The Analogue Computer Simulation of Integrated Chemical Plant and Controller Systems.

By

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SUMMARY.

A systematic approach to the generation of a simplified model is presented. The individual sections of the systematic approach:

1. Model Building.
2. Simulation.
3. Simplification.
4. Use

are discussed in detail.

A dynamic model of the catalytic tubular reactor for the dehydrogenation of iso-propanal to acetone is developed. This model was successfully simulated on an analogue computer. The results obtained from the analogue computer simulation were successfully analysed to produce a considerably simplified dynamic model of the reactor.

At each stage in the systematic approach the theory, and practice as applied to the reactor model, is presented.

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Chapter One.

Introduction.

The rapidly increasing use of automatic control and optimisation in the process industries has led to an increased demand for accurate but simple mathematical models of the dynamics of the processes involved. The emphasis here is on the word 'simple', since while there is no difficulty in the formulation of a mathematical model, the model is often prohibitively complex.

Unfortunately there is no completely satisfactory means yet known, of simplifying a complex model. Linearisation is the only universal method. This of course suffers from the limitation that theoretically its accuracy is only within infinitesimal limits. Although often practically satisfactory, proof of this fact, which is difficult to obtain, is usually required.

The introduction of the analogue computer has added a means of handling both simple and complex models. Methods such as frequency response, enable comparison for compatability of the different models. Furthermore, these methods which are described later, can be used to obtain simplified mathematical representations of a system in a form amenable to analysis for optimal performance of control systems.

The object of the work was to simulate an integrated network of process plant items, using a limited amount of analogue computer equipment.

Chapter Two.

Model Building.

2.1 Introduction.

There are two ways of building a model. These are firstly the collection of data from an existing plant and its analysis, and secondly the quantitative method based on reasonable assumptions. The importance of the latter becomes prime when considering design, as at that time there may well be means of obtaining actual operating data.

The means of the quantitative method is well published and the applicable rules proved successfully. Basically the requirement to formulate a model is a mathematical description based upon reasonable assumptions of ideality, plug flow or complete mixing in reactors, and the application of the laws of conservation, mass, energy and momentum, to a differential increment.

The object of this chapter is to show how the quantitative method was used to obtain the mathematical model and also how the model must be simplified prior to solution by analogue computer.

2.2 Choice of the Tubular Reactor.

For the purpose of the study undertaken it was necessary to take, as an example, an existing system. It was accordingly decided to study the production of Acetone from Isopropanol by dehydration in a catalytic tubular reactor. The reaction involved is gas phase and reversible, being first order in the forward direction and second order in the reverse.

$$\text{Isopropanol} \rightleftharpoons \text{Acetone} + \text{Hydrogen} \qquad 2.1$$

$$(CH_3)_2CHOH(gas) \rightleftharpoons (CH_3)_2CO(gas) + H_2(gas) \qquad 2.2$$

The reason for the decision was that help and information of the type required for the study was made available by the Ministry of Technology Warren Spring Laboratories, where a plant of the type mentioned was being studied as an experiment in direct digital control. The system of non-linear partial differential equations of the mathematical model also contains most of the difficulties typical of chemical engineering systems.

2.3 Tubular Reactor Model.

The assumption upon which the mathematical derivation of the tubular reactor model is based, is that of plug flow. Plug flow means that the fluid in its passage along the tube undergoes no longitudinal mixing. Hence the fluid moves as if it were a solid bar or plug along the tube. This assumption alone would leave the model with the complexity of concentration and temperature gradients in a radial direction. The temperature gradients occur because of the heat transfer at the tube surface and the finite non-zero resistance to heat flow of the fluid. The concentration gradients are dependent on the temperature gradients because of the different reaction rates at different temperatures. If there were no heat transfer between the fluid and the tube wall no gradients would exist. This is because the heat generated by the chemical reaction taking place within the fluid would be constant across a radial cross-section.

It is necessary to overcome this complexity by assuming either infinite thermal conductivity within the fluid, or complete lateral mixing. The former while arranging for no radial temperature gradients, will infer no longitudinal temperature gradients, which is more than is required. The latter allows for both temperature and concentration gradients along the length of the reactor, while negating any radial gradients. Hence complete lateral mixing will be assumed.

The velocity profiles across the diameter of the tube of the true and assumed cases show (FIG 2.1), that if the flow is turbulent, the assumption of plug flow is very good indeed.

The accuracy of the assumption of complete lateral mixing is more difficult to compare with the true case. It is however, a method of averaging which is usually an acceptable simplification.

Applying these assumptions to an increment of reactor length for an increment of time yields the transient mass and heat balances as derived in Appendix 1. These represent the mathematical model.

$$\frac{\partial b}{\partial L} = A\varepsilon\left(\rho(\text{rate}) - \frac{\partial \rho}{\partial t}\right) \qquad 2.3$$

$$\frac{\partial x_A}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial x_A}{\partial L} = -(1 + x_A)(\text{rate}) \qquad 2.4$$

$$(c_A x_A + c_B x_B + c_c x_c)\left(\frac{\partial \theta}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial \theta}{\partial L}\right)$$

$$= \frac{q_o a_\omega + q_s a_s}{A\varepsilon\rho} - (\text{rate})(\Delta H_o + (c_B + c_c - c_A)(2\theta - \theta_o)) \qquad 2.5$$

The chemical reaction (equations 2.1 and 2.2) has the following form of kinetics:

$$\text{rate} = k_F x_A - k_R x_B x_c \qquad 2.6$$

where the values of the rate constants are given by the Arrhenius relationship:

$$k_I = P_I \exp(-E/RT) \qquad 2.7$$

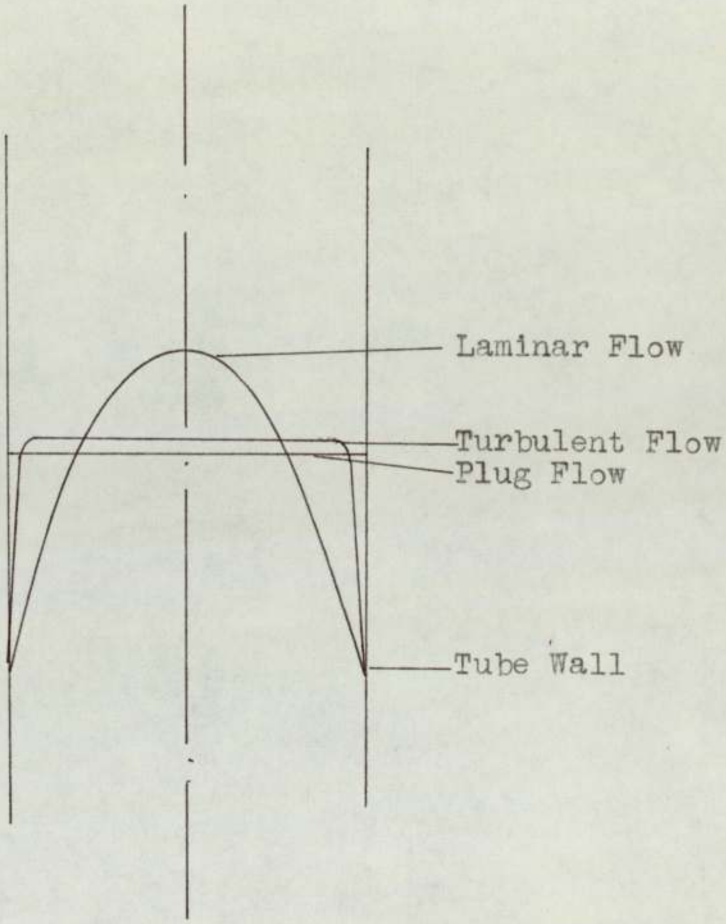


FIGURE 1 Velocity Profiles

In the case under consideration heat transfer takes place from a heating medium in a jacket surrounding the tube, and also to the catalyst packed into the tube. For both heat transfer cases it will be assumed that the heat transfer coefficient is constant with respect to the fluid properties and actual measured values will be used. The equations for the heat transferred, as derived in Appendix 1, are as follows:

between the heat transfer medium and the fluid in the reactor,

$$q_\omega a_\omega = U_\omega a_\omega \left(\theta - \theta_c \right) \qquad 2.8$$

between the fluid in the reactor and the catalyst

$$\frac{d\theta_s}{dt} = C_1 \left(\theta_s - \theta \right) \qquad 2.9$$

The importance of the fact that coefficient 'C_1' in equation 2.9 is constant, will be seen later.

2.4 The Continuous Stirred Tank Reactor Model.

The model is derived in Appendix 2. The conditions in the reactor make the contents an intimate mixture of the gaseous reactants and products, and the solid catalyst. For the real reactor it is assumed that the catalyst is packed to a voidage below the level required for free movement. Hence the practical significance of the model is not immediately apparent. It is shown later, however, that the tubular reactor can be approximated to a series of stirred tank reactors. The comparative ease of analogue computer simulation of the model of this series of reactors gives this model its importance.

The basic assumption for the theory of a continuous stirred tank reactor is that the contents of the reactor are completely mixed so that the mixture has no concentration or temperature gradients in any direction. The outlet stream must, therefore, have properties identical to the properties of the contents of the tank.

The second assumption is a simplification. It is assumed that there is no variation, due to temperature variation, of the total mass contained in the tank. This is, of course not true, but if only small variations in temperature occur, then the effect of the assumption is minimal. This assumption is equivalent to assuming constant molar density. It is shown later, how the vast heat capacity of the catalyst present allows only minor fluctuations in temperature and therefore, density.

The derivation of the heat and mass balances are shown in Appendix 2 and yield the following mathematical model:-

$$b_{OUT} = b_{IN} + (\text{rate})\, V/\rho \qquad 2.10.$$

$$\frac{dx_{A\,OUT}}{dt} = -(1 + x_{AOUT})(\text{rate}) + \frac{b_{IN}}{V/\rho}(x_{A\,IN} - x_{AOUT}) \qquad 2.11.$$

$$\frac{d\theta_{OUT}}{dt} = \frac{q_W A_W + q_S A_S}{V/\rho c} + \frac{b_{IN}}{V/\rho}(\theta_{IN} - \theta_{OUT}) - \frac{(\text{rate})}{c}\left\{\Delta H_0 + (c_B + c_C - c_A)(2\theta_{OUT} - \theta_0)\right\} \qquad 2.12.$$

Since the reaction is the same, the kinetics are identical to those for the tubular reactor. The heat transfer equations are as follows:-

$$q_W A_W = U_W A_W (\theta_C - \theta_{OUT}) \qquad 2.13.$$

$$\frac{d\theta_S}{dt} = C_1 (\theta_S - \theta_{OUT}) \qquad 2.14.$$

2.5 The Difference Approximation.

Before a comparison of the two models (sections 2.3 and 2.4) can be made, the method of solution of the partial differential equation of the tubular reactor model must be considered. The method used was by analogue computer and since the analogue computer cannot integrate in two dimensions simultaneously a technique had to be found for reducing the tubular reactor model to a form which could be handled.

The difference approximation for derivatives with respect to one dimension, based upon Taylor's Series expansions, yields satisfactory results. By expansions a number of different difference approximations can be found. Whichever one is used however, the result will always be in the form of a simplified model of the tubular reactor as a series of differential difference equations.

The first Taylor's series expansion used is:-

$$Y_{(x-\Delta x)} = Y_x - \Delta X \frac{\partial Y_x}{\partial X} + \frac{(\Delta X)^2}{2!} \frac{\partial^2 Y_x}{\partial X^2} - \ldots\ldots \qquad 2.15.$$

The first and simplest difference equation is derived from equation 2.15 by neglecting terms of the order of ΔX^2 , giving:-

$$\frac{\partial Y_x}{\partial X} = \frac{Y_{x-\Delta x} - Y_x}{\Delta X} \qquad 2.16.$$

The next step is to take another expansion as follows:-

$$y_{(x+\Delta x)} = y_x + \Delta X \frac{\partial y_x}{\partial X} + \frac{\Delta X^2}{2!} \frac{\partial^2 y_x}{\partial X^2} + \ldots \qquad 2.17.$$

Subtracting equation 2.17 from 2.15 gives the second difference approximation:-

$$\frac{\partial y_x}{\partial X} = \frac{y_{x+\Delta x} - y_{x-\Delta x}}{2\Delta X} \qquad 2.18.$$

By further additions of Taylor's series ~~expanions~~ expansions for the general term $y_{x \pm N\Delta X}$ a series of difference approximations is formed. By careful choice they can be arranged in order of apparent accuracy, in that the first term neglected is of increasingly higher order in ΔX. As ΔX is small, the higher the power to which it is raised, the smaller the term in which it occurs will be. Considering the first two approximations (equations 2.16 and 2.18) it can be seen that the first term neglected in 2.18 is $\frac{2\,(\Delta X)^2}{3!} \frac{\partial^3 y_x}{\partial X^3}$ while that for 2.16 is $\frac{\Delta X}{2!} \frac{\partial^2 y_x}{\partial X^2}$. The expected errors involved should mean that equation 2.18 represents the more accurate approximation.

There is however, the consideration of the application of these approximations, and the effect they have on the solution of equations to which they are applied. Consider, therefore, as an example the solution of the following equation:-

$$\frac{\partial Y}{\partial X} + \frac{\partial Y}{\partial W} = C \qquad 2.19$$

Using the two difference approximations on the 'X' dimension yields:-

$$\frac{dY_x}{dW} = C - \frac{Y_x - Y_{x-\Delta x}}{\Delta X} \qquad 2.20$$

using equation 2.16, and

$$\frac{dY_x}{dW} = C - \frac{Y_{x+\Delta x} - Y_{x-\Delta x}}{2\Delta X} \qquad 2.21$$

using equation 2.18.

Equation 2.20 shows that the simplest approximation leads to negative feedback in the individual equations, whereas equation 2.21 shows that the second approximation does not. It is possible therefore, that in equation 2.21 there may be oscillation introduced by the approximation which is not in the original system. Because of negative feedback in equation 2.20, oscillation will not occur unless it is a property of the original system.

Another important consideration is that of the boundary conditions. Equation 2.20 has only one imaginary boundary, denoted by $Y_{x-\Delta x}$ at the initial stage, and represents the input. Equation 2.21, on the other hand, has two imaginary boundary conditions, an initial, or input, and a final value denoted by $y_{x+\Delta x}$ at the final stage. Higher order approximations using a greater number of the Taylor series expansions require more boundary conditions.

For these reasons it was decided to use the approximation given in equation 2.16.

2.6 The Difference Step.

2.6.1 Introduction.

One facet of the difference approximation which does not appear in the literature is the use of varying step lengths along the differenced dimension. The reason is perhaps that the method is used mainly in conjuction with digital computation, in which case the waste of storage space in using a number of different difference step lengths would be prohibitive and unduly complex. For analogue computer solution however, each step length is part of a coefficient to be set on a coefficient potentiometer, and therefore, no further difficulty is encountered in using different step lengths.

The following short study (section 2.6) was made, to determine the theoretical errors in the final output stage for a simple linear model, and the empirical errors for a non-linear system. The aim of the study was to determine whether or not an advantage could be gained by varying the difference step length.

To analyse the empirical results obtained, a graphical technique is proposed, which shows how the minimum final stage error can be obtained.

2.6.2 Theory For a Simple Case.

For a theoretical analysis of the errors involved in a linear system, consider the solution of the following equation both analytically and by differencing:-

$$\frac{dY}{dX} = AY \qquad 2.22$$

For a constant value of input signal to $Y_{(0)}$ the analytical solution is:-

$$Y = Y_{(0)} \exp(-AX) \qquad 2.23$$

If the differencing relationship given in equation 2.16 is used, i.e. $\frac{dY}{dX} = (Y_x - Y_{x-\Delta x})/\Delta X$ the following equation is obtained:-

$$Y_x = \frac{Y_{x-\Delta x}}{1 + A\Delta X} \qquad 2.24$$

Reduction of the series of equations 2.24 to relate the output Y_x to the system input $Y_{(0)}$ gives:-

$$Y_N = \frac{Y_{(0)}}{\prod_{i=1}^{N}(1 + A\Delta X_i)} \qquad 2.25$$

Hence, given a limiting value of the 'X' dimension equal to X, say, where

$$X = \sum_{i=1}^{N} \Delta X_i \qquad 2.26$$

there is an error on the output Y in the difference approximation, given by:-

$$\text{error} = Y_{(0)} \left(\frac{1}{\prod_{i=1}^{N} (1 + A\Delta X_i)} - \exp(-AX) \right) \quad 2.27$$

Analytical minimisation of this error is achieved by setting the partial derivatives of the error, with respect to the N individual values of ΔX_i, equal to zero, then solving the N simulaneous equations obtained. Generally the partial derivatives are given by:-

$$\frac{\partial(\text{error})}{\partial \Delta X_j} = A Y_{(0)} \left(\exp(-AX) - \frac{1}{(1 + A\Delta X_j) \prod_{i=1}^{N} (1 + A\Delta X_i)} \right)$$

$$2.28$$

Setting $\frac{\partial(\text{error})}{\partial \Delta X_j} = 0$ and taking the ratio of any two equations in the set 2.28 gives:-

$$\frac{1 + A\Delta X_k}{1 + A\Delta X_l} = 1 \qquad 2.29$$

$$\text{or} \qquad \Delta X_k = \Delta X_l \qquad 2.30$$

Since this is true for all values of l and k, then for minimum final error all increments must be equal. The fact that this is a minimum and not a maximum is shown visually in Fig. 3.

