied by Box and Jenkins (5) to a gas furnace and a chemical process.

The plant testing is normally very costly and time consuming, especially when the rate of response is very slow, and because many disturbances should be considered. A good example of this is a high purity fractionator column where the composition effects are on the order of hours, and where many disturbances such as feed composition, enthalpy, and flow rates, etc., must be taken into account. As an alternative to the plant testing, theoretical prediction of processes is often considered.

Systems modeled by distributed equations such as heat exchangers, tubular reactors, etc., could in principle be locally linearized (if the model is nonlinear), and an analytical expression of the transfer function obtained. Inspection of these analytical expressions of the transfer functions (12, 32) reveals that in general they are too complicated to deal with directly. Besides the complexity of transfer functions for counter current processes with split boundary conditions, the process of obtaining these expressions is very involved and becomes much worse as the number of dependent variables increases. It has been a common practice to resort to some approximation technique to represent the dynamics of the system by a simpler form of transfer function. One popular approach is fitting the frequency response data into an appropriate form of transfer function. Either the experimental techniques (direct sinusoidal or pulse testing) which were discussed
earlier, or the frequency domain solution technique, which are given in the latter part of this chapter can be used to obtain the frequency response data.

Planchard and Gonzalez (11) have shown that the following transfer function

\[ G(s) = \frac{1 - XKP \times \exp(-\tau_0 s)}{(1+\tau_1 s)(1+\tau_2 s)} \]  

(3-1)

where \( XKP = 1 - \) steady state gain
\( \tau_0 = \) dead time
\( \tau_1 \) and \( \tau_2 = \) time constants
gives good time fit to the response of heat exchangers in the face of changes in the boundary conditions. They have also shown that the following transfer function is a suitable one

\[ G(s) = GN \frac{\exp(-\tau_0 s)}{(1+\tau_1 s)(1+\tau_2 s)} \]  

(3-2)

where \( GN = \) steady state gain.

For some other suitable form of transfer function models the reader is referred to (18, 32).

In this research two different identification techniques were used. One is the Taylor diffusion model that is treated by Gould (12) and Rosenbrock (27). The technique, where it applies, reduces a system of simultaneous hyperbolic partial differential equations to a single parabolic partial differential equation. The method is analytical, and the resulting transfer functions are expressed in terms of their decomposition into modes. The other identification technique used was the frequency domain solution technique due to Foss and Sinai (31) and
Bollinger (4). The technique is numerical and its merit has been confirmed experimentally by Foss and Sinai. This method is used to obtain the frequency response data as a comparison base to validate the Taylor diffusion model. In the next chapter, it is used to obtain the frequency response of the feedforward invariance controllers directly without resort to any approximation of the system transfer functions. Here, the Taylor diffusion model is developed first, and the frequency domain solution technique is presented.

B. Taylor Diffusion Model

There are three basic assumptions that are the foundation of the Taylor model. As stated by Gould (12), these are:

1. After a disturbance of any kind, in a coordinate system moving with a mean velocity \( v \), equilibrium is achieved much more rapidly in the radial direction than in the axial direction.

2. For systems involving more than two simultaneous partial differential equations, axial gradients tend to be the same at every instant for all streams at a given point along the axis of the system.

3. The sum of all transfer terms in all equations is zero.

By the transfer term it is meant the term describing the disappearance of energy, momentum or mass to another system or form. In the system under study these terms are the transfer of energy from the shell to the tube side by convection and condensation of water as the result of mass transfer. To satisfy assumption number 3, both sides of equation (2-10) were multiplied by \( \lambda \). The necessity of assumptions 1 and 2 will become clearer as the model is developed.

To develop the model, the system of equations (2-26) is
considered. These equations, after $\delta V_c$ and $\delta V_g$ are set equal to zero, in the original spatial coordinate $Z$ take the following form:

\[
H_1 \frac{\partial}{\partial t} \delta T_c = H_1 \frac{\partial}{\partial Z} \delta T_c + k_1 (\delta V_g - \delta V_c)
\]

\[
H_2 \frac{\partial}{\partial t} \delta T_g = -H_2 \frac{\partial}{\partial Z} \delta T_g + k_1 (\delta T_c - \delta T_g) + k_2 [S_2(Z) \delta m - S_3(Z) (\delta T_c + \delta T_g)]
\]

\[
H_3 \frac{\partial}{\partial t} \delta m = -H_3 \frac{\partial}{\partial Z} \delta m + k_2 [S_3(Z) (\delta T_c + \delta T_g) - S_2(Z) \delta m]
\]

(3-3)

If the variation of sensitivity coefficients $S_2(Z)$ and $S_3(Z)$ are moderate over the length of the heat exchanger, then it is feasible to approximate them by their mean values. If the mean values are represented by $\overline{S}_2$ and $\overline{S}_3$, they can be calculated as follows:

\[
\overline{S}_2 = \frac{1}{L} \int_0^L S_2(Z) dZ
\]

(3-4)

\[
\overline{S}_3 = \frac{1}{L} \int_0^L S_3(Z) dZ
\]

It is easy to show that equations (3-4) in the normalized coordinate, $y = Z/L$, takes the following form:

\[
\overline{S}_2 = \int_0^1 S_2(y) dy
\]

(3-5)

\[
\overline{S}_3 = \int_0^1 S_3(y) dy
\]
Substituting the sensitivity coefficients for their mean value, equations (3-3) become

\[ H_1 \frac{\partial}{\partial t} \delta T_c = H_1 \frac{V}{c} \frac{\partial}{\partial z} \delta T_c + k_1 (\delta T_g - \delta T_c) \]

\[ H_2 \frac{\partial}{\partial t} \delta T_g = -H_2 \frac{V}{g} \frac{\partial}{\partial z} \delta T_g + k_1 (\delta T_c - \delta T_g) + k_2 [\bar{S}_2 \delta m - \bar{S}_3 (\delta T_c + \delta T_g)] \]

\[ H_3 \frac{\partial}{\partial t} \delta m = -H_3 \frac{V}{g} \frac{\partial}{\partial z} \delta m + k_2 [\bar{S}_3 (\delta T_c + \delta T_g) - \bar{S}_2 \delta m] \]  \hspace{1cm} (3-6)

Assume the moving coordinate that satisfies assumption number one and forces the system of equations (3-6), after being transformed to the moving coordinate system, into equilibrium takes the following form:

\[ x = Z + vt \]
\[ t' = t \]

It can be shown (12), that the derivatives of equations (3-6) in the new coordinate system take the following form:

\[ \frac{\partial}{\partial t} (\ast) = v \frac{\partial}{\partial x} (\ast) + \frac{\partial}{\partial t'} (\ast) \]

\[ \frac{\partial}{\partial z} (\ast) = \frac{\partial}{\partial x} (\ast) \]  \hspace{1cm} (3-7)

Here, (\ast) stands for the dependent variables \( \delta T_c, \delta T_g, \) and \( \delta m. \)

Combination of equations (3-6) and (3-7) yields
\[ H_1 \frac{\partial}{\partial t} \delta T_c = H_1 (\overline{V_c} - v) \frac{\partial}{\partial x} \delta T_c + k_1 (\delta T_g - \delta T_c) \]

\[ H_2 \frac{\partial}{\partial t} \delta T_g = -H_2 (\overline{V_g} + v) \frac{\partial}{\partial x} \delta T_g + k_1 (\delta T_c - \delta T_g) + k_2 [\overline{S_2} \delta m - \overline{S_3} (\delta T_c + \delta T_g)] \]

\[ H_3 \frac{\partial}{\partial t} \delta m = -H_3 (\overline{V_g} + v) \frac{\partial}{\partial x} \delta m + k_2 [\overline{S_3} (\delta T_c + \delta T_g) - \overline{S_2} \delta m] \] (3-8)

The system of equations (3-8) will be at equilibrium if the proper value can be found for \( v \). Assuming this, then equations (3-8) reduce to

\[ H_1 (\overline{V_c} - v) \frac{\partial}{\partial x} \delta T_c + k_1 (\delta T_g - \delta T_c) = 0 \]

\[ -H_2 (\overline{V_g} + v) \frac{\partial}{\partial x} \delta T_g + k_1 (\delta T_c - \delta T_g) + k_2 [\overline{S_2} \delta m - \overline{S_3} (\delta T_c + \delta T_g)] = 0 \]

\[ -H_3 (\overline{V_g} + v) \frac{\partial}{\partial x} \delta m + k_2 [\overline{S_3} (\delta T_c + \delta T_g) - \overline{S_2} \delta m] = 0 \] (3-9)

To evaluate the proper value of \( v \), a mean variable \( \delta T_m \) is defined as follows:

\[ \delta T_m = \frac{H_1 \delta T_c + H_2 \delta T_g + H_3 \delta m}{H} \] (3-10)

where \( H = H_1 + H_2 + H_3 \)

Now the second assumption is invoked, but instead of setting the axial gradients in equations (3-8) or (3-9) equal to each other and equal to the axial gradient of the mean variable \( \delta T_m \), a more general relation is defined as follows:
By setting $\eta_1 = \eta_2 = \eta_3 = 1$ in equations (3-11), the formulation reduces to the standard procedure used by Gould (12) to develop the Taylor model for a double pipe heat exchanger with no mass transfer.

Setting $\eta_1 = \eta_2 = 1$, and $\eta_3 = \bar{s}_3$, the modeling is similar to the one used by the same author to develop the Taylor model for a packed column with two dependent variables. No explanation was given by Gould in this latter case. No mathematical justification can be given, as stated by Rosenbrock (27), in developing the Taylor model. The problem of choosing the proper value for $\eta_1$, $\eta_2$, and $\eta_3$ is based on physical intuition rather than on a mathematical basis. The success of the technique depends entirely on the values chosen for $\eta_1$, $\eta_2$, and $\eta_3$. Several approximations were used to evaluate $\eta_1$, $\eta_2$, and $\eta_3$, and are discussed later. For the moment, assume that values for $\eta_1$, $\eta_2$, and $\eta_3$ have been chosen. If equations (3-9) are added and the derivatives are substituted for their equivalence in equations (3-11), the result is

$$
\left[ \eta_1 H_1 (\overline{V} - v) - \eta_2 H_2 (\overline{\rho} + v) - \eta_3 H_3 (\overline{\rho} + v) \right] \frac{\partial}{\partial x} \delta T_m = 0 \quad (3-12)
$$

Equation (3-12) is satisfied for all values of $\delta T_m$ if the term in the bracket is equal to zero. Setting the term in the bracket equal to zero and solving for $v$ the result, which gives the proper value of $v$...
that forces the system of equations (3-8) into equilibrium, is

\[
v = \frac{\zeta_1 H_1 \bar{V} - \zeta_2 H_2 \bar{g} - \zeta_3 H_3 \bar{g}}{\zeta_1 H_1 + \zeta_2 H_2 + \zeta_3 H_3} \quad (3-13)
\]

The procedure to find the relationship between the dependent variables \(\delta T_c, \delta T_g, \delta m,\) and the mean variable \(\delta T_m\) is as follows:

1. Substitute \(\frac{\partial}{\partial x} \delta T_c\) in the first equation of the set of equations (3-9) by \(\zeta \frac{\partial}{\partial x} \delta T_m\), then solve for \(\delta T_g\). The result is

\[
\delta T_g = \delta T_c - \frac{\zeta_1 H_1}{k_1} (\bar{V} - v) \frac{\partial}{\partial x} \delta T_m \quad (3-14)
\]

2. Add the first two equations of the set of equations (3-9), then substitute each derivatives by its equivalence from equations (3-11). Substitute for \(\delta T_g\) using equation (3-14), and then solve for \(\delta m\). The result is

\[
\delta m = 2 \frac{\tilde{S}_3}{\tilde{S}_2} \delta T_c - \left[ \frac{\zeta_1 H_1}{k_1} \frac{\tilde{S}_3}{S_2} + \frac{\zeta_2 H_2}{k_2 \tilde{S}_2} (\bar{V} - v) - \frac{\zeta_2 H_2}{k_2 \tilde{S}_2} (\bar{V} + v) \right] \frac{\partial}{\partial x} \delta T_m 
\]

3. Combine equations (3-10), (3-14), and (3-15). The result is

\[
\delta T_c = C_1 \delta T_m - C_2 \frac{\partial}{\partial x} \delta T_m \\
\delta T_g = C_3 \delta T_m - C_4 \frac{\partial}{\partial x} \delta T_m \\
\delta m = C_5 \delta T_m - C_6 \frac{\partial}{\partial x} \delta T_m 
\]

