DYNAMICS OF A CONTINUOUS STIRRED TANK REACTOR FOR DIFFERENT REACTION ORDERS

by

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A Thesis submitted to the University of Aston in Birmingham for the degree of Doctor of Philosophy.

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June 1980

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SUMMARY

The work studies the effect of reaction order on the dynamic behaviour of a jacketted stirred tank reactor under the action of controllers, and hence develops control schemes which improve the performance.

Initially theoretical work determined system stability and behaviour mainly for planning the experiments. Reaction orders 2,1,0 and -1 were studied on the system for various control schemes and disturbances.

The experimental work involved a partial simulation technique in which the mass balance of an exothermic chemical reaction was simulated by a digital computer. The computer calculated the heat generation depending on the reaction order and other operating and reaction rate parameters. Appropriate signals applied to the immersion heaters provided in the vessel liberated the corresponding heat. The cooling water flowrate was the manipulative variable and its setting calculated by the computer for the control scheme chosen.

The transient response of the system for each experimental run was plotted and compared with the corresponding total simulation result. For this comparison the complete plant was simulated by a set of differential equations and samplers.

Invariance of tank temperature and concentration for load disturbances was achieved by a control strategy derived from the state equations. This strategy was an improvement on feedback control.

Decoupling of tank temperature from the other two state variables was achieved by a control scheme involving an iterative procedure for the calculation of coolant flowrate.

The open loop unstable operating point was stabilised by proportional feedback control. The limit-cycle at the open loop stable and unstable points was generated by a feedback control scheme. Conditions for the existence of a limit-cycle were established by the second method of Liapunov and the harmonic contents of these nonlinear oscillations determined. The effect of oscillations was determined by comparing the time average conversion with the steady-state peformance.

Key Words: Partial-Simulation; Stability; Invariance; Decoupling; Limit-Cycle

ACKNOWLEDGEMENTS

In recognition of the help and advice received the author wishes to extend his sincere gratitude to:

Mr. A.R. Cooper of the Department of Chemical Engineering, for his valuable help, moral support and supervision and his patient review of the manuscript.

Dr. B. Gay of the Department of Chemical Engineering, for his advice and help on computing.

The Commonwealth Scholarship Commission in the United Kingdom for provision of the scholarship.

Mr. D. Bleby for his assistance with electrical and electronic problems.

DEDICATED TO MY FAMILY

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NOMENCLATURE

A	Liapunov matrix
A_{ij}	elements of matrix A
B	positive definite symmetric matrix
C	Concentration of reactants (kg/m^3)
C_p	specific heat of feed (kJ/kg K)
D, D_1, D_2, D_3	exponential decay constant (s)
D_{max}	maximum value of D (s)
D_s	digital signal
E	activation energy (kJ/kg mole)
F	feed flowrate (m^3/s)
H	Heat (J/s)
I	unit matrix
IAE	integral of absolute error
J	Jacobian matrix
J_{ij}	elements of matrix J
K	multiplication factor
K_1	$= k_o C_o^{n-1}$
K_2	$= K_c \times 10^6$
K_3	$= \frac{\bar{F}}{V K_1 \alpha_{SS}^n} + e^{-Q/\beta_{SS}}$
K_4	$= k/V$
K_C	proportional gain (m^3/s)
K_L	Liapunov value
Q	$= \frac{E \Delta H C_o}{R \rho C_p}$
Q_1	counter rate
R	Universal gas constant (kJ/kg mole K)

RAS	Region of asymptotic stability
$R(X,Y)$	$= K_1((X+\alpha_{SS})^n e^{\frac{-Q}{(\beta_{SS}+Y)}} - \alpha_{SS}{}^n e^{-\frac{Q}{\beta_{SS}}})$
S	= Laplace transform
$S_1, S_2 \ldots$	inequality constraints for stability
T	tank temperature (K)
T_I	integral time $/K_c (s^2/m^3)$
Tr	Trace of a matrix
T_D	differential time $\times K_c (m^3)$
UA	heat transfer conductance (kJ/s K)
V	reactor volume (m^3)
V_L	Liapunov function
V_S	supply voltage
X	dimensionless perturbation in concentration = $\bar{C}/C_o$
X_o, X_1, X_2	harmonic contents in C during limit-cycling (kg/m^3)
Y	dimensionless perturbation in temperature = $\bar{T}b$
Y_o, Y_1, Y_2	harmonic contents in T during limit-cycling (K)
Z	dimensionless perturbation in jacket temperature = $\bar{T}_c b$
Z_o, Z_1, Z_2	harmonic contents in T_c during limit-cyling (K)
a_i	constants of polynomial
b	$= \frac{\rho Cp}{\Delta H C_o}$ (K^{-1})

$f(x)$	system of equations
k	Arrehnius type reaction rate constant $= k_o e^{-E/RT}$
k_o	frequency factor
n	reaction order
sf	stable focus
sn	stable node
t	time (s)
uf	unstable focus
un	unstable node
α	trigger angle
α_1	$= (\pi-\alpha)$
α_{ss}	dimensionless steady-state concentration $= C_{ss}/C_o$
β_{ss}	dimensionless steady-state temperature $= T_{ss}b$
β_{oss}	dimensionless steady-state feed temperature $= T_{oss}b$
β_o	dimensionless perturbation in feed temperature $= \bar{T}_o b$
γ_{ss}	dimensionless steady-state jacket temperature $= T_{c\,ss}b$
γ_{oss}	dimensionless steady-state coolant temperature $= T_{coss}b$
γ_o	dimensionless perturbation in coolant temperature $= \bar{T}_{co}b$

$\lambda_1, \lambda_2, \lambda_3$	eigenvalues of matrix J
ρ	density of feed (kg/m^3)
ΔH	heat of exothermic reaction (kJ/kg)
τ	residence time in the tank = V/F (s)
τ_c	residence time in the jacket = V_c/F_c (s)
τ_1	$= 1/_{\tau} + 1/_{\tau_o}$ (s^{-1})
τ_2	$= 1/_{\tau_c} + 1/_{\tau_I}$ (s^{-1})
τ_3	$= 1/_{\tau_o} + 1/_{\tau_I}$ (s^{-1})
$1/_{\tau_o}$	$= \frac{UA}{V\rho C_p}$ (s)
$1/_{\tau_I}$	$= \frac{UA}{V_c \rho_c C_{pc}}$ (s)
τ_m	Time constant of measuring element (s)
τ_s	Sampling time (s)
τ_v	Time constant of control valve (s)
w	angular velocity (radians/ s)
ϕ_i	load disturbance
$\| \|$	modulus of or determinant of a matrix

Subscripts

SS	steady-state
Cal	calculated
act	actual
S	open loop stable point
U	open loop unstable point
O	inlet condition
c	pertaining to coolant stream

m	values output from measuring elements
UL	upper limit on flowrate

Combinations of these subscripts are also possible.

Superscripts

*	sampled values
-	perturbation
T	transpose of a matrix
.	differential with respect to time

CHAPTER 1

INTRODUCTION

The study of the effect of reaction order on the dynamics of a continuous stirred tank reactor (C.S.T.R.) is important because a stable system for a particular reaction order can become unstable as the order is changed. This has special relevance when complex homogeneous or heterogeneous rate equations are simplified to yield one reaction order for a certain set of assumptions, but a different one for another set of assumptions. The reaction order is also affected by the operating conditions. For example in solid catalysed reactions the order is different not only for different types of catalyst surface but also for different impurities. In homogeneous liquid phase reactions large excess of one reactant or product during the reaction process can change the order.

A purely theoretical study of the transient behaviour of a C.S.T.R. sometimes deviates too much from practicality while in complete experimentation, practical difficulties reduce the range of study. Hence in the present study, a partial simulation technique which combines both experiment and theory is used. Thus the mass balance of an irreversible exothermic chemical reaction is simulated using a digital computer, and based upon the current rate of reaction, the computer calculates the reaction heat generation and sends the appropriate signal to the immersion heaters situated in the reactor.

Reaction heat is thus released and the actual heat transfer to a surrounding cooling jacket takes place. With water as the reaction as well as the cooling medium various reaction orders can be simulated by the digital computer with little difficulty.

A general theoretical study of the system stability is carried out for all integer reaction orders ranging from -4 to 4. However experiments and complete theoretical work is carried out for reaction orders -1, 0, 1 and 2.

The transient behaviour of the reactor is obtained with and without the action of control on the cooling water flowrate. Theoretical nonlinear stability analyses are carried out by the use of Krasovskii's theorem and the effect of various controller configurations on the region of asymptotic stability (RAS) is determined and also verified experimentally. More importance has been placed on complicated control configurations of the decoupling and invariance type because of their superiority over conventional type controls and because they have not found their way into chemical process control due to lack of proper understanding.