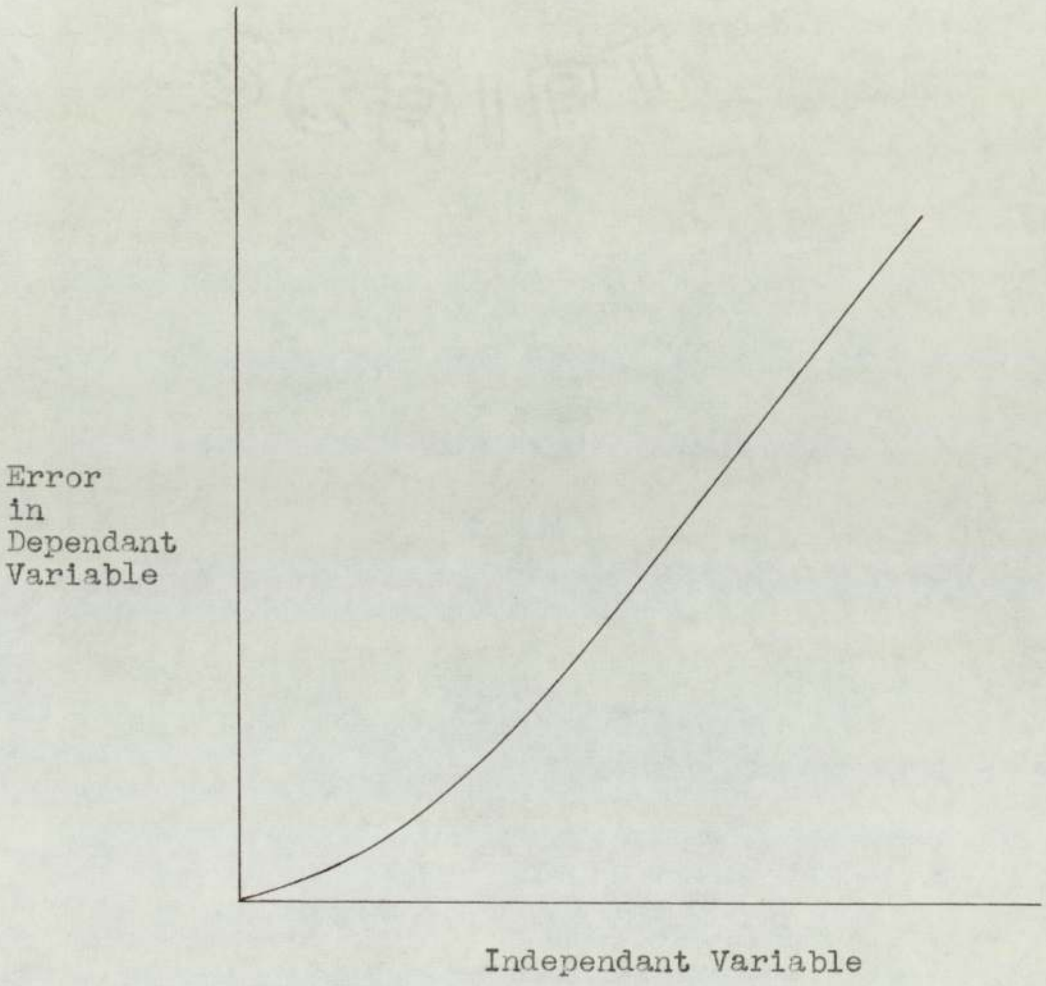


FIGURE 2 Single Stage Error

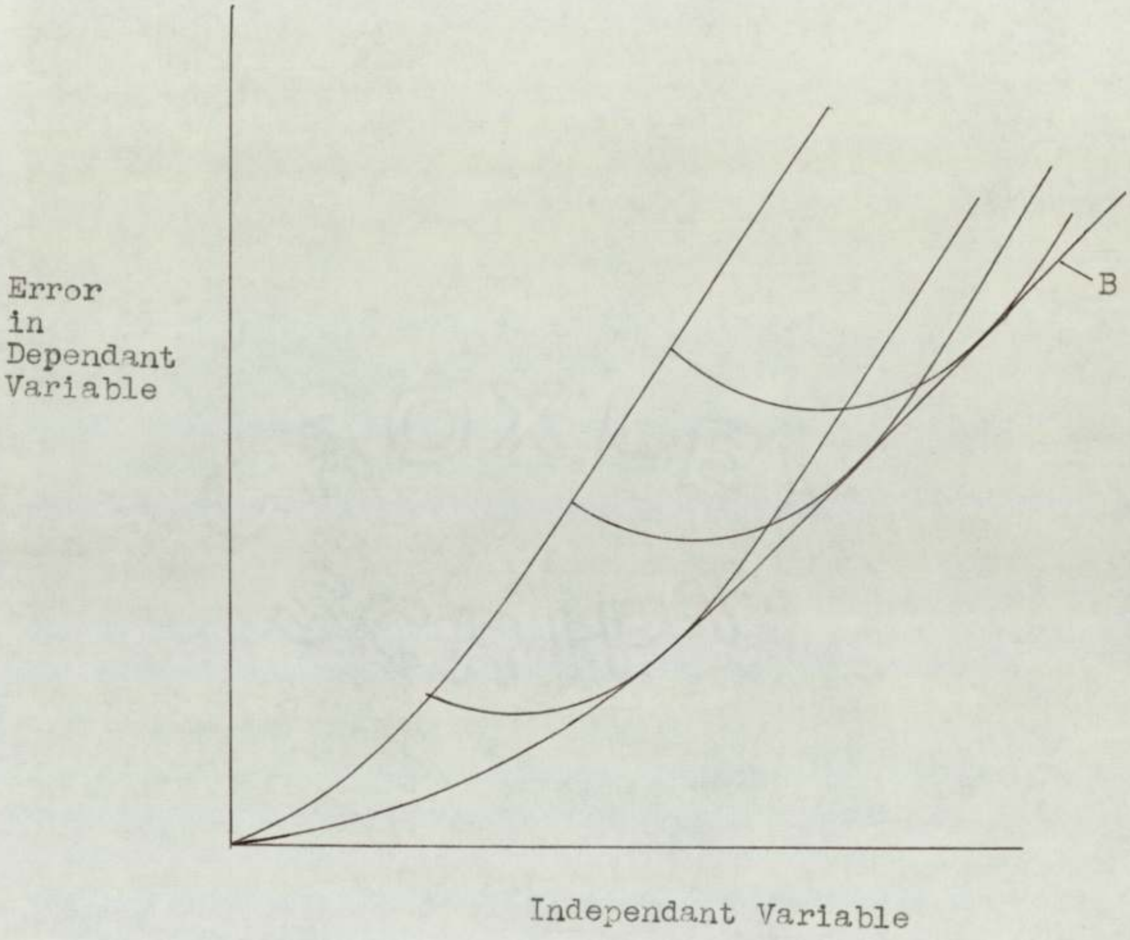


FIGURE 3 Two Stage Errors

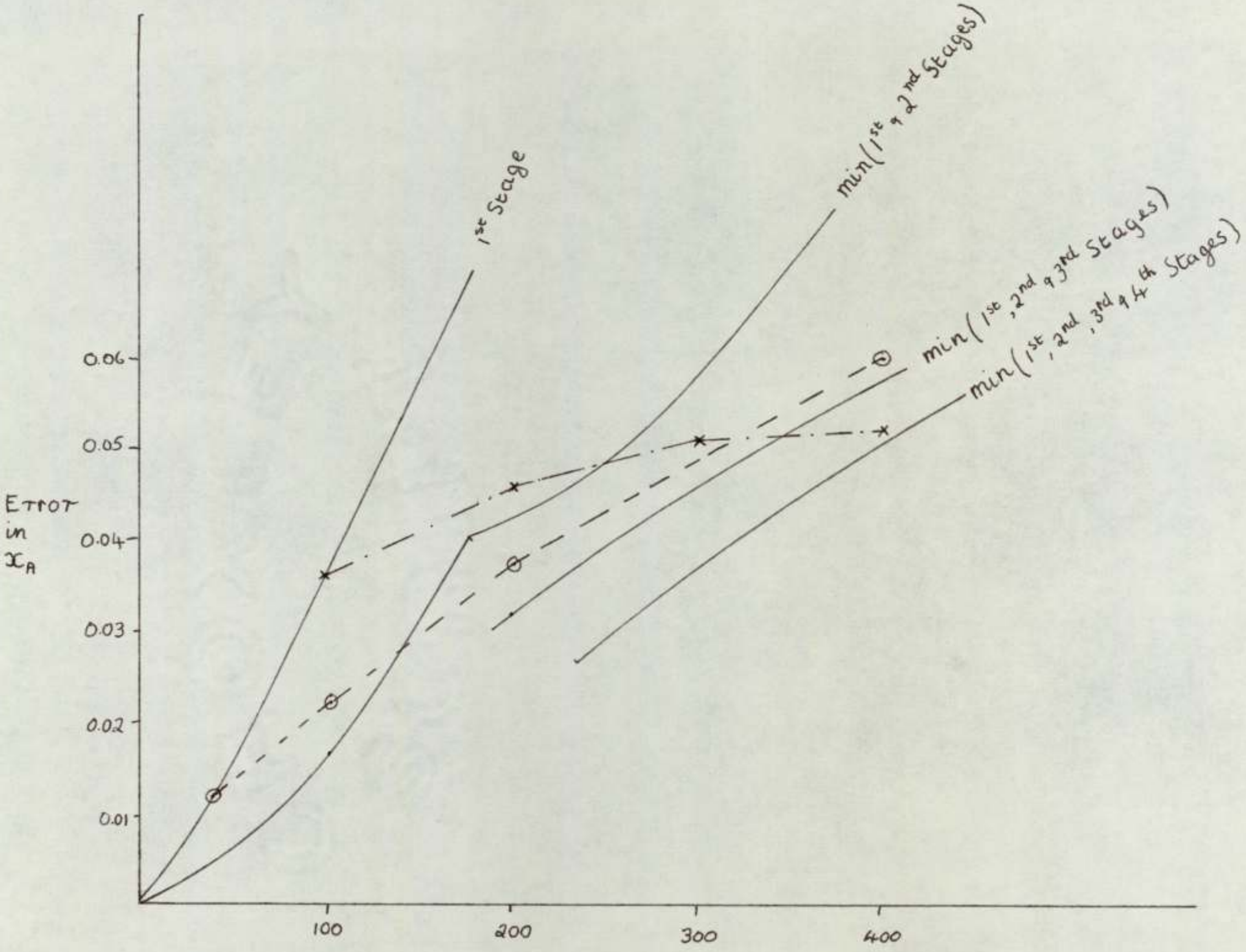


FIGURE 4 Multiple Stage Minimum Errors

2.6.3 Graphical Representation.

For the system previously discussed (section 2.6.2) a plot may be made of the error on the output of an N stage approximation, versus the fractional length of the individual stages of the total length. For a one stage process this yields a single curve Fig.2. The equation of this line is equation 2.27 for $i = 1$

$$\text{i.e.} \quad (\text{error}) = Y_{(0)} \left(\frac{1}{1 + A\Delta X} - \exp(-A\Delta X) \right) \qquad 2.31$$

For a two stage process the series of curves shown in Fig.3 is obtained. The general equation of this set is again given by equation 2.27, this time for $i = 2$

$$\text{i.e.} \quad (\text{error}) = Y_{(0)} \left(\frac{1}{(1 + A\Delta X_1)(1 + A\Delta X_2)} - \exp(-A(\Delta X_1 + \Delta X_2)) \right) \qquad 2.32$$

Interpolation between these curves shows that there exists a curve tangential to all the second stage curves. This represents the minimum error obtainable using two stages. This minimum error curve (marked 'B', Fig.3) has the equation:-

$$(\text{error}) = \min_{\Delta X_1, \Delta X_2} \left\{ Y_{(0)} \left(\frac{1}{(1 + A\Delta X_1)(1 + A\Delta X_2)} - \exp(-A(\Delta X_1 + \Delta X_2)) \right) \right\} \qquad 2.33$$

As shown in section 2.6.2 the minimum is known to be $\Delta X_1 = \Delta X_2$ and equation 2.33 becomes:-

$$(error) = y_{(0)}\left(\frac{1}{(1 + A\Delta X)^2} - exp(-A2\Delta X)\right) \qquad 2.34$$

For stages beyond the second stage similar curves to 'B' (Fig.3) exist. These represent minimum error segmentation of all the steps in the differenced dimension. They are obtained empirically for the N^{th} stage by taking values lying on the similar curve for the $(N-1)^{th}$ stage. Points above the minimum error curve for the $(N-1)^{th}$ stage cannot give minimum error values for the N^{th} stage.

To find the minimum final error of an N stage process requires that all N minimum error curves be plotted. Taking the minimum final error shown by the plot and back-tracking gives the optimum lengths for all the stages. This is in fact, a specialised statement of the Principle of Optimality. The technique is, therefore, a graphical Dynamic Programming approach to the problem.

2.6.4 Application of the Analysis.

An analysis of the type described in section 2.6.3 was undertaken on the simulation described in section 3.6. Since there was no readily obtainable analytical solution to the mathematical model involved, a steady state solution by digital computer was used to make a comparison. The program and results of the digital calculation, together with the results of the analysis are given in Appendix III.

It was possible to divide the length dimension into a greater number of segments for the digital calculation than for the analogue simulation. The results of the digital calculation were therefore, accepted as being more accurate. In fact, it was found that beyond one hundred divisions no perceptible increase in accuracy was obtained. Therefore, the division of the length dimension into a hundred was said to give the accurate solution.

2.6.5 Summary of Results.

The optimal fractional lengths for the simulation (section 3.6) were obtained. They were found to be approximately 3/10, 2/10, 2/10 and 3/10, for the 1st, 2nd, 3rd and 4th segments respectively.

By way of comparison, the diagram Fig.4 shows the errors obtained for two other methods of dividing the length dimension. Firstly the length was divided into four equal stages. The use of this close approximation to optimal conditions increases the error by only 4%. The second method was division into segments of equal fractional conversion. Using the digital solution as a guide the length fractions are: 2/20, 3/20. 5/20 and 10/20. Under these conditions the final error is increased by 20% over that for optimal conditions. In fact, a more accurate result could be obtained by using an optimal three stage process.

2.6.6 Conclusion.

As shown the increase in error in using equal stages for a four stage process is negligible. Hence this arrangement is used in the simulation.

2.7 Comparison of Models.

The model of the tubular reactor is to be simplified by differencing using equation 2.16. Equal differencing steps are to be used as suggested in section 2.6.6. The result is the following model.

$$b_{OUT} = b_{IN} + (rate)A\varepsilon\rho\Delta l \qquad 2.35$$

$$\frac{dx_{AOUT}}{dt} = -(1 + x_{A.OUT})(rate) + \frac{b_{IN}}{A\varepsilon\rho\Delta l}(x_{AIN} - x_{AOUT}) \qquad 2.36$$

$$\frac{d\theta_{OUT}}{dt} = \frac{q_w A_w + q_s A_s}{A\varepsilon\rho c\Delta l} + \frac{b_{IN}}{A\varepsilon\rho\Delta l}(\theta_{IN} - \theta_{OUT})$$

$$- \frac{(rate)}{c}\Big(\Delta H_0 + (c_B + c_C - c_A)(2\theta - \theta_0)\Big) \qquad 2.37$$

$$q_w A_w = U_w A_w(\theta_c - \theta_{OUT}) \qquad 2.38$$

$$\frac{d\theta_s}{dt} = C_1(\theta_s - \theta_{OUT}) \qquad 2.39$$

Since the term $A\varepsilon\Delta l$ is the volume of the reactants and products, it equals V. Likewise the term $A(1-\varepsilon)\Delta l$ is the volume of the catalyst. These equations are therefore, identical to the set for the stirred tank reactor section 2.4

Hence the method of differencing reduces the tubular reactor to a series of stirred tank reactors.

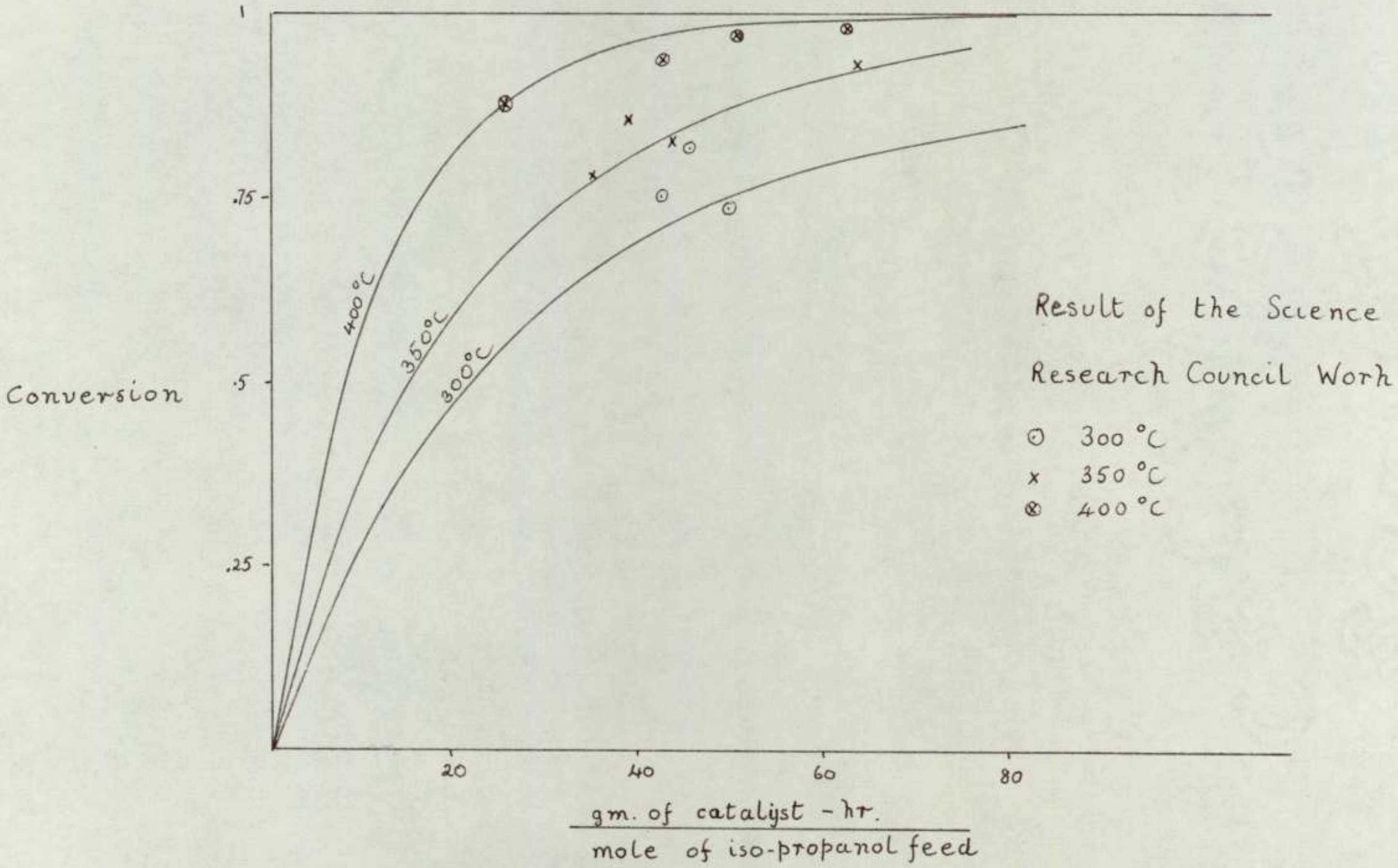


FIGURE 5 Comparison of Theoretical and Laboratory Results

2.8 Comparison with the Real System.

Information on steady state operation was given by Science Research Council's Warren Springs Laboratories and was compared with that obtained from the digital simulation (Appendix IV). Comparison was made Fig.5. It shows the good agreement between the model and the pilot plant at steady state conditions, and over a wide range of working temperatures. Unfortunately data on transient behaviour was not available.

Chapter Three

Simulation

3.1 Introduction.

The word simulation has a very wide meaning. Here it refers to systems undergoing change. A simulation is therefore, a system whose behaviour is analogous to another, with respect to the variation of the properties of the original system, along the dimensions of space, hence also the word analogue.

The greater majority of analogues are for special purposes. These include physical models and pilot plants. Most of these suffer the major difficulty of scale factors, due to the need to use in the model values of the dimensionless groups describing the system identical to those of the plant. An example is the model of a large liner where the characteristic length in the Reynold's Number may be smaller by a factor of 1000. To find the conditions required, that is a Reynold's Number equal to that for the liner, may require a fluid of extreme properties.

Two types of general purpose analogue computer exist, a mechanical one, invented by Bush in 1927, which was slow in operation and difficult to program, and the electronic analogue computer, which superseded the mechanical one just after the Second World War. The most important advantage of the electronic analogue computer is that the varying properties are scaled into voltages, and scaling problems of the type described above do not occur.

The purpose of this chapter is to discuss the relative merits of the different means of simulating a system, with special reference to the partial differential equations of the model of the tubular reactor derived in chapter two.

3.2 Description of Apparatus.

The apparatus used was a parallel hybrid computer made by Electronic Associates Limited, and called the TR-48 Hybrid Computer. It is a solid state machine and hence the TR, an abbreviation of transistor, in the name. It consists of the following two major sections. Firstly, the most important section is the analogue, built for a basic complement of 48 amplifiers, but using certain refinements is capable of expansion up to 54 amplifiers. Secondly the logic and electronic mode control section, to enable control of the analogue section.

The total complement of analogue equipment on the machine used is given in Table 1. As is shown, there are 44 amplifiers available. Of these, ten are track/store amplifiers, eight are contained in two blocks of quad amplifiers which may be used as inverters or as high gain amplifiers, but not as summers. The remaining 26 are general purpose amplifiers. In addition to these there are ten inverters contained in the variable diode function generation units.

The 16 integrator networks all have variable time constant facilities, achieved by using four condensers in each network. These have the values 9 μF, 1 μF, .09 μF and .01 μF. Appropriate selection of different combinations of these condensers yield four time constants of 1 sec., 100 ms., 10 ms. and 1 ms.. The usefulness of this aspect of the TR-48 is seen later when dealing with frequency response analysis.

A recent addition to the control system of the TR-48 has enabled the addition of 30 servo-setting potentiometers which, together with 30 hand setting potentiometers, make up the complement of 60 potentiometers. The new control system enables the read-out to print or papertape of the values of potentiometer coefficients, amplifier outputs and the summing junction potentials of integrator networks. The addition also enables the setting of the servo-setting potentiometers from the keyboard of the teleprinter used or via paper-tape through the tape reader.

Another recent addition is a specialised TR-20 console, by the same maker, containing two four-cup servo multipliers and eight inverters. This unit can be slaved to the main computer. Patching connections between the two are via trunk connections which terminate in the face of both patching areas.

The logic and electronic mode control complements are given in Table 2. A complete description of the function, and some of the simple uses of the individual components are given in the makers handbook.

Only one type of unit sends signals from the analogue section to the logic. These are the comparitors which compare two analogue voltages and give as an output,logic signals relative to the values of the two voltages.

Three types of unit are controlled by the electronic mode control. They are:-

1. Integrators
2. Track/store amplifiers
3. The digital/analogue switches and relays.

The integrators are controlled by switching them from operate to reset mode and vice versa. This type of operation is most useful for high speed repetative calculation and iteration. The track/ store amplifiers are used as a form of analogue storage and are controlled so as to follow the sum of the voltages on their summing junctions. When switched into the store mode they hold on their output the instantaneous value at the time of switching, until returned to the track mode. The switches including the relays are either open or closed depending upon their logical inputs.

Full use was made in the work of all the above facilities of the machine, and were used in conjunction with the following three input - output devices:-

1. Oscilloscope
2. Teleprinter.
3. Variplotter.

All are adequately described by the makers handbooks.

TABLE 1

TR-48 Analogue Components.

Component		Number.
Amplifiers:	General Purpose	16
	Track/store	10
	Quad. inverters	8
Integrator Networks		16
Trunks		1
Readout panel		1
Function switches		4
Quarter Square Multipliers		4
Variable diode function Generators		5
Square Root function Generator		1
Potentiometers:	Servo-Setting	30
	Hand-Setting	30
Comparitors		6
Digital/Analogue switches		12
Relays		6

TABLE 2.

TR-48 Logic Components.

Component	Number
General Purpose Registers	4
AND Gate Blocks	5
MONO STABLE Blocks	1
DIFFERENTIATOR Blocks	1
Electronic Mode Control Block	1
Track/store - Integrator Block	1
Relay - Switch Block	1
Indicator Block	1
Comparitor Block	1

3.3 Breaking-in the TR-48.

The analogue computer used in the work was delivered approximately one year after the work was begun. After it had been checked-out by the engineers, work with it could start. Because of its newness, a system of testing each piece of apparatus was found necessary. In the first few months a considerable number of units became unstable or blew-out. These were repaired at frequent intervals by visiting engineers.

It is significant perhaps, that during the first three months no really reliable results could be obtained.

At a later period when the work was proceeding satisfactorily the computer was sent back to the manufacturers for certain modifications. These were the inclusion of the servo-setting potentiometers and the connections to the read-in and read-out facility. These modifications were in fact, prototypes, and the result was to cause a further breaking-in period.

On a number of occasions it became necessary to completely rewire the program in order to by-pass units which became unstable. The amplifiers were particularly prone to instability and the final program used a number borrowed from a similar machine to cover periods when unstable amplifiers had to be sent back to the makers for repair.

During this period it was found that in most cases unstable amplifiers could be rendered stable by moving them to another location in the computer. This in fact, was a short term measure recommended by the manufacturers. Its effect was however found to be long term and the next stage of the breaking-in process was to find the most suitable locations in the computer for the amplifier units. This juggling process was time consuming but led to much greater amplifier stability.

A further recommendation by the engineers was to exchange the transistors in pairs of amplifier units so as to gain stability by matching components. This also, was found very useful in rendering unstable amplifiers stable again.