(3-16)
The coefficients $C_1$ through $C_6$ are

$$C_1 = \frac{H}{H_1 + H_2 + 2 \frac{S_3}{S_2} H_3}$$

$$C_2 = \frac{1}{C_1} \left[ \frac{\zeta_1 H_1 H_2}{k_1} + \frac{\zeta_1 H_1 H_3}{k_1} \frac{S_3}{S_2} + \frac{\zeta_1 H_1 H_2}{k_2 S_2} (\bar{V}_c - V) + \frac{\zeta_2 H_2 H_3}{k_2 S_2} (\bar{V}_g + V) \right]$$

$$C_3 = C_1$$

$$C_4 = C_2 + \frac{\zeta_1 H_1}{k_1} (\bar{V}_c - V)$$

$$C_5 = C_1 \left\{ \begin{array}{c} \frac{S_3}{S_2} \\ \frac{S_3}{S_2} \end{array} \right\}$$

$$C_6 = C_2 \left\{ \begin{array}{c} \frac{S_3}{S_2} \\ \frac{S_3}{S_2} \end{array} \right\} + \left\{ \frac{\zeta_1 H_1 S_3}{k_1 S_2} + \frac{\zeta_1 H_1}{k_2 S_2} \right\} (\bar{V}_c - V) - \frac{\zeta_2 H_2}{k_2 S_2} (\bar{V}_g + V)$$

Addition of both sides of equations (3-6) results in

$$H \frac{\partial}{\partial t} \delta T_m = H_1 \bar{V} \frac{\partial}{\partial z} \delta T_c - H_2 \bar{V} \frac{\partial}{\partial z} \delta T_g - H_3 \bar{V} \frac{\partial}{\partial z} \delta m$$

(3-18)

Here use has been made of $H_1 \delta T_c + H_2 \delta T_g + H_3 \delta m = H \delta T_m$ from the definition of the mean variable $\delta T_m$ by equation (3-10). It is shown by equations (3-7) that $\frac{\partial}{\partial x} (*) = \frac{\partial}{\partial z} (*)$, thus the independent variable $x$ in equations (3-16) can be replaced by $Z$. After making this substitution,
independent variable \( x \) by \( Z \) results in the following:

\[
\frac{\partial}{\partial Z} \delta T_c = C_1 \frac{\partial}{\partial Z} \delta T_m - C_2 \frac{\partial^2}{\partial Z^2} \delta T_m
\]

\[
\frac{\partial}{\partial Z} \delta T_g = C_3 \frac{\partial}{\partial Z} \delta T_m - C_4 \frac{\partial^2}{\partial Z^2} \delta T_m
\]  \( \text{(3-19)} \)

\[
\frac{\partial}{\partial Z} \delta m = C_5 \frac{\partial}{\partial Z} \delta T_m - C_6 \frac{\partial^2}{\partial Z^2} \delta T_m
\]

Combination of equation (3-18) with equations (3-19) yields

\[
\frac{\partial}{\partial t} \delta T_m + v_m \frac{\partial}{\partial Z} \delta T_m = \alpha_T \frac{\partial^2}{\partial Z^2} \delta T_m
\]  \( \text{(3-20)} \)

where

\[
v_m = \frac{-C_1 H_1 \overline{v} + (C_3 H_2 + C_4 H_3) \overline{v}}{H} \]

\( \text{(3-21)} \)

\[
\alpha_T = \frac{-C_2 H_1 \overline{v} + (C_4 H_2 + C_5 H_3) \overline{v}}{H}
\]

Equation (3-20), with its coefficients defined by equations (3-21), is the Taylor diffusion model of the system under study.

Equation (3-20) can be normalized as follows:

\[
\theta = v_m \frac{t}{L}, \quad y = \frac{Z}{L}
\]  \( \text{(3-22)} \)

Carrying out the transformation, the result is

\[
\frac{\partial}{\partial \theta} \delta T_m + \frac{\partial}{\partial y} \delta T_m = \frac{1}{P_T} \frac{\partial^2}{\partial y^2} \delta T_m
\]  \( \text{(3-23)} \)

where

\[
P_T = L \frac{v_m}{\alpha_T}
\]  \( \text{(3-24)} \)
In order to solve equation (3-23), two boundary conditions and one initial condition are needed. The boundary conditions are derived from equations (3-16). If the steady states defined in equations (2-15) are the final steady states, then the boundary conditions will be homogeneous. These, in normalized spatial coordinate \( y \), are:

\[
\begin{align*}
\delta T_m(1, \theta) - \alpha \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=1} &= 0, & \alpha = \frac{c_2}{c_1 L} \\
\delta T_m(0, \theta) - \beta \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=0} &= 0, & \beta = \frac{c_4}{c_3 L} \\
\delta T_m(0, \theta) - \gamma \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=0} &= 0, & \gamma = \frac{c_6}{c_5 L}
\end{align*}
\] (3-25, 3-26, 3-27)

Only two boundary conditions, one at each side, are needed, consequently two sets of boundary conditions can be used. These are

\[
\begin{align*}
\delta T_m(1, \theta) - \alpha \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=1} &= 0 \\
\delta T_m(0, \theta) - \beta \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=0} &= 0
\end{align*}
\] (3-28)

and

\[
\begin{align*}
\delta T_m(1, \theta) - \beta \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=1} &= 0 \\
\delta T_m(0, \theta) - \gamma \frac{\partial}{\partial y} \delta T_m(y, \theta) \bigg|_{y=0} &= 0
\end{align*}
\] (3-29)

With every set of boundary conditions (equations (3-28) and (3-29)) there is one solution of equation (3-23) associated with it. Gould (12) suggests that both sets of solutions should be obtained and if there is any discrepancy between the two, the best one should be
chosen.

The initial condition can be calculated in two different ways which were discussed in the previous chapter in obtaining initial incremental distribution. One was based on the solution of nonlinear steady state equations (2-21), and the other one was based on the linearized steady state equations derived from the system of equations (2-23) by setting the time derivatives equal to zero. The latter one was used in this study because the frequency domain solution technique which is used as a comparison basis to study the merits of the Taylor model is a linear technique.

Once the initial distribution (initial condition) of the incremental variables $\delta T_c(y,0_\pm)$, $\delta T_g(y,0_\pm)$, and $\delta m(y,0_\pm)$ are obtained, the initial condition for the Taylor model (equation (3-23)) can be obtained by the use of equation (3-10) as follows:

$$\delta T_m(y,0_\pm) = \frac{1}{H} \left| H_1 \delta T_c(y,0_\pm) + H_2 \delta T_g(y,0_\pm) + H_3 \delta m(y,0_\pm) \right| \quad (3-30)$$

Having specified the initial and boundary conditions, the Taylor model (equation (3-23)) can be solved by the classical method of separation of variables. The detail of the procedure is given by Gould (12). After the solution of equation (3-23) is obtained, equations (3-16) are used to obtain the incremental variables. As was mentioned earlier, there are two sets of boundary conditions associated with equation (3-23), therefore there will be two sets of solutions. Following Gould's procedure, these solutions are:
1. The solution associated with the boundary conditions specified by equations (3-28)

\[ \tilde{T}_c(0,s) = C_1 \sum_{i=1}^{\infty} \frac{a_i \eta_i \xi_i}{(1-\beta_p)} \frac{1}{s+\nu_i} \]

\[ \tilde{T}_g(1,s) = C_3 \sum_{i=1}^{\infty} \frac{a_i \eta_i \exp(p) [(1-\beta_p)^2 + (\beta \xi'_i)^2]}{(1-\beta_p)} \times (\sin \xi'_i) \frac{1}{s+\nu_i} \]

\[ \tilde{m}(1,s) = C_5 \sum_{i=1}^{\infty} a_i \eta_i \exp(p) \left[ \frac{1}{1-\gamma_p + \frac{\beta \gamma \xi'_i}{1-\beta_p}} \sin \xi'_i + \frac{\beta - \gamma}{1-\gamma_p} \xi'_i \cos \xi'_i \right] \times \frac{1}{s+\nu_i} \]

(3-31)

2. The solution associated with the boundary conditions specified by equations (3-29)

\[ \tilde{T}'_c(0,s) = C_1 \sum_{i=1}^{\infty} \frac{a'_i \eta'_i (\gamma-\alpha) \xi'_i}{1-\gamma_p} \frac{1}{s+\nu'_i} \]

\[ \tilde{T}'_g(1,s) = C_3 \sum_{i=1}^{\infty} a'_i \eta'_i \exp(p) \left[ \frac{1}{1-\beta_p + \frac{\beta \gamma \xi'_i}{1-\gamma_p}} \sin \xi'_i + \frac{\gamma - \beta}{1-\gamma_p} \xi'_i \cos \xi'_i \right] \]

\[ \tilde{m}'(1,s) = C_5 \sum_{i=1}^{\infty} \frac{a'_i \eta'_i \exp(p)}{1-\gamma_p} \left[ \frac{1}{(1-\gamma_p)^2 + (\gamma \xi'_i)^2} \right] (\sin \xi'_i) \times \frac{1}{s+\nu'_i} \]

(3-32)

Here a tilde over the variables denotes the Laplace transformation of incremental variables. The first argument inside the parenthesis stands for the normalized spatial coordinate \( y \), and the second one is
the Laplacian operator \( s \) (e.g., \( \hat{\mathcal{L}}_C(0,s) = L[\delta T_C(y=0,t)] \)). The unit of time \( t \) is in minutes.

The parameters of equations (3-31) and (3-32) are:

\[
p = \frac{P_T}{2}
\]

\[
\nu_1 = \left( \frac{P_T}{2} \right)^2 \left[ 0.5 + 2 \left( \frac{\xi_1}{P_T} \right)^2 \right] (v_m/L)
\]

\[
\nu_1' = \left( \frac{P_T}{2} \right)^2 \left[ 0.5 + 2 \left( \frac{\xi_1'}{P_T} \right)^2 \right] (v_m/L)
\]

(3-33)

\( C_1, C_3, \) and \( C_5 \) are defined by equations (3-17). \( \alpha, \beta, \) and \( \gamma \) are given by equations (3-25) through (3-27). \( \xi_1 \) and \( \xi_1' \) are called the eigenvalues or characteristic values of the problem (radians) and they are the roots of the following equations:

\[
\xi_1 \cot \xi_1 + \frac{(1-\beta \rho)(1-\alpha \rho) + \alpha \beta \xi_1^2}{\beta-\alpha} = 0
\]

(3-34)

\[
\xi_1' \cot \xi_1' + \frac{(1-\gamma \rho)(1-\alpha \rho) + \alpha \gamma \xi_1'^2}{\gamma-\alpha}
\]

After \( \xi_1 \) and \( \xi_1' \) are evaluated, the normalized factor \( \eta_1 \) and \( \eta_1' \) are calculated using the following equations:

\[
2 \eta_1^{-2} = \left[ \frac{\beta \xi_1}{(1-\beta \rho)} + 1 \right] + \left[ \frac{\beta \xi_1}{(1-\beta \rho)} - 1 \right] \frac{\sin 2\xi_1}{2\xi_1} + \frac{2\beta}{1-\beta \rho} \sin^2 \xi_1
\]

(3-35)

\[
2 \eta_1'^{-2} = \left[ \frac{\gamma \xi_1'}{(1-\gamma \rho)} + 1 \right] + \left[ \frac{\gamma \xi_1'}{(1-\gamma \rho)} - 1 \right] \frac{\sin 2\xi_1'}{2\xi_1'} + \frac{2\gamma}{1-\gamma \rho} \sin^2 \xi_1'
\]
Once $\xi_i$, $\xi'_i$, $\eta_i$, and $\eta'_i$ are calculated, $a_i$ and $a'_i$ are evaluated by the following formula:

\[
a_i = \int_{0}^{1} \exp(-2py) \phi_i(y) \delta T_m(y,0_{-}) \, dy
\]

\[
a'_i = \int_{0}^{1} \exp(-2py) \phi'_i(y) \delta T_m(y,0_{-}) \, dy
\]

where $\phi_i(y)$ and $\phi'_i(y)$ are the orthonormal set by which the initial distribution $\delta T_m(y,0_{-})$ is expanded. These are:

\[
\phi_i(y) = \eta_i \exp(py) \left[ \sin \xi_i y + \frac{\beta \xi_i}{1-\beta p} \cos \xi_i y \right]
\]

\[
\phi'_i(y) = \eta'_i \exp(py) \left[ \sin \xi'_i y + \frac{\gamma \xi'_i}{1-\gamma p} \cos \xi'_i y \right]
\]

C. System Transfer Functions

In this study the transfer functions relating the changes in outlet mass fraction of water to the changes in input variables (entering coolant temperature, gas temperature, mass fraction of water, coolant velocity, and gas velocity) were evaluated. These transfer functions are represented by $G_1(s)$ through $G_5(s)$ respectively. The derivation of the transfer function, relating the changes in mass fraction of water at the outlet to the changes in inlet gas temperature, is given here ($G_2(s)$). The development of the other transfer functions is the same. The procedure is also the same for transfer functions relating the other output variables (outlet coolant and gas temperature) to
the above input variables.