Operation of the reactor system only at a stable operating point or only in a perfectly stabilised mode reduces the scope for changing the system performance. The stabilising of an open loop unstable operating point with the help of simple proportional controllers opens up a new range of operating points. Inducing sustained oscillations at an inherently stable operating point for constant input conditions sometimes helps in improving the system performance to a certain degree. This nonlinear oscillation, known as limit-cycling, is studied for different reaction orders and their fundamental harmonics evaluated.

The effect of inlet conditions, like feed and coolant temperatures and flowrates on the operating points is also theoretically studied in order to take into account the day to day changes in water temperature.

The transient behaviour and analysis of the reactor alone is carried out in Chapter 3, while the effects of lags and delays introduced by measuring elements and valves are considered when total simulation of the complete plant is performed in Chapter 7. The experimental runs are compared with total simulation. Various computer programs for analysis, simulation and control, and experimental work are also developed.

Although SI units are used throughout this report, CGS units are used in the computer programs for theoretical, total simulation and experimental work.

CHAPTER 2

LITERATURE SURVEY

2.1 INTRODUCTION

The aim of the work was to study stable and unstable operation of a C.S.T.R. and to investigate control schemes not hitherto applied to chemical reactor systems.

In order to generate interesting cases of stable and unstable reactor operation, the effect of various parameters including reaction order on the dynamic behaviour of a chemical reactor was sought in the literature. The survey included the effect of operating conditions on the order of a chemical reaction.

The implementation of the open loop and the controlled schemes used established techniques of partial simulation, in which the reaction and mass balances were simulated on a computer and the thermal effects existed in plant items.

The literature survey therefore covered the following areas of interest

(i) The effect of various parameters on the order of chemical reaction.

(ii) Theoretical simulation studies on a C.S.T.R. both with and without control to predict the transient responses and multiple operating points.

(iii) Transient experimental work carried out in a C.S.T.R.

(iv) The partial simulation technique as a tool of study, using either an analogue or a digital computer.

(v) Stability analysis of a C.S.T.R. and calculation of the maximum region of stability.

(vi) Operation of the C.S.T.R. at an unstable equilibrium point, as an alternative to the inherently stable point.

(vii) Decoupling of a multivariable interacting nonlinear system.

(viii) Advantages of the Invariance type control.

(ix) Limit-cycling in a stirred tank reactor and its effect on overall performance.

2.2 EFFECT OF PARAMETERS ON ORDER OF REACTION

The order of a given chemical reaction can change with a number of factors including temperature, presence of impurities, type of catalyst and energy level of products. For a particular set of conditions there will be a complete reaction mechanism involving the order. Some examples of variation of order with conditions are given below[1].

In the following liquid phase reaction

$$2I^- + S_2O_8^{-2} \rightarrow I_2 + 2\ SO_4^{-2}$$

the order is two for high concentrations of iodide ions while it is three for low concentrations.

In the decomposition of ammonia on platinum catalyst the rate equation is given by

$$\frac{-d\{NH_3\}}{dt} = k_1\ \{NH_3\}/\{H_2\}$$

while on iron catalyst it is

$$-\frac{d\{NH_3\}}{dt} = k_2\{NH_3\}\ \{H_2\}^{3/2}$$

The presence of O_2 as an impurity in the formation of hydrogen chloride changes the rate equation from

$$\frac{d\{HCl\}}{dt} = k_2\ \{Cl_2\}\ \{CH_4\}$$

to $$\frac{d\{HCl\}}{dt} = k_1\ \{Cl_2\}^2 / \{O_2\}$$

Sometimes the large excess of one reactant or product during the reaction process can change the order. Thus in the following reaction[2]

$$HCO\ Co\ (CO)_4 + PH_3 \rightarrow HCO\ Co\ (CO)_3\ PH_3 + CO$$

the rate is first order in HCO Co $(CO)_4$ for large concentrations of phosphine while the rate equation becomes

$$k_1\ \{HCO\ Co\ (CO)_4\}\ \frac{\{PH_3\}}{\{CO\}}$$

for small concentrations of it. This type of behaviour is also observed in liquid phase reactions between acylcobalttetra-carbonyls with hydrogen, olefines, dienes or acetylenes.

It is also seen that the pseudo reaction order for complex reactions changes depending upon the type of assumptions made. Thus negative order type reactions are possible, where one of the components inhibits the main reaction. Generally reaction orders never exceed a value of three because of the greater loss of entropy in the activated state and the small probability of collision of three or more molecules at the same time to form the activated complex.

2.3 DYNAMICS OF A C.S.T.R.

2.3.1 Theoretical Study

The theoretical dynamic behaviour of a C.S.T.R. with exothermic reaction has been analysed by many authors. The types of dynamic behaviour possible for a first order reaction are classified according to the system parameters like heat transfer coefficient , activation energy, Dam Köhler number and adiabatic temperature rise by Uppal and Ray[3]. Several kinds of "jump phenomena" like coalescence of limit-cycles with separatrices or merging of two limit-cycles are explained with respect to the parameters. A consecutive first order reaction scheme was analysed by Hlavacek et al[4]. Multiplicity and stability were theoretically analysed in the parametric plane.

A brief communication on the effect of reaction rate on the open loop stability of chemical reactors by the classical approach was presented by Luyben[5]. The importance of assuming the correct mixing effects in a C.S.T.R. was emphasised by Dudukovic[6]. The author concludes that even though micromixing effects are secondary for normal reaction rate equations, they are significant in self inhibited rate expressions which have a maximum rate at some intermediate reaction concentration. Certain micromixing patterns may give rise to unexpected multiple steady-state at intermediate degree of segregation when only a single steady-state is possible at the maximum mixedness condition.

2.3.2 Experimental Work

Though there are some papers available in the literature that deal with the experimental study of continuous stirred tank reactor performance they all deal with the second order exothermic reaction between sodium-thiosulphate and hydrogen peroxide. The studies by Vejtasa et al[7], Chang and Schmitz[8,9] and Schmitz et al[10] covered the following aspects

(i) steady-state and transient behaviour of the system.

(ii) stabilisation of an unstable point by means of feedback control.

(iii) the construction of phase-plane diagrams showing experimental limit-cycles.

(iv) effect of cooling jacket wall thickness on the dynamics.

The hydrolysis of acetyl chloride was studied in a reactor by Baccaro et al[11] mainly to establish the existence of limit-cycles for the particular system.

2.3.3 Partial Simulation Technique

From the literature it can be seen that very little experimental work has been carried out on reactor dynamics because the experiments involve high cost and sophisticated instrumentation. Apart from that, a suitable reaction system has to be chosen so that the system behaviour can be studied within the range of instruments. This is partly overcome without too much deviation from practicality by the partial simulation technique where the chemical reaction and mass balance are simulated with the aid of an analogue or digital computer while the heat effects are actually studied on the plant.

Initial work in the Chemical Engineering Department at Aston on the partial simulation technique was carried out with an analogue computer to simulate the reaction and material balance and it was changed later to a digital computer because of the many disadvantages that are typical of an analogue computer. The principal work covered in the Department follows.

The three authors who used analogue simulation were Chao[12], who studied the optimal and adaptive control of a C.S.T.R, Alpaz[13], who attempted the simulation of a plug flow reactor with a series of C.S.T.Rs and Buxton[14], who studied the single loop control of a C.S.T.R. acting through a cooling coil. These authors used a conventional type of controller in their work.

H. Farabi[15] was first to study the advantages of cascade control over a single loop control on a jacketted C.S.T.R. for a first order reaction using the partial simulation technique with the aid of a digital computer for the mass balance and also for the control action. The use of a digital computer to generate the controller action helps to simulate complicated controller configurations that can hardly be tried on conventional controllers.

2.4 STABILITY ANALYSIS

A vast amount of theoretical work has been carried out on the general stability behaviour of a stirred tank reactor. The papers can be broadly classified into two groups according to the method employed. They are Krasovskii's theorem for nonlinear systems and other classical methods for linear and non-linear systems which also include the phase-space technique. In the latter method system stability is analysed by solving the system equations numerically and deducing the transient behaviour for large perturbations. The only article worth mentioning is a communication paper by Berger et al[16] that tries to extend this technique to a series cascade of reactors.