B.I.T. Number

1	2	3	4		N	N+1	
			B.I.T. Content				Clock Pulse
1	0	0	0		0	0	1
0	1	0	0		0	0	2
0	0	1	0		0	0	3
0	0	0	0		0	1	N+1
1	0	0	0		0	0	N+2

FIGURE 6 Sequence for Binary Shift Register

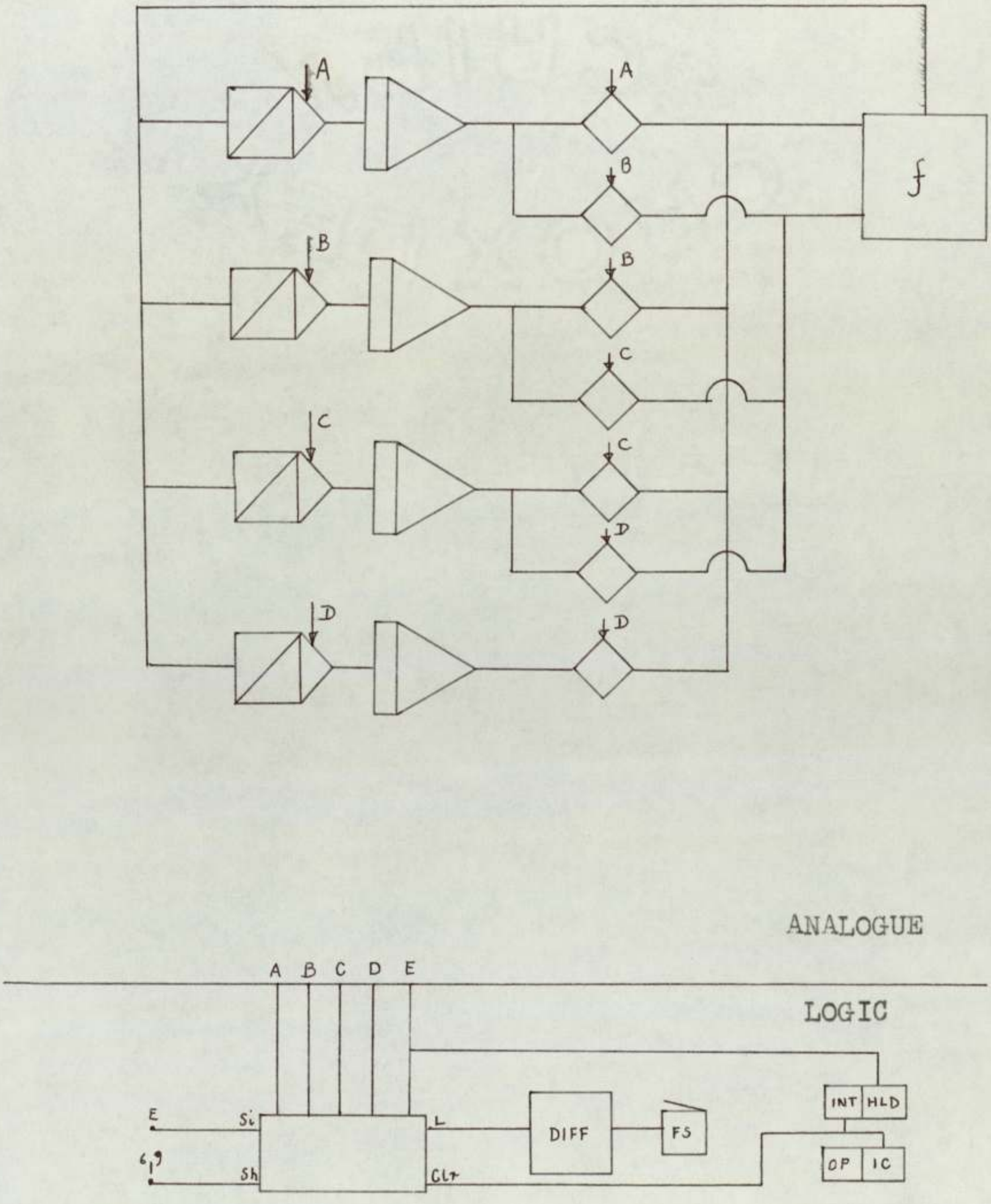


FIGURE 7 Time Sharing by Multiplexing

3.4 Methods of Simulating Partial Differential Equations.

The mathematical model obtained for the tubular reactor contains the difficulty of being based on a set of partial differential equations. A number of techniques have been developed for the simulation of models of this form.

One important group of techniques is based on the reduction of two-dimensional partial differntial equations by 'pseudo - Laplace transforms'. The mathematical treatment of a simple tubular heat exchanger uses the pseudo - Laplace transform to enable replacement of the partial derivative of the length dimension. The reason that this method is applicable is that only the output properties are of real interest and values of properties at intermediate points along the length dimension are unimportant.

Resulting from this analysis the model contains a time delay. This is in fact, as difficult to simulate as the original set of partial differential equations. There are however, a number of specially built units to enable simulation of the time delay. There are also a number of simple approximations which can be used. The means of solution fall into two groups, electronic and mechanical. The electronic are generally based upon algebraic approximations for the time delay and include for example, the well known Padé approximation. The mechanical means are special units designed to delay for a period of time the passage of an electric current. They include a rotating drum surrounded by condensers which charge and discharge as the drum rotates with the delay time being determined by the time taken for the condenser to rotate from input to the output points. Also used is a double headed tape recorder, where the delay time is the time taken for the tape to traverse the gap between the two heads.

An extension of this pseudo Laplace analysis by Davies transforms the equations into an infinite series of simultaneous equations. By this method the accuracy of the results obtained is dependant upon the number of equations taken before truncation. Davies showed that reasonable accuracy could be obtained by truncation after five equations. The method however, introduces non-linearities even where the original system is linear. Also it is difficult if not impossible to use on non-linear systems.

The simplest method of simulating partial differential equations is the method known as 'By Parallel'. This method entails setting up the complete set of simultaneous ordinary differential equations obtained by application of one of the difference approximation techniques. It is called by parallel because of the ability of the analogue computer to simultaneously solve the complete set of equations. One great disadvantage of this method is the need for a large quantity of analogue equipment. For example, if the original partial differential equation has a single non-linearity such as a multiplication of two varying properties, the differential difference approximation consisting of N stages, has N non-linearities, and will require N multipliers for the simulation. Real systems in fact, have many non-linearities often of considerable complexity and hence a very large amount of non-linear analogue equipment would be required for their simulation. For the system under consideration (chapter 2), using four difference steps, some 32 multipliers and 250 amplifiers would be needed. This is unfortunately far beyond the range of the available equipment.

An extension to the 'Parallel' method can be made when dealing with a hybrid computer. This is the technique known as 'time sharing by multiplexing'. This extremely useful technique enables the solution of the N differential difference equations with little more equipment than is required to solve just one of them.

The method is more consistent with the ideas of digital computation, in that it is a continuous system of updating values. It encompasses the use of some of the extra analogue equipment complement of the parallel hybrid computer as well as parts of the logic section. Most important is the need in multiplexing to use the hybrid machine's ability to store analogue information.

As the name states, a number of analogue components are to be shared in time between the individual difference equations. The programming required to achieve this is best described in two parts, the multiplexer, derived from the logic section, and the analogue equipment which uses the signals generated by the multiplexer to achieve the time sharing.

The multiplexer consists simply of a binary shift register into which a single '1' is placed at the most significant end on the first clock pulse of the calculation. On each successive clock pulse the '1' is shifted to the next less significant place. At the last stage the '1' is fed back to the beginning of the register. The shift sequence is shown in Fig.6. The number of bits required is N + 1, where N is the number of difference increments used.

The output of each stage is used directly as the control signal for the electronic mode control of the controlled analogue equipment.

For the analogue stage consider the solution of the single differential difference equation:-

$$\frac{dY_i}{dt} = f(Y_i , Y_{i-1}) \qquad 3.1$$

The method uses the same set of analogue equipment to compute all of the individual values of the derivatives $\frac{dY_i}{dt}$. This is achieved by a process of switching successive values of the components Y_i and Y_{i-1} into the single equipment block which then computes $\frac{dY_i}{dt}$. Each value of a derivative is stored on the subsequent clock pulse by a track/store amplifier.

On the completion of this series of computations the 'N' values of derivatives have been computed and stored. For a single increment of time all the integrators are allowed to integrate on the appropriate derivative values. This is achieved by using the N + 1th bit of the shift register to control the electronic hold of the machine. On completion of this time period a new set of derivative values is calculated and stored. It can easily be seen that the solution thus derived is a series of straight lines. If however, the time increment, during which integration takes place, is sufficiently small the solution will approximate adequately to the true solution, in that the output device would not be able to detect the difference.

The only restriction on the function 'f' is that it may not itself contain any derivatives. The circuit for this type of calculation is shown in Fig.7.

The simulation of a stirred tank reactor was investigated. This, as shown in chapter 2, is identical to the simulation of a single increment of the differenced approximation. Hence it is not representative of the whole reactor, but only of a part of it.

The proposed ultimate aim was to simulate the total number of units which make up the complete chemical plant. This simulation was to be carried out using a very limited quantity of analogue equipment. Therefore, the initial aim was to reduce the complex model to a dynamically simpler equivalent form.

Considering simplification to be of prime importance, partial simulation offers a means of obtaining suitable information from which the simplified model can be built.

3.5 Comparison of the Advantages and Disadvantages of the Methods.

Comparison of the methods is in terms of three important properties:-

a) Applicability.
b) Time taken.
c) Equipment requirement.

As discussed in section 3.4 the method using pseudo-Laplace transforms may not be applicable to non-linear systems, and the tubular reactor is of course, non-linear, but all the other methods are applicable.

In considering time two aspects are important. The first is the time required for programming and debugging. Obviously the smaller and simpler the program the shorter will be the time required for this part. Secondly is the operating time. Of the methods discussed only the last shows a divergence in this respect. In this case, for N difference steps, a study requires N times as many runs and takes N times as long to complete.

For a study involving limited equipment availability methods using less equipment are to be preferred. The parallel method is extremely demanding in this respect and excessive simplification would be needed to allow its use. The method of time sharing by multiplexing requires a considerable quantity of such devices as logically controlled switches. This is particularly true in the case of multiple order systems. In the case of the tubular reactor the individual segment is third order and individual derivatives are a function of up to five property values. It was found that with respect to switches the requirement was in excess of the number available. This leaves the position where partial simulation is needed if a study is to include all the non-linearities in the mathematical model.

3.6 Simulation of an Individual Increment.

The implementation of the simulation presents no difficulty. The circuit diagram is shown in FIG.8, and Tables 3 and 4 show the individual amplifier outputs and the potentiometer settings respectively. Included in FIG.8 is the sinusoidal circuit used for frequency response analysis.

Before implementation can be started, the means of simulating each individual non-linearity must be known. Also the model must be scaled so that the ranges of the variables of the problem can be set within the range of the machine.

Most of the non-linearities in the tubular reactor problem are simple multiplications and do not require special analysis. One however, is more difficult. This is the value of the forward reaction rate coefficient given by the Arrhenius relationship equation 2.7. Although it is possible to obtain an absolute circuit (FIG.9) for this relationship the equipment requirement of the circuit is too great to allow its use.

The absolute circuit is obtained by implementing the differentiated rate equation. The rate equation is:

$$k = P \exp(-E/RT) \qquad 3.2$$

Differentiating with respect to 'T' gives

$$\frac{dk}{dT} = + \frac{Ek}{RT^2} \qquad 3.3$$

The analogue computer will however only integrate with respect to

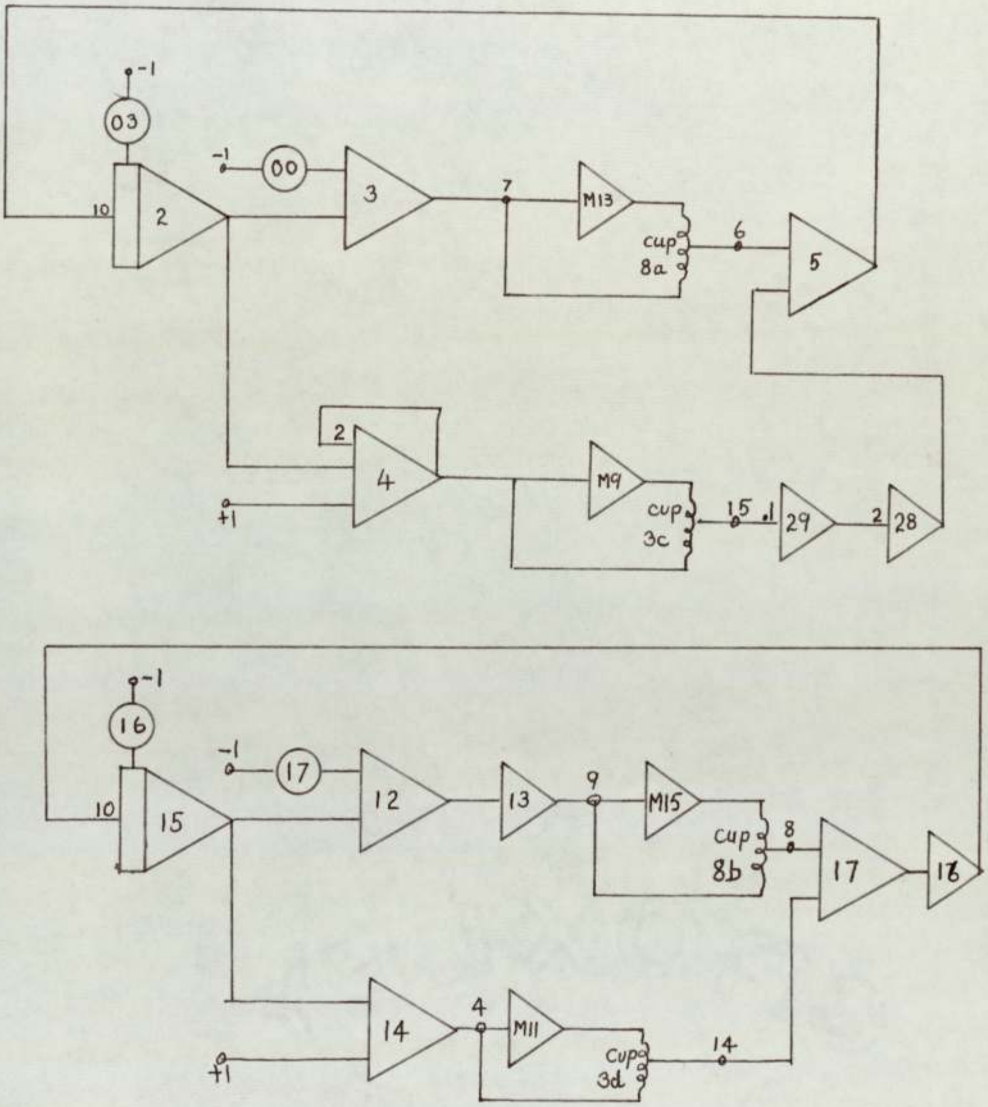


FIGURE 8(a) Circuit Diagram

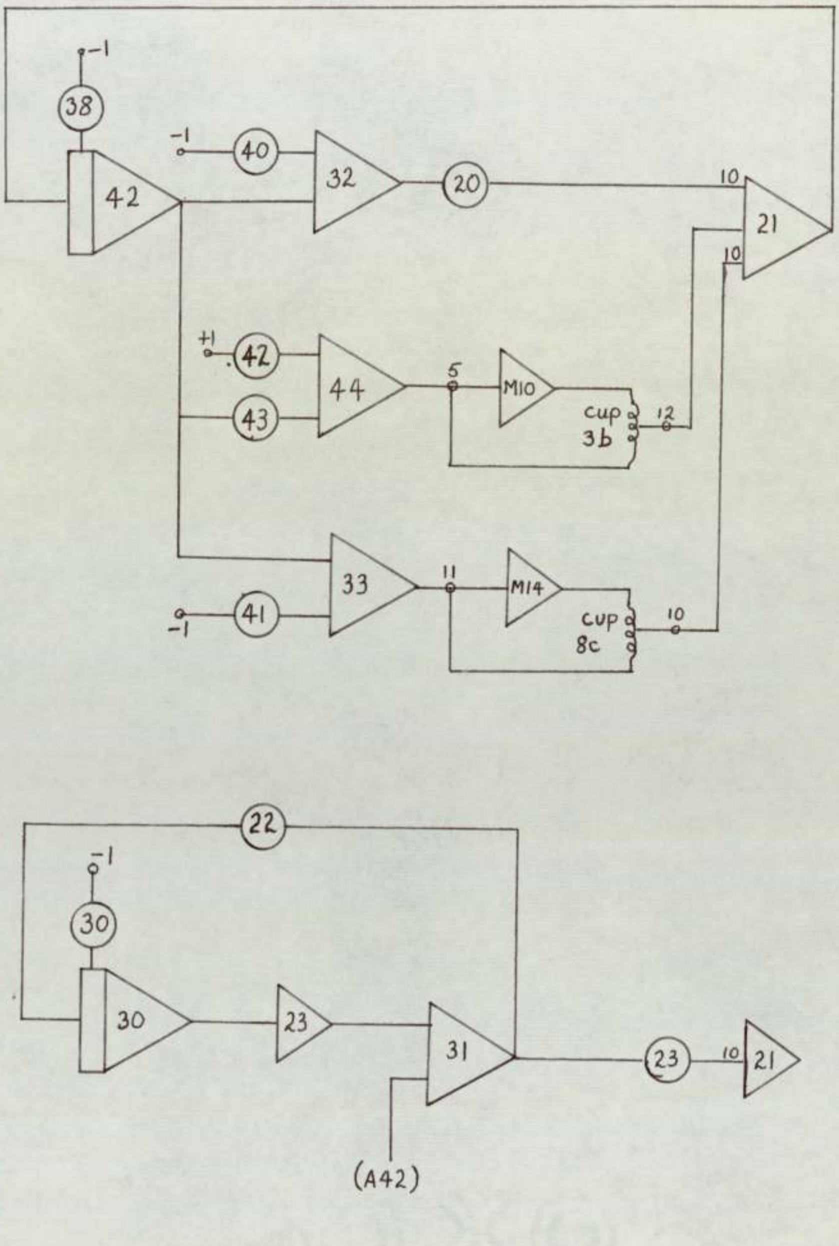


FIGURE 8(b) Circuit Diagram

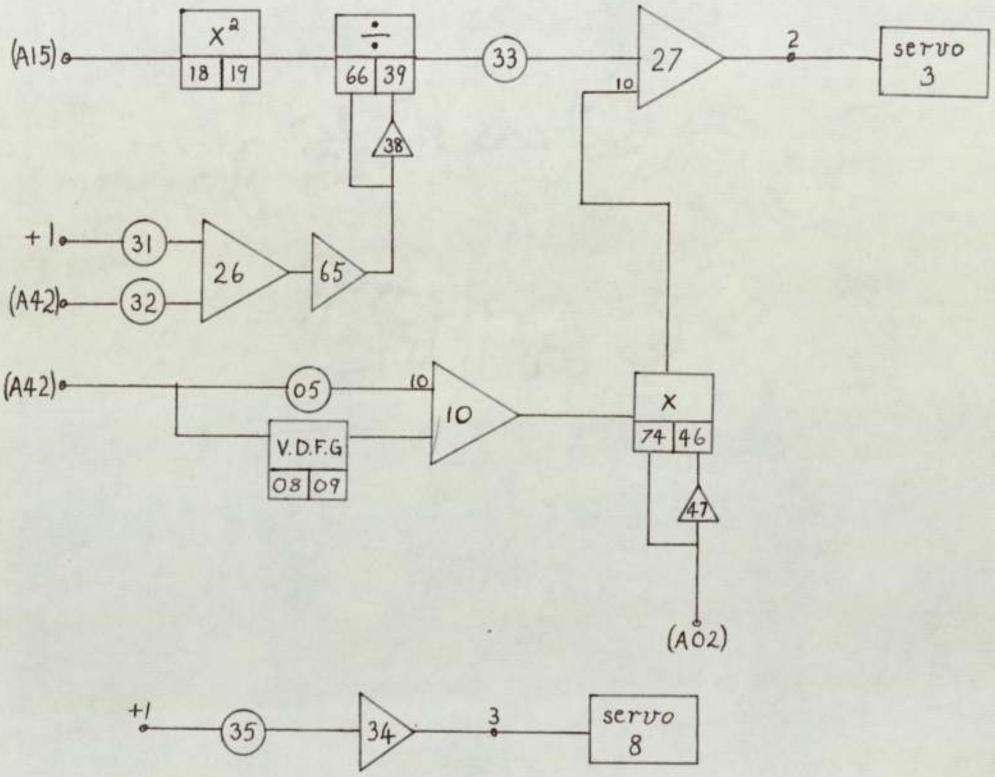


FIGURE 8(c) Circuit Diagram

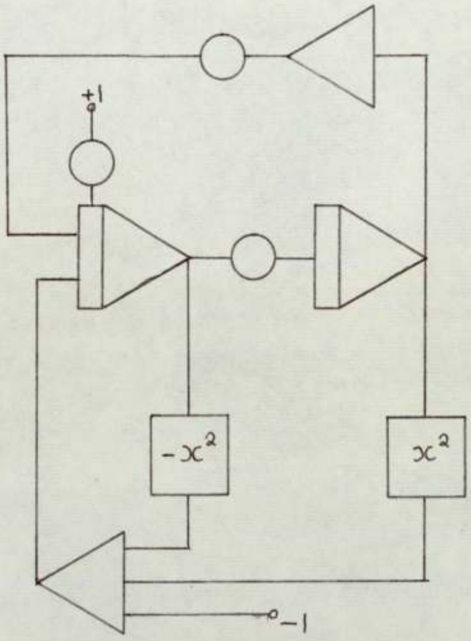


FIGURE 8(d) Circuit Diagram

time, as the remainder of the problem is to be run with time as the independant variable. Hence using the identity:

$$\frac{dk}{dt} = \frac{dk}{dT} \cdot \frac{dT}{dt} \qquad 3.4$$

the resulting relationship for the differential of the rate constant is:

$$\frac{dk}{dt} = \frac{+Ek}{RT^2} \frac{dT}{dt} \qquad 3.5$$

Since the values of θ and $\frac{d\theta}{dt}$ are available on the machine, the values of T and $\frac{dT}{dt}$ can be computed from:

$$T = \theta + 273 \qquad 3.6$$

and

$$\frac{dT}{dt} = \frac{d(\theta + 273)}{dt} = \frac{d\theta}{dt} \qquad 3.7$$

The absolute circuit is thus obtained by implementing the following equation:

$$\frac{dk}{dt} = \frac{+Ek}{R(\theta + 273)^2} \frac{d\theta}{dt} \qquad 3.8$$

as in FIG.9.