Assume the system is initially at steady state. At time t=0, the inlet gas temperature changes. Recalling the definition of total variables in Chapter II (equations (2-15)), the outlet mass fraction of water at any time t is

\[ m(l,t) = \overline{m}(l) + \delta m(l,t) \quad (3-38) \]

where \( \overline{m}(l) \) is the final value of the mass fraction of water at the outlet (y=1). If the initial value of the outlet mass fraction of water \( m(l,0) \) is subtracted from both sides of equation (3-38), the result is

\[ \Delta m(l,t) = \overline{m}(l) - \overline{m}(l,0) + \delta m(l,t) \quad (3-39) \]

Taking the Laplace transform of both sides of equation (3-39) yields

\[ L_t[\Delta m(l,t)] = \frac{\overline{m}(l) - \overline{m}(l,0)}{s} + \overline{m}(1,s) \quad (3-40) \]

If it is assumed that the change which caused all this was a step change in inlet gas temperature from \( T_g(0,0) \) to \( T_g(0) \), then the inlet gas temperature change may be written as:

\[ \Delta T_g(0,t) = [T_g(0) - T_g(0,0)] u(t) \quad (3-41) \]

where \( u(t) \) is the unit step function. Taking the Laplace transform of both sides of equation (3-41) yields

\[ L_t[\Delta T_g(0,t)] = \frac{T_g - T_g(0,0)}{s} \quad (3-42) \]
Therefore the transfer function that relates the changes in the outlet mass fraction of water to the changes in the inlet gas temperature is obtained by dividing equation (3-41) by equation (3-42). The result is

\[ G_2(s) = \frac{L_t[\Delta m(l,t)]}{L_t[\Delta T_g(0,t)]} = G_2(0) + \frac{s}{T_g(0) - T_g(0,0_-)} \dot{m}(l,s) \quad (3-43) \]

The significance of the result is that the steady state gain

\[ G_2(0) = \frac{\bar{m}(l) - m(l,0_-)}{T_g(0) - T_g(0,0_-)} \]

is correct because of the manner in which the incremental distributions were defined. Substitution for \( \dot{m}(l,s) \), by using the corresponding equation in the system of equations (3-31) and (3-32), results in

\[ G_2(s) = G_2(0) + s \sum_{i=1}^{\infty} \frac{K_i}{s + \nu_i} \]

\[ G_2'(s) = G_2(0) + s \sum_{i=1}^{\infty} \frac{K_i'}{s + \nu_i'} \quad (3-44) \]

where

\[ K_i = \frac{1}{T_g(0) - T_g(0,0_-)} C_s a_i \eta_i \exp(p) \left[ \left( \frac{1 - \gamma p + \beta \xi_i^2}{1 - \beta p} \right) \sin \xi_i \right. \]

\[ \left. + \frac{\beta - \gamma}{1 - \beta p} \xi_i \cos \xi_i \right] \]

\[ K_i' = \frac{1}{T_g(0) - T_g(0,0_-)} C_s a_i' \eta_i' \exp(p) \frac{1}{1 - \gamma p} \left[ \left( 1 - \gamma p \right)^2 + \left( \gamma \xi_i' \right)^2 \right] \sin \xi_i' \quad (3-45) \]
D. General Procedure and Results

The first step is the solution of the steady state equations (2-21) associated with its boundary conditions given in Chapter II. Once the steady state solution is obtained, the sensitivity coefficients $S_2(y)$ and $S_3(y)$ are evaluated; consequently their mean values $S_2$ and $S_3$ are obtained using equations (3-5). The trapezoidal rule was used to evaluate $S_2$ and $S_3$. The values obtained were:

$$S_2 = 0.43313 \quad S_3 = 0.16036 \times 10^{-2}$$

The second step involves obtaining the initial distributions of the dependent variables. It was mentioned earlier that the linearized steady state equations are used to obtain initial distributions of the dependent variables. If the linearized equations are used, the steady state gains of the transfer functions obtained from the Taylor model and the frequency domain solution technique will be exactly the same. The linearized steady state equations are obtained simply by setting the time derivatives in equations (2-23) equal to zero. By doing so, the result in terms of sensitivity coefficients is

$$\frac{H_1}{L} \frac{d}{dy} \delta T_C + k_1(\delta T_g - \delta T_C) + H_1S_1(y) \delta V_C = 0$$

$$-\frac{H_2}{L} \frac{d}{dy} \delta T_g + k_1(\delta T_C - \delta T_g) + k_2[S_2(y) \delta m - S_3(y)(\delta T_C + \delta T_g)] - H_2S_4(y) \delta V_g = 0$$

$$-\frac{H_3}{L} \frac{d}{dy} \delta m + k_2[S_3(y)(\delta T_C + \delta T_g) - S_2(y) \delta m] - H_3S_5(y) \delta V_g = 0$$

(3-46)
The boundary conditions and the velocity changes associated with equations (3-46) are given in Table 3.

<table>
<thead>
<tr>
<th></th>
<th>( \delta T_c (1,0_-) )</th>
<th>( \delta T_g (0,0_-) )</th>
<th>( \delta m (0,0_-) )</th>
<th>( \delta V_c (0_-) )</th>
<th>( \delta V_g (0_-) )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.0</td>
<td>0.0</td>
<td>0.05</td>
<td>0.05V_c</td>
<td>0.1V_g</td>
</tr>
</tbody>
</table>

The numerical technique, to solve equations (3-46) with the associated boundary conditions given in Table 3, is the same as the one discussed in Chapter II, Section D. Once \( \bar{S}_2, \bar{S}_3 \), and the initial distributions are obtained, the next step involves choosing the values of \( \zeta_1, \zeta_2, \) and \( \zeta_3 \) defined by equations (3-11). The following cases were studied in this research:

Case I: \( \zeta_1 = \zeta_2 = \zeta_3 = 1 \)

Case II: \( \zeta_1 = 1 \), \( \zeta_2 = \frac{\delta T_g (y,0_-)}{\partial y} \)

Case III: \( \zeta_1 = \zeta_2 = 1 \), \( \zeta_3 = \bar{S}_3 \)
Here the bar over the variables or derivatives denotes averaging over the length of the system. Equation (3-30) is used to evaluate \( \delta T_m(y,0_-) \), and the averaging procedure is similar to the one used to evaluate \( \bar{s}_2 \) and \( \bar{s}_3 \) (the trapezoidal rule). Cases II and IV are derived from equations (3-11) by which \( \zeta_1 \), \( \zeta_2 \), and \( \zeta_3 \) are defined. Case I is the standard procedure as used by Gould (12) to develop the Taylor model of heat exchangers with no mass transfer, and Case III is similar to the one used by the same author in developing the Taylor model of a packed column with two dependent variables. After the appropriate values are assigned to \( \zeta_1 \), \( \zeta_2 \), and \( \zeta_3 \), the rest of the parameters (\( \nu \) by equation (3-13), \( C_1 \) through \( C_6 \) by equations (3-17), \( \alpha \), \( \beta \), and \( \gamma \) defined by equations (3-25) through (3-26), etc.) may be calculated. In evaluating the transfer functions, the following steps were taken:

1. The roots of equations (3-34), which are the eigenvalues or characteristic values of the problem (in radians) were obtained. The first six roots are reported in this study. These roots were evaluated numerically using the Regula-Falsi technique.

2. After the eigenvalues (\( \xi_i \) and \( \xi'_i \)) are obtained, equations (3-35) are used to obtain the corresponding values for \( \eta_i \) and \( \eta'_i \).

3. \( a_i \) and \( a'_i \) are evaluated by using equations (3-36). The
trapezoidal rule was used in evaluating $a_i$ and $a_i'$ numerically. Note that $\delta T_m(y,0,-)$ had already been calculated and it is available.

4. Once $\xi_i$, $\xi_i'$, $\eta_i$, $\eta_i'$, $a_i$, and $a_i'$ are obtained, $K_i$ and $K_i'$ are calculated by the use of equations (3-45) when the input variable is the inlet gas temperature. For the other input variables the same equations can be used except the term \[ \frac{1}{T_g(0) - T_g(0,0,-)} \] should be substituted by the proper term (e.g. \[ \frac{1}{m(0) - m(0,0,-)}, \frac{1}{V_c(0) - V_c(0,-)} \]) etc.). $v_i$ and $v_i'$ are calculated by using equations (3-33).

The results are summarized in Tables 4 through 9.
Table 4. Parameters of the Transfer Function $G_1(s)$

$G_1(s) = \frac{L_t[\Delta m(1,t)]}{L_t[\Delta T_c(1,t)]} = G_1(0) + s \sum K_i \frac{s}{s + v_i}$

<table>
<thead>
<tr>
<th>Case No.</th>
<th>i</th>
<th>$\xi_i$</th>
<th>$\xi_i'$</th>
<th>$v_i$</th>
<th>$v_i'$</th>
<th>$K_i$</th>
<th>$K'_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
<td>1.6088</td>
<td>1.6512</td>
<td>7.1834</td>
<td>7.5669</td>
<td>-0.2235 x $10^{-1}$</td>
<td>-0.2283 x $10^{-1}$</td>
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<tr>
<td></td>
<td>2</td>
<td>4.7202</td>
<td>4.7353</td>
<td>61.806</td>
<td>62.204</td>
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<td>-0.7503 x $10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>7.8524</td>
<td>7.8616</td>
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<td>171.44</td>
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<td>-0.7692 x $10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>10.988</td>
<td>10.994</td>
<td>334.90</td>
<td>335.30</td>
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<td>-0.8396 x $10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>14.124</td>
<td>14.129</td>
<td>553.37</td>
<td>553.77</td>
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<td>-0.8115 x $10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>17.261</td>
<td>17.265</td>
<td>826.47</td>
<td>826.87</td>
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<td>-0.8431 x $10^{-1}$</td>
</tr>
<tr>
<td>II</td>
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<td>0.5665</td>
<td>0.6126</td>
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<td>-0.2606 x $10^{-2}$</td>
</tr>
<tr>
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<td>5.7868</td>
<td>1.3752</td>
<td>1.5132</td>
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<td>-0.1772 x $10^{-3}$</td>
</tr>
<tr>
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<td>3</td>
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<td>8.7392</td>
<td>2.8266</td>
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<tr>
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<td>14.764</td>
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<td>17.819</td>
<td>11.322</td>
<td>11.662</td>
<td>-0.7896 x $10^{-3}$</td>
<td>-0.4458 x $10^{-3}$</td>
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</tbody>
</table>
Table 4 (continued)

Steady state gain $G_1(0) = 0.37843 \times 10^{-2}$

<table>
<thead>
<tr>
<th>Case No.</th>
<th>$i$</th>
<th>$\xi_1$</th>
<th>$\xi'_1$</th>
<th>$v_1$</th>
<th>$v'_1$</th>
<th>$K_i$</th>
<th>$K'_i$</th>
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<tr>
<td>III</td>
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<td>2.9432</td>
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<tr>
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<td>$0.1307 \times 10^{-2}$</td>
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<td>14.913</td>
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<td>$-0.1759 \times 10^{-2}$</td>
<td>$-0.2576 \times 10^{-2}$</td>
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<tr>
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<td>17.962</td>
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<td>9.0751</td>
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<tr>
<td>IV</td>
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<td>2.5519</td>
<td>0.6122</td>
<td>0.7650</td>
<td>$-0.1861 \times 10^{-2}$</td>
<td>$-0.2269 \times 10^{-2}$</td>
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<tr>
<td></td>
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<tr>
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<td>8.0662</td>
<td>8.2851</td>
<td>6.6269</td>
<td>6.9852</td>
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<tr>
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<td>11.320</td>
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<td>12.942</td>
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<tr>
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<td>30.748</td>
<td>$-0.3035 \times 10^{-2}$</td>
<td>$-0.2953 \times 10^{-2}$</td>
</tr>
</tbody>
</table>
Table 5. Parameters of the Transfer Function $G_2(s)$

\[ G_2(s) = \frac{L_t[\Delta m(1,t)]}{L_t[\Delta T(0,t)]} = G_2(0) + s \sum \frac{K_i}{s + \nu_i} \]

<table>
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Table 5 (continued)

Steady state gain $G_2(0) = 0.69974 \times 10^{-3}$

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Table 6. Parameters of the Transfer Function $G_3(s)$

$$G_3(s) = \frac{L_t[\Delta m(1,t)]}{L_t[\Delta m(0,t)]} = G_3(0) + s \sum \frac{K_i}{s + \nu_i}$$

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Table 6 (continued)

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Table 7. Parameters of the Transfer Function $G_4(s)$

$$G_4(s) = \frac{L_t[\Delta m(l,t)]}{L_t[\Delta v_c(t)]} = G_4(0) + s \sum \frac{K_i}{s + \nu_i}$$

Steady state gain $G_4(0) = -0.15095 \times 10^{-1}$

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<td>-0.1229 ( \times 10^{-1} )</td>
<td>-0.1404 ( \times 10^{-1} )</td>
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<tr>
<td></td>
<td>4</td>
<td>10.949</td>
<td>14.054</td>
<td>-38.649</td>
<td>-63.654</td>
<td>-0.1328 ( \times 10^{-1} )</td>
<td>-0.2900 ( \times 10^{-2} )</td>
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<tr>
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<td>17.212</td>
<td>-64.087</td>
<td>-95.453</td>
<td>-0.3311 ( \times 10^{-2} )</td>
<td>-0.6941 ( \times 10^{-2} )</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>17.251</td>
<td>20.364</td>
<td>-95.886</td>
<td>-133.61</td>
<td>-0.6532 ( \times 10^{-2} )</td>
<td>-0.9363 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>
Table 8. Parameters of the Transfer Function $G_5(s)$

$$G_5(s) = \frac{L_t[\Delta m(1,t)]}{L_t[\Delta V_g(t)]} = G_5(0) + s \sum \frac{K_i}{s + v_i}$$