Krasovskii's theorem for nonlinear systems has been applied by many authors. The important step in the application of this theorem is the construction of a positive definite Liapunov function and it is generally agreed in the literature that this is the most difficult step. While Berger et al[17,18] assume unit matrix as the Liapunov matrix and study the positive definiteness of

$-\left[J^T + J \right]$, Jacques et al[19] assume a Liapunov matrix of the form

$$\begin{bmatrix} 1 & S \\ S & \gamma \end{bmatrix}$$

and maximise it with an inequality constraint

$$(\gamma - S^2) > 0.$$

Tarbell[20] tries to arrive at a Liapunov function from the fundamentals of thermodynamics but finally admits that the theorem of minimum entropy production does not apply to the near equilibrium C.S.T.R. steady-state due to the presence of convective heat exchange between the reactor and the surroundings.

Lueck and Meguine[21] give an algorithm to update the Liapunov matrix calculated initially, using the Jacobian matrix.

The various steps involved are

1) Calculate J at the origin ($x=o$) and check whether the necessary condition for stability is satisfied.

2) Solve $J^T A + AJ = -I$ for A and check whether A is positive definite.

3) maximise K_L in the equation $V_L = f^T A f = K_L$ satisfying the condition $-\dot{V}_L = -f^T \{J^T A + AJ\} f \geq 0$

4) find J at this new point ($x=x^*$) where the $V_L = K_L$ contour touches $-\dot{V}_L = 0$.

5) Check whether the roots of J are on the left half of the plane and if so go to step (2).

The algorithm does not always yield the largest A matrix because the J matrix calculcated from step (4) will invariably fail the test in step (5) because of the fact that the $x=x^*$ point will generally be outside the separatrices formed by the conditions for the real parts of roots of J to be on the left half of the plane.

Berger and Lapidus[22] try to maximise the time derivative of the Liapunov function on the closed Liapunov hyper surface but they simplify the problem by assuming a unit matrix as the Liapunov matrix. Davidson and Kurak[23] outline a very cumbersome method which involves very high computational time. The Liapunov function is found by maximising the volume of the stable region for the system

$$x^T A x = 1$$

2.5 UNSTABLE OPERATING POINTS

Operating a reactor at the unstable point is an attractive alternative for many reasons. Various techniques have been used for this by many authors. These include simple proportional control[24], relay feedback control[25] as control strategies for operation at the unstable equilibrium point. Chang and Schmitz[9], in their experimental study, used P + I control at the unstable point in the chemical reaction between sodium-thiosulphate and hydrogen peroxide. They also describe the problems involved in shifting the system operating point from the inherently stable point to the open loop unstable point. Horak et al[51] describe the effect of using various manipulated variables in the control of a C.S.T.R. at its open loop unstable point. The reasonable manipulated variables used by these authors were flowrate of coolant or feed, outlet flowrate of products or inlet temperature of coolant. Apart from these they also mention other manipulated variables which are not practical.

2.6 INTERACTION AND DECOUPLING OF STATE VARIABLES

A physical system is defined as multivariable when it has a number of inputs and outputs. The most important characteristic of such a system is that they will be generally interacting and coupled, a condition that occurs when there are inputs which simultaneously affect more than one output. The C.S.T.R. with a cooling jacket is a typical example of such a system.

A system which is defined by the set of differential equations:

$$\dot{x}_i = f_i(x_1, x_2 \dots x_n) + \phi_i \qquad (2.1)$$

$$i = 1, 2 \dots n$$

is said to be decoupled if it can be expressed as

$$\dot{x}_i = -D_i \, x_i \qquad i = 1 \dots n \qquad (2.2)$$

where D_i's are constants and ϕ_i's are disturbances entering the system. The value of D_i determines the speed of response.

No work has been reported so far on the practical study of the noninteracting type of control on a C.S.T.R. Furthermore very few papers exist for the theoretical study of these control configurations on any chemical process system. Mesarovic[26] and Meerov[27] lay the foundations for a multivariable control system theory.

Decoupling of a multivariable interacting system has been analysed by many authors, though most of them simplify the problem by linearising the state equations.

Foster et al[28] and Ballinger and Lamb[29] present a method to decouple a C.S.T.R. system by feedback and feedforward compensators. Shean Lin Liu[30] developed a decoupling technique which can be applied to nonlinear systems over the entire state space, taking into account the constraints on process input variables. Hutchinson and McAvoy[31] apply this technique for the time optimal control of a noninteracting system. Tokumaru et al[32] obtain the necessary conditions for noninteraction using variational methods.

2.7 INVARIANCE CONTROL

The principle of invariance, when applied to a control system, will give the calculated relationships permitting selection of parameters of the system, so that one of its generalised coordinates will be independent of one or several disturbing influences applied to the system. Petrov[33] has dealt with the general aspects of the principle of invariance for both linear and nonlinear systems.

Consider a dynamic system represented by the following set of differential equations

$$a_{i1}\, x_1 + a_{i2}\, x_2 \; \cdots\cdots + a_{in} x_n = f_i(t) \tag{2.3}$$

where $$a_{i1} = A_{i1} \frac{d^2}{dt^2} + B_{i1} \frac{d}{dt} + C_{i1} \tag{2.4}$$

and A, B, C are constants (zero or non-zero). Under conditions of absolute invariance of the unknown function x_i (t) of the system (2.3) from the arbitrary forcing function $f_i(t)$ the minor D_{ij} of the principal determinant

Δ becomes identically equal to zero. If the conditions of invariance of one of the variables x_j are realised in the system, defining its behaviour relative to a certain disturbing effect, $f_i(t)$, then in the absence of other disturbing effects and zero initial conditions, the variable x_j will be equal to zero. It follows that influences of this variable on other generalised coordinates of the system will be absent.

An essential requirement for the realisation of these conditions of invariance is that there must be identical matching of the set of solutions of the equations of the original system and the system broken at the output of the element, defined by the generalized coordinates x_j (at the point of measurement of the variable x_j) during realization of conditions of invariance and zero initial conditions and when all influences are equal to zero. Another necessary condition is that, there must be at least two channels for propagation of the influences between the point of application of the external effect and the point of measurement of magnitude, whose relation to this effect must be secured (Dual channel concept).

The only paper available in the literature which applies this principle to the control of a chemical process system is by Haskins et al[34]. The authors tried a theoretical application of this principle to the control of a heat exchanger acted upon by sinusoidal disturbances in inlet temperature and found it to be very successful.

2.8 LIMIT-CYCLES

The study of the oscillatory nature of a C.S.T.R. response for constant input conditions has attracted several authors.

Oscillations were observed experimentally by Baccaro et al[10] in the hydrolysis of acetyl chloride while Chang et al[8] observed similar behaviour in the reaction between sodium thiosulphate and hydrogen peroxide in a C.S.T.R. A limit-cycle was also observed by Heemskerk et al[35] in the acid catalysed hydrolysis of 2,3 epoxy propanol-1. Both the hydrolyses are first order in nature. Apart from generating limit-cycles the authors do not analyse these nonlinear oscillations.

In addition to these three papers, the following deal with the theoretical aspects of limit-cycles.

Luus et al[36] use an averaging technique to determine the time average of state variables while Beek[37] uses a truncated power series type expansion to obtain the variation of state variables with time. Douglas et al[38], Dorawala et al[39] and Gaitonde et al[40] study theoretically the effect of oscillations on the final conversion and conclude that sometimes oscillations can improve the time average conversion by as much as 20%.

The existence of a limit-cycle is established in two dimensional systems by the use of Bendixon's theorem[41] while the theory of Bifurcation is used by many authors to establish it in higher dimensional systems.

2.8.1 Theory of Bifurcation

Since the C.S.T.R. with a cooling jacket is a three dimensional system the bifurcation theorems have to be used for establishing the existence of limit-cycles.

Minorsky[42] defines two kinds of bifurcation in a parametric space. The bifurcation of the first kind occurs whenever the limit-cycle nearest to the singular point shrinks in size indefinitely and when the parameter reaches the bifurcation value, the limit-cycle coalesces with the singular point with the result that the latter changes its stability while the limit-cycle disappears. The bifurcation of the second kind occurs whenever two adjoining cycles approach indefinitely giving rise to a semistable cycle which disappears thereafter. The two kinds of bifurcation mentioned are reversible.

Ku et al[43,44] and Jonnada et al[45] establish analytical criteria for the existence of a limit-cycle in high dimensional systems using Bifurcation theorems in parametric space. The analytical criteria are derived from the direct method of Liapunov. They also classify the limit-cycle into soft excitation and hard excitation types depending upon their behaviour with respect to the parameter under consideration. No papers were found which make use of the theory of bifurcation for establishing the existence of a limit-cycle in a chemical process system.

2.9 CONCLUSIONS

From the literature survey carried out it could be seen that though a thorough understanding of the C.S.T.R has been carried out theoretically by many authors, experimental work has been done mainly on the second order exothermic reaction between sodiumthiosulphate and hydrogen peroxide. No experimental work on C.S.T.R. dynamics has been reported in the literature for zero or negative reaction orders.