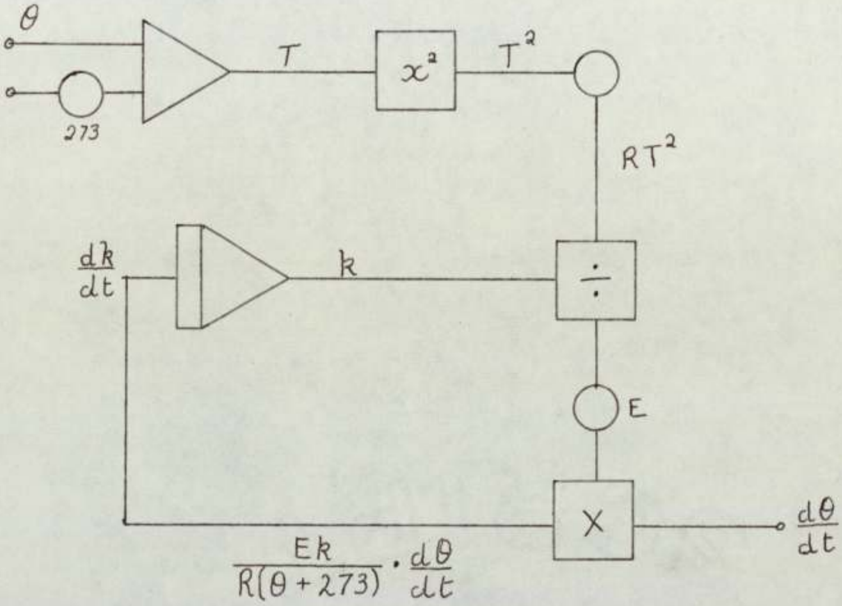


FIGURE 9 Absolute Circuit for Arrhenius' Relationship

A simpler and less equipment demanding method would be to use a variable diode function generator to generate the function of the rate constant. The shape of the curve however, does not allow a very accurate duplication to be made. A better method, suggested by Korn and Korn, uses the variable diode function generator to give an output equal to the error between the real function and a straight line drawn between two selected points on the curve. For best results the two points should be selected at opposite ends of the temperature scale to be used. Table 6 shows the function values and the errors between the function and the straight line. The curve generated by the variable diode function generator is shown in FIG.10.

The scaling of this problem is the scaling of the two dependant variables concentration and temperature. The scaling of concentration was achieved in the basic theory by using only mole fractions, hence further scaling is unnecessary. The scaling of temperature presents the difficulty of requiring prior knowledge of the maximum temperature to be achieved by the system. In this case an approximate maximum temperature is known, as it will probably be equal to the temperature of the heating fluid. Allowing for a variation in the value of the temperature of the heating fluid, a maximum of 500°C is assumed. Setting this maximum as equivalent to one machine unit gives the range 0 - 1 machine unit equivalent to 0 - 500°C.

One further property which was considered as requiring scaling was the rate constant. It was found however, that the rate constant

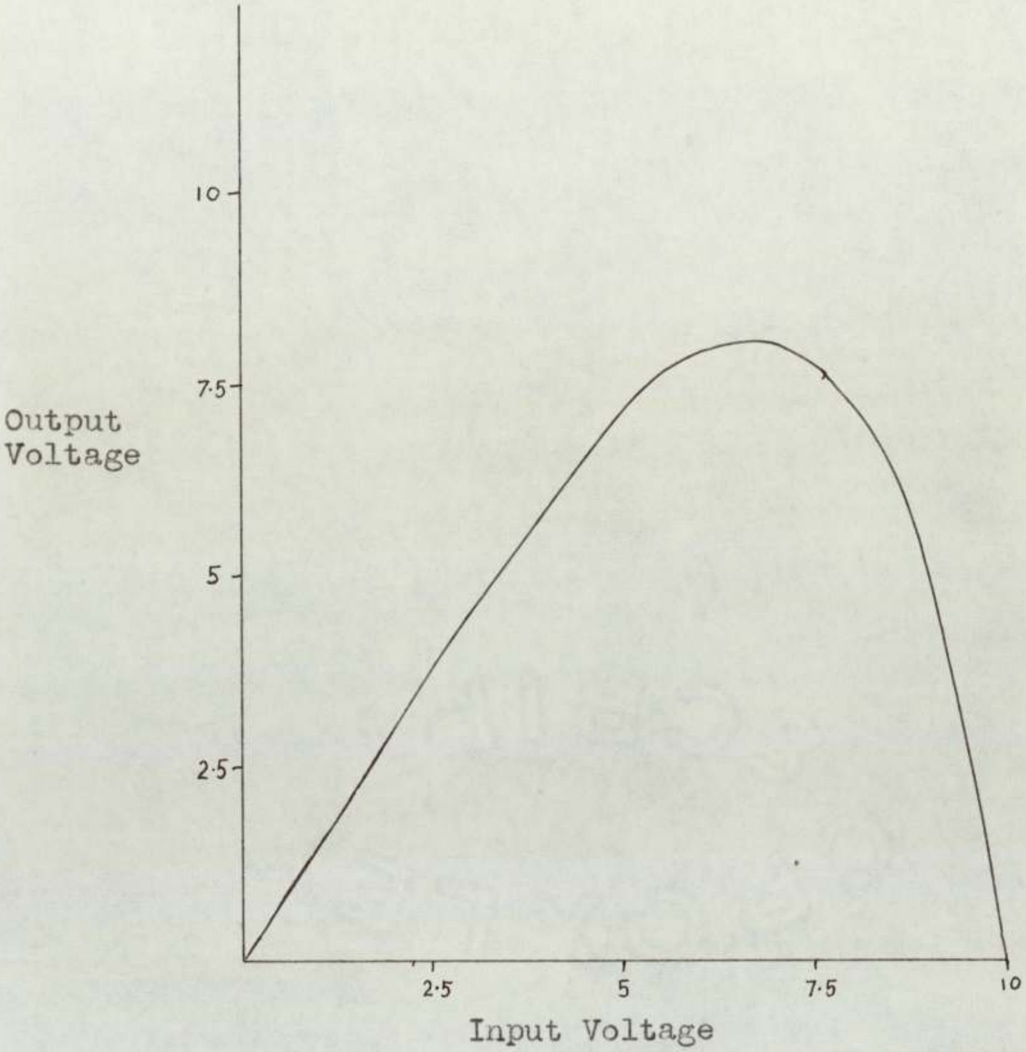


FIGURE 10 Diode Function Generator Setting

would only require scaling if the reactor temperature were to exceed 475°C. This, in effect, set a working maximum temperature of 475°C on the simulation. This was found to be adequate for the study.

CHAPTER FOUR

SIMPLIFICATION.

4.1 Introduction.

The importance of simplification of a mathematical model for an analogue computer study is related to the requirements involved. If the simulation is to be of a single piece of equipment, simplification may well be unimportant. If a number of individual units are to be simulated simultaneously on a computer of limited size, simplification becomes of prime importance.

Two methods of simplification of the model of the tubular reactor will be dealt with here. They are:

1. Theoretical simplification by linearisation.
2. Building a simple empirical model from experimental observations.

4.2 Linearisation.

Linearisation of the model of the tubular reactor about its steady state operating conditions, using Taylor's series expansion should yield equations which are a reasonable approximation for small perturbations. The original model expressed in general form for a single incremental difference step is:

$$\frac{dx_A}{dt} = f_1(x_A,\ x_{AIN},\ x_B,\ \theta,\ b) \qquad 4.1$$

$$\frac{dx_B}{dt} = f_2(x_B,\ x_{BIN},\ x_A,\ \theta,\ b) \qquad 4.2$$

$$\frac{d\theta}{dt} = f_3(\theta,\ \theta_{IN},\ x_A,\ x_B,\ b,\ \theta_c,\ \theta_s) \qquad 4.3$$

$$\frac{d\theta_s}{dt} = f_4(\theta,\ \theta_s) \qquad 4.4$$

Although this model is fourth order it can be reduced to third order by a simple but realistic assumption.

The assumption is that the reactor feed concentration is of constant composition. This will, in fact, be very nearly true since the feed is to be an azeotropic mixture of isopropanol and water.

Under such conditions there will be a simple algebraic relationship between the concentrations, in mole fractions, of reactants and products.

The reaction under consideration is of the type:

$$A = B + C$$

If one mole of A enters and m moles react we have:

1 - m moles of A
m moles of B
m moles of C

If throughout there were m_i moles of an inert present, then the total moles present at the finish is $1 + m + m_i$.

Hence the mole fraction of A (x_A) is:

$$x_A = \frac{1 - m}{1 + m + m_i} \qquad 4.5$$

and of B (x_B) is:

$$x_B = \frac{m}{1 + m + m_i} \qquad 4.6$$

From equation 4.5:

$$m = \frac{1 - x_A - m_i x_i}{1 + x_A} \qquad 4.7$$

Substituting into 4.6:

$$x_B = \frac{1}{2 + m_i} - \frac{1 + m_i}{2 + m_i} \cdot x_A \qquad 4.8$$

For a constant value of m_i this yields the straight line relationship:

$$x_B = \hat{A}_1 + \hat{A}_2 x_A$$

(where $\hat{A}_1$ and $\hat{A}_2$ are constants)

Using this relationship reduces the model to a dynamic third order system of the form:

$$\frac{dx_A}{dt} = f_1(x_A, x_{AIN}, \theta, b) \qquad 4.9$$

$$\frac{d\theta}{dt} = f_2(x_A, \theta, \theta_{IN}, \theta_S, \theta_C, b) \qquad 4.10$$

$$\frac{d\theta_S}{dt} = f_3(\theta, \theta_S) \qquad 4.11$$

Application of a first order approximation of a Taylor's series expansion to equations 4.9 and 4.10 yields:

$$\frac{dx_A}{dt} = x_A\left(\frac{\partial f_1}{\partial x_A}\right)_{t=0} + x_{AIN}\left(\frac{\partial f_1}{\partial x_{AIN}}\right)_{t=0} + \theta\left(\frac{\partial f_1}{\partial \theta}\right)_{t=0} + b\left(\frac{\partial f_1}{\partial b}\right)_{t=0} \qquad 4.12$$

$$\frac{d\theta}{dt} = x_A\left(\frac{\partial f_2}{\partial x_A}\right)_{t=0} + \theta\left(\frac{\partial f_2}{\partial \theta}\right)_{t=0} + \theta_S\left(\frac{\partial f_2}{\partial \theta_S}\right)_{t=0}$$

$$+ \theta_{IN}\left(\frac{\partial f_2}{\partial \theta_{IN}}\right)_{t=0} + \theta_C\left(\frac{\partial f_2}{\partial \theta_C}\right)_{t=0} + b\left(\frac{\partial f_2}{\partial b}\right)_{t=0} \qquad 4.13$$

Since equation 4.11 is already in a linear form, application of Taylor's series expansion will yield an equation identical to the original. Hence equation 4.11 is the third equation of the model.

Calculation of the coefficients of the linearised model is by differentiation of the functions of equations 4.9 and 4.10. Hence the following coefficients are obtained. Thus for equation 4.12:

$$\left(\frac{\partial f_1}{\partial x_A}\right)_{t=0} = -(1 + x_{AO})\left(k_{FO} + 2k_{RO}\rho_0 \hat{A}_1\hat{A}_2 - 2k_{RO}\rho_0 \hat{A}_2^2 x_{AO}\right) - (\text{rate}_0) - \frac{b_0}{V\rho_0} \qquad 4.14$$

$$\left(\frac{\partial f_1}{\partial x_{AIN}}\right)_{t=0} = \frac{b_0}{V\rho_0} \qquad 4.15$$

$$\left(\frac{\partial f_1}{\partial b}\right)_{t=0} = \frac{x_{AINO} - x_{AO}}{V\rho_0} \qquad 4.16$$

$$\left(\frac{\partial f_1}{\partial \theta}\right)_{t=0} = -(1 + x_{AO})\left(\frac{k_{FO}x_{AO}E}{R(273+\theta_0)^2} + \frac{k_{RO}\, x_{BO}^2\, 273}{22400(273+\theta_0)^2}\right) + \frac{b_0(x_{AINO} - x_{AO})22400}{273\, V} \qquad 4.17$$

Similarly for equation 4.13:

$$\left(\frac{\partial f_2}{\partial x_A}\right)_{t=0} = -\left(\frac{\Delta H_0 + 2\Delta c\,\theta_0}{c}\right)\left(k_{FO} + 2k_{RO}\rho_0\hat{A}_1\hat{A}_2 - 2k_{RO}\rho_0\hat{A}_2^2\,x_{AO}\right) \qquad 4.18$$

$$\left(\frac{\partial f_2}{\partial \theta_{IN}}\right)_{t=0} = \frac{b_0}{V\rho_0} \qquad 4.19$$

$$\left(\frac{\partial f_2}{\partial \theta_c}\right)_{t=0} = \frac{U_w a_w}{V\rho_0 c} \qquad 4.20$$

$$\left(\frac{\partial f_2}{\partial \theta_s}\right)_{t=0} = \frac{U_s a_s}{V\rho_0 c} \qquad 4.21$$

$$\left(\frac{\partial f_2}{\partial b}\right)_{t=0} = \frac{(\theta_{INO} - \theta_0)}{V\rho_0} \qquad 4.22$$

$$\left(\frac{\partial f_2}{\partial \theta}\right)_{t=0} = -\frac{b_0}{V\rho_0} + \frac{b_0(\theta_{INO} - \theta_0)22400}{273\,V} - \frac{U_w a_w + U_s a_s}{V\rho_0 c}$$

$$+ \frac{22400}{273\,Vc}\left(U_w a_w(\theta_{co} - \theta_0) + U_s a_s(\theta_{so} - \theta)\right)$$

$$- \frac{2\Delta c(\text{rate}_0)}{c}$$

$$- \left(\frac{\Delta H_0 + 2\Delta c\,\theta_0}{c}\right)\left(\frac{k_{FO}x_{AO}\,E}{R(273+\theta_0)^2} + \frac{273\,k_{RO}(x_{BO})^2}{22400(273+\theta_0)^2}\right) \qquad 4.23$$

4.3 Methods of Dynamic Analysis.

4.3.1 Introduction.

The empirical methods of analysing system dynamics to obtain models are best divided into groups. Each group is defined by a different input signal. Four types of input are available:

1. Step.
2. Ramp.
3. White noise.
4. Sinusoid.

For each type of input signal a number of methods of analysing the results have been developed.

4.3.2. The Step Change.

The outputs of systems which have undergone a step change on their input are known as process reaction curves. The shapes of these curves are well known for a multitude of systems. They are amenable to a number of simple forms of analysis.

The simplest is the fitting of the unknown process reaction curve to an equivalent for a series of N equally sized stirred tank reactors. For this analysis the unknown process reaction curve must be compared with a previously prepared plot of a number of process reaction curves of different known values of N. The simplicity of this as an overall method is in the next stage of the analysis. The reason for the simplicity is that the inverse of the transfer function obtained for the equivalent N stage process is a known power series of time, and hence the solution is easily found.

Another graphical method, using constructional techniques enables an approximation to the model to be made in the form of either a first or second order dynamic delay together with a time delay.

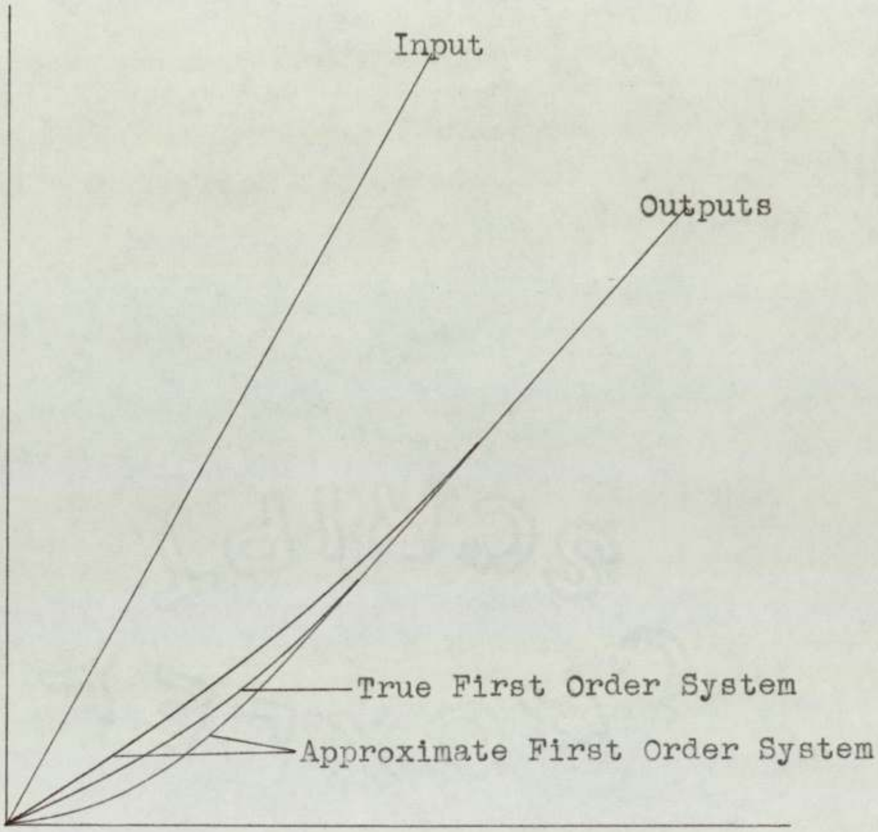


FIGURE 11 Response to a Ramp

4.3.3 The Ramp

The unrestricted nature of a continuous ramp change does not allow its use on all types of system. It would be of little use in dealing with the variation of any property having limits (e.g. concentration). It can be useful in determining certain parameters of systems of known dynamic characteristics. It is especially useful in showing the difference between the following two first order dynamic systems:

$$(1) \qquad \frac{K}{(Ts + 1)}$$

$$(11) \qquad \frac{K(T_1 s + 1)}{(T_2 s + 1)(T_3 s + 1)}$$

The output curve (FIG 11) has three characteristics.

1 Initial Slope

2 Final Slope

3 The intersection of the asymtote to infinity and the time axis.

System (1) above has only two variable constants, whereas system (11) has four. Hence one of the characteristics in system (1) is dependant upon the other two. In system (11) all three can vary independently. Hence system (1) is a special case of systems of type (11) and can be readily identified.

4.3.4 White Noise.

The use of white noise as an input for analytical purposes arises from the fact that many systems in their natural environment will be subjected to an input signal upon which is superinposed some form of random disturbance. Disturbances of this type are called noise, and completely random disturbances having zero correlation and covering a complete spectrum are called white noise.

The analysis must correlate the probability functions of input and output signals. Such a problem is extremely complex and may be used only in the simplest cases. The development of spectral density analysis has enabled such correlation to be achieved by comparison. Using this method a system which has white noise as its natural input may be continuously analysed in its natural environment. Thus the method is of specific interest in control problems where random input signals exist.

4.3.5 The Sinusoid.

Frequency response analysis is based upon the use of a sinusoidal input signal. The bounded nature of a sinusoid allows a system to sustain this type of continuously changing input for an unlimited period of time. The unlimited duration of the signal means that a system can reach a pseudo-steady state of continuous variation. The implication of reaching the steady state is that the analysis need not deal with transients.

Three methods of analysing sinusoidal signals are:

1. Root Locus.
2. Nyquist Diagrams.
3. Bode Diagrams.

The Root locus method is a purely theoretical method used for studying control stability of systems. The Nyquist diagram is used for a similar purpose but is of greater experimental importance. The Bode diagram, also of experimental importance, is used primarily for comparing the properties of different types of dynamic systems. It is through the use of the Bode diagram that frequency response analysis can be used to determine a mathematical model of the dynamics of a system.

4.3.6 The Bode Diagram.

The Bode diagram is a double plot of both phase lag and amplitude attenuation ratio versus the frequency of the input sine wave. The phase angle scale is linear while both amplitude ratio and frequency are logarithmic. Both plots are of interest, although the information obtained from one is duplicated in the other.

The main attribute of the phase angle versus frequency plot is in the asymptotic values of phase angle as the frequency tends to both zero and infinity. The angular difference between the two values is representative of the order of the system. For a first order system this difference equals 90°, and generally for an n^{th} order system the difference is $90n^\circ$. Hence a system's order could be obtained from a plot of experimental results.

This information is duplicated in the amplitude ratio versus frequency plot but by a different parameter. It is obtained exclusively from the gradient of the asymptote as frequency tends to infinity. The asymptote as frequency tends to zero gives the value of the gain of the system. This alone makes this plot more useful.