<table>
<thead>
<tr>
<th>Case No.</th>
<th>$i$</th>
<th>$\xi_i$</th>
<th>$\xi'_i$</th>
<th>$v_i$</th>
<th>$v'_i$</th>
<th>$K_i$</th>
<th>$K'_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
<td>1.6088</td>
<td>1.6512</td>
<td>7.1834</td>
<td>7.5669</td>
<td>-0.8781$x 10^{-3}$</td>
<td>-0.8942$x 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>4.7202</td>
<td>4.7353</td>
<td>61.806</td>
<td>62.204</td>
<td>-0.1558$x 10^{-2}$</td>
<td>-0.1542$x 10^{-2}$</td>
</tr>
<tr>
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<td>3</td>
<td>7.8524</td>
<td>7.8616</td>
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<td>171.44</td>
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<td>-0.3558$x 10^{-3}$</td>
</tr>
<tr>
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<td>10.988</td>
<td>10.994</td>
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<td>-0.4728$x 10^{-3}$</td>
<td>-0.4697$x 10^{-3}$</td>
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<tr>
<td></td>
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<td>14.124</td>
<td>14.129</td>
<td>553.37</td>
<td>553.77</td>
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<td>17.261</td>
<td>17.265</td>
<td>826.47</td>
<td>826.87</td>
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<td>-0.2436$x 10^{-3}$</td>
</tr>
<tr>
<td>II</td>
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<td>1.2812</td>
<td>0.61344</td>
<td>-0.7529</td>
<td>-0.1923</td>
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<td>0.8753$x 10^{-4}$</td>
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<td>-9.0911</td>
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<td>0.2620$x 10^{-3}$</td>
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<td>3</td>
<td>7.8066</td>
<td>7.7434</td>
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<td>-26.598</td>
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<td>0.6814$x 10^{-4}$</td>
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<tr>
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<td>4</td>
<td>10.963</td>
<td>10.918</td>
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<td>-52.852</td>
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<td>0.8048$x 10^{-4}$</td>
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<tr>
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<td>14.078</td>
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<td>-87.856</td>
<td>0.2121$x 10^{-4}$</td>
<td>0.1990$x 10^{-4}$</td>
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<td></td>
<td>6</td>
<td>17.260</td>
<td>17.232</td>
<td>-132.05</td>
<td>-131.61</td>
<td>0.4065$x 10^{-4}$</td>
<td>0.4202$x 10^{-4}$</td>
</tr>
</tbody>
</table>

Steady state gain $G_5(0) = 0.15398 \times 10^{-3}$
Table 8 (continued)

<table>
<thead>
<tr>
<th>Case No.</th>
<th>i</th>
<th>$\xi_i$</th>
<th>$\xi'_i$</th>
<th>$v_i$</th>
<th>$v'_i$</th>
<th>$K_i$</th>
<th>$K'_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>III</td>
<td>1</td>
<td>2.7193</td>
<td>2.9432</td>
<td>0.6201</td>
<td>0.6541</td>
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<td>-0.1648 x $10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>5.5418</td>
<td>5.9001</td>
<td>1.2454</td>
<td>1.3554</td>
<td>0.1813 x $10^{-3}$</td>
<td>0.2084 x $10^{-3}$</td>
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<tr>
<td></td>
<td>3</td>
<td>8.4741</td>
<td>8.8795</td>
<td>2.3477</td>
<td>2.5364</td>
<td>-0.1206 x $10^{-3}$</td>
<td>-0.1690 x $10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>11.481</td>
<td>11.884</td>
<td>3.9567</td>
<td>4.2098</td>
<td>0.9176 x $10^{-4}$</td>
<td>0.1476 x $10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>14.532</td>
<td>14.913</td>
<td>6.0853</td>
<td>6.3866</td>
<td>-0.6924 x $10^{-4}$</td>
<td>-0.1263 x $10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>17.610</td>
<td>17.962</td>
<td>8.7386</td>
<td>9.0751</td>
<td>0.5728 x $10^{-4}$</td>
<td>0.1122 x $10^{-3}$</td>
</tr>
<tr>
<td>IV</td>
<td>1</td>
<td>1.4899</td>
<td>1.3711</td>
<td>-3.0840</td>
<td>-2.6131</td>
<td>0.3850 x $10^{-3}$</td>
<td>0.3681 x $10^{-3}$</td>
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<tr>
<td></td>
<td>2</td>
<td>4.6892</td>
<td>4.6555</td>
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<td>-30.041</td>
<td>0.7736 x $10^{-3}$</td>
<td>0.7896 x $10^{-3}$</td>
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<tr>
<td></td>
<td>3</td>
<td>7.8433</td>
<td>7.8232</td>
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<td>-84.817</td>
<td>0.1949 x $10^{-3}$</td>
<td>0.1933 x $10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>10.991</td>
<td>10.977</td>
<td>-167.41</td>
<td>-166.98</td>
<td>0.2415 x $10^{-3}$</td>
<td>0.2445 x $10^{-3}$</td>
</tr>
<tr>
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<td>5</td>
<td>14.137</td>
<td>14.126</td>
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<td>-276.52</td>
<td>0.5781 x $10^{-4}$</td>
<td>0.5619 x $10^{-4}$</td>
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<tr>
<td></td>
<td>6</td>
<td>17.282</td>
<td>17.273</td>
<td>-413.89</td>
<td>-413.46</td>
<td>0.1281 x $10^{-3}$</td>
<td>0.1297 x $10^{-3}$</td>
</tr>
</tbody>
</table>
E. Laplace Transform

Obtaining the frequency response data, by applying the complex domain solution technique, requires the Laplace transformation of the linearized system of equations (2-26). To carry out this transformation, the use of the following theorems is necessary. These, as stated by Gould (12), are:

"Theorem 1. If \( f(y,t) \) is transformable with respect to \( t \), and has the transform \( F(y,s) \) and if the limits
\[
\lim_{y \to y_0} f(y,t) \quad \text{and} \quad \lim_{y \to y_0} F(y,s)
\]
both exist, then
\[
L_t \lim_{y \to y_0} [f(y,t)] = \lim_{y \to y_0} F(y,s)
\]

Theorem 2. If \( f(y,t) \) is transformable with respect to \( t \) and has the transform \( F(y,s) \) and if \( \frac{\partial f(y,t)}{\partial y} \) exists, then
\[
L_t \left[ \frac{\partial f(y,t)}{\partial y} \right] = \frac{\partial F(y,s)}{\partial y}
\]

Theorem 3. If \( f(y,t) \) is transformable with respect to \( t \) and has the transform \( F(y,s) \) and if \( f(y,0) \) is the initial value of \( f(y,t) \), then
\[
L_t \left[ \frac{\partial f(y,t)}{\partial t} \right] = sF(y,s) - f(y,0)
\]

Theorem 1 states the conditions for commutativity of the transform operation and a limiting process. Theorem 2 is a corollary of theorem 1 in the special case of partial differentiation with respect to a
second independent variable. Theorem 3 is merely a recasting of the well known real differentiation theorem in the case of partial differentiation of a function of several variables (including time) with respect to time."

Theorems 2 and 3 take the following form for higher order derivatives:

\[ L_t \left( \frac{\partial^n f(y,t)}{\partial y^n} \right) = \frac{\partial^n F(y,s)}{\partial y^n} \]

\[ L_t \left( \frac{\partial^n f(y,t)}{\partial t^n} \right) = s^n F(y,s) - s^{n-1} f(y,0) - s^{n-2} f'(y,0) - \ldots - f^{n-1}(y,0) \]

Here \( f'(y,0), \ldots, f^{n-1}(y,0) \) are the derivatives with respect to time evaluated at \( t=0 \).

To carry out the transformation of the system of equations (2-26) to the Laplace domain, the steady states are assumed to be initial steady states. This assumption results in zero initial distributions of the incremental variables. It is always possible to make this assumption, since in any Laplace transformation the initial conditions may be set equal to zero. Then, after obtaining the solution on the basis of this assumption, the final solution is simply obtained by adding the initial condition to the above solution.

Application of theorems 2 and 3 to the system of equations (2-26) yields
\[
\frac{dT_c}{dy} = \frac{L}{H_1 V_c} \left[ (H_1 s + k_1) \tilde{T}_c - k_1 \tilde{T}_g - H_1 S_1(y) \tilde{\phi}_c(s) \right]
\]

\[
\frac{dT_g}{dy} = \frac{L}{H_2 V_g} \left[ (k_1 - k_2 S_3(y)) \tilde{T}_c - (H_2 s + k_1 + k_2 S_3(y)) \tilde{T}_g 
+ k_2 S_2(y) \tilde{m} - H_2 S_4(y) \tilde{\phi}_g(s) \right]
\]

\[
\frac{d\tilde{m}}{dy} = \frac{L}{H_3 V_g} \left[ k_2 S_3(y) \tilde{T}_c + k_2 S_3(y) \tilde{T}_g - (H_3 s + k_2 S_2(y) \tilde{m}
- H_3 S_5(y) \tilde{\phi}_g(s) \right]
\]

(3-47)

Here \(S_1(y)\) through \(S_5(y)\) are the sensitivity coefficient defined by equations (2-24).

**F. Frequency Response**

The method used to obtain the frequency response of the heat exchanger system is the complex domain solution technique as reported by Foss and Sinai (38). To implement the technique, the Laplacian operator \(s\) is substituted by \(j\omega\) (where \(j = \sqrt{-1}\), and \(\omega\) is the frequency in radians/min.) into equations (3-47). All the dependent variables, \(\tilde{T}_c(y,j\omega), \tilde{T}_g(y,j\omega), \tilde{m}(y,j\omega)\), and the velocities \(\tilde{\phi}_c(j\omega)\) and \(\tilde{\phi}_g(j\omega)\) are now complex variables. These variables may be represented by their real and imaginary components as follows:
\[ \begin{align*}
\dot{\tilde{c}} &= TCR + jTCI \\
\tilde{g} &= TGR + jTGI \\
\tilde{m} &= MR + jMI \\
\dot{\tilde{v}}_c &= VCR + jVCI \\
\dot{\tilde{v}}_g &= VGR + jVGI
\end{align*} \]

(3-48)

Here it is understood that all the variables on the right hand side of equations (3-48) are functions of the spatial coordinate \( y \) except the velocity components which are independent of \( y \). These complex variables are substituted into the system of equations (3-47). The result is

\[ \begin{align*}
\frac{j}{d^2y} TCI + \frac{d}{dy} TCR &= \frac{L}{H_1 V_c} \left[ (jH_1 \omega + k_1)(TCR + jTCI) \\
&- k_1(TGR + jTGI) - H_1 S_1(y)(VCR + jVCI) \right] \\
\frac{j}{d^2y} TGI + \frac{d}{dy} TGR &= \frac{L}{H_2 V_g} \left[ (k_1 - k_2 S_3(y))(TCR + jTCI) \\
&- (jH_2 \omega + k_1 + k_2 S_3(y))(TGR + jTGI) \\
&+ k_2 S_2(y)(MR + jMI) - H_2 S_4(y)(VGR + jVGI) \right] \\
\frac{j}{d^2y} MI + \frac{d}{dy} MR &= \frac{L}{H_3 V_g} \left[ k_2 S_3(y)(TCR + jTCI) + k_2(TGR + jTGI) \\
&- (jH_3 \omega + k_2 S_3(y))(MR + jMI) - H_3 S_5(y)(VGR + jVGI) \right] \\
\end{align*} \]

(3-49)

Multiplying the terms in the brackets, substituting \( j^2 = -1 \) wherever it appears, and finally setting the real and imaginary parts in both sides of quality signs equal to each other (definition of equality of
two complex variables) yields

\[
\frac{d}{dy} TCI = \frac{L}{H_1 V_c} \left[ k_1 TCI + H_1 \omega TCR - k_1 TGI - H_1 S_1 (y) VCI \right]
\]

\[
\frac{d}{dy} TCR = \frac{L}{H_1 V_c} \left[ - H_1 \omega TCI + k_1 TCR - k_1 TGR - H_1 S_1 (y) VCR \right]
\]

\[
\frac{d}{dy} TGI = \frac{L}{H_2 V_g} \left[ (k_1 - k_2 S_3 (y)) TCI - (k_1 + k_2 S_3 (y)) TGI - H_2 \omega TGR \\
+ k_2 S_2 (y) MI - H_2 S_4 (y) VGI \right]
\]

\[
\frac{d}{dy} TGR = \frac{L}{H_2 V_g} \left[ (k_1 - k_2 S_3 (y)) TCR + H_2 \omega TGI - (k_1 + k_2 S_3 (y)) TGR \\
+ k_2 S_2 (y) MR - H_2 S_4 (y) VGR \right]
\]

\[
\frac{d}{dy} MI = \frac{L}{H_3 V_g} \left[ k_2 S_3 (y) TCI + k_2 S_3 (y) TGI - k_2 S_2 (y) MI - H_3 \omega MR \\
- H_3 S_5 (y) VGI \right]
\]

\[
\frac{d}{dy} MR = \frac{L}{H_3 V_g} \left[ k_2 S_3 (y) TCR + k_2 S_3 (y) TGR + H_3 \omega MI - k_2 S_2 (y) MR \\
- H_3 S_5 (y) VGR \right]
\]

Equations (3-50) form a system of six ordinary differential equations with split boundary conditions. To obtain the frequency response data, these equations must be solved simultaneously for every frequency \( \omega \). The boundary conditions are specified according to the input variable whose effect on the output variable is being sought.