The partial simulation technique, in spite of its advantages over theoretical simulation or complete experimental work has not been fully exploited so far in understanding the reactor system. Though decoupling and invariance type control have been tried up to a certain extent on electrical systems they have never been tried on chemical process equipment mainly due to their complexities and the fact that a digital (or analogue) computer has to be used as controller.

From the literature it is seen that order for a particular reaction system can change depending upon many parameters. The effect of reaction order on dynamics of a C.S.T.R. offers an interesting study due to the fact that order affects dynamic behaviour appreciably and very few engineers give importance to the effect of order on dynamics of a C.S.T.R. for design purposes.

The stability and limit-cycle behaviour of the C.S.T.R. has been analysed by many authors in a two dimensional plane. These studies in three dimensional phase space introduce many complexities and require new techniques that have never been tried before.

Experimental work reported on the generation of limit-cycles has been only at the open loop stable operating point. There has been no work which compares limit-cycles generated at the open loop stable and unstable points.

No work has been reported so far on stability analysis by the Krasovskii's theorem in a region with multiple equilibrium (singular) points, though such a situation is possible in chemical reactor systems. The Liapunov function in such situations should be chosen with care so that it does not violate the necessary condition, which is that the value should be zero only at x equal to zero (origin) and tend to infinity as x tends to infinity.

The present work not only tries to emphasise the advantages of the partial simulation technique but also makes use of the powerfulness of the digital computer to act as a controller. So control schemes which have not been applied for chemical process systems so far are tried out.

CHAPTER 3

THEORETICAL DEVELOPMENTS

3.1 INTRODUCTION

This chapter deals with the theoretical studies carried out on the system in order to build up an understanding of its dynamic behaviour and hence to design the experimental programme. The stability of the reactor system was analysed for different reaction orders and equations for cooling water flowrate were derived for a number of control strategies.

3.2 MATHEMATICAL FORMULATION

An Arhenius type exothermic n^{th} order irreversible chemical reaction is assumed to take place in a jacketted continuous stirred tank reactor. Neglecting the heat losses to the surroundings and assuming complete mixing in both the reactor and the jacket the mass and energy balances in the reactor and energy balance in the jacket can be written as

$$F\,(C_o - C) - Vk\,C^n = V\frac{dC}{dt} \qquad (3.1)$$

$$F\rho C_p (T_o - T) - UA\,(T - T_c) + \Delta HVkC^n = V\rho C_p \frac{dT}{dt} \qquad (3.2)$$

$$F_c\,\rho_c C_{pc} (T_{co} - T_c) + UA\,(T - T_c) = V_c\,\rho_c C_{pc} \frac{dT_c}{dt} \qquad (3.3)$$

$$\text{where } k = k_o\,e^{-E/RT} \qquad (3.4)$$

The parameters heat of reaction, frequency factor and initial concentration are given in Appendix (5.6) and are chosen so that the operating temperatures are between 293 and 318 K to match the operating range of instruments on the experimental equipment. The same parameter values are used in the experimental work. The heat transfer conductance chosen for the theoretical studies is an average value obtained from tests on the equipment. The activation energy is chosen depending upon the order of reaction so that the system has an operating temperature near to 305 K. The values of activation energy chosen for various reaction orders are also given in Appendix (5.6).

3.3 STEADY-STATE EQUATIONS

At steady-state the right hand sides of equations (3.1) to (3.3) are equated to zero. The equation so arising from (3.2) can be split into two parts as heat generation and heat removal to arrive at the following set of steady-state equations.

$$\text{Heat Generation} = \Delta H V k_o C^n e^{-E/RT} \tag{3.5}$$

$$\text{Heat removal} = F\rho C_p (T-T_o) + UA\,(T-T_c) \tag{3.6}$$

$$FC + Vk_o C^n e^{-E/RT} = FC_o \tag{3.7}$$

$$T_c = (F_c \rho_c C_{pc} T_{co} + UAT)/(F_c \rho_c C_{pc} + UA) \tag{3.8}$$

Equation (3.5) when plotted against T is S-shaped, and depends on the order of reaction; the heat removal line plotted against T is independent of reaction order. The number of times the heat removal line cuts the heat generation curve determines the total number of operating points some of which are stable and some unstable. The lower operating point is generally stable and next higher

TABLE 3.1 INLET CONDITIONS

$F = 5 \times 10^{-5} m^3/s$

$F_c = 4 \times 10^{-5} m^3/s$

$T_o = 288.1$ K

$T_{co} = 288.1$ K

TABLE 3.2 OPERATING POINTS FOR VARIOUS REACTION ORDERS

Reaction	T_{SS} (K)	C_{SS} (kg/m^3)	T_{cSS} (K)	Nature of operating point
-1	296.1	19.636	291.95	S
-1	305.1	19.215	296.27	U
0	301.1	19.405	294.35	S
0	306.1	19.163	296.75	U
1	304.5	19.221	296.17	S
1	312.1	18.889	299.63	U
2	305.1	19.218	296.27	S
2	339.0	17.65	312.56	U

one, if it exists, is unstable.

3.4 EFFECT OF REACTION ORDER ON OPERATING POINTS

For the set of inlet conditions in Table (3.1) the steady-state equations (3.5) to (3.8) are solved for integer orders ranging from -1 to 2 and the results presented in Table (3.2). The computer program for obtaining these operating points, written in BASIC for HP 2000 is given in Appendix (1.1).

It can be seen from Table (3.2) that the unstable operating temperature and hence the difference between unstable and stable operating temperatures increases with increase in positive or negative order.

3.5 STATE EQUATIONS FOR TRANSIENT STUDIES

The set of differential equations (3.1) to (3.3) can be written assuming all the inputs as zero, in a form which is suitable for transient analysis as

$$\frac{dX}{dt} = -\frac{X}{\tau} - K_1\{(X+\alpha_{SS})^n e^{-Q/(Y+\beta_{SS})} - \alpha_{SS}^n e^{-Q/\beta_{SS}}\} \quad (3.9)$$

$$\frac{dY}{dt} = -\tau_1 Y + Z/\tau_o + K_1\{(X+\alpha_{SS})^n e^{-Q/(Y+\beta_{SS})} - \alpha_{SS}^n e^{-Q/\beta_{SS}}\} \quad (3.10)$$

$$\frac{dZ}{dt} = -\tau_2 Z + Y/\tau_I + \frac{\bar{F}_c}{V_c}(\gamma_{OSS} - \gamma_{SS} - Z) \quad (3.11)$$

where X, Y and Z are the state variables in dimensionless perturbations of tank concentration, tank temperature and jacket temperature respectively.

$\bar{F}_C$ is the control variable, the perturbation of coolant flow from its steady-state value. It thus has a zero value for open loop and otherwise depends on the control strategy chosen. An upper limit on cooling water flowrate is used in the theoretical work to correspond to the finite coolant pump capacity on the equipment.

The Jacobian matrix J defined by

$$J = \frac{\partial f_i}{\partial x_j} \qquad j = 1,2 \,.....\, n \qquad i = 1,2 \,.....\, n$$

for the above system

$$J = \begin{bmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{bmatrix}$$

where $J_{21} = K_1 \; n \; (X + \alpha_{SS})^{n-1} e^{-Q/(\beta_{SS} + Y)}$

$$J_{11} = -\,{}^{1}/_{\tau} - J_{21}$$

$$J_{12} = -\,K_1 \; (X + \alpha_{SS})^{n} e^{-Q/(\beta_{SS} + Y)} \; \frac{Q}{(\beta_{SS} + Y)^2}$$

$$J_{22} = -\,\tau_1 - J_{12}$$

$$J_{13} = o$$

$$J_{23} = {}^{1}/_{\tau_o}$$

$$J_{31} = o$$

$$J_{32} = {}^{1}/_{\tau_I} + \frac{\partial \bar{F}c}{V_c \partial Y} \; (\gamma_{OSS} - \gamma_{SS} - Z)$$

$$J_{33} = -\,\tau_2 + \frac{\partial \bar{F}c}{V_c \partial Z} \; (\gamma_{OSS} - \gamma_{SS} - Z) - \frac{\bar{F}c}{V_c} \qquad (3.12)$$