For an n^{th} order system the gradient passes from zero to n, and hence it will pass through all integer values between zero and n. The tangents to the curve and having integer values of gradient have two special properties. Firstly the verticals drawn from the intersection of two adjacent tangents to the curve are all the same length and equal to $\frac{1}{2}\log 2$. Secondly the values of frequency at the intersections of all of these tangents with that of gradient zero yield sufficient information to give all of the time constants.

The former of the above points represents a simple means of drawing the tangents, and a useful guide to systems having transfer functions which do not follow the form:

$$\frac{K}{\prod_{i=1}^{N}(s + a_i)}$$

but may indicate the more general form:

$$\frac{K \prod_{i=1}^{N}(s + b_i)}{\prod_{j=1}^{M}(s + a_j)}$$

4.4 Frequency Response Practice.

Apart from the system to be analysed two other pieces of apparatus are required for frequency response analysis. They are:

1. A means of generating an input sinusoid.
2. A means of observing and mesuring the output sinusoid.

There would appear to be little difficulty in generating a sinusoid on an analogue computer since it is the solution of the simple differential equation:

$$\frac{d^2y}{dt^2} = -y \quad (\text{where at } t=0, y=0 \text{ and } \frac{dy}{dt}=1)$$

However, this equation is critically stable and a minor inaccuracy in components will cause the computer solution to be unstable. To overcome this effect a number of limiting circuits have been devised to maintain a constant amplitude. This type of circuit often gives a sinusoid with slightly squared peaks. A far better means of correcting any amplitude variation is to use the natural corrective circuit contained in the equation:

$$\sin^2 t + \cos^2 t = 1 \qquad 4.24$$

where an error may be obtained from:

$$\text{error} = 1 - \sin^2 t - \cos^2 t \qquad 4.25$$

It was found that using this equation to give a feed back error signal, a sinusoid with no measurable inaccuracy could be maintained for more than 100 cycles. It was considered that the advantage in increased accuracy achieved outweighed the increase in required equipment.

The simplest measurement of the output signal is to record, from any voltage measurement equipment, the voltage difference between peaks.

There are however, two methods of obtaining the measurement more easily.

1. The Quadrature component method.
2. The null phase method.

These methods are most useful where noise is a problem, and one rather wasteful on apparatus where it does not occur, as on an analogue computer.

Finally the range of frequency to be used is determined by the flexibility of the computer. With the TR - 48's multiple time constant integration networks, a total of six logarithic cycles range may be obtained. Since the time constants of the problem have a range of only one to a hundred the available range is more than ample.

4.5 The Network Analogy.

A preliminary investigation was carried out on the simulation. This revealed two properties of the system which could be used to further simplify the model.

1. The dynamics relating the reactor inlet temperature and the heating medium temperature to the reactor outlet variables were essentially the same. This is to be expected since physical properties are assumed constant.

2. The reactor flow rate was very nearly independant of the other inlet variables. This, too, is expected since any changes will be caused by changes of mass in the reactor.

The preliminary investigation also enabled the order of the transfer functions relating inlet and outlet variables to be obtained. The results suggested that:

1. $\frac{\text{Outlet temperature}}{\text{Inlet temperature}}$ and $\frac{\text{Outlet concentration}}{\text{Inlet concentration}}$

were first order.

2. $\frac{\text{Outlet temperature}}{\text{Inlet concentration}}$ and $\frac{\text{Outlet concentration}}{\text{Inlet temperature}}$

were second order.

However, a closer investigation of these results revealed that the first order systems were not truly first order. In FIG. 12, the Bode diagram of a first order system is shown. The distance marked $\mathcal{X}$ should be $\frac{1}{2}\log 2$. In the experimental plots it was found that the equivalent lengths were not $\frac{1}{2}\log 2$. This suggests that although the systems were basically first order, other

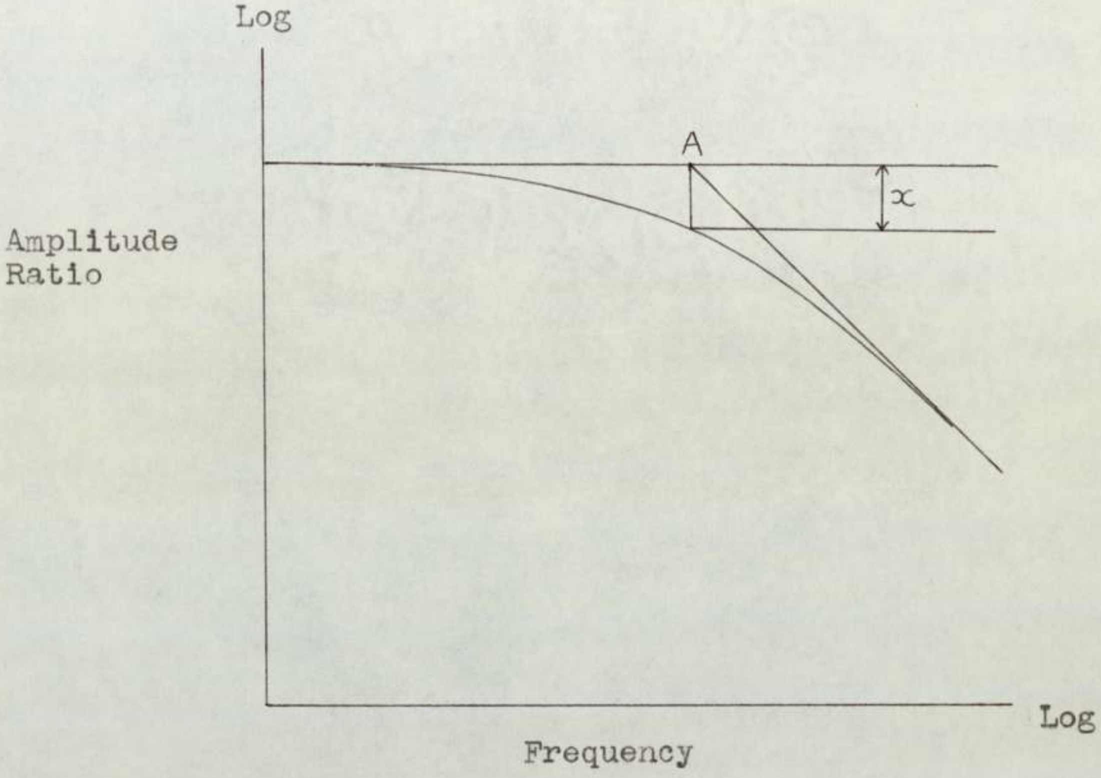


FIGURE 12 BOde Diagram of a
First Order System

components existed which should be accounted for.

To attempt to accommodate the discrepancies the following form of transfer function was used:

$$f(s) = \frac{K(T_1 s + 1)}{(T_2 s + 1)(T_3 s + 1)} \qquad 4.26$$

The difficulty of obtaining the individual values of the time constants now arises, and a statistical method was tried.

For a transfer function as given in equation 4.26 the amplitude ratio (A.R) is given by:

$$(A.R) = K \sqrt{\left(\frac{1 + (\omega T_1)^2}{(1 + (\omega T_2)^2)(1 + (\omega T_3)^2)} \right)} \qquad 4.27$$

From frequency response values of (A.R), ω and K were obtained.

Rearranging equation 4.27:

$$\frac{\left(\frac{(A.R)}{K}\right)^2 - 1}{\omega^2} = T_1^{\,2} - \left(\frac{(A.R)}{K}\right)^2 (T_2^{\,2} + T_3^{\,2}) - \omega^2 \left(\frac{(A.R)}{K}\right)^2 T_2^{\,2} T_3^{\,2} \qquad 4.28$$

This may be likened to the linear equation:

$$Y = A_1 + A_2 X_1 + A_3 X_2 \qquad 4.29$$

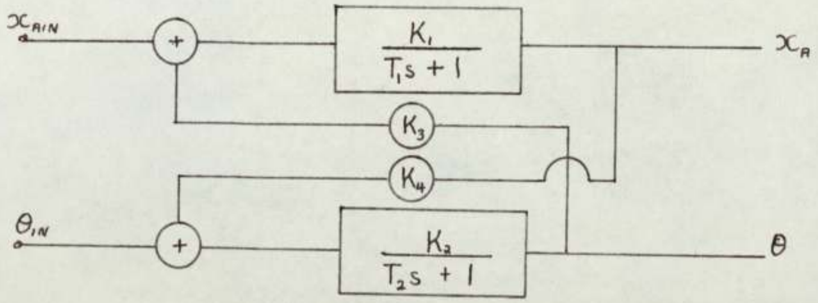


FIGURE 13 Simple Network

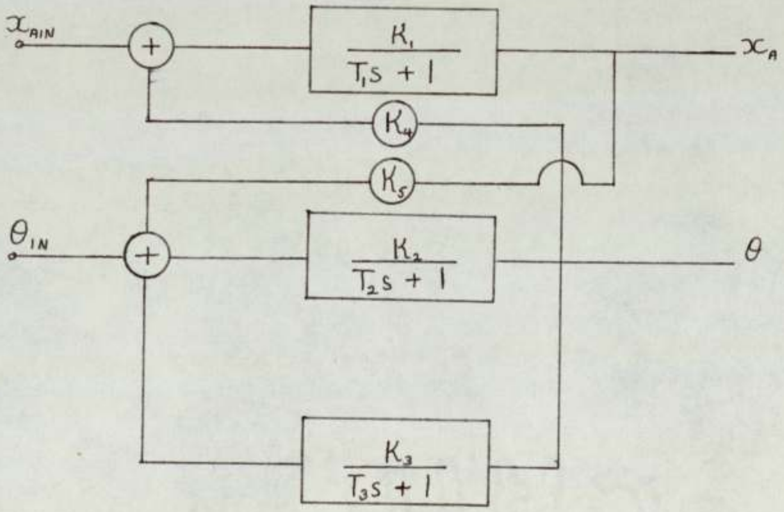


FIGURE 14 Modified Network

where

$$A_1 = T_1^2 \;,\; A_2 = T_2^2 + T_3^2 \;,\; A_3 = T_2^2 T_3^2 \qquad 4.30, .31, .32$$

Values of A_1, A_2 and A_3 obtained from the method of least squares can be substituted in equations 4.30, 4.31 and 4.32 to give values of T_1, T_2 and T_3. However, the accuracy of the values obtained is suspect because of the vast ranges of the variables Y, X_1 and X_2. The method was tried with the result that the values of the time constants were found to be too sensitive to the value of 'K' to be of any practical use.

It was noted that the value of the term $\dfrac{T_1}{T_2 T_3}$ was constant with respect to 'K' even though the individual values of T_1, T_2 and T_3 varied. The value of this term is the value of 'ω' at the point 'A' in FIG 12 and may be found graphically.

The failure of the statistical method led to the need to look at the system to enable identification. The symmetry showed that there was a simple network equivalent of the system, FIG 13. Analysis of the network and comparison with the simulation showed a further inadequacy. In all cases at the steady state there was a tendency to drift which could not be explained by computer drift. Closer analysis of the original mathematics showed the drift to be caused by the influence of the large heat capacity of the catalyst upon the system. Modification of the network to include this catalyst effect gave the network (FIG 14) which was to be used as the working simplified model.

For the network FIG 14

$$\bar{\theta} = \frac{K_2}{(T_2 s + 1)}\left(K_5\, \bar{x}_A + \bar{\theta}_{IN} + \frac{K_3 \bar{\theta}}{(T_3 s + 1)} \right) \qquad 4.33$$

$$\bar{x}_A = \frac{K_1}{(T_1 s + 1)}\left(\bar{x}_{AIN} + \dot{K} \bar{\theta} \right) \qquad 4.34$$

which yield

$$\frac{\bar{\theta}}{\bar{\theta}_{IN}} = \frac{K_2 (T_1 s + 1)(T_3 s + 1)}{f(s)} \qquad 4.35$$

$$\frac{\bar{\theta}}{\bar{x}_{AIN}} = \frac{K_1 K_2 K_5 (T_3 s + 1)}{f(s)} \qquad 4.36$$

$$\frac{\bar{x}_A}{\bar{x}_{AIN}} = \frac{K_1 \left((T_2 s + 1)(T_3 s + 1) - K_2 K_3 \right)}{f(s)} \qquad 4.37$$

$$\frac{\bar{x}_A}{\bar{\theta}_{IN}} = \frac{K_1 K_2 K_4 (T_3 s + 1)}{f(s)} \qquad 4.38$$

where $f(s) = (T_1 s+1)(T_2 s+1)(T_3 s+1) - K_1 K_2 K_3 (T_3 s+1) - K_2 K_3 (T_1 s+1)$ 4.39

Hence the four gains

$$\frac{K_2^*}{A} \quad , \quad \frac{K_1 K_2^* K_5}{A} \quad , \quad \frac{K_1}{A} \text{ and } \frac{K_1 K_2^* K_5}{A}$$

where

$$K_2^* = \frac{K_2}{1 - K_2 K_3} \qquad 4.40$$

$$A = 1 - K_1 K_2^* K_4 K_5 \qquad 4.41$$

and the four intercepts of the tangents to infinity and zero will be

$$\frac{A}{T_2(1-K_2K_3)} \, , \, \frac{A}{T_1T_2(1-K_2K_3)} \, , \, \frac{A}{T_1} \, , \, \frac{A}{T_1T_2(1-K_2K_3)}$$

For practical purposes these expressions do not yield sufficient information to obtain a solution.

Considering the original model it is obvious that for the added loop in FIG 14 to be the catalyst effect then the value of K_3 must be unity, and the value of T_3 must be given by the constant 'C_1' in equation 2.9.

Using this information together with the four gain equations leaves only two further equations for a solution. These are obtained from the intercept values of the first order systems.

The advantage of neglecting the values of the other two intercepts is that of accuracy. These intercepts would be obtained from dynamic records of second order systems with very low gains. The measurement of the very small amplitude of the output sinusoids would cause a great loss in accuracy.

4.6 Results.

In the preliminary investigation it was noted that there was occasionally a small degree of non-repeatability. This was found to be caused by:

1. Reading error
2. Potentiometer drift.

To obviate this in the final set of results the following sequence was used for obtaining values of amplitude ratio for different values of frequency.

1. The potentiometers were set up.
2. The computer started and a reading taken.
3. The computer reset.
4. 2 and 3 repeated a further nine times.
5. The potentiometers checked.

If at any time an odd reading was taken, or if at the end the potentiometers did not check, then the results were discarded and the sequence repeated.

In order to take the readings the ascilloscope scale was calibrated against the machine scale.

The final values obtained by frequency response are given in Tables 8 and 9 and are also shown in FIG 15. The calculated values of the constants in the model section 4.5 are given in Tables 10 and 11.

TABLE 3

Potentiometer Settings.

Potentiometer Number	Value	Typical Values.
00	x_{AIN}	.8666
03	x_{AO}	.5506
05	.14	.1400
16	x_{BO}	.1826
17	x_{BIN}	.0000
20	$u_w a_w / V\rho c$	.7750
22	$U_s a_s / \rho_s c_s (1-\varepsilon) A$	.0050
23	$a_s / V\rho c$	.3800
30	θ_{SO}	.5506
31	.556	.5560
32	.303	.3030
33	.333	.3332
35	$b / V\rho$	.2540
38	θ_o	.6320
40	θ_c	.8000
41	θ_{IN}	.6000
42	$\Delta H / c$	.6500
43	$2\Delta c / c$	.3200

TABLE 4

Amplifier Outputs.

Amplifier Number	Output
02	x_A
03	$x_A - x_{AIN}$
04	$-(1 + x_A)/2$
05	$-dx_A/dt$
10	$-1.4\theta - f(\theta)$
12	$x_{BIN} - x_B$
13	$x_B - x_{BIN}$
14	$1 - x_B$
15	x_B
16	$-dx_B/dt$
17	$+dx_B/dt$
21	$-d\theta/dt$
23	$-\theta_s$
26	$-(\bar{A}_1 + \bar{A}_2\theta)$
27	(rate)
28	$-.1(\text{rate})(1 + x_A)/2$
29	$\cdot 1(\text{rate})(1 + x_A)/2$
30	θ_s
31	$\theta_s - \theta$
32	$\theta_c - \theta$
33	$\theta_{IN} - \theta$
34	$-.1\, b/V\rho$

Table 4 (Cont'd)

Amplifier Number	Output
42	θ
44	$-(\Delta H - 2\Delta c\theta)/c$
65	$\bar{A}_1 + \bar{A}_2\theta$

TABLE 5

Physical and Chemical Properties.

Total cross-sectional area of reactor = 46.5 cm^2

Surface area of catalyst = 200 cm^2/cm

Surface area of wall = 87.2 cm^2/cm

Voidage = 0.4

Density of catalyst = 2 gm/cm^3

Specific heat of catalyst = 2 cal/gm $^\circ$C

Specific heat of isopropanol = 41 cal/gm mole $^\circ$C

Specific heat of acetone = 40 cal/gm mole $^\circ$C

Specific heat of hydrogen = 8 cal/gm mole $^\circ$C

Heat transfer coefficient at catalyst surface = .003 cal/cm^2 sec $^\circ$C

Heat transfer coefficient at wall = .0014 cal/cm^2 sec $^\circ$C

Forward reaction rate constant term = 4,950,000 sec^{-1}

Forward reaction activation energy = 13,300 cal/gm mole

Reverse reaction rate constant term = 148,000 cm^3/sec gm mole

Reverse reaction activation energy = zero

Enthalpy of reaction at 20°C = 13,000 cal/gm mole

Length of reactor = 400 cms

TABLE 6

Value of the setting points on the diode function generator.

Input Voltage	Output Voltage
0	0
2	2.8
4	5.54
5	6.77
6	7.70
6.5	7.94
7	7.94
7.5	7.74
8	7.28
9	4.75
10	0

The straight line used is:

$$\text{Output} = 1.4\ (\text{Input})$$

The difference between this straight line and the curve obtained from the above setting is used to generate the term $\exp(-E/RT)$ as used in the reaction kinetics.

TABLE 7

Oscilloscope Calibration

Computer Voltmeter Reading	Oscilloscope Scale Reading
.0000	.0000
.1000	.1000
.2000	.2000
.3000	.3000
.4000	.4000
.5000	.5000
.6000	.6000
.7000	.7010
.8000	.8010
.9000	.9020
1.0000	1.0010

Since the magnitude of the errors is so small they may be neglected.

TABLE 8

Steady State Gains.

Segment Number.	$\frac{\theta}{\theta_{IN}}$	$\frac{x_B}{x_{BIN}}$	$\frac{\theta}{x_{BIN}}$	$\frac{x_B}{\theta_{IN}}$
1	.172	.604	.029	.346
2	.216	.661	.037	.261
3	.254	.665	.050	.196
4	.271	.665	.057	.146

TABLE 9

Frequency Response Results.

Segment 1

Frequency of Input	Amplitude Ratio	
cycles/second	θ/θ_{IN}	X_A/X_{AIN}
.0001	.172	.604
.000316	.172	
.001	.150	.604
.00178	.120	
.00316	.082	
.00564	.060	
.01	.052	.604
.1	.050	.600
1.0	.047	.600
1.78		.545
3.16	.046	.444
5.64		.348
10.0	.044	.250
17.8	.042	
31.6	.040	
56.4	.029	
100.0	.018	.025

Segment 2.