To obtain the effect of each input variable on the output
variables, the real part of this input variable is set equal to a constant or simply one and its imaginary part plus the real and imaginary parts of all other input variables are set equal to zero. This is equivalent to having the system forced by a delta function since the Fourier transform of delta function is real and equal to its strength. If the constant is taken to be one, the resulting frequency response data will be that of the transfer function, otherwise the magnitude should be divided by the constant.

In order to obtain the frequency response of the transfer functions $G_i(s)$ through $G_5(s)$ (defined in Tables 4 through 8), using the complex domain solution technique, the conditions given in Table 9 were imposed on the system of equations (3-50). Once the system of equations (3-50) are solved for discrete values of $\omega$, the magnitude and phase angle is calculated as follows:

$$|G_i(j\omega)| = \sqrt{(MR(y=1))^2 + (MI(y=1))^2}/\text{FORCV}$$

$$\angle G_i(j\omega) = \tan^{-1}(MI(y=1)/MR(y=1))$$

(3-51)

Here FORCV is the forcing variable and it is equal to the non-zero element of each column in Table 9.

After obtaining the magnitude and the phase angle, one may try to fit the data into a particular transfer function model. Some of the models which have been suggested by different authors were discussed in Section A of this chapter. Once the transfer function model is chosen, some criteria such as integral of squared time error, integral of squared error, etc., may be minimized with respect to the parameters of the model. One criteria which is commonly used is the
minimization of the integral of squared error defined as:

\[
\text{ISE} = \int_0^\infty [f(t,y) - h(t,y)]^2 \, dt \quad (3-52)
\]

where

\[ f(t,y) = \text{actual time response of the system} \]
\[ h(t,y) = \text{the time response of the transfer function model}. \]

Table 9. Conditions Imposed on Equations (3-50)

<table>
<thead>
<tr>
<th>Conditions to obtain:</th>
<th>( G_1(j\omega) )</th>
<th>( G_2(j\omega) )</th>
<th>( G_3(j\omega) )</th>
<th>( G_4(j\omega) )</th>
<th>( G_5(j\omega) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCI ( y=1 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TCR ( y=1 )</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TGI ( y=0 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TGR ( y=0 )</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>MI ( y=0 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>MR ( y=0 )</td>
<td>0</td>
<td>0</td>
<td>0.05</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>VCI</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>VCR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.05( V_c )</td>
<td>0</td>
</tr>
<tr>
<td>VGI</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>VGR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.1( V_g )</td>
</tr>
</tbody>
</table>

Schnell, utilizing Parseval's theorem, has shown that the frequency domain equivalent of equation (3-52) is given by:

\[
\text{ISEF} = \int_0^\infty [G^2 - 2GH \cos(\theta - \psi) + H^2] \, d\omega \quad (3-53)
\]

where

\[ G = |F(j\omega)| = \text{actual magnitude of system frequency response} \]
\[ H = |H(j\omega)| = \text{the magnitude of the transfer function model} \]
\[ \theta = \text{actual phase angle of the system frequency response} \]
\[ \psi = \text{the phase angle of transfer function model.} \]

The approximation of the system's dynamics by a particular model is not being performed in this research; however, equation (3-53) is used, in the next chapter, to evaluate the controller parameters from its frequency response data.

Regardless of the input variable whose effect on the output variable is being sought, the system of equations (3-50) has split boundary conditions. There are two unspecified conditions at \( y=0 \) (TCE, and TCR). Equations (3-50), subject to conditions given in Table 9, were solved numerically. Gill's modification of the fourth order Runge-Kutta were used. The shooting method, as was discussed in Section D of Chapter II, was used. The algorithm to adjust the assumed initial conditions is the well known Newton-Raphson method which is developed, for the general case of \( n \) unknown initial conditions, in Appendix B. The Jacobian matrix \( J \) was evaluated numerically with the increment of 0.05. Its inversion was carried out by the Gauss-Jordan elimination method (6), and a general computer routine that gives the inverse of the matrix as well as the increment vector of missing initial conditions is taken from the same reference.

For all frequency \( \omega \), the assumed initial conditions (TCI(\( y=0 \)), and TCR(\( y=0 \))) at the start of the solution were set equal to zero. The tolerance used was, as before, equal to \( 10^{-6} \). The heat exchanger was divided into 80 equal segments to carry out any numerical solution in this study except for the solution of partial differential equations in which the system was divided into 40 equal segments. The computer
program for the solution of the system equations was validated by a problem with known analytical solution (12).

G. Discussion of the Results

In section B of this chapter, three basic assumptions which are the foundation of the Taylor diffusion model were given. The first two are the vital ones, and the third one limits the class of system that can be treated by the Taylor model. To satisfy the later assumption for the system under study, both sides of equation (2-10) were multiplied by \( \lambda \). It was mentioned in the earlier part of this chapter that physical intuition may be needed in developing the model for more complicated systems. Additionally, it is reported by Gould (12) and Rosenbrock (27) that the Taylor diffusion approximation of a heat exchanger represents adequately the dynamics of the system as long as the number of transfer units (e.g., \( N_1 = k_1L/H_1V_c \), \( N_2 = k_1L/H_2V_c \)) are greater than two. Once use is made of the first assumption in transforming the system's equations into a moving coordinate which forces the system into equilibrium, the second assumption must be invoked to obtain the velocity by which the coordinate is moving. This assumption cannot always be satisfied. Here, the need for physical intuition or the requirement for the magnitude of the number of transfer units become essential. In this study, an attempt was made to eliminate these limitations. This was accomplished by modifying the second assumption through introduction of new parameters (e.g., \( \zeta_1 \), \( \zeta_2 \), and \( \zeta_3 \) defined by equations (3-11)).

A systematic approach was chosen in developing the Taylor diffusion model. A weighted mean variable was first defined (equation (3-10)).
Use was made of the first assumption to transform the system's equation into a moving coordinate system traveling by an undefined mean velocity. To evaluate this velocity, the modified second assumption (equation (3-11)) was invoked. The main problem was in the estimation of these additional parameters ($\zeta_1$, $\zeta_2$, and $\zeta_3$). In section D of this chapter, the general procedure of obtaining the transfer functions $G_1(s)$ through $G_5(s)$ was given. The form and the corresponding data of these transfer functions are given in Tables 4 through 8. Four different cases were investigated in evaluating the parameters $\zeta_1$, $\zeta_2$, and $\zeta_3$. These are given in section D. Case I is based on the unmodified second assumption. Case III is on the basis of physical intuition. Cases II and IV were obtained as follows. The idea stems from equations (3-11) where they are first introduced. If these relations are always satisfied approximately, then they must be so initially. Additionally, it is shown by equations (3-7) that the axial gradients in the actual and moving coordinate are equal. Consequently one may use the same relationship (equations (3-11)) to obtain these parameters by using the initial steady state solution. If the parameters do not exhibit extreme nonlinearity, they may be substituted by their mean value. This was done in Case IV of this study. In Case II, one of these parameters ($\zeta_1$) was arbitrarily set equal to one, and the other two were obtained as follows. Consider equations (3-11), since the left hand side of these equations are the same then the right hand side must equal to each other

$$\zeta_1 \frac{\partial \delta T}{\partial y} = \zeta_2 \frac{\partial \delta T}{\partial y} = \zeta_3 \frac{\partial \delta m}{\partial y}.$$ 

Since $\zeta_1$ has been specified, then $\zeta_2$ and $\zeta_3$ can be calculated by using the initial steady state solution to evaluate the axial gradients. In this case evaluation of
the axial gradient of the weighted variable $\frac{\partial \delta m}{\partial y}$ is not necessary. Systems where these parameters exhibit extreme nonlinearity are discussed in Chapter V. By the approach chosen in this study, one need not be concerned about using physical intuition in satisfying the second assumption.

To study the relative merits of the individual cases, the plots of the magnitude and the phase angle of the transfer functions $G_1(s)$ through $G_5(s)$ versus frequency $\omega$ were obtained. The results are shown in Figures 3-1 through 3-32. In each figure, there are four different curves. One curve represents the result of the complex domain solution which is used as a comparison base to validate the relative accuracy of the individual cases of each transfer function. The other three curves are the result of Taylor diffusion approximation associated with one set of boundary conditions (equations (3-28)) and retaining three through five eigenvalues. The plots of the other set of transfer functions obtained by the use of boundary conditions (equations (3-29)) were not obtained, since the two sets of transfer functions are approximately equal. Case I resulted in a set of transfer functions which exhibit quite different characteristics than that of the actual ones. This further strengthens the significance of the second assumption. Cases II through IV adequately represent the dynamics of the system. Note that for the transfer functions $G_4(s)$ and $G_5(s)$ relating the output variable $\delta m(y=1,t)$ to the coolant and gas velocity, only the plots for Cases I and III are reported here since Cases II and IV resulted in unstable transfer functions (see Tables 7 and 8). This is not surprising since the axial gradients exhibit such a severe nonlinearity that
the averaging of the parameters $\zeta_1$, $\zeta_2$, and $\zeta_3$ loses its significance. Here, it is understood that in Cases II and IV, the parameters $\zeta_1$, $\zeta_2$, and $\zeta_3$ are evaluated separately for each transfer function (in Case II, $\zeta_1$ is set equal to one). In other words, the steady state equations (3-46) subject to the corresponding conditions given in Table 3 must be solved to obtain initial distributions. On the contrary, these parameters are constant in Cases I and III for all the transfer functions. Cases II and IV give satisfactory results for all the inputs other than the velocities, and the results of Case III are satisfactory for all the inputs. Consequently one may conclude that once the $\zeta_1$ parameters are evaluated using the technique of Case II or IV, that for any input other than the velocity they may be used to obtain the transfer function relating the output variable to the velocity.
COMPARISON BETWEEN MAGNITUDE OF $G_1(s)$ OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-1

MAGNITUDE OF $G_1(s)$

FREQUENCY IN RADIANS/MIN.
COMPARISON BETWEEN PHASE ANGLE OF G1(S) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-2
COMPARISON BETWEEN MAGNITUDE OF $G_1(s)$ OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE II

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-3
COMPARISON BETWEEN PHASE ANGLE OF G1(S) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE II

LEGEND
- COMPLEX DOMAIN SOL.  O THREE EIG. VALUES
Δ FOUR EIG. VALUES + FIVE EIG. VALUES

Figure 3-4
COMPARISON BETWEEN MAGNITUDE OF $G_1(s)$ OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND
- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-5
COMPARISON BETWEEN PHASE ANGLE OF $G_1(S)$ OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-6
COMPARISON BETWEEN MAGNITUDE OF $G_1(S)$ OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE IV

LEGEND

- COMPLEX DOMAIN SOL.
- FOUR EIG. VALUES
- THREE EIG. VALUES
- FIVE EIG. VALUES

Figure 3-7

MAGNITUDE OF $G_1(S)$

FREQUENCY IN RADIANS/MIN.
Figure 3-8

Figure 3-8
COMPARISON BETWEEN MAGNITUDE OF $G_2(s)$ OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE I

**Legend**
- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

**Figure 3-9**

MAGNITUDE OF $G_2(s)$ vs. FREQUENCY IN RADIANS/MIN.
Comparison between phase angle of C2(s) obtained from complex domain solution and Taylor model case I.

Legend:
- Complex Domain Sol.
- Three Eig. Values
- Four Eig. Values
- Five Eig. Values

Figure 3-10

Phase angle of C2(s) in degrees

Frequency in radians/min.
Comparison between Magnitude of $G_2(s)$ obtained from Complex Domain Solution and Taylor Model Case II

**Legend**

- □ Complex Domain Sol.
- △ Four EIG. Values
- ○ Three EIG. Values
- + Five EIG. Values

**Figure 3-11**

Frequency in Radians/Min.