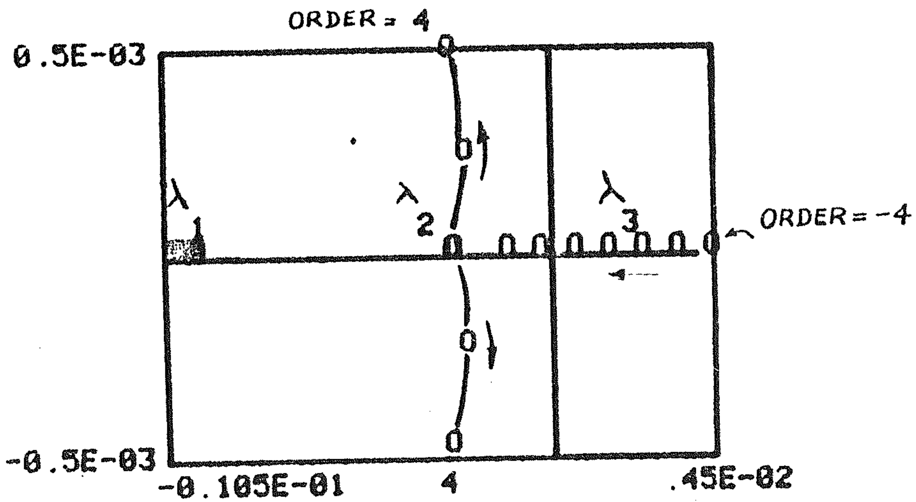


FIG.3.1 EIGENVALUES OF CHARACTERISTIC MATRIX FOR VARIOUS REACTION ORDERS AT 305K

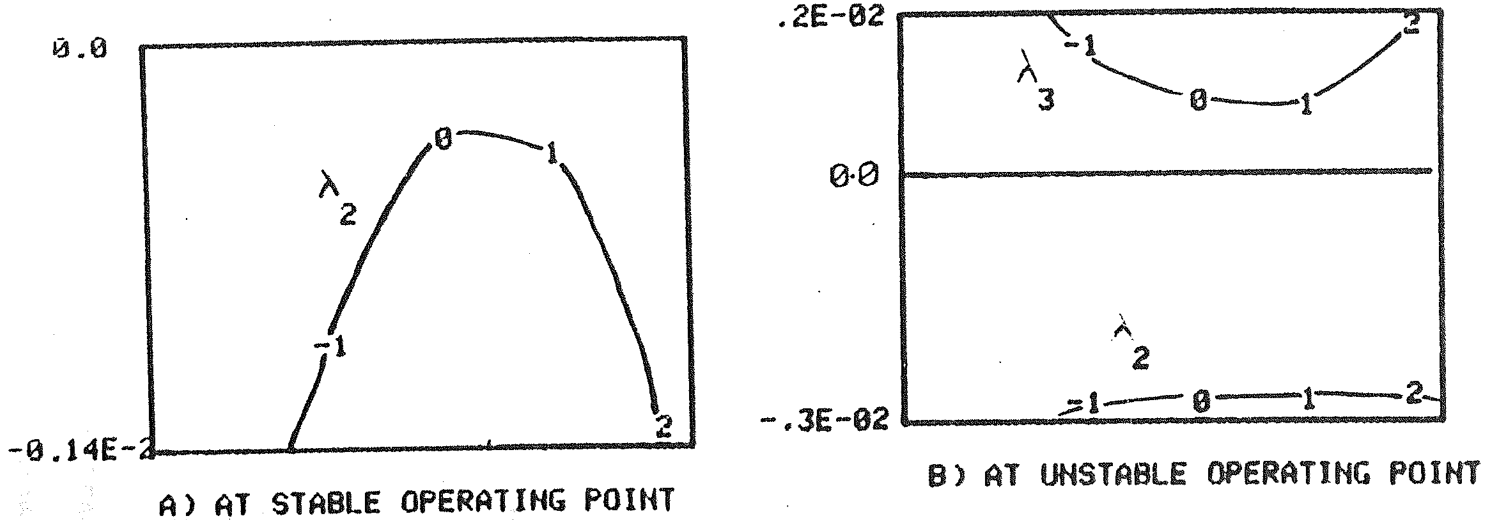


FIG.3.2 EIGENVALUES AT OPEN LOOP STABLE AND UNSTABLE POINTS FOR VARIOUS REACTION ORDERS

3.6 EFFECT OF REACTION ORDER ON THE LINEARISED SYSTEM

The Jacobian matrix calculated at the origin can be termed as the characteristic matrix of the linearised system. This matrix determines the system behaviour at the origin (operating points).

The nature of the eigenvalues of this characteristic matrix determines the stability of the origin. The eigenvalues of the characteristic matrix are plotted against reaction order at the operating point near 305 K in Fig. (3.1). It can be seen from the figure that one of the eigenvalues is on the right-half of the plane for negative order systems thereby indicating instability. As the order is increased the system becomes stable for reaction order one. A further increase in order makes the eigenvalues complex, indicating oscillations in the system behaviour.

From Table (3.2) it can be seen that systems with reaction order -1 to 2 have a stable and an unstable operating point. The eigenvalues calculated at these points are plotted in Fig. (3.2). From Fig. (3.2a) it can be seen that zero order seems the least stable of the four systems.

3.7 EFFECT OF INLET PARAMETERS

3.7.1 Effect on Operating Points

The operating parameters like reactant flowrate and inlet temperature, cooling water flowrate and temperature have an effect on the equilibrium points and the stability of the system. A brief theoretical study of this effect

TABLE 3.3 OPERATING POINTS FOR VARIOUS REACTION ORDERS FOR A DIFFERENT SET OF CONDITIONS

Reaction order	T_{SS} (K)	C_{SS} (kg/m^3)	T_{cSS} (K)	Nature of operating point
-1	303.1	19.59	297.43	S
-1	310.2	19.27	300.82	U
0	305.1	19.51	298.4	S
0	315.1	19.06	303.25	U
1	305.8	19.49	298.0	S
1	325.5	18.66	306.28	U
2	306.1	19.476	298.9	S
2	363	17.07	322.25	U

$F = 80$ ml/s $= 8 \times 10^{-5}$ m^3/s

$F_c = 50$ ml/s $= 5 \times 10^{-5}$ m^3/s

$T_O = 294.1$ K

$T_{CO} = 292.1$ K

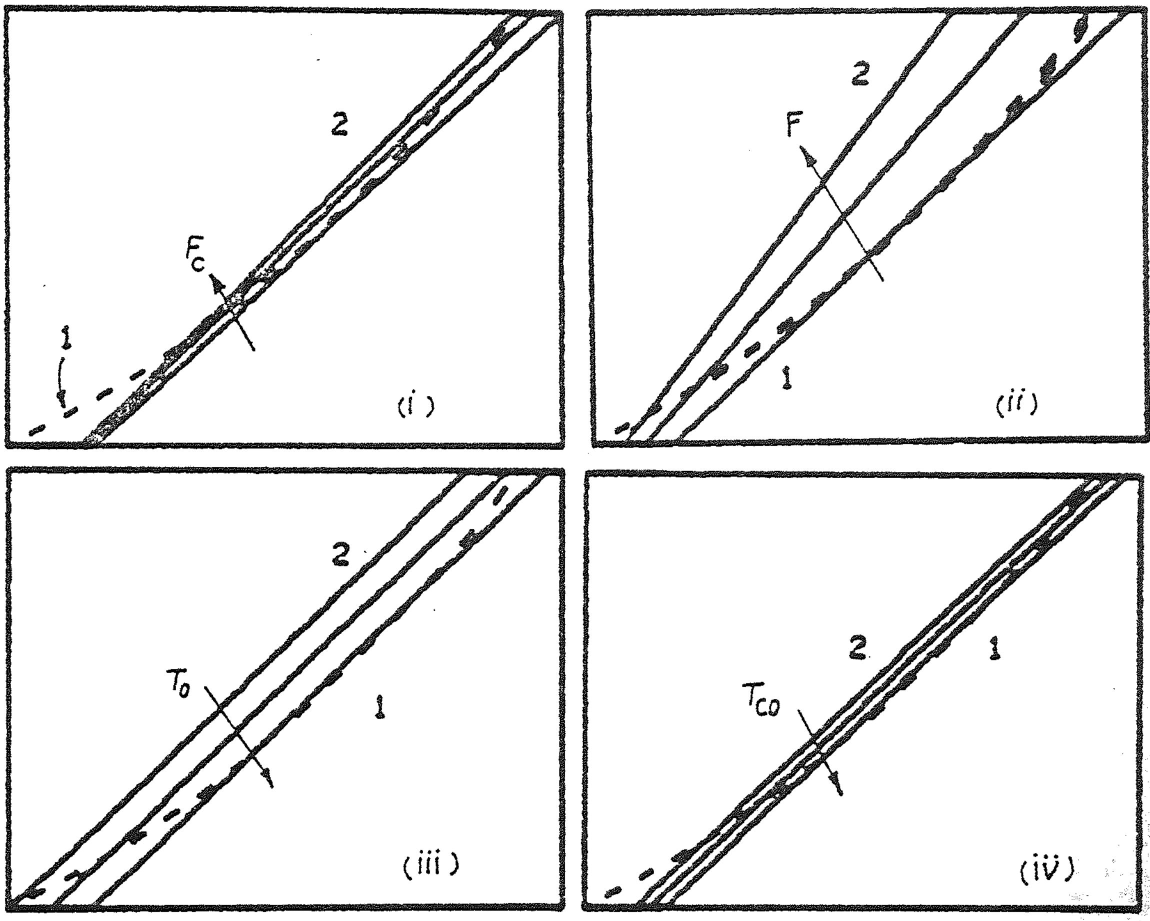
is made in order to take into account the day to day changes in water temperature expected in the experimental work. Increase in water temperature moves the equilibrium temperature upwards while increasing the flowrates has the opposite effect.