Frequency of Input	Amplitude Ratio	
	θ/θ_{IN}	$\dot{x}_A/x_{AIN}$
.0001	.216	.661
.001	.180	.661
.01	.055	.660
.1	.055	.660
1.0	.055	.610
1.78		
3.16		.500
5.64		.400
10.0	.052	.280
17.8		.165
31.6	.048	
56.4	.038	
100.0	.024	.028

Segment 3

Frequency of Input	Amplitude Ratio	
	θ/θ_{IN}	x_A/x_{AIN}
.0001	.254	.665
.001	.205	.665
.01	.075	.660
.1	.070	.660
1.0	.060	.600
3.16		.550
5.64		.425
10.0	.060	.316
17.8		.175
31.6	.055	
56.4	.040	
100.0	.025	.030

Segment 4

Frequency of Input	Amplitude Ratio	
	θ/θ_{IN}	x_A/x_{AIN}
.0001	.271	.665
.001	.230	.665
.01	.090	.665
.1	.070	.660
1.0	.060	.605
3.16		.600
5.64		.475
10.0	.060	.320
31.6	.055	
56.4	.048	
100.0	.025	.030

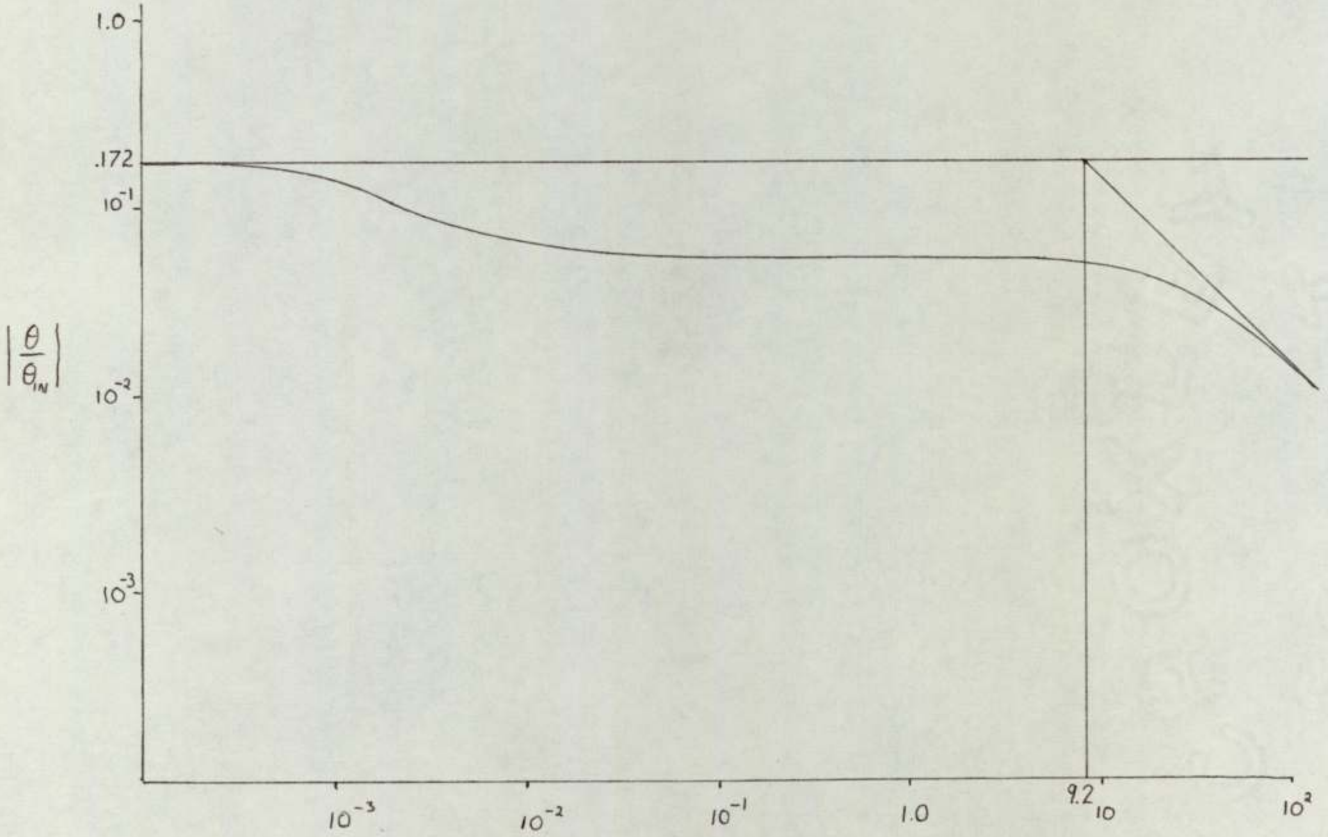


FIGURE 15(a) Results Segment 1

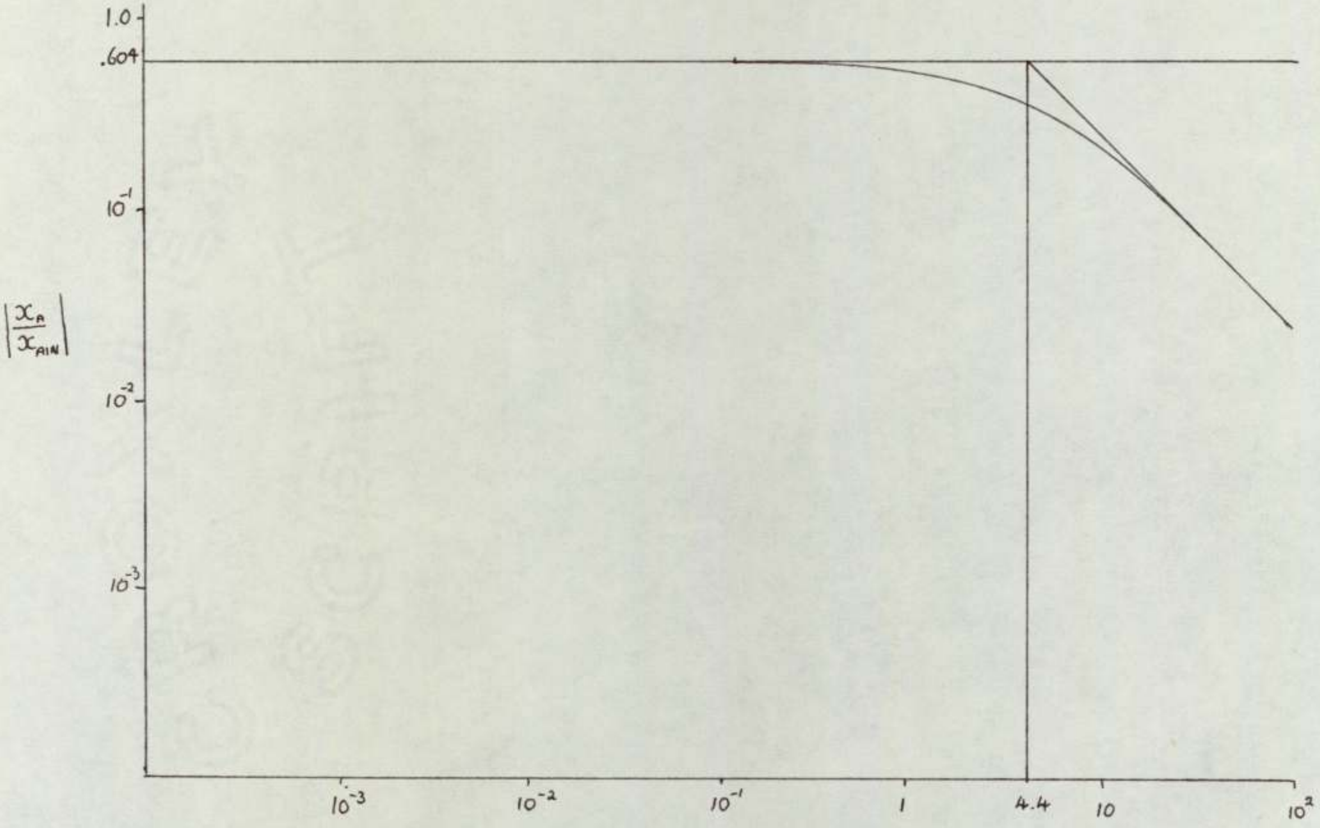


FIGURE 15(b) Results Segment 1

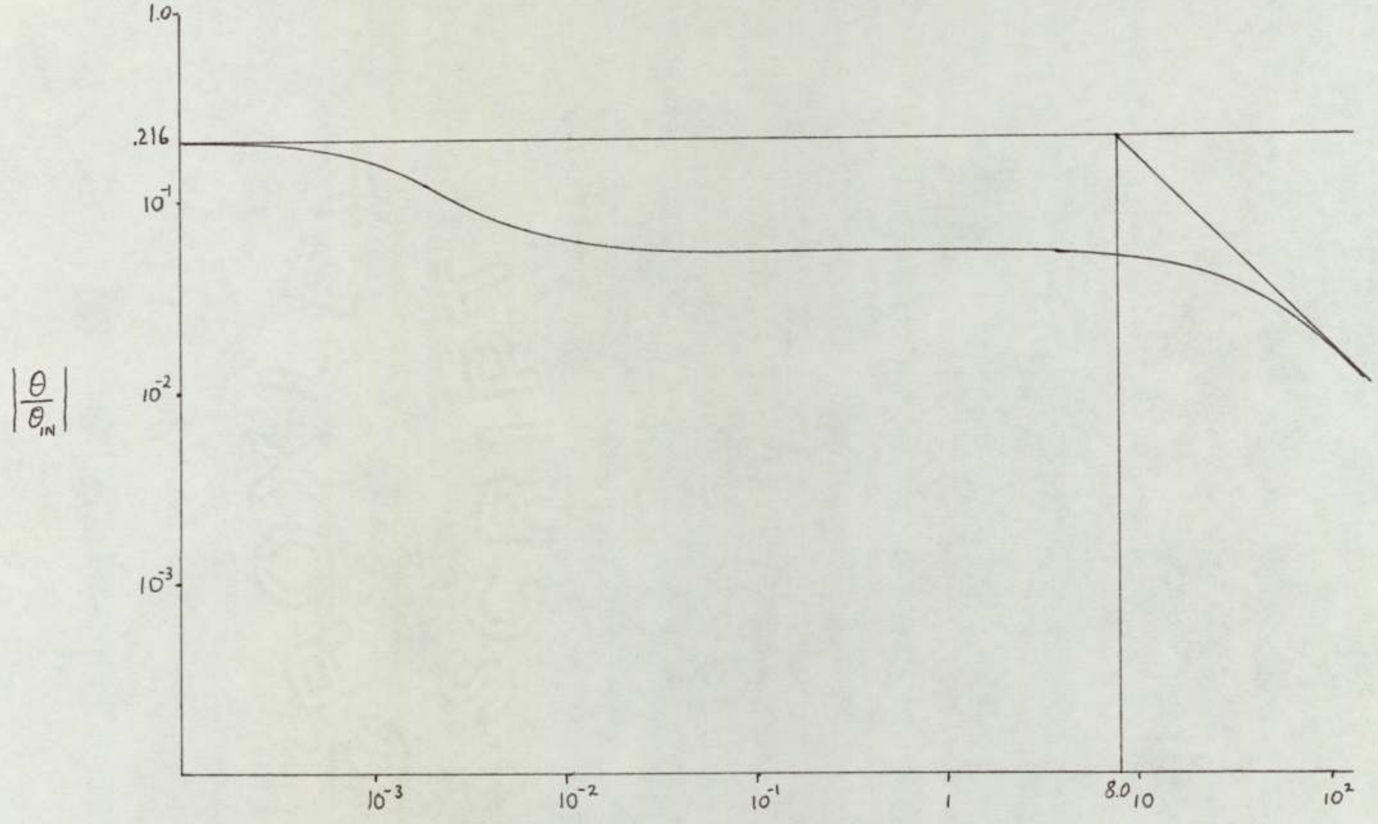
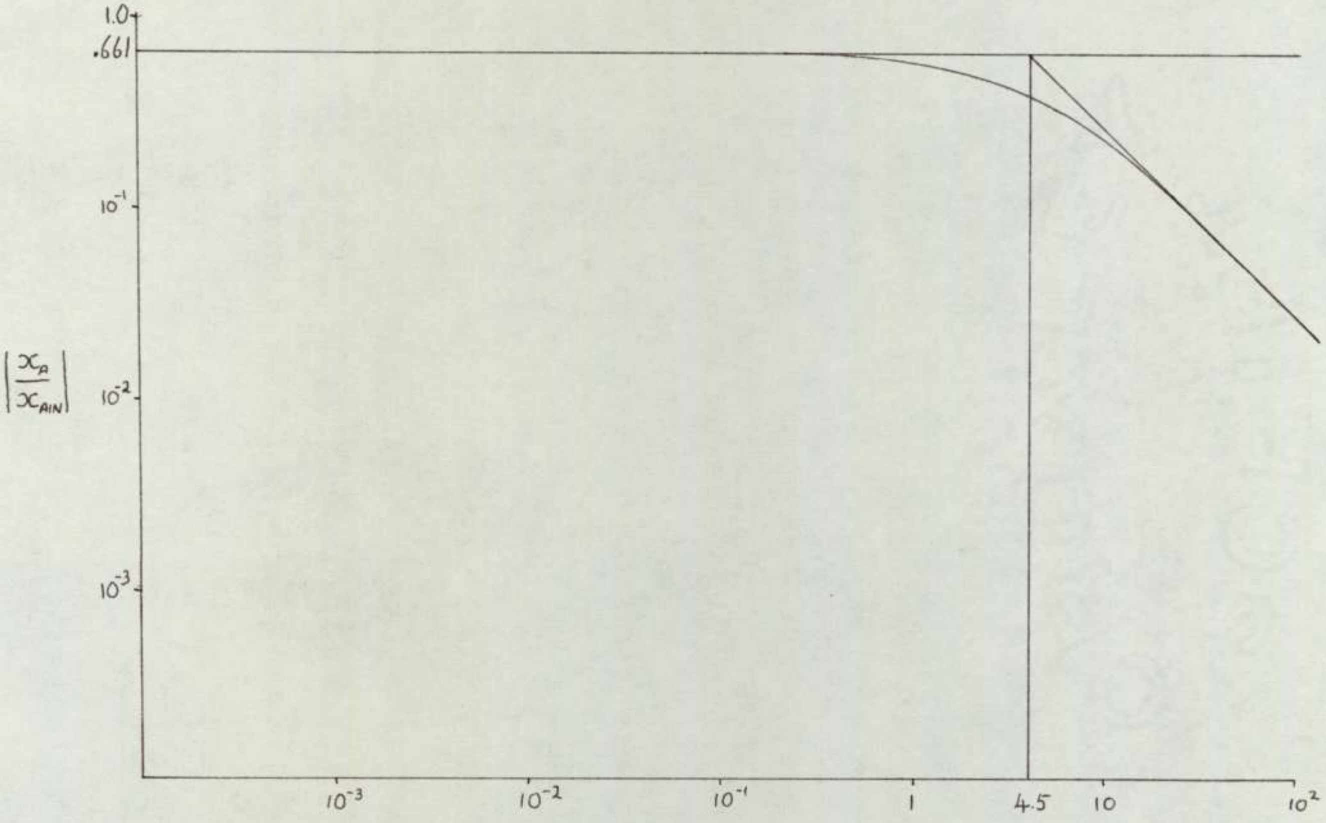


FIGURE 15(c) Results Segment 2



Frequency Rad./sec.

FIGURE 15(d) Results Segment 2

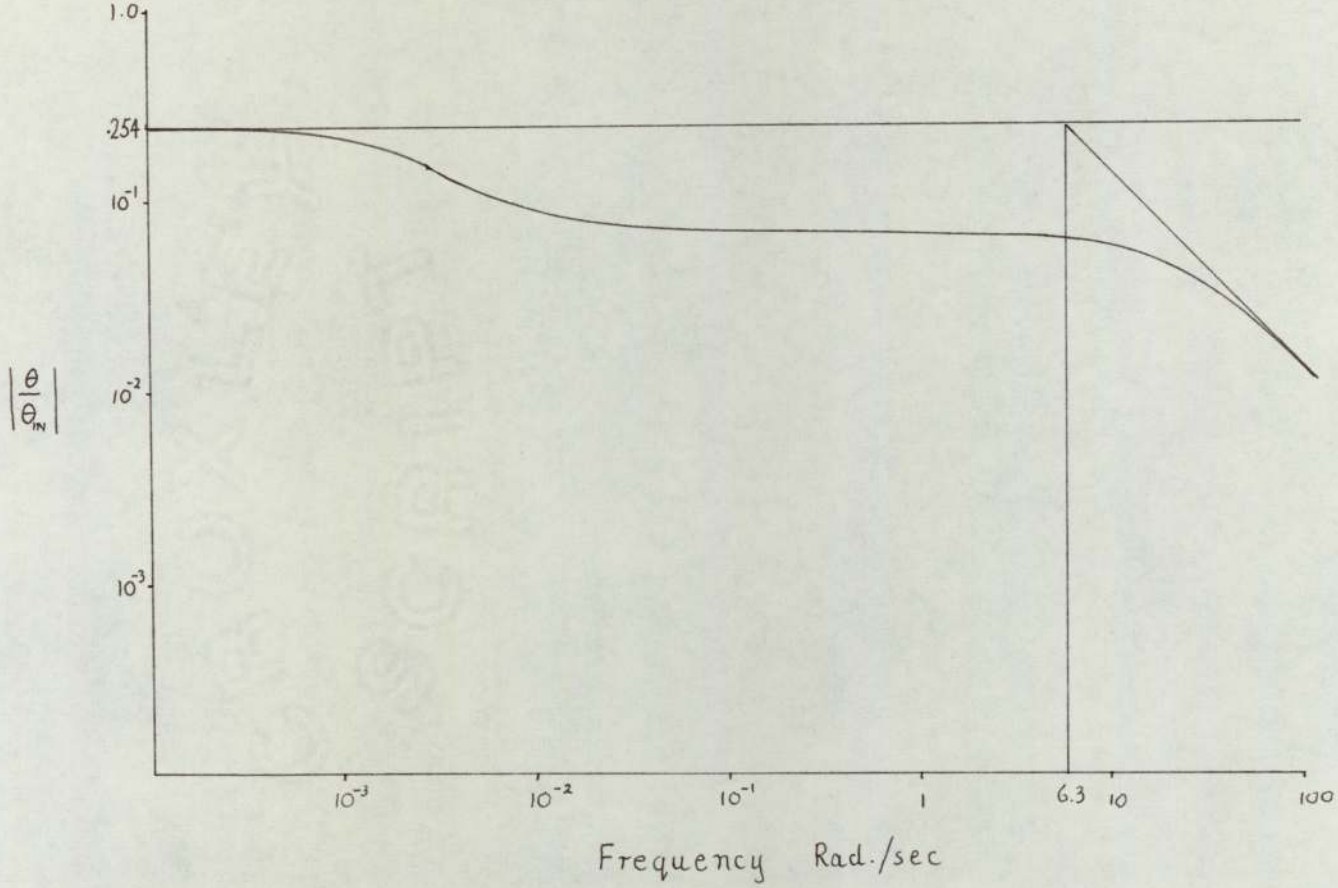


FIGURE 15(e) Results Segment 3

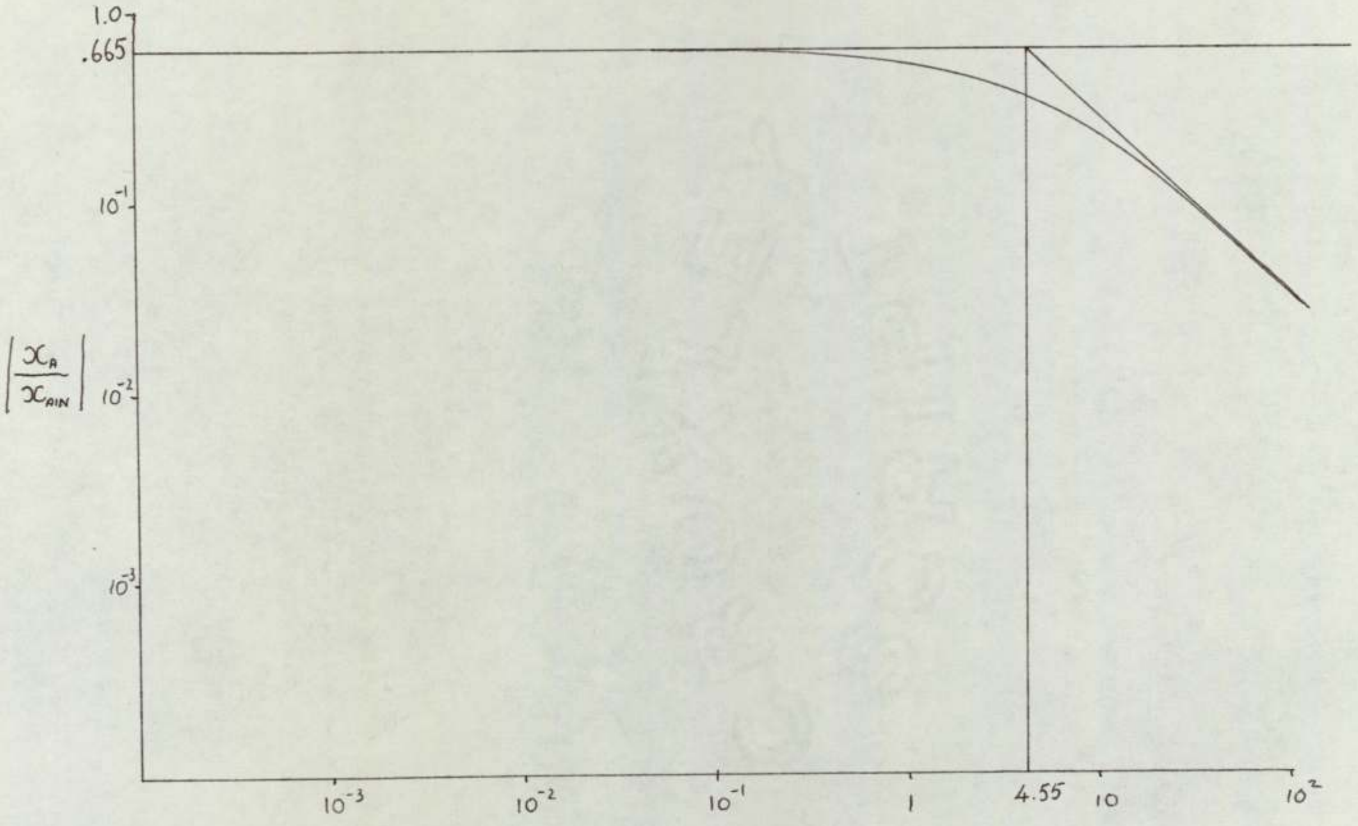


FIGURE 15 (f) Results Segment 3

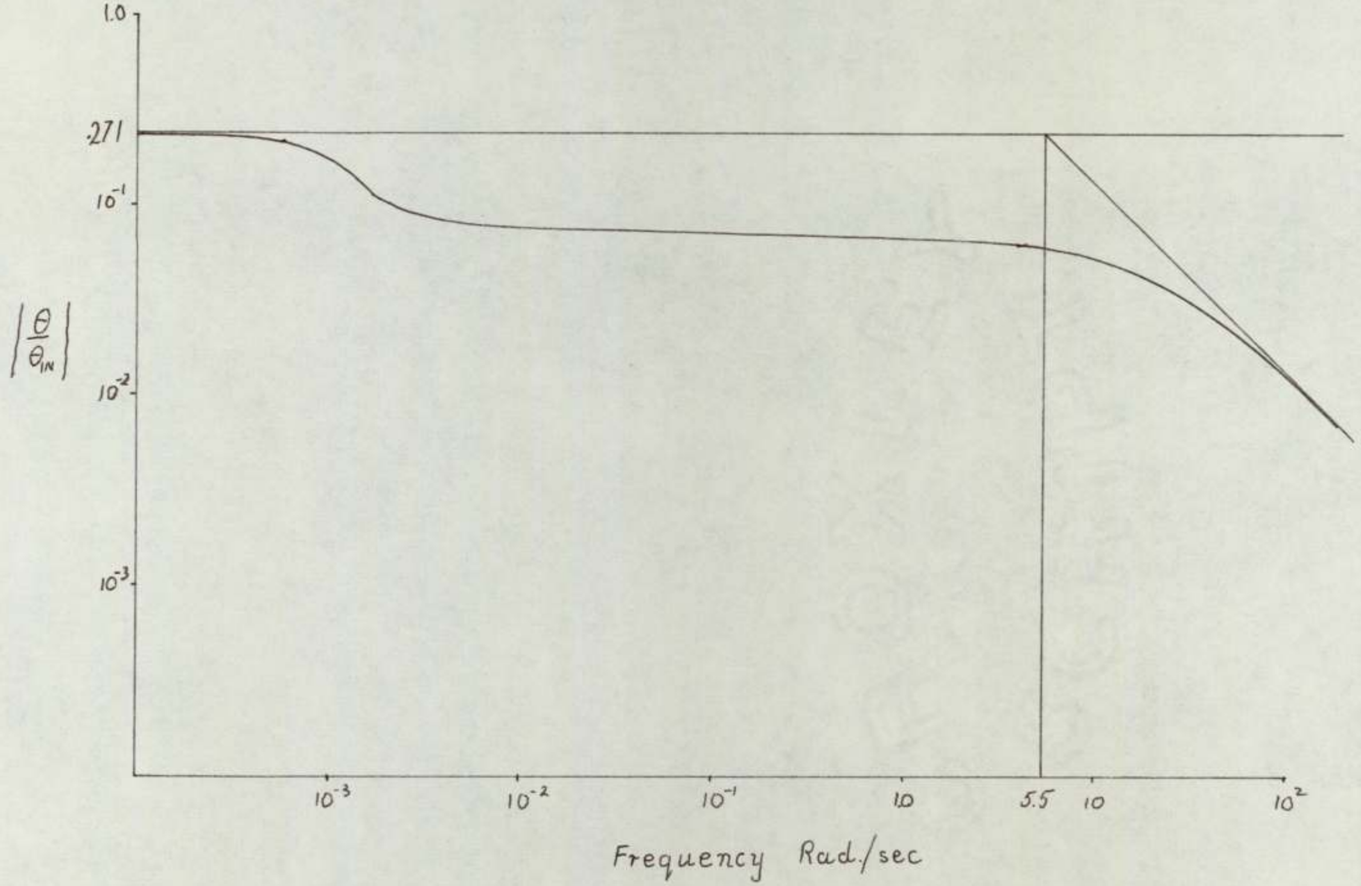


FIGURE 15(q) Results Segment 4

TABLE 10

Constants Obtained for the segments of the Model.