Magnitude of $G_2(s)$
COMPARISON BETWEEN PHASE ANGLE OF G2(s) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE II

LEGEND

- COMPLEX DOMAIN SOL.
- FOUR EIG. VALUES
- THREE EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-12
COMPARISON BETWEEN MAGNITUDE OF G2(S) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND
- COMPLEX DOMAIN SOL. • THREE EIG. VALUES
Δ FOUR EIG. VALUES + FIVE EIG. VALUES

Figure 3-13
COMPARISON BETWEEN PHASE ANGLE OF $G_2(s)$ OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE III

<table>
<thead>
<tr>
<th>LEGEND</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>⊙ COMPLEX DOMAIN SOL.</td>
<td>○ THREE EIG. VALUES</td>
</tr>
<tr>
<td>▲ FOUR EIG. VALUES</td>
<td>+ FIVE EIG. VALUES</td>
</tr>
</tbody>
</table>

![Graph showing phase angle comparison]

**Figure 3-14**

**Legend**
- ⊙ Complex Domain Sol.
- ○ Three EIG. Values
- ▲ Four EIG. Values
- + Five EIG. Values

**Axes:**
- Y-axis: Phase Angle of $G_2(s)$ in Degrees
- X-axis: Frequency in Radians/Min.
COMPARISON BETWEEN MAGNITUDE OF G2(s) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE IV

LEGEND

□ COMPLEX DOMAIN SOL.
△ FOUR EIG. VALUES
○ THREE EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-15

MAGNITUDE OF G2(s)

FREQUENCY IN RADIANS/MIN.
COMPARISON BETWEEN PHASE ANGLE OF G2(S) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE IV

LEGEND
- COMPLEX DOMAIN SOL.
△ FOUR EIG. VALUES
○ THREE EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-16

FREQUENCY IN RADIANS/MIN.

PHASE ANGLE OF G2(S) IN DEGREES
Comparison between magnitude of $g_3(s)$ obtained from complex domain solution and Taylor model case I.

**Legend**
- $\circ$ Complex domain sol.
- $\triangle$ Four eig. values
- $\diamond$ Three eig. values
- $+$ Five eig. values

![Diagram showing comparison of magnitudes](image)

Figure 3-17
COMPARISON BETWEEN PHASE ANGLE OF G3(S) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND

- COMPLEX DOMAIN SSL.  ○ THREE EIG. VALUES
△ FOUR EIG. VALUES  △ FIVE EIG. VALUES

Figure 3-18

FREQUENCY IN RADIANS/MIN.

PHASE ANGLE OF G3(S) IN DEGREES

100.00 -180.00 -120.00

10° 10³ 10⁶ 10⁴ 10² 10⁰ 10⁻² 10⁻⁴ 10⁻⁶
COMPARISON BETWEEN MAGNITUDE OF G3(s) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE II

LEGEND

○ COMPLEX DOMAIN SOL.
▲ FOUR EIG. VALUES
○ THREE EIG. VALUES
◆ FIVE EIG. VALUES

Figure 3-19

MAGNITUDE OF G3(S) VS FREQUENCY IN RAD/SEC.
Figure 3-20
COMPARISON BETWEEN MAGNITUDE OF G3(s) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND
- COMPLEX DOMAIN SOL.
- FOUR EIG. VALUES
- THREE EIG. VALUES
- FIVE EIG. VALUES

Figure 3-21

MAGNITUDE OF G3(S)

FREQUENCY IN RAD/SEC
COMPARISON BETWEEN PHASE ANGLE OF G3(S) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND

○ COMPLEX DOMAIN SOL.
● FOUR EIG. VALUES
○ THREE EIG. VALUES
● FIVE EIG. VALUES

Figure 3-22

FREQUENCY IN RADIANS/Min.
COMPARISON BETWEEN MAGNITUDE OF G3(S) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE IV

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
△ FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-23

MAGNITUDE OF G3(S)

10^0

10^2

10^4

10^6

10^8

10^10

10^12

FREQUENCY IN RADIANS/MIN.
COMPARISON BETWEEN PHASE ANGLE OF G3(S) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE IV

LEGEND

○ COMPLEX DOMAIN SOL.

△ FOUR EIG. VALUES

○ THREE EIG. VALUES

+ FIVE EIG. VALUES

Figure 3-24
COMPARISON BETWEEN MAGNITUDE OF G_4(S) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-25
COMPARISON BETWEEN PHASE ANGLE OF $G(\omega)$ OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND
- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-26

PHASE ANGLE OF $G(\omega)$ IN DEGREES

FREQUENCY IN RAD/SEC

FREQUENCY IN RADIANS/MIN.

Figure 3-26
COMPARISON BETWEEN MAGNITUDE OF G\(_4\)(s) OBTAINED FROM COMPLEX
domain solution and Taylor model case III

**LEGEND**
- **Complex domain sol.**
- **Four eig. values**
- **Three eig. values**
- **Five eig. values**

![Graph showing comparison between magnitude of G\(_4\)(s) obtained from complex domain solution and Taylor model case III.](image)

Figure 3-27
COMPARISON BETWEEN PHASE ANGLE OF $G_4(S)$ OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-28
COMPARISON BETWEEN MAGNITUDE OF G5(S) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND

- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
- FOUR EIG. VALUES
- FIVE EIG. VALUES

Figure 3-29
COMPARISON BETWEEN PHASE ANGLE OF G5(S) OBTAINED FROM COMPLEX DOMAIN SOLUTION AND TAYLOR MODEL CASE I

LEGEND

- COMPLEX DOMAIN SOL.
-△ FOUR EIG. VALUES
-○ THREE EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-30

PHASE ANGLE OF G5(S) IN DEGREES

FREQUENCY IN RADIANS/MIN.
COMPARISON BETWEEN MAGNITUDE OF G5(S) OBTAINED FROM COMPLEX
DOMAIN SOLUTION AND TAYLOR MODEL CASE III

LEGEND
- COMPLEX DOMAIN SOL.
- THREE EIG. VALUES
△ FOUR EIG. VALUES
+ FIVE EIG. VALUES

Figure 3-31
Comparison between phase angle of $G_5(s)$ obtained from complex domain solution and Taylor model case III

Legend
- Complex domain sol.
- Three eig. values
- Four eig. values
- Five eig. values

Figure 3-32

Phase angle of $G_5(s)$ in degrees

Frequency in radians/min
CHAPTER IV

INVARINANCE CONTROLLERS

A. Introduction

The direct application of the technique of Chapter I for designing invariance controllers to a distributed parameter system requires a knowledge of the transfer functions relating input to output variables. Because of the complexity of the analytical expression of these transfer functions, it has been a common practice to approximate the dynamics of the system by simpler transfer function models. The case where the input variables occur as changes in the boundary conditions has been investigated by different researchers, and a variety of transfer function models have been suggested. These were discussed in section A of Chapter III. The literature search revealed little effort in developing transfer functions for this type of systems where the input is the fluid velocity and therefore no particular transfer function model has been suggested previously.

For the system under study, the manipulated variable is the coolant fluid velocity. The load disturbances are changes in inlet gas and coolant temperature, inlet mass fraction of water, and gas velocity. The controlled variable is the outlet mass fraction of water \( \delta m(y=1,t) \) which is to be held invariant in the face of the above disturbances entering the system.

In this research neither the transfer functions obtained from
the Taylor diffusion model, nor the discrete frequency response data of the transfer functions obtained from the complex domain solution technique were used in designing invariance controllers. The transfer functions obtained from the Taylor diffusion model are valid in the low frequency region. Consequently, if one uses them to design invariance controllers, the controllers so designed will be seriously in error during upsets which contain significant energy having high frequency content. This was the principal reason that these transfer functions were not used to design invariance controllers. A frequency response technique for designing a feedforward controller for a distillation column has been suggested by Luyben (24). The technique is principally the same as the one given in Chapter I. It requires the frequency response data of the transfer functions relating the disturbance and manipulated variable to the output variable. This technique was modified in this study and was applied to the determination of invariant controllers. Here the frequency response data of the manipulated variable which makes the output variable invariant is first obtained. These data are obtained by solving the complex domain equations, developed in the previous chapter, with the appropriate boundary conditions. This technique will be explained in detail later in the following section.

In order to study the effectiveness of these controllers, the time response of the controlled variable (outlet mass fraction of water) to step changes in load disturbances were obtained both with and without the invariant controller. These responses were compared graphically. Additionally, the following criterion was evaluated to quantitatively
define the controller effectiveness:

\[ E = \frac{I_u - I_c}{I_u} \times 100 \]  

(4-1)

where \( E \) is the controller efficiency, \( I_u \) is the integrated absolute value of the output variable which is to be held invariant but under conditions of no control, and \( I_c \) is the integrated absolute value of this same output variable under conditions of control. In other words, if the output variable is truly invariant, then \( I_c = 0 \), and \( E = 100 \).

B. Design of Invariance Controllers

Regardless of how the invariance controllers are defined, the manipulated variable obtained by the use of these controllers results in zero output (controlled) variable in the face of a measurable disturbance entering the system. Consider the system under study where the controlled variable is the outlet mass fraction of water \( \delta m(y=1,t) \), and the manipulated variable is the coolant fluid velocity \( \delta V_c(t) \). Invariance conditions of \( \delta m(y=1,t) = 0 \) in the time domain is equivalent to \( \tilde{m}(y=1,s) = 0 \) in the Laplace domain. The same condition, in the frequency domain, is satisfied if both real and imaginary parts of \( \tilde{m}(y=1,j\omega) \) are simultaneously zero. Consequently if one can find the frequency components of the manipulated variable \( \tilde{V}_c(j\omega) \) that results in zero components of \( \tilde{m}(y=1,j\omega) \), then this can be related to the frequency response of the invariant controller as explained below.

In this study, only invariance feedforward controllers were designed and their effectiveness was investigated. Representing the invariance feedforward controllers by \( GC_1(s) \), \( GC_2(s) \), \( GC_3(s) \), and \( GC_5(s) \)
which correspond to the input variables $\tilde{T}_c(y=1,s)$, $\tilde{T}_g(y=1,s)$, $\tilde{m}(y=0,s)$, and $\tilde{V}_g(s)$ respectively; then the general control equation may be defined as follows

$$\tilde{V}_c(s) = G_{C_1}(s) \tilde{T}_c(y=1,s) + G_{C_2}(s) \tilde{T}_g(y=0,s) + G_{C_3}(s) \tilde{m}(y=0,s) + G_{C_5}(s) \tilde{V}_g(s)$$

(4-2)

In order to obtain the frequency response of the individual controllers, one may set all but one input variable equal to zero. This practice is feasible, since the system's mode, which is used to obtain $\tilde{V}_c(j\omega)$ that makes the output variable invariant, is linear and the superposition principle is valid. Consider one particular case where the non-zero input variable is $\tilde{T}_c(y=1,s)$, then equation (4-2) reduces to

$$\tilde{V}_c(s) = G_{C_1}(s) \tilde{T}_c(y=1,s)$$

(4-3)

Suppose that $V_c(j\omega)$ which makes the outlet mass fraction of water invariant in the face of changes in inlet cooling temperature $\tilde{T}_c(y=1,s)$ has been obtained; then the magnitude and the phase angle of the controller $G_{C_1}(j\omega)$ are simply obtained by:

$$|G_{C_1}(j\omega)| = \frac{|\tilde{V}_c(j\omega)|}{|\tilde{T}_c(y=1,j\omega)|}$$

(4-4)

$$\angle G_{C_1}(j\omega) = \angle \tilde{V}_c(j\omega) - \angle \tilde{T}_c(y=1,j\omega)$$

The following section describes the determination of $\tilde{V}_c(j\omega)$ which makes the controlled variable invariant.
C. Determination of Invariance $\tilde{\tilde{V}}_c(j\omega)$
and the Invariance Controllers

The general system equations, in the frequency domain, were derived in the previous chapter. These are equations (3-50) which were used to obtain the frequency response data of the transfer functions $G_1(j\omega)$ through $G_5(j\omega)$. These equations are:

$$\frac{d}{dy} TCI = \frac{L}{H_1c} [k_1 TCI + H_1 TCR - k_1 TGI - H_1 S_1(y) VCI]$$

$$\frac{d}{dy} TCR = \frac{L}{H_1c} [- H_1 TCI + k_1 TCR - k_1 TGR - H_1 S_1(y) VCR]$$

$$\frac{d}{dy} TGI = \frac{L}{H_2g} [(k_1 - k_2 S_3(y)) TCI - (k_1 + k_2 S_3(y)) TGI - H_2 \omega TGR$$

$$+ k_2 S_2(y) MI - H_2 S_4(y) VGI]$$

$$\frac{d}{dy} TGR = \frac{L}{H_2g} [(k_1 - k_2 S_3(y)) TCR + H_2 \omega TGI - (k_1 + k_2 S_3(y)) TGR$$

$$+ k_2 S_2(y) MR - H_2 S_4(y) VGR]$$

$$\frac{d}{dy} MI = \frac{L}{H_3g} [k_2 S_3(y) TCI + k_2 S_3(y) TGI - k_2 S_2(y) MI - H_3 \omega MR$$

$$- H_3 S_5(y) VGI]$$

$$\frac{d}{dy} MR = \frac{L}{H_3g} [k_2 S_3(y) TCR + k_2 S_3(y) TGR + H_3 \omega MI - k_2 S_2(y) MR$$

$$- H_3 S_5(y) VGR]$$

The technique of obtaining the frequency response data of $\tilde{\tilde{V}}_c(j\omega)$ which makes the controlled variable invariant is similar to the one
described in section F of Chapter III, but with a different set of conditions imposed on equations (4-5). These conditions are given in Table 10. Note that in every column, the last two rows are set equal to zero which are the requirements for invariance in the frequency domain. In contrast to the conditions given in Table 9 of Chapter II, which were imposed on equations (3-50) to obtain the frequency response data of the transfer functions, two additional conditions are added here. These are MR(y=1) = 0, and MI(y=1) = 0. There are two additional unknowns (VCR and VCI) which must be determined to satisfy the above two conditions.