The operating points for various reaction orders are obtained for different sets of initial conditions and tabulated in Table (3.3). For all further theoretical work only the first set of conditions in Table (3.1) and the operating points in Table (3.2) are considered.

3.7.2 Effect on Stability

Parameters like inlet temperature, inlet coolant flowrate and temperature, change only the heat removal, while tank inlet flowrate affects both the heat generation and heat removal. The unstable operating point is a point above which the heat generation is greater than the heat removal and the system goes out of bounds. So the region between the stable and the unstable operating points, where heat removal is greater than heat generation, can be considered as the stability region, as a first approximation.

The inlet parameters affect the stability region in different ways. Increase in tank inlet temperature decreases the intercept of the heat removal line and hence the stability region. Increase in jacket inlet temperature affects the heat removal line in a similar manner but to a lesser degree. Increase in the tank flowrate increases both heat generation and removal.



1 = Heat generation

2 = Heat removal

X axis = Operating temperature

Y axis = Heat gen./ removed

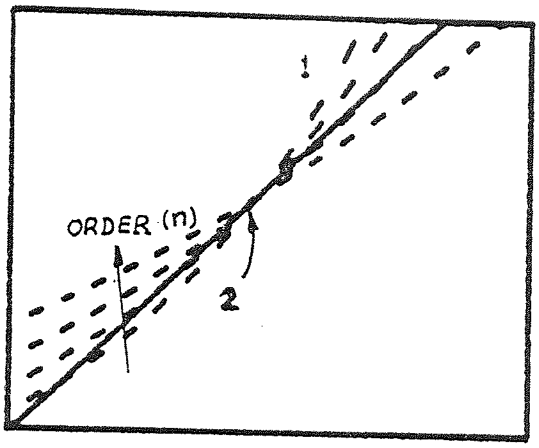
(i) Effect of coolant flowrate (F_c)

(ii) Effect of feed flowrate (F)

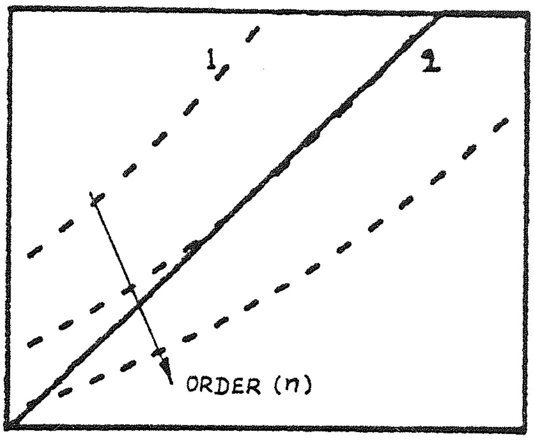
(iii) Effect of feed inlet temperature (T_o)

(iv) Effect of coolant inlet temperature (T_{co})

FIG.3.3(a) EFFECT OF OPERATING PARAMETERS ON HEAT GENERATION AND REMOVAL



FOR DIFFERENT E VALUES (refer App(5.6))



FOR CONSTANT E VALUE

1 = Heat generation

2 = Heat removal

X axis = Operating temperature

Y axis = Heat gen./ removed

FIG.3.3(b) EFFECT OF REACTION ORDER ON HEAT GENERATION AND REMOVAL

However, the increase in heat generation is generally less than the increase in heat removal and hence, there is an increase in the stability region.

Reaction order affects only the heat generation. If the activation energy is constant for all reaction orders then increase in order will decrease heat generation (assuming not much change in concentration) and hence positive orders will be more stable than negative orders. However, in the present study activation energy decreases as order is increased and although the previous argument cannot be extended to this case, mathematically it can be stated that

$$|n| \text{ is more stable than } |n-1|.$$

The effect of various parameters on heat generation and heat removal is shown in Fig. (3.3). The difference between the unstable and stable operating points for various orders and different inlet conditions is tabulated in Table (3.4). Since the various parameters interact with one another the temperature difference is not linearly dependent on the various parameters.

For all inlet conditions the difference in stable and unstable state temperatures is highest for reaction order two. The temperature difference for order one is higher than that of order zero. Except for conditions one and three the difference is higher for order one than for the negative order.

TABLE 3.4 DIFFERENCE BETWEEN STABLE AND UNSTABLE OPERATING POINTS FOR VARIOUS OPERATING CONDITIONS

Reaction orders	DIFFERENCE(IN K) FOR VARIOUS CONDITIONS							
	1	2	3	4	5	6	7	8
-1	9	11	8	16	14	10	17	21
0	5.1	9	2	17	16	9	18	23
1	7.2	13	7	23	21	16	25	32
2	34	39	37	51.3	49.3	45.1	54.5	62.2

Conditions	$F(m^3/s)$ $\times 10^{-6}$	$F_c(m^3/s)$ $\times 10^{-6}$	T_O (K)	T_{CO} (K)
1	50	40	288.1	288.1
2	50	50	288.1	288.1
3	50	50	288.1	290.1
4	60	40	288.1	288.1
5	60	40	288.1	290.1
6	60	40	290.1	288.1
7	60	50	288.1	288.1
8	70	40	288.1	288.1

3.8 STABILITY ANALYSIS OF THE UNCONTROLLED SYSTEM

The stability analysis of the system for various reaction orders is carried out by two methods. The first method is by the application of Krasvoskii's theorem and obtaining the region of asymptotic stability (RAS) using a quadratic Liapunov function. The second method involves actually solving the system equations for various starting conditions and determining the stability region. The limitations of the first method are revealed on plotting the results of both the methods.

3.8.1 By Krasvoskii's Theorem

The stability of the nonlinear system and the region of asymptotic stability can be determined by the application of Krasvoskii's theorem.

The theorem states that for a system defined by

$$\dot{x} = f(x)$$

where f has continuous partial derivatives, if a quadratic function of the form

$$V_L = f^T A f$$

Could be defined with the following properties

(i) A is positive definite symmetric matrix

(ii) $V_L = o$ only at $x = o$

(iii) $V_L \to \infty$ as $x \to \infty$

and if $\dot{V}_L = \frac{dV_L}{dt} = f^T\{J^T A + AJ\}f$ is negative then the system is asymptotically stable at $x=o$ and V_L is the Liapunov function of the system. The largest region that is within the volume $V_L = K_L$ and satisfies everywhere along its surface $\dot{V}_L < o$ is the region of asymptotic stability of the system.

Instead of inspecting the sign of the scalar quantity $\dot{V}_L$, the stability of the system can be determined by looking at the definiteness of the matrix $\{J^T A + AJ\}$. The conditions for the stability of the CSTR system can be obtained from the conditions for the negative definiteness of this matrix. To start with, a simple symmetrix matrix can be assumed for A(viz I, the identity matrix). Then for the system to be stable, $-\{J^T + J\}$ should be positive definite. Applying Sylvester's theorem (see Appendix (3.5))to this expression, the following conditions are obtained for the stability of the system.

$$S_1 = -2 J_{11} > 0 \quad (3.13)$$

$$S_2 = 4 J_{11} J_{22} - (J_{12} + J_{21})^2 > 0 \quad (3.14)$$

$$S_3 = -2 J_{11}\{(4 J_{22} J_{33} - (J_{23}+J_{32})^2\}+2 J_{33}(J_{12}+J_{21})^2 > 0 \quad (3.15)$$

$$S_4 = -2 J_{22} > 0 \quad (3.16)$$

$$S_5 = -2 J_{33} > 0 \quad (3.17)$$

$$S_6 = 4 J_{22} J_{33} - (J_{23} + J_{32})^2 > 0 \quad (3.18)$$

These six inequality conditions when plotted in the X,Y plane for different orders divide the region into stable and unstable regions. The stable region obtained by this technique is highly conservative because not only the definiteness of $\{J^T A + AJ\}$ alone is considered but a unit matrix is used as the Liapunov matrix. Fig. (3.4) gives the plot of equations (3.13)-(3.18) for various orders;