Segment Number	K_1	K_2	K_3	K_4	K_5
1	.545	.132	1.0	4.33	.363
2	.615	.168	1.0	2.34	.331
3	.625	.193	1.0	1.52	.389
4	.630	.204	1.0	1.08	.420

TABLE 11

Time Constants Obtained for the segments of the Model.

Segment Number	T_1	T_2	T_3
1	.204	.112	186
2	.205	.140	186
3	.206	.184	186
4	.206	.216	186

CHAPTER FIVE

USE OF THE MODEL.

5.1 Introduction.

The use of the model obtained for the reactor would be for simulation together with similar models of other process plant items in an integrated system. It has been found however, that the time involved in developing a number of similar models for other process plant units would be too great.

This section therefore, will deal with the uses of the whole or integrated model. The major use of the model would be in the control field, either for studying and comparing different control configurations, or for determining such optimal characteristics of start-up and shut-down trajectories as may exist.

Because of recent interest in feed-forward control it was felt that this aspect should be studied from the point of view of the applicability and use of simulation to the design of feed-forward controllers. One particular facet presented difficulty in the simulation domain. It was found that it was necessary to formulate a simulation of differentiation. Therefore, a study of differentiators was made.

The final section of this chapter discusses the methods of determining optimal start-up and shut-down trajectories.

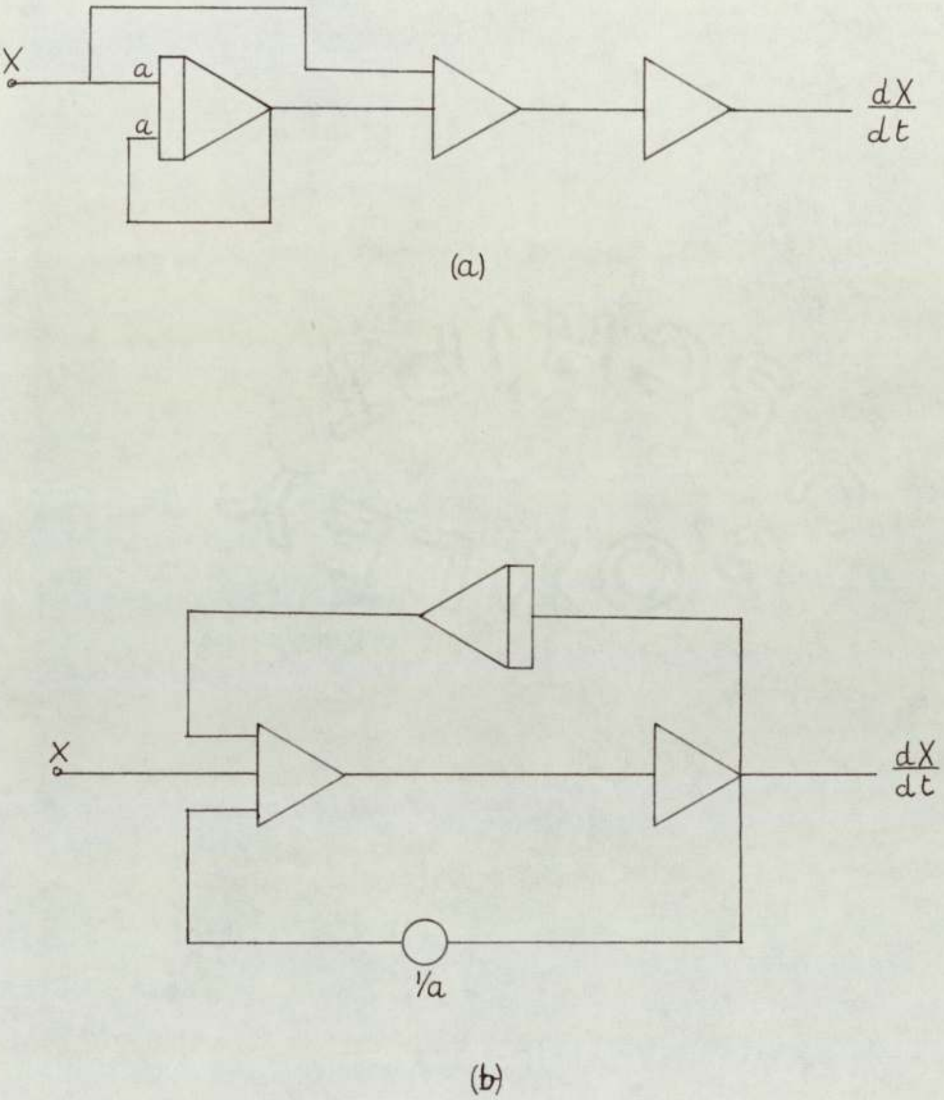


FIGURE 16 Differenciators

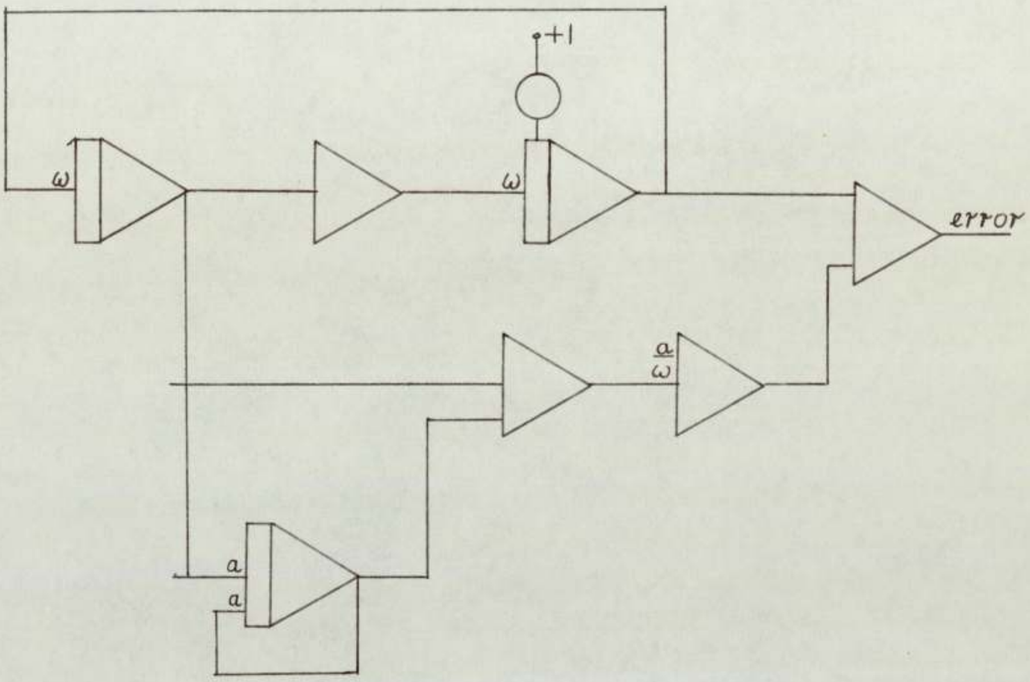


FIGURE 17 Differenciation of a Sinusoid

5.2 Simulation of a Differentiator.

There has not been found a natural phenomenon which has the property of being a differentiator. Hence, it would seem that there was no need to consider this when dealing with simulations. There is however, the fact that the control of certain processes may be greatly improved if control based on the derivative of a property is included.

To test this hypothesis requires the use of an electronic circuit which differentiates a signal. Such a circuit has been found to exist. It is however, of little practical use since it is a perfect differentiator and will give an output which is the real derivative of the input. In using an analogue computer the signals are not pure, they have a certain amount of noise associated with them. The true differentiator differentiates the noise as well as the signal and the result is erroneous. Furthermore, one special class of signals, the step change, has an infinite value for its derivatives. Thus this important class of signals could not be used with the true differentiator.

Two circuits which approximate to differentiators have been used and are shown FIG 16. The first of these, FIG 16A, has been studied both theoretically and using the analogue computer to demonstrate the order of magnitude of the errors involved.

For the demonstration the sine wave was found to be a useful function.

1. It is a continuous finite bounded function.

2. The gain of the differentiator appeared to be unity.
3. The approximation had a small phase lag compared with the real derivative.
4. The final steady error was a sinusoid of small amplitude.

The transfer function of the approximation circuit is:

$$X_{(s)} = \frac{as\,I_{(s)}}{(s + a)} \qquad 5.1$$

The transform of the sine wave is:

$$\mathcal{L}\,\sin(\omega t) = \frac{\omega}{s^2 + \omega^2} \qquad 5.2$$

Therefore, the output of the approximation is:

$$Y_{(s)} = \frac{a\omega s}{(a + s)(s^2 + \omega^2)} \qquad 5.3$$

or

$$Y_{(t)} = \omega\left(\frac{\cos\left(\omega t - \tan^{-1}\left(\frac{\omega}{a}\right)\right) - e^{-at}}{\left(1 + \left(\frac{\omega}{a}\right)^2\right)^{1/2}}\right) \qquad 5.4$$

Comparing this with the true derivative of

$$Y_{(t)} = \omega\cos\omega t \qquad 5.5$$

shows:

1. The initial exponential in the term e^{-at}
2. The gain of $1/\left(1 + \left(\frac{\omega}{a}\right)^2\right)^{1/2}$ which is close to 1 if $\left(\frac{\omega}{a}\right)$ is small.
3. The phase lag in the term $\tan^{-1}\left(\frac{\omega}{a}\right)$ which is small if $\left(\frac{\omega}{a}\right)$ is small.
4. The final steady state sinusoid produced by the difference between the two signals.

The experimental results were obtained for $\omega = 1$ and $a = 10$ thus:

$$\left(\frac{\omega}{a}\right) = .1 \tag{5.6}$$

Under these conditions the maximum value in the final steady sinusoid was of the order of 0.1 per cent of the original signal and therefore, of the same order as the errors inherent in the apparatus.

5.3 Feed Forward Control.

One of the possible uses of a dynamic model is for the construction of a feed forward controller. The advantage of the feed forward control is that in theory it is possible to control a system using it, so that the output did not vary from its set-point whatever happened to the input. This is of course, absolute control.

There are two conditions necessary for the construction of a working absolute controller.

1. A model which is completely accurate.
2. All input variables must be identified and measured continuously.

In practice neither can be obtained. Also, in the practical use of feed forward control, the system would contain dynamic delays. The feed forward controller needed to nullify the effect of these delays would have to contain a differentiator. The difficulties in this area have been discussed in section 5.2. Attempts to construct feed forward controllers have still been successful.

Feed forward control on its own is of little use except when the above conditions are met. Where approximations have to be made, whether in the model or in the controller's circuits, it must be in addition to feed-back control. The implimentation can be made in two ways:

1. The addition of the feed forward and feed back signals.

2. The variation of the feed-back set point by the feed forward unit.

There appears to be little difference between these two methods.

5.4 Optimal Trajectories.

Apart from the use of optimal theory to find the optimal steady state of a plant, there is the further consideration of optimal start-up and shut-down. Start-up and shut-down is important in plants where catalyst deterioration takes place, and frequent changes of catalyst are necessary. The model required for an analysis of this kind must be:

1. Dynamic
2. Accurate over the start-up range.

For this purpose the linearised model is not sufficient because of its limited range of accuracy. A model obtained by frequency response analysis, where the amplitude of the test signal covered the start-up range, would be better. In the case of the example model reactor there is one possible point which could cause an error. A simplifying assumption of constant density with respect to temperature was made. If this model were to be used for the purpose of obtaining optimal trajectories across large ranges of temperature it may be necessary to relax this assumption.

The classical method of finding these trajectories, using the Calculus of Variation, from which is derived the Euler-Lagrange equation, gives the answer for very simple processes. Unfortunately, this method involves the well known two-point boundary value problem. The following three methods of overcoming the two-point boundary value problem have been highlighted in recent years:

1. The gradient methods introduced almost simultaneously by Kelly and Bryson.
2. Pontryagin's Maximum Principle.
3. Bellman's Dynamic Programming.

The gradient methods use the well known Method of Steepest Descent, and as usual no account is taken of the possible differences between two stationary points on the hypersurface of a performance index. This inability can lead to spurious results.

Pontryagin's Maximum Principle is the most powerful of the techniques. It will handle both linear and non-linear systems. Also the method enables some knowledge of the optimum to be found without solving all the mathematics involved. Perhaps however, most of its advantages are lost in its complexity.

Dynamic Programming can be shown to be related to the Maximum Principle using Calculus of Variation. It has been the subject of mounting interest, having been used successfully a number of times. It suffers one disadvantage, it can only handle linear systems.

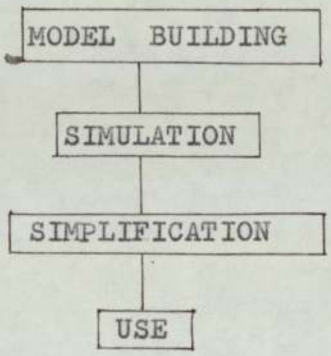
CHAPTER SIX

Conclusions.

Only one conclusion can be drawn from the results:-

> A systematic approach to the generation of a simplified model has been developed. The available techniques of each stage in the system have been discussed. By use of a single example, the systematic approach has been used successfully to generate a simplified model of an item of process plant.

The Systematic Approach To Model Simplification.



Each of the first three stages of the systematic approach has within it a series of techniques. Each will have its own merits in a given situation.

It is not suggested that every process plant item, if handled in the same way as the example given, would give the best results. What is intended is that the systematic approach should be followed using the most applicable technique at each stage. By this method all plant items could be studied and simplified models obtained. With models simplified to the level of the example given it would be possible to simulate simultaneously more than one process plant item even with the apparatus limitations discussed.

It may now be noted that we are at the second stage in the systematic approach. The fourth box (i.e. USE) in fact, has become another complete cycle of the systematic approach. The power of the technique of continuously cycling through the systematic approach is that it can lead to unlimited simplification. Whereas the initial model of the example reactor was impossible to simulate on the available equipment a single cycle of the systematic approach rendered it a reasonable proposition. Extrapolating to a complete chemical plant, a few such cycles would turn this very large and complex model into one of reasonable size, and one which could be simulated with the limited equipment available.

BIBLIOGRAPHY.

This thesis is basically the application of other fields of technology to Chemical Engineering problems. It will be noticeable therefore, that the literature cited is mainly from standard texts in these other fields of technology. These texts not only cover individual points relevant to the argument presented here, but also the more general principles of the applicable theory. Because of this pointed references are not made within the text but will be discussed here.

CHAPTER TWO.

This chapter is the application of mathematics to Chemical Engineering. Applications of this sort are well known to the Chemical Engineer. The following two references are to general texts which lay out the general mathematical principles as well as the philosophics behind the theory.

1. "Mathematical Modelling in Chemical Engineering."
   R.G.E.FRANKS WILEY 1966.
2. "Mathematics for Chemical Engineers."
   V.G.JENSON and G.V.JEFFREYS. Interscience.

CHAPTER THREE.

In the description of the apparatus (Section 3.2) it was stated that the best description could be obtained from the Manufacturers handbooks.

The oscilloscope was supplied with its handbook published by the manufacturer namely Solartron Ltd. The Hybrid computer together with its peripherals was supplied by Electronic Associates Ltd., who also supplied the following handbooks:

"TR - 48 Hybrid Computer Handbook."

"1100 Series Variplotter Handbook."

"R33 Teleprinter Handbook."

In section 3.4 reference is made to Davies paper:

"Simulation of a simple tubular heat Exchanger"

W.D.T. Davies PR. Cont. and Auto. Vol. 13 No.8. Aug. 1966.

and also the use of 'pseudo-laplace' transforms:

"Dynamic Response of a Heat Exchanger to flow rate changes."

F.J.Stermole and M.A.Larson. I. & E.C. Vol.2. p.62. 1963.

For a more general set of papers showing how simulation can and has been used a collection has been published:

"Simulation", edited by J.Mcleod.

McGraw Hill. 1966.

CHAPTER FOUR.

The control theory presented here can be found in most control texts. One familiar to Chemical Engineers is:

P. Harriot

"Process Control". McGraw Hill.

Another important work is by the originator of the Root locus technique Walter G. Evens:

Walter G. Evens

"Control - Systems Dynamics". McGraw Hill.

The methods discussed in section 4.4 can be found in:

Cowley P.E.A. ASME Trans. 79 4 pp 823-832.

CHAPTER FIVE.

Three papers on feed forward control show its usefulness. Firstly on an industrial scale:

McMullein E.C. and Shinsky F.G.

Control Eng. 11 3 p.69

And for a theoretical background:

Tierney J.W, et al.

Control Eng. 4 pp 166 - 75 Sept. 1967.

Harris J.T., Schechter R.S. 18FC Process D9D

2 3 245 July 1963.

Finally the major works in the field of Optimisation theory.

1. Kelly H.J. AM Rocket Society Journal
   30 10 Oct. 1960.

2. Bryson A.E. et al Journal of Aerospace Sciences.
   29 April 1962.

3. Pontryagin L.S. et al Interscience
   "Mathematical Theory of Optimal Processes"

4. Bellman R.F. Princeton University Press.
   "Dynamic Programming."

LIST OF TABLES.

LIST OF FIGURES.

NOMENCLATURE.

$A, \hat{A}$	Arbitrary constant.
A	Area. Unsuffixed cross sectional areas of reactor Suffixed other surface areas.
a	Surface area /unit length
B	Arbitrary Constant
b	Mass flow rate (molar)
C	Arbitrary constant
c	Specific Heat (molar)
$\mathcal{E}$	Voidage
E	Internal Energy.
f	Function
ΔH	Enthalpy of reaction.
k	Reaction rate constants
m	Arbitrary number of moles
q	Quantity of heat per unit time
(rate)	Rate of reaction
R	Gas constant
t	Time
T	Absolute temperature
U	Heat transfer coefficient
V	Volume
W	Arbitrary variable
ω	Frequency
X	Arbitrary variable
x	Concentration (mole fraction)

Y	Arbitrary Variable
θ	Temperature °C
ρ	Density (molar)

Suffixes

IN	Input
OUT	Output
A	Reactant (usually Isopropanol)
B	Product (usually Acetone)
C	Product (usually Hydrogen)
o	Datum value and for $t = 0$
s	Catalyst
c	Tube wall
F	Forward
R	Reverse
1, 2, etc.	Stage number.

Prefix

Δ	Incremental part.

APPENDIX 1

The Theoretical Model of the Tubular Reactor.