Table 10. Conditions Imposed on Equations (4-5) to Obtain the Frequency Response of Invariant Controllers

<table>
<thead>
<tr>
<th></th>
<th>GC₁(jω)</th>
<th>GC₂(jω)</th>
<th>GC₃(jω)</th>
<th>GC₅(jω)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCR(y=1)</td>
<td>1.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TCI(y=1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TGR(y=0)</td>
<td>0</td>
<td>1.0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>TGI(y=0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>MR(y=0)</td>
<td>0</td>
<td>0</td>
<td>0.05</td>
<td>0</td>
</tr>
<tr>
<td>MI(y=0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>VGR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.1 (\bar{V}_g)</td>
</tr>
<tr>
<td>VGI</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>MR(y=1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>MI(y=1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Equations (4-5) subject to conditions of Table 10 were solved numerically for discrete values of frequency. In solving equations (4-5) with the associated conditions, there are four unknowns which
must be determined. These are two missing boundary conditions, TCR and TCI at initial point \( y=0 \), and two coolant velocity components, VCR and VCI, to satisfy the invariance conditions. The shooting technique was used in solving the equations (4-5). These four unknowns were assumed initially (they were set equal to zero) for every frequency, and the equations were solved. If the computed conditions did not match the ones given in Table 10, the assumed unknowns were adjusted and the solution was repeated. Gill's modification of fourth order Runge-Kutta was used to solve the system of equations (4-5). A Newton-Raphson technique, developed in Appendix B, was used to adjust the assumed unknowns. Here the error vector has four elements which are the differences between the computed TCR, TCI, MR, and MI at \( y=1 \) and the corresponding ones given in Table 10. The Jacobian is a 4x4 matrix and was evaluated numerically. The increment used to evaluate the Jacobian was taken equal to 0.05. The tolerance used was equal to \( 10^{-6} \).

Once VCR and VCI are obtained, the magnitude and the phase angle of \( \tilde{V}_c(j\omega) \) may be calculated by

\[
|\tilde{V}_c(j\omega)| = \sqrt{VCR^2 + VCI^2}
\]

\[
\angle\tilde{V}_c(j\omega) = \tan^{-1} \frac{VCI}{VCR}
\]

Then equations (4-4) were used to obtain the frequency response data of the controller \( GC_1(j\omega) \) as explained above. The procedure to obtain the other controllers is exactly the same.

The magnitude and the phase angle of each controller are plotted versus frequency \( \omega \) in Figures 4-1 through 4-8. Also shown in the same
MAGNITUDE OF THE CONTROLLER DESIGNED FOR INLET COOLANT TEMPERATURE CHANGES

LEGEND
- THEORETICAL
- APPROXIMATE

Figure 4-1
PHASE ANGLE OF THE CONTROLLER DESIGNED FOR INLET COOLANT TEMPERATURE CHANGES

LEGEND

□ THEORETICAL
○ APPROXIMATE

Figure 4-2

FREQUENCY IN RADIANS/MIN.
MAGNITUDE OF THE CONTROLLER DESIGNED FOR INLET GAS TEMPERATURE CHANGES

LEGEND

O THEORETICAL
O APPROXIMATE

Figure 4-3

FREQUENCY IN RADIANS/MIN.
PHASE ANGLE OF THE CONTROLLER DESIGNED FOR INLET GAS TEMPERATURE CHANGES

LEGEND

- THEORETICAL
- APPROXIMATE

Figure 4-4

FREQUENCY IN RADIANS/MIN.
MAGNITUDE OF THE CONTROLLER DESIGNED FOR INLET GAS MAS FRACTION OF WATER CHANGES

LEGEND

THEORETICAL
APPROXIMATE

Figure 4-5

FREQUENCY IN RADIANS/MIN.
PHASE ANGLE OF THE CONTROLLER DESIGNED FOR INLET GAS MAS FRACTION OF WATER CHANGES

LEGEND

□ THEORETICAL
○ APPROXIMATE

Figure 4-6

FREQUENCY IN RADIANS/MIN.
MAGNITUDE OF THE CONTROLLER DESIGNED FOR GAS VELOCITY CHANGES

LEGEND

- THEORETICAL
- APPROXIMATE

Figure 4-7

FREQUENCY IN RADIANS/MIN.
PHASE ANGLE OF THE CONTROLLER DESIGNED FOR GAS VELOCITY CHANGES

LEGEND

- THEORETICAL
- APPROXIMATE

Figure 4-8

PHASE ANGLE OF CONTROLLER CC5 IN DEGREES

-200.00
-150.00
-100.00
-50.00
0.00

FREQUENCY IN RADIANS/MIN.
figure are the plots of the magnitude and the phase angle of the approximate transfer function of the corresponding controller. The magnitude of the analytical controllers exhibit the characteristic of a first order lead term. They start increasing very slowly in the low frequency region. This behavior eliminates the existence of any predictor elements associated with the controller. This indicates that the controllers are physically realizable. As the frequency increases, the phase angle increases and reaches a maximum, then starts decreasing (except for $GC_5(j\omega)$). This behavior indicates the existence of a dead time element associated with the controllers. Although the approximation of these controllers by PD controller plus a dead time element would result in a better fit, because of practical hardware considerations they were approximated by a conventional PD controller. In approximating these controllers, the equivalence of the integral of square error in the frequency domain (equation (3-53)) was minimized. It must be mentioned that the portion of the controller's frequency response data between frequencies $\omega=0$ to $\omega=10$ were used in their approximation. The parameters of the controllers are given in Table 11.

Table 11. The Parameters of Invariance Controllers

$$GC_i(s) = K_i(1 + T_{di}s)$$

<table>
<thead>
<tr>
<th>$i$</th>
<th>$K_i$</th>
<th>$T_{di}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.25069</td>
<td>0.14280</td>
</tr>
<tr>
<td>2</td>
<td>$0.46355 \times 10^{-1}$</td>
<td>0.24794</td>
</tr>
<tr>
<td>3</td>
<td>$0.24509 \times 10^{2}$</td>
<td>0.24852</td>
</tr>
<tr>
<td>5</td>
<td>$0.10201 \times 10^{-1}$</td>
<td>0.86078</td>
</tr>
</tbody>
</table>
As is evident from Figures 4-1 through 4-8, the fit is fairly good in the low frequency region but becomes poor at high frequencies. This suggests that, in time domain, the response of the controlled variable under the conditions of control behaves rather poorly at initial time and improves as time increases. This is further strengthened by inspection of Figures 4-9 through 4-12 where the responses of the controlled variable \( \delta m(y=1,t) \) to a step change in the input variable are plotted versus time under the conditions of control and no control. If one is interested in the high frequency region as well as the low frequency region, a dead time element may be combined with the PD controller. In this case minimization of the integral of square error becomes a two-dimensional optimization problem.

In obtaining the time domain response, the system of linear partial differential equations (2-26) were solved numerically. The finite difference for these equations are given in Appendix A. The shooting technique was used to solve the system of equations. The Newton-Raphson method was used to adjust the assumed missing boundary condition at initial point \( \delta T_c(y=0,t) \). The controller efficiency \( \bar{E} \) defined by equation (4-1) was also evaluated for data of Figures 4-9 through 4-12. In evaluation of the controller efficiency, \( I_u \) and \( I_c \) were evaluated by using the trapezoidal rule. The results are given in Table 12.
COMPARISON BETWEEN UNCONTROLLED AND CONTROLLED SYSTEM RESPONSE TO STEP CHANGE IN TC (Y=1, T)=3

LEGEND

- UNCONTROLLED
- CONTROLLED

Figure 4-9
COMPARISON BETWEEN UNCONTROLLED AND CONTROLLED SYSTEM RESPONSE TO STEP CHANGE IN TG(Y=0,T) = 3

LEGEND

- UNCONTROLLED
- CONTROLLED

Figure 4-10
COMPARISON BETWEEN UNCONTROLLED AND CONTROLLED SYSTEM
RESPONSE TO STEP CHANGE IN M(Y=0,T)=0.05

LEGEND

■ UNCONTROLLED  ○ CONTROLLED

Figure 4-11
COMPARISON BETWEEN UNCONTROLLED AND CONTROLLED SYSTEM
RESPONSE TO STEP CHANGE IN VG=2% OF GAS VELOCITY

LEGEND
○ UNCONTROLLED ○ CONTROLLED

Figure 4-12

TIME IN MINUTES

OUTLET MASS FRACTION OF WATER M(Y=1, 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7})
Table 12. Controller's Efficiency $E$

<table>
<thead>
<tr>
<th>Controllers</th>
<th>$I_u$</th>
<th>$I_c$</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>$GC_1(s)$</td>
<td>$0.99439 \times 10^{-1}$</td>
<td>$0.54928 \times 10^{-2}$</td>
<td>94.4</td>
</tr>
<tr>
<td>$GC_2(s)$</td>
<td>$0.17868 \times 10^{-1}$</td>
<td>$0.55012 \times 10^{-3}$</td>
<td>90.8</td>
</tr>
<tr>
<td>$GC_3(s)$</td>
<td>$0.15747$</td>
<td>$0.48537 \times 10^{-2}$</td>
<td>90.5</td>
</tr>
<tr>
<td>$GC_5(s)$</td>
<td>$0.72277 \times 10^{-1}$</td>
<td>$0.85086 \times 10^{-2}$</td>
<td>88.2</td>
</tr>
</tbody>
</table>
CHAPTER V

SUMMARY AND CONCLUSION

In this study, a shell and tube heat exchanger was modeled by a set of three nonlinear simultaneous partial differential equations. The equations were locally linearized about the steady state operating conditions. The system's equations were modified to satisfy the third assumption, given in section B of Chapter III, to formulate the problem by a Taylor diffusion model.

To design the invariance controllers for the system under study, two different approaches were considered. One was based upon the transfer functions obtained using the Taylor diffusion approximation. The technique was generalized through introduction of new parameters via modification of the second assumption (section B of Chapter III). Two different techniques were proposed to estimate the new parameters. These are given in section D of Chapter III. Modification of the second assumption enables one not to be concerned about using physical intuition or the requirements for the magnitude of the number of transfer units. The results and the feasibility of the techniques were discussed in detail in section G of Chapter III. Although the results proved to be promising, these transfer functions were not used to design invariant controllers. The primary reason was that the transfer functions derived adequately represented the dynamics of the system only in the low frequency region. Consequently the invariance
controllers designed based upon these transfer functions would be seriously in error during upsets which contain significant energy having high frequency content.

On the basis of the findings in this research, the following procedure is recommended in developing the Taylor diffusion model to any arbitrary problem:

1. Check to see if the problem satisfies the third assumption (the sum of all transfer terms in all equations must be zero). Many problems, in their original form, do not satisfy this assumption and further modification may be necessary.

2. If the system's equations are nonlinear, linearize the equations about the steady state operating conditions. Substitute the sensitivity coefficients by their mean value if they are not severely nonlinear. If this is so, divide the system into several sections. The mean value for the sensitivity coefficients associated with the velocities need not be evaluated.

3. Develop the Taylor diffusion model using the modified second assumption (see equation (3-11)).

4. Obtain the axial gradients based upon the initial steady state distributions to estimate the parameters $\xi_1$, $\xi_2$, ..., etc., either by the technique of Case I or II.

The results may further be improved if the initial distributions obtained from the solution of the nonlinear steady state equations are used.

A procedure was developed for the design of invariant controllers based upon the determination of the analytical frequency response of
the controllers themselves. Here the frequency response data of the manipulated variable that makes the controlled variable invariant were first obtained. By defining the manipulated variable in terms of the input variable, the frequency response data of the invariance controllers were obtained. As was discussed in the previous chapter, the magnitude of the controllers exhibits the characteristic of a first order lead term. The behavior of the phase angles indicates that a small dead time element is also associated with the controllers. The frequency response data of the controllers were used to approximate the controller transfer function by minimizing the integral square error criteria in the frequency domain (equation (3-52)). A conventional PD controller was used as a model for all the invariant controllers since this type hardware is readily available. The approximation of the controllers by conventional PD controller is adequate in the low frequency region while it becomes poor at higher frequencies. This manifests itself in initial dynamic variance in \( \delta m \) for step changes in the incoming disturbances. The response of the system improves considerably as time increases. It was suggested, in Chapter IV, that the combination of a dead time element with the PD controller may result in a better response at initial time as well as the final time. The controllers may be further refined if the controller gain is substituted by the gain obtained from the solution of nonlinear steady state equations.