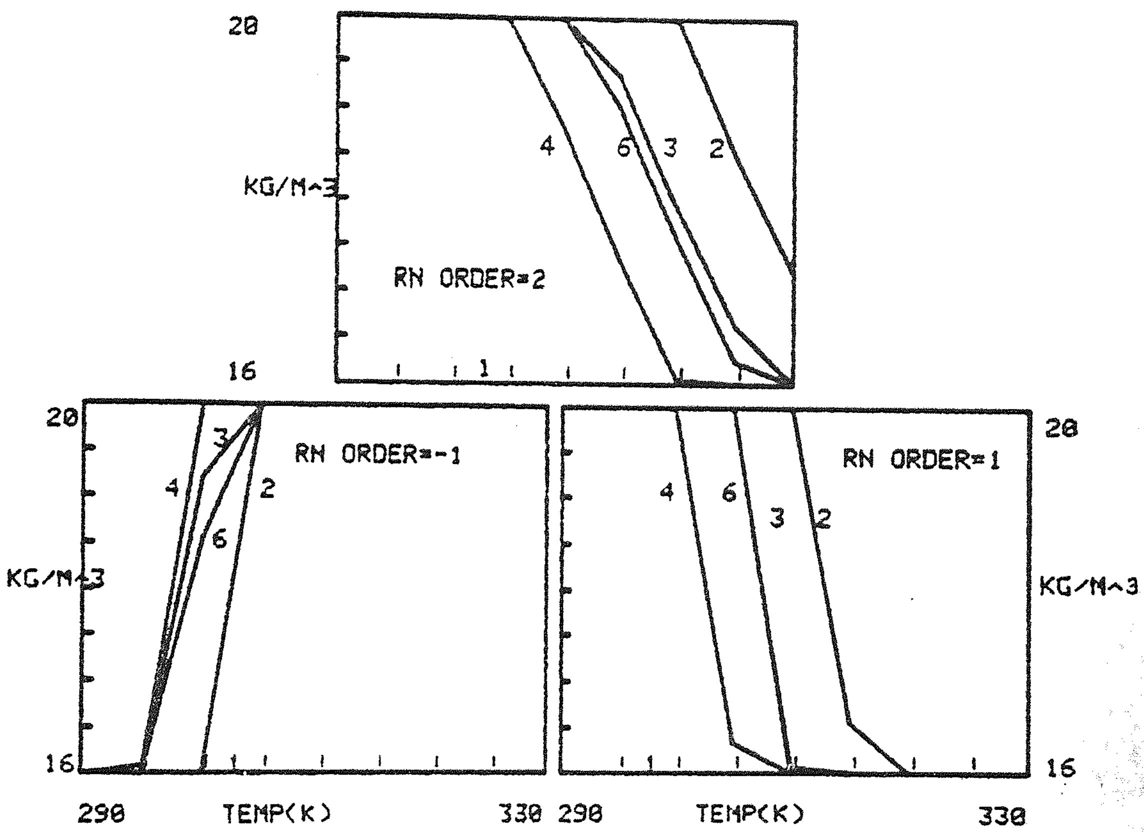


FIG.3.4 SEPARATRICES 1 TO 6 FOR VARIOUS REACTION ORDERS
(OPEN LOOP) (A= I)

reaction order zero is not considered because the matrix elements are independent of X.

When equation (3.12) is substituted into equation (3.13) and rearranged a lower limit for X is obtained for order -1 and second order reactions as

$$X > \left[\frac{-1}{\tau\ K_1 n\ e^{-Q/(Y + \beta_{SS})}} \right] \tag{3.19}$$

Similarly condition (3.16) can be rewritten as an upper limit

$$X < \left[\frac{\tau_1 (Y + \beta_{SS})^2}{Q\ K_1 e^{-Q/(Y + \beta_{SS})}} \right]^{1/n} - \alpha_{SS} \tag{3.20}$$

Equation (3.20) is valid for all orders not equal to zero.

A larger stability region can be obtained if a different A matrix other than the identity matrix is chosen. Then the six conditions for $-\{J^T A + AJ\}$ to be positive definite are

$$S_1 = -2\ J_{11}A_{11} - 2\ J_{21}\ A_{12} > 0 \tag{3.21}$$

$$S_2 = -2\ J_{22}A_{22} - 2\ J_{32}A_{23} - 2\ J_{12}A_{12} > 0 \tag{3.22}$$

$$S_3 = -2\ J_{33}A_{33} - 2\ J_{23}A_{23} > 0 \tag{3.23}$$

$$S_4 = S_1 S_2 - S_7^2 > 0 \tag{3.24}$$

$$S_5 = S_3 S_4 - 2\ S_7^2\ S_8 S_9 - S_1 S_9^2 - S_2 S_8^2 > 0 \tag{3.25}$$

$$S_6 = S_2 S_3 - S_9^2 > 0 \tag{3.26}$$

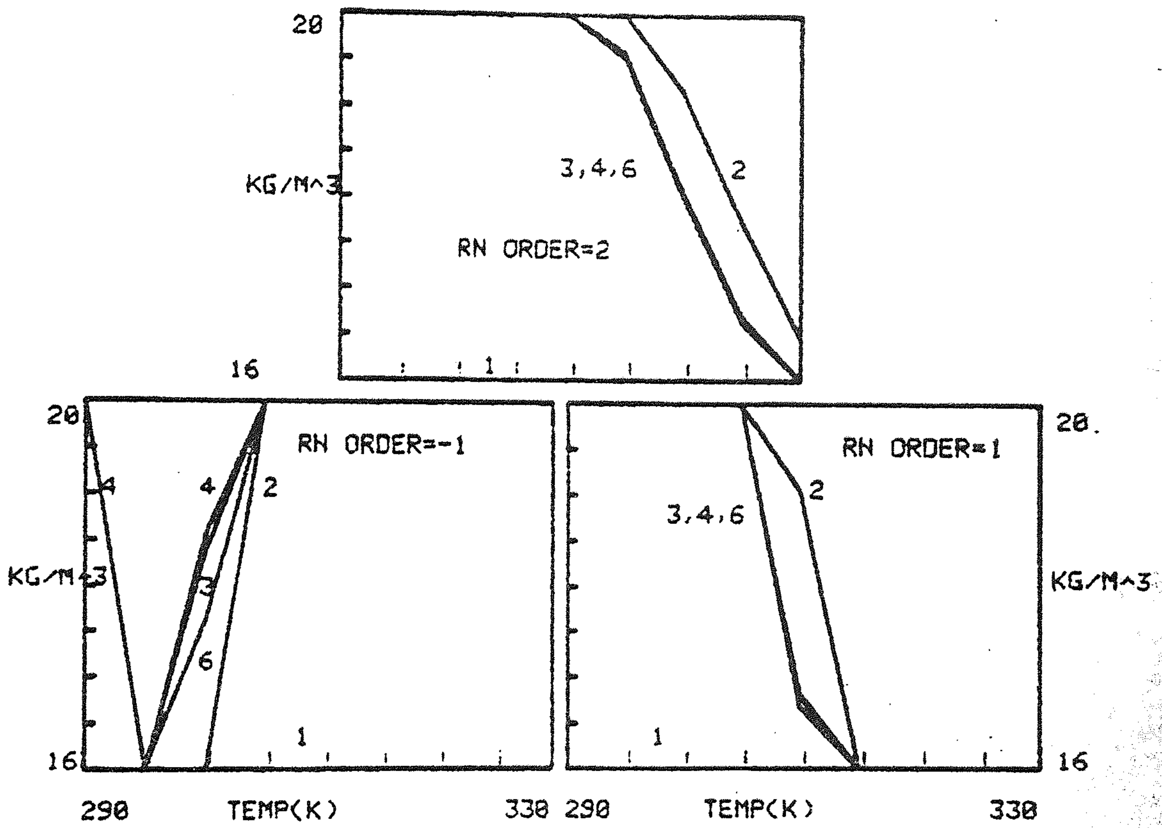


FIG.3.5 SEPARATRICES 1 TO 6 FOR VARIOUS REACTION ORDERS
(OPEN LOOP) (REFER TABLE(3.5) FOR A MATRICES)

where $S_7 = A_{12}(J_{11} + J_{22}) + J_{21}A_{22}+A_{11}J_{12} + A_{13}J_{32}$

$$S_8 = A_{13}(J_{11} + J_{33}) + A_{12}J_{23} + J_{21}A_{23}$$

and $S_9 = A_{23}(J_{22} + J_{33}) + A_{22}J_{23} + J_{32}A_{33} + J_{12} A_{13}$

Fig. (3.5) gives the plot of equations (3.21)-(3.26). It can be seen that the region of stability is increased appreciably from that of Fig. (3.4). The A matrix for each order in Fig. (3.5) is obtained by an optimisation procedure described later in this sub-section.