Consider mass balances over a time δt on an increment δl of reactor length (FIG 18) for:

1. Total mass.
2. Individual components.

and for the reaction

$$A \rightleftharpoons B + C \qquad \text{A1.1}$$

Total moles in = $b\,\delta t$

Total moles out = $(b + \delta b)\delta t$

Accumulation = $A\varepsilon\,\delta\rho\,\delta l$

Reaction = $\rho\,\delta l\,A\varepsilon\,(\text{rate})\,\delta t$

The mass balance is:

In - Out = Accumulation – Reaction A1.2

Hence

$$b\delta t - (b + \delta b)\delta t = A\varepsilon\,\delta\rho\,\delta l - A\varepsilon\rho\,\delta l\,\delta t\,(\text{rate}) \qquad \text{A1.3}$$

or

$$\frac{\delta b}{\delta l} = A\varepsilon\,\frac{\delta\rho}{\delta t} - A\varepsilon\rho\,(\text{rate}) \qquad \text{A1. 4}$$

In the limit

$$\frac{\partial b}{\partial l} = A\varepsilon\left(\rho(\text{rate}) - \frac{\partial\rho}{\partial t}\right) \qquad \text{A1. 5}$$

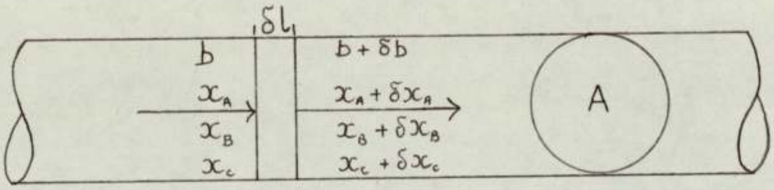


FIGURE 18 The Tubular Reactor

Moles of A in = $b\,x_A\,\delta t$

Moles of A out = $(b + \delta b)(x_A + \delta x_A)\delta t$

Accumulation = $A\varepsilon\,\delta L\,\delta(\rho x_A)$

Reacted = $-A\varepsilon\rho\,\delta L\,\delta t\,(\text{rate})$

Hence, as above:

$$b\,x_A\,\delta t \quad - \quad (b + \delta b)(x_A + \delta x_A)\delta t$$

$$= \quad A\varepsilon\,\delta L\,\delta(\rho x_A) \;+\; A\varepsilon\rho\,\delta L\,\delta t\,(\text{rate}) \qquad \text{A1.6}$$

or

$$-x_A\frac{\delta b}{\delta L} - b\frac{\delta x_A}{\delta L} - \frac{\delta b\,\delta x_A}{\delta L} = A\varepsilon\frac{\delta(\rho x_A)}{\delta t} + A\varepsilon\rho(\text{rate}) \qquad \text{A1.7}$$

In the limit

$$\frac{\partial x_A}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial x_A}{\partial L} = -(\text{rate}) - x_A\left(\frac{1}{A\varepsilon\rho}\frac{\partial b}{\partial L} + \frac{1}{\rho}\frac{\partial\rho}{\partial t}\right) \qquad \text{A1.8}$$

$$\text{i.e.}\quad \frac{\partial x_A}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial x_A}{\partial L} = -(1 + x_A)(\text{rate}) \qquad \text{A1.9}$$

Similar equations have been obtained for components B and C by reversing the sign of the 'reacted' term indicating that the component is formed by the reaction and not destroyed.

Hence

$$\frac{\partial x_B}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial x_B}{\partial l} = (1 - x_B)(rate) \qquad A1.10$$

and

$$\frac{\partial x_c}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial x_c}{\partial l} = (1 - x_c)(rate) \qquad A1.11$$

Also, for an inent the 'reacted' term is not present and hence:

$$\frac{\partial x_I}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial x_I}{\partial l} = - x_I(rate) \qquad A1.12$$

Summation of these expressions gives:

$$x_A + x_B + x_c + x_I = 1 \qquad A1.13$$

which must be true by the definition of mole fraction, and serves as a check on the above working.

Consider also a heat balance over the increment on the reaction stream:

Heat in = $bc\theta$

Heat out = $(b + \delta b)(c + \delta c)(\theta + \delta\theta)$

Accumulation = $\frac{\partial}{\partial t}(\delta l\, \varepsilon A \rho c \theta)$

Due to Reaction = $\varepsilon A \rho\, \delta l\, (rate) \Delta H$

In from Wall = $U_\omega a_\omega (\theta_c - \theta)\delta l$

Out to catalyst = $U_s a_s (\theta - \theta_s)\delta l$

Hence

$$-bc\,\delta\theta \; - \; c\theta\,\delta b \; - \; b\theta\,\delta c$$

$$+\,\delta l\left(U_\omega a_\omega\left(\theta_c - \theta\right) + U_s a_s\left(\theta - \theta_s\right)\right)$$

$$= \delta l\, A\varepsilon\, \frac{\partial(c\rho\,\theta)}{\partial t} \; + \; \delta l\, A\varepsilon\rho\, \Delta H\,(\text{rate} \qquad \text{A1.14}$$

Let

$$q_\omega a_\omega \;=\; U_\omega a_\omega\left(\theta_c - \theta\right) \qquad \text{A1.15}$$

$$q_s\, a_s \;=\; U_s\, a_s\left(\theta - \theta_s\right) \qquad \text{A1.16}$$

Then in the limit:

$$\frac{q_\omega a_\omega + q_s a_s}{A\varepsilon\rho} = \frac{b}{A\varepsilon\rho}\,\frac{\partial(\theta c)}{\partial l} + \frac{\partial(\theta c)}{\partial t}$$

$$+\;\theta c\left(\frac{1}{\rho}\frac{\partial\rho}{\partial t} + \frac{1}{A\varepsilon\rho}\frac{\partial b}{\partial l}\right) + \Delta H\,(\text{rate}) \qquad \text{A1.17}$$

Since $$\Delta H \;=\; \Delta H_o + \left(c_B + c_C - c_A\right)\left(\theta - \theta_o\right) \qquad \text{A1.18}$$

Then

$$\left(c_A x_A + c_B x_B + c_C x_C\right)\left(\frac{\partial\theta}{\partial t} + \frac{b}{A\varepsilon\rho}\frac{\partial\theta}{\partial l}\right) = \frac{q_\omega a_\omega + q_s a_s}{A\varepsilon\rho}$$

$$+\;(\text{rate})\left(\Delta H_o + \left(c_B + c_C - c_A\right)\left(2\theta - \theta_o\right)\right) \qquad \text{A1.19}$$

Also considering a heat balance on the catalyst:

Heat from gas to catalyst = $U_s a_s (\theta - \theta_s) \delta l \, \delta t$

Heat increase within catalyst = $\rho_s c_s (1 - \varepsilon) A \, \delta l \, \delta t$

Hence

$$\frac{\delta \theta_s}{\delta t} = \frac{U_s a_s}{\rho_s c_s (1-\varepsilon) A} (\theta - \theta_s) \qquad A1.20$$

APPENDIX II

The Stirred Tank Reactor Model.

To obtain the Mathematical model both heat and mass balances must be considered. In deriving these balances, an approximating assumption that there is no accumulation due to expansion of gas is made. This is in fact the equivalent of stating constant molar density.

For the overall mass balance:

Moles in = $b_{IN}\,\delta t$

Moles out = $b_{OUT}\,\delta t$

Change due to reaction = $V\rho\,(rate)\,\delta t$

Therefore $$b_{OUT} = b_{IN} + V\rho\,(rate) \qquad A2.1$$

For the individual component balances:

Moles in = $b_{IN}\,x_{AIN}\,\delta t$

Moles out = $b_{OUT}\,x_{A}\,\delta t$

Change due to reaction = $V\rho\,(rate)\,\delta t$

Accumulation = $V\rho\,\delta x_{A}$

Therefore for a component destroyed by the reaction:

$$b_{IN}\,x_{AIN} - b_{OUT}\,x_{A} = V\rho\,(rate) + V\rho\,\frac{dx_{A}}{dt} \qquad A2.2$$

or

$$\frac{dx_{A}}{dt} = -(1 + x_{A})(rate) + \frac{b_{IN}}{V\rho}\,(x_{AIN} - x_{A}) \qquad A2.3$$

and for a component made in the reaction:

$$\frac{dx_B}{dt} = (1 - x_B)(rate) + \frac{b_{IN}}{V\rho}(x_{BIN} - x_B) \qquad A2.4$$

For a heat balance on the reaction stream:

Heat in $= b_{IN}\, c_{IN}\, \theta_{IN}$

Heat out $= b_{OUT}\, c\ \theta$

Accumulation $= \dfrac{d(V\rho c \theta)}{dt}$

Due to the reaction $= V\rho\,(rate)\,\Delta H$

In from heated surface $= q_\omega A_\omega$

Out to catalyst $= q_s A_s$

Hence

$$b_{IN}\, c_{IN}\, \theta_{IN} - b_{OUT}\, c\, \theta + q_\omega A_\omega + q_s A_s$$

$$= V\rho \frac{d(\theta c)}{dt} + (rate)\, V\rho\, \Delta H \qquad A2.5$$

Using the identities:

$$c = c_A x_A + c_B x_B + c_C x_C \qquad A2.6$$

$$\Delta H = \Delta H_o + (c_B + c_C - c_A)(\theta - \theta_o) \qquad A2.7$$

and substituting individual component and overall mass balances gives:

$$\frac{d\theta}{dt} = \frac{q_{\omega} A_{\omega} + q_s A_s}{V\rho c} + \frac{b_{IN}}{V\rho}(\theta_{IN} - \theta)$$

$$- \frac{(\text{rate})}{c}\left(\Delta H_0 + (c_B + c_C - c_A)(2\theta - \theta_0)\right) \qquad A2.8$$

For a heat balance on the catalyst

Heat from gas to catalyst = $U_s A_s (\theta - \theta_s) \delta t$

Heat increase within catalyst = $\rho_s c_s (1 - \varepsilon) V \delta\theta_s$

Hence

$$\frac{d\theta_s}{dt} = \frac{U_s A_s}{\rho_s c_s (1 - \varepsilon) V}(\theta - \theta_s) \qquad A2.9$$

APPENDIX III

The following table is the collection of the results obtained from the analysis described in Section 2.6.

Results for a Single Stirred Tank Reactor.

Length of Tubular reactor of equivalent Volume Δl_1 cms	x_A mole fraction	x_B mole fraction	$\frac{\theta}{500}$	b moles/sec
40	.7080	.0880	.6186	.1088
60	.6412	.1276	.6242	.1130
80	.5926	.1560	.6280	.1167
100	.5506	.1826	.6320	.1200
120	.5094	.2046	.6350	.1229
140	.4780	.2230	.6380	.1255
160	.4490	.2394	.6410	.1280

Results for Two Stirred Tank Reactors in Series.

Length Equivalent of First Stage Δl_1	Length Equivalent of Second Stage Δl_2	x_A	x_B	$\frac{\theta}{500}$	$b^{(1)}$
160	40	.3816	.2858	.6486	
	60	.3526	.3032	.6516	
	80	.3306	.3155	.6540	
	100	.3102	.3182	.6564	
	120	.2924	.3378	.6586	
	140	.2788	.3462	.6608	.1449
	160	.2646	.3542	.6628	.1463
140	40	.4044	.2634	.6462	
	60	.3736	.2822	.6496	
	80	.3562	.2964	.6520	
	100	.3282	.3086	.6544	
	120	.3082	.3202	.6566	.1416
	140	.2928	.3298	.6588	
	160	.2780	.3380	.6610	

(1) Values of b are calculated at points to be used for estimating third and fourth stages only.

Δl_1	Δl_2	x_A	x_B	$\frac{\theta}{500}$	b
120	40	.4314	.2476	.6444	
	60	.3988	.2676	.6482	
	80	.3740	.2822	.6506	.1349
	100	.3488	.2966	.6530	.1368
	140	.3286	.3084	.6554	
	160	.3112	.3184	.6572	
100	40	.4632	.2304	.6414	
	60	.4276	.2522	.6452	
	80	.4001	.2682	.6480	.1328
	100	.3750	.2830	.6506	.1352
	120	.3518	.2964	.6530	
	140	.3330	.3078	.6548	
	160	.3132	.3190	.6570	
80	40	.4960	.2094	.6382	
	60	.4550	.2340	.6422	.1269
	80	.4266	.2512	.6452	
	100	.3990	.2676	.6482	.1327
	120	.3740	.2820	.6506	
	140	.3538	.2940	.6528	
	160	.3328	.3062	.6550	

Δl_1	Δl_2	x_A	x_B	$\frac{\theta}{500}$	b
60	40	.5338	.1872	.6354	.1209
	60	.4894	.2142	.6394	
	80	.4560	.2338	.6426	
	100	.4260	.2518	.6456	
	120	.4000	.2672	.6484	
	140	.3770	.2800	.6506	
	160	.3550	.2934	.6530	
40	40	.5870	.1558	.6316	
	60	.5360	.1864	.6356	.1144
	80	.4990	.2080	.6390	
	100	.4652	.2286	.6422	
	120	.4358	.2460	.6452	
	140	.4120	.2602	.6478	
	160	.3870	.2736	.6504	

Results for Three Stirred Tank Reactors in Series.

Δl_1 = 160 cms , Δl_2 = 160 cms

Δl_3	x_A	x_B	$\frac{\theta}{500}$
60	.2182	.3782	.6678
80	.2084	.3840	.6696
100	.1990	.3896	.6710
120	.1910	.3936	.6712
140	.1832	.3984	.6738
160	.1762	.4020	.6750

Δl_1 = 160 cms. , Δl_2 = 140 cms.

60	.2296	.3730	.6680
80	.2186	.3790	.6698
100	.2080	.3852	.6716
120	.1978	.3910	.6732
140	.1914	.3950	.6742
160	.1836	.4000	.6758

Δl_1 = 140 cms. , Δl_2 = 120 cms

Δl_3	x_A	x_B	$\frac{\theta}{500}$
60	.2508	.3520	.6644
80	.2384	.3596	.6666
100	.2266	.3666	.6684
120	.2156	.3730	.6702
140	.2068	.3780	.6714
160	.1976	.3834	.6730

Δl_1 = 120 cms. , Δl_2 = 100 cms.

60	.2804	.3348	.6612
80	.2650	.3440	.6634
100	.2510	.3522	.6652
120	.2386	.3592	.6672
140	.2280	.3656	.6688
160	.2170	.3716	.6704

Δl_1 = 120 cms. , Δl_2 = 80 cms.

Δl_3	x_A	x_B	$\frac{\theta}{500}$	
60	.2974	.3236	.6568	
70	.2906	.3276	.6576	(b = .1430)
80	.2818	.3330	.6590	(b = .1431)
100	.2670	.3420	.6614	
120	.2548	.3482	.6634	
140	.2438	.3538	.6654	
160	.2324	.3596	.6660	

Δl_1 = 100 cms. , Δl_2 = 80 cms.

60	.3180	.3140	.6564	
80	.2994	.3250	.6586	
100	.2820	.3354	.6606	
120	.2670	.3440	.6626	
140	.2550	.3516	.6644	
160	.2426	.3584	.6666	
70	.3070	.3180	.6574	(b = .1417)

Δl_1 = 80 cms , Δl_2 = 100 cms

Δl_3	x_A	x_B	$\frac{\theta}{500}$	
60	.3170	.3126	.6552	(b =.1406)
80	.2990	.3236	.6572	
100	.2824	.3330	.6594	
120	.2690	.3412	.6614	
140	.2560	.3484	.6634	
160	.2452	.3550	.6658	

Results for Four Stirred Tank Reactors in Series.

$\Delta l_1 = 120$ cms. , $\Delta l_2 = 80$ cms. , $\Delta l_3 = 80$ cms

Δl_4	x_A	x_B	$\frac{\theta}{500}$
40	.2818	.3330	.6590
60	.2320	.3616	.6680
80	.2210	.3668	.6692
100	.2098	.3738	.6706
120	.2000	.3792	.6736
140	.1938	.3846	.6742
160	.1838	.3892	.6758

$\Delta l_1 = 120$ cms. , $\Delta l_2 = 80$ cms. , $\Delta l_3 = 70$ cms.

60	.2374	.3548	.6644
80	.2256	.3604	.6662
100	.2142	.3686	.6678
120	.2042	.3746	.6692
140	.1960	.3798	.6700
160	.1880	.3854	.6720

$\Delta l_1 = 100$ cms , $\Delta l_2 = 80$ cms , $\Delta l_3 = 70$ cms

Δl_4	x_A	x_B	$\frac{\theta}{500}$
60	.2480	.3490	.6624
80	.2358	.3562	.6640
100	.2238	.3644	.6662
120	.2152	.3706	.6672
140	.2070	.3774	.6698
160	.1984	.3824	.6706

$\Delta l_1 = 80$ cms , $\Delta l_2 = 100$ cms , $\Delta l_3 = 60$ cms

60	.2560	.3446	.6608
80	.2428	.3542	.6630
100	.2300	.3612	.6652
120	.2200	.3690	.6678
140	.2110	.3730	.6680
160	.2020	.3798	.6694

Results for the Two Special Cases.

$\Delta l_1 = 40$ cms

x_A	x_B	$\frac{\theta}{500}$	b
.7080	.0880	.6186	.1088
$\Delta l_1 = 40$ cms , $\Delta l_2 = 60$ cms			
.5360	.1864	.6356	.1144
$\Delta l_1 = 40$ cms , $\Delta l_2 = 60$ cms , $\Delta l_3 = 100$ cms			
.3658	.2852	.6532	.1281
$\Delta l_1 = 40$ cms , $\Delta l_2 = 60$ cms , $\Delta l_3 = 100$ cms , $\Delta l_4 = 200$ cms			
.2092	.3776	.6720	
$\Delta l_1 = 100$ cms , $\Delta l_2 = 100$ cms , $\Delta l_3 = 100$ cms			
.2700	.3430	.6620	.1458
$\Delta l_1 = 100$ cms , $\Delta l_2 = 100$ cms , $\Delta l_3 = 100$ cms , $\Delta l_4 = 100$ cms			
.2030	.3814	.6716	

The following table shows the results of a run on the digital program given in Appendix 4. The run was made as the base case for the study in Section 2.6

Reactor lengths Δl. cms	x_A mole fraction	x_B mole fraction	θ °C
0	.8667	.0000	300.0
20	.7788	.0470	307.6
40	.6988	.0899	311.8
60	.6287	.1274	314.7
80	.5678	.1601	817.1
100	.5145	.1886	319.1
120	.4678	.2136	320.0
140	.4265	.2357	322.7
160	.3899	.2553	324.3
180	.3572	.2728	325.7
200	.3279	.2885	327.1

Δl	x_A	x_B	θ °C
220	.3016	.3026	328.5
240	.2778	.3154	329.7
260	.2562	.3269	330.9
280	.2367	.3374	331.9
300	.2188	.3470	333.0
320	.2026	.3557	334.0
340	.1877	.3637	334.9
360	.1741	.3710	335.8
380	.1616	.3777	336.6
400	.1501	.3838	337.4
420	.1395	.3895	338.1
440	.1298	.3947	338.8
460	.1208	.3995	339.5
480	.1125	.4039	340.1
500	.1048	.4080	340.7

APPENDIX IV

Comparison of Steady State Theory with Practical Results.

The computer program given here was written to simulate steady state conditions for the reactor at different flow rates and temperature conditions. This was done to compare the accuracy of the model with results obtained by The Science Research Council's Warren Springs Laboratories. FIG.5 shows the comparison of the computer results with those obtained by The Science Research Council.

The following sequence of instructions is the program written for the department's P.D.S. 1020 computer.

```
 INP
C003 -
1031 +
L002 -
A017 -
C028 -
L017 -
D028 -
D018 -
C008 -
M019 -
M001 -
M001 -
C029 -
L021 -
D022 -
D028 -
 EXP
C030 -
L020 -
D030 -
M000 -
S029 -
C009 -
```

L003 -

D012 -

D008 -

C010 -

L009 -

D010 -

C011 -

L016 -

S000 -

M011 -

M014 -

A000 -

C004 -

L015 -

S001 -

M011 -

M014 -

A001 -

C005 -

L027 -

M002 -

A026 -

M011 -

D024 -

S029 -

M014 -

```
A002 -
C006 -
L012 -
M008 -
M009 -
A003 -
C007 -
L004 -
C000 -
L005 -
C001 -
L006 -
C002 -
L007 -
C003 -
1000 +
C/R 000
L000 -
TYPE
L001 -
TYPE
L002 -
TYPE
L003 -
TYPE
JMP 003
RET
```

The following sequence is used to load the initial values of variable into the P.D.S. 1020.

```
INP         .8333
C000 -
INP         .0000
C001 -
INP         300
C002 -
INP         18.6
C012 -
INP         1.0
C014 -
C015 -
INP         -1.0
C016 -
INP         273
C017 -
INP         22400
C018 -
INP         2460
C019 -
INP         82500
C020 -
INP         13300
C021 -
INP         1.987
```

```
C022 -

INP          .8

C023 -

INP          45

C024 -

INP          310

C025 -

INP          13000

C026 -

INP          10

C027 -

INP          40

C031 -
```

The following table gives the results obtained from the runs on the computer for different temperatures.

Reactor Temperature = 300 °C

$\frac{\text{gm of catalyst - hr}}{\text{moles of iso-propanol feed}}$	x_A	x_B	fractional conversion.
7.15	.5277	.1666	.24
14.3	.3742	.2504	.40
21.45	.2807	.3014	.52
28.6	.2188	.3350	.60
35.8	.1757	.3587	.67
43	.1445	.3756	.72
50.1	.1215	.3882	.76
57.3	.1041	.3977	.74
64.5	.0909	.4049	.81
71.5	.0807	.4105	.83
78.6	.0728	.4148	.85
85.7	.0606	.4181	.86
93	.0618	.4208	.87

Reactor Temperature = 350 °C

$\frac{\text{gm. of catalyst - hr}}{\text{moles of iso-propanol feed}}$	x_A	x_B	fractional conversion
7.15	.4408	.2140	.33
14.3	.2779	.3029	.52
21.45	.1879	.3520	.65
28.6	.1326	.3821	.74
35.8	.0965	.4018	.81
43	.0721	.4152	.85

Reactor Temperature = 400 °C

7.15	.2813	.3010	.52
14.3	.1327	.3821	.74
21.45	.0688	.4169	.83
28.6	.0379	.4338	.92
35.8	.0222	.4424	.95
43	.0140	.4469	.97
50.1	.0096	.4492	.98
57.3	.0073	.4505	.98