A mathematical model of an actual process is usually an approximation. To eliminate the effects of modeling and linearization error, a conventional feedback element may be necessary. It is felt that the
combination of invariance controllers and a feedback element designed by using the transfer functions obtained from the Taylor diffusion model would compensate for modeling inaccuracies.
NOMENCLATURE

\( A_c \) Cross sectional area to the coolant fluid, \( \text{ft}^2 \)

\( A_g \) Cross sectional area to the gas, \( \text{ft}^2 \)

\( A_i, A_o \) Inside and outside tube area, \( \text{ft}^2/\text{ft} \)

\( a' \) Constant (equation (2-14))

\( a_i, a_i' \) Defined by equations (3-36)

\( C_p, C_p', C_g \) Specific heat of a fluid, the coolant and the gas, Btu/lbs \(^\circ\)F

\( C_{m_p} \) Molal specific heat of gas, Btu/lb mole, \(^\circ\)F

\( C_1, C_2 \ldots \) Defined by equations (3-17)

\( C' \) A constant (equation (2-14))

\( D_i \) Diameter or equivalence diameter, \( \text{ft} \)

\( D_g \) Binary diffusivity of water vapor with hydrogen, \( \text{ft}^2/\text{hr} \)

\( d' \) Constant (equation (2-14))

\( E \) Defined by equations (2-22) and (4-1)

\( G(s) \) Transfer function

\( G_i \) Mass fluid velocity, \( \text{lbs/hr ft}^2 \)

\( G_{C_1(s)}, G_{C_2(s)} \ldots \) Invariance feedforward transfer functions

\( \text{GN} \) Steady state gain

\( G_1(s), G_2(s) \ldots \) Transfer functions relating the output to inputs (see Tables 4, 5, \ldots)

\( H \) \( H_1 + H_2 + H_3 \)

\( H_1, H_2, H_3 \) Defined by equations (2-13)

\( h, h_c, h_g \) Individual heat transfer coefficients of a fluid, the coolant and the gas side, Btu/hr \( \text{ft}^2 \) \(^\circ\)F

\( I_u, I_c \) Defined by equations (4-1)
\( \mathbf{J} \)  

The Jacobian matrix, defined by equation (B-2)

\( j \)  

\( \sqrt{-1} \)

\( K^* g \)  

Mass transfer coefficient, lb mole/min. ft\(^2\) atm.

\( K_i, K'_i \)  

Defined by equations (3-45)

\( k, k_c, k_g \)  

Thermal conductivity of a fluid, the coolant fluid and the gas, Btu/hr ft °F

\( k^* g \)  

Mass transfer coefficient, lb mole/hr ft\(^2\) atm.

\( k_1, k_2 \)  

Defined by equations (2-13)

\( L \)  

Length of the system, ft

\( MI \)  

The imaginary part of \( \tilde{m}(y,j\omega) \)

\( MR \)  

The real part of \( \tilde{m}(y,j\omega) \)

\( m \)  

Local mass fraction of water at steady state, lbs water/lbs gas

\( \dot{m} \)  

Local mass fraction of water at steady state, lbs water/lbs gas

\( \tilde{m} \)  

Laplace transform of \( \delta m(y,t) \)

\( P \)  

Total pressure of the system, atm. Also defined by equations (3-33)

\( P_g \)  

Local partial pressure of water, atm.

\( P_\lambda \)  

Local vapor pressure of water, atm.

\( \overline{P_g}, \overline{P_\lambda} \)  

\( P_g \) and \( P_\lambda \) at steady state

\( Pr \)  

Prandtl modulus, dimensionless

\( P_T \)  

Defined by equation (3-24)

\( P_{cr} \)  

Critical pressure of water, atm.

\( R \)  

Ideal gas constant

\( S \)  

Perimeter of the tube, ft

\( S_c \)  

Schmidt modulus, dimensionless

\( S_1, S_2 \ldots \)  

Sensitivity coefficients defined by equations (2-24)
\( \bar{S}_2, \bar{S}_3 \) Average value of \( S_1 \) and \( S_2 \)

\( s \) Laplacian operator

\( T \) Temperature, °R or °k

\( T_c, T_g \) Local coolant and gas temperature, °F

\( \bar{T}_c, \bar{T}_g \) \( T_c \) and \( T_g \) at steady state

\( \tilde{T}_c, \tilde{T}_g \) Laplace transform of \( \delta T_c(y,t) \) and \( \delta T_g(y,t) \)

\( TCI, TGI \) The imaginary part of \( \tilde{T}_c(y,jw) \) and \( \tilde{T}_g(y,jw) \)

\( TCR, TGR \) The real part of \( \tilde{T}_c(y,jw) \) and \( \tilde{T}_g(y,jw) \)

\( t \) Time, min.

\( U \) Overall heat transfer coefficient, Btu/min. ft\(^2\) °F

\( u \) Overall heat transfer coefficient, Btu/hr ft\(^2\) °F

\( V \) General dependent variable to be a function of time and space

\( v \) Defined by equation (3-13)

\( V_c, V_g \) Coolant and gas velocity, ft/min.

\( \bar{V}_c, \bar{V}_g \) \( V_c \) and \( V_g \) at steady state

\( \tilde{V}_c, \tilde{V}_g \) Laplace transform of \( \delta V_c(t) \) and \( \delta V_g(t) \)

\( v_m \) Defined by equations (3-21)

\( VCI, VGI \) The imaginary parts of \( \tilde{V}_c(jw) \) and \( \tilde{V}_g(jw) \)

\( VCR, VGR \) The real parts of \( \tilde{V}_c(jw) \) and \( \tilde{V}_g(jw) \)

\( x \) The moving coordinate \( X + vt \). See also equation (2-14)

\( y \) Dimensionless distance \( Z/L \)

\( Z \) Distance, ft

\( \alpha \) \( C_2/C_1L \)

\( \alpha_T \) Defined by equation (3-21)

\( \beta \) \( C_4/C_3L \)
$\gamma \quad c_6/c_5 L$

$\delta \quad \text{An operator indicating deviation from steady state (e.g., } \delta_T, \delta T_g, \delta m)\text{)}$

$\Delta \quad \text{Increment (e.g., } \Delta Z)\text{)}$

$\zeta_1, \zeta_2, \zeta_3 \quad \text{Defined by equations (3-11)}$

$\eta_1, \eta_2, \ldots, \eta_1', \eta_2' \ldots \text{ Equations (3-35)}$

$\theta \quad v_t/L$

$\lambda \quad \text{Heat of evaporation of water, Btu/lbs}$

$\mu, \mu_w \quad \text{Viscosity, ft/hr}$

$\nu_1, \nu_2, \ldots, \nu_1', \nu_2' \ldots \text{ Equations (3-33)}$

$\xi_1, \xi_2, \ldots, \xi_1', \xi_2' \ldots \text{ Equations (3-34)}$

$\rho_c, \rho_g \quad \text{Coolant and gas density, lbs/ft}^3$

$\tau_0, \tau_1, \tau_2 \quad \text{Dead time and time constants}$

$\phi_1, \phi_2, \ldots, \phi_1', \phi_2' \ldots \text{ Equations (3-37)}$

$\omega \quad \text{Frequency, radians/min.}$
REFERENCES


34. Vershinin, V. D., "Relations Between Adjoins Corresponding to Elements of a Determinant, and Their Application to Invariance Theory," Avt. i Telem., Vol. 23, No. 4, pp. 441-446, April 1962.


APPENDIX A

FINITE DIFFERENCE EQUATIONS OF THE SYSTEM

The centered difference equations for the system of partial
differential equations (2-26) are developed here. Referring to Figure
2-8, the cross point indicates the location about which the finite
difference equations are written. To derive these equations, the time
and space derivatives in equations (2-26) were substituted for by
their equivalence from equations (2-25). The dependent variables \( \delta T_c \),
\( \delta T_g \) and \( \delta m \) were substituted by the average taken over the four grid
points surrounding the cross point. The results are:

\[
\begin{align*}
\left[ \frac{H_1}{2\Delta t} - \frac{H_V}{L} \frac{1}{2\Delta y} + \frac{k_1}{4} \right] & \delta T_{i,n+1} - \frac{k_1}{4} \delta T_{g_{i,n+1}} + 0 \times \delta m_{i,n+1} = D^1_i \\
- \frac{k_1 - k_2 S_3}{4} \delta T_{c_{i,n+1}} & + \left[ \frac{H_2}{2\Delta t} + \frac{H_V}{L} \frac{1}{2\Delta y} + \frac{k_1 + k_2 S_3}{4} \right] \delta T_{g_{i,n+1}} \\
- \frac{k_2 S_2}{4} \delta m_{i,n+1} & = D^2_i \\
- \frac{k_2 S_3}{4} \delta T_{c_{i,n+1}} & - \frac{k_2 S_3}{4} \delta T_{g_{i,n+1}} \left[ \frac{H_3}{2\Delta t} + \frac{H_V}{L} \frac{1}{2\Delta y} + \frac{k_2 S_2}{4} \right] \delta m_{i,n+1} = D^3_i
\end{align*}
\]

\[(A-1)\]

where
For each time increment, the system of simultaneous algebraic
equations must be solved for $i=1,R$. There is one unspecified boundary
condition at initial point $i=0$. This is $\delta T_{c_{0,n+1}}$. The shooting tech-
nique was used to solve these systems of equations. In other words,
$\delta T_{c_{0,n+1}}$ is assumed. Then the system of equations (A-1) are solved
for $i=1,R$. Once the solution is obtained, the computed $\delta T_{c_{R,n+1}}$ is
compared with the specified one to see if the assumed value for
$\delta T_{c_{0,n+1}}$ has yielded the right solution. If not, the assumed value is
adjusted until the right solution is obtained. The Newton-Raphson
technique was used to adjust the assumed value for $\delta T_{c_{0,n+1}}$. It is
also understood that the sensitivity coefficients $S_1$ through $S_5$ are
evaluated at the cross point (e.g., $S_1 = \frac{S_1(i\Delta y) + S_1((i-1)\Delta y)}{2}$).
APPENDIX B

NEWTON RAPHSON TECHNIQUE

An error column vector $e$ of dimension $n$ is defined where its elements are the difference between the computed boundary conditions and the ones specified by the problem. Representing the assumed initial conditions by column vector $x^i$ where the superscript $i$ stands for iteration number. The error vector corresponding to the assumed initial conditions $x^i$ would be $e(x^i)$. Suppose that the next assumed initial condition is $x^{i+1}$, then the corresponding error vector will be $e(x^{i+1})$. Expanding $e(x^{i+1})$ in terms of Taylor series and keeping the first two terms yields

$$e(x^{i+1}) = e(x^i) + \left( \frac{\partial e}{\partial x} \right)_{x=x^i} \Delta x$$

(B-1)

Here $\Delta x = x^{i+1} - x^i$, and $\left( \frac{\partial e}{\partial x} \right)_{x=x^i}$ is called Jacobian matrix and it is an $nxn$ matrix given by

$$J = \left( \frac{\partial e}{\partial x} \right)_{x=x^i} = \left[ \begin{array}{cccc}
\frac{\partial e_1}{\partial x_1} & \frac{\partial e_1}{\partial x_2} & \cdots & \frac{\partial e_1}{\partial x_n} \\
\frac{\partial e_2}{\partial x_1} & \frac{\partial e_2}{\partial x_2} & \cdots & \frac{\partial e_2}{\partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial e_n}{\partial x_1} & \frac{\partial e_n}{\partial x_2} & \cdots & \frac{\partial e_n}{\partial x_n}
\end{array} \right]$$

(B-2)
where

\[ e_j, \ j=1,n \] are the elements of the error vector \( e \)

\[ x_j, \ j=1,n \] are the elements of the initial condition vector \( x \)

The increment vector \( \Delta x \) is simply obtained by setting the error vector \( e(x^{i+1}) \) equal to zero vector. By doing so, and then solving for \( \Delta x \) yields

\[ \Delta x = - J^{-1} e(x^i) \]  \hspace{1cm} (B-3)

once the increment \( \Delta x \) is calculated, the next value of the initial condition would be:

\[ x^{i+1} = x^i + \Delta x \]  \hspace{1cm} (B-4)

After \( x^{i+1} \) is calculated the system of equations is solved, and the procedure is repeated until the convergence with respect to some tolerance is reached.
Mohammad Reza Karbassian was born on January 28, 1938. He entered Tehran Polytechnic, Tehran, Iran, in September of 1959 and was awarded a Bachelor of Science degree in chemical engineering in 1963. He worked a year and a half for Tehran Cement Company in Tehran, and came to the United States in January, 1966.

After completing one term of English language and orientation, he enrolled in the Graduate School of Louisiana State University in September, 1967. He received the degree of Master of Science in Chemical Engineering in 1970, and is presently a candidate for the degree of Doctor of Philosophy in the Department of Chemical Engineering.
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Major Field: Chemical Engineering

Title of Thesis: Application of the Principal of Invariance to a Distributed Parameter System

Approved:

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Major Professor and Chairman

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Dean of the Graduate School

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March 2, 1973