The Liapunov function considered so far is not a true monotonically increasing function for the C.S.T.R. system under consideration because f and hence V_L are equal to zero not only at the origin but also at the open loop unstable point. So far no work has been reported on determining Liapunov functions near multiple equilibrium (singular)points. In order to make V_L a true monotonically increasing function, a Liapunov function of the form

$$V_L = f^T Af + x^T Ax/10^7 = K_L$$

is considered, which is zero only at the origin and is not equal to zero at any other singular point in the space. A value of 10^7 is chosen so that the two terms on the right hand side are of the same magnitude. To obtain the largest RAS, this function has to be maximised under the inequality constraint

$$\dot{V}_L = f^T\{J^T A + AJ\} f + 2f^T Ax < 0$$

at all points on the surface of the contour. A digital computer program written in FORTRAN for CDC 7600 is presented in Appendix (1.3) and the various steps involved in the calculating procedure are given below.

Step 1: Calculate the Jacobian matrix J at X, Y, Z = 0.

Step 2: Check whether the eigenvalues of J have negative real parts; this is a necessary condition for stability.

The checking procedure is given in Appendix (3.1)

Step 3: Solve the equation

$J^T A + AJ = -B$ for matrix A, where B is a positive definite symmetric matrix (input by the user).

The solving method is given in Appendix (3.2)

Step 4: Check whether A is positive definite using Sylvester's theorem (Appendix (3.5))

Step 5: Assume a small Liapunov function value K_L

Step 6: For different values of X and Y calculate Z by solving the equation $f^T A f + x^T A x/10^7 = K_L$.

Calculate $\dot{V}_L$ and check whether $\dot{V}_L < 0$.

Also calculate the volume of the ellipsoid.

The procedure is described in Appendix (3.3)

Step 7: If $\dot{V}_L < 0$ at all points, increment K_L and repeat step 6 until the largest K_L that obeys the condition is obtained; otherwise go to Step 9.

Step 8: Calculate J at another X, Y and Z and go to Step 2.

Step 9: With A obtained so far maximise the volume of the Liapunov contour by repeating steps 5-7 by varying the elements of A using the logical search technique described in Appendix (3.4).

The flow chart of the program is given in Appendix (2.1). The largest volume obtained and the corresponding A matrix for various orders are tabulated in Table (3.5).

It can be seen from the Table (3.5) that the RAS of the second order system is largest and that of the zero order one is the smallest. Also the volume of the RAS of the -1 order system is larger than that of the first order system. The region of stability (RS) tabulated in the table is the region which encloses the RAS and is separated from the RAS by a small band where $\dot{V}_L > 0$. A semi-stable limit-cycle can be considered to be situated there separating the RAS and the equilibrium point from the remainder of the RS. So any trajectory starting outside this semi-stable limit-cycle but within RS will move towards it, while a trajectory below the limit-cycle will move towards the equilibrium point. An unstable limit-cycle may be considered to separate the RS from the remainder of the phase space. All orders other than -1 possess this RS.

The stability region was determined using the program for proportional type control of the tank temperature and plotted.

TABLE 3.5 LIAPUNOV MATRIX AND REGION OF STABILITY FOR VARIOUS REACTION ORDERS (OPEN LOOP)

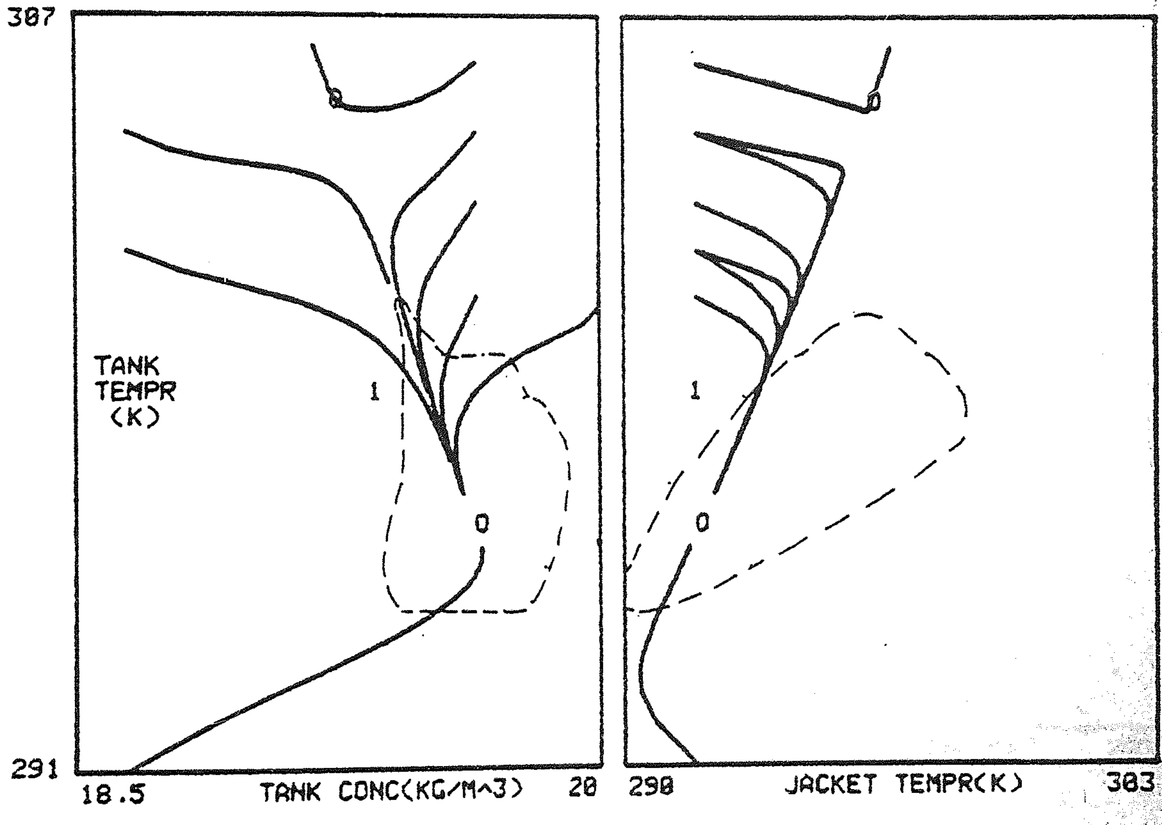
Reaction order	A Matrix (upper diagonal elements)			RAS K_L/Volume	RS K_L/Volume
-1	0.2411×10^{7}	$-.6897 \times 10^{7}$	$-.2378 \times 10^{7}$		
		0.6553×10^{8}	0.1655×10^{8}	0.19×10^{-2}/	—
			0.4636×10^{7}	0.2205×10^{-4}	
0	0.2249×10^{8}	$-.5796 \times 10^{7}$	$-.4176 \times 10^{7}$		
		0.4844×10^{8}	0.1242×10^{8}	0.27×10^{-2}/	0.37×10^{-2}/
			0.5938×10^{7}	0.6359×10^{5}	0.101×10^{-4}
1	0.3921×10^{7}	$-.6107 \times 10^{7}$	$-.1561 \times 10^{6}$		
		0.2599×10^{9}	0.6239×10^{8}	0.64×10^{-2}/	0.86×10^{-2}/
			0.2033×10^{8}	0.2051×10^{-4}	0.3167×10^{-4}
2	0.2019×10^{8}	$-.619 \times 10^{7}$	$-.934 \times 10^{5}$		
		0.606×10^{8}	0.153×10^{8}	0.203×10^{-1}	0.237×10^{-1}/
			0.916×10^{7}	0.422×10^{-4}	0.54×10^{-4}

3.8.2. By Numerical Integration

The stability region of the system can also be determined by numerically integrating the set of system equations (3.9)-(3.11) for different initial conditions. Though this technique is time consuming it gives the exact behaviour of the system around the operating point. A program is written in SLAM (Simulation Language for Analog Modelling) for the ICL 1904S computer to study the dynamic behaviour of the C.S.T.R. The listing of this program is not given since it is similar to the one described in Chapter 7 (Total Simulation of the plant). The program calculates the values of the state variable at different time intervals by the Fourth order Runge-Kutta Fixed step method. The program can also be used to study the effect of control on the dynamic behaviour of the system by incorporating the type of control required from those available in the program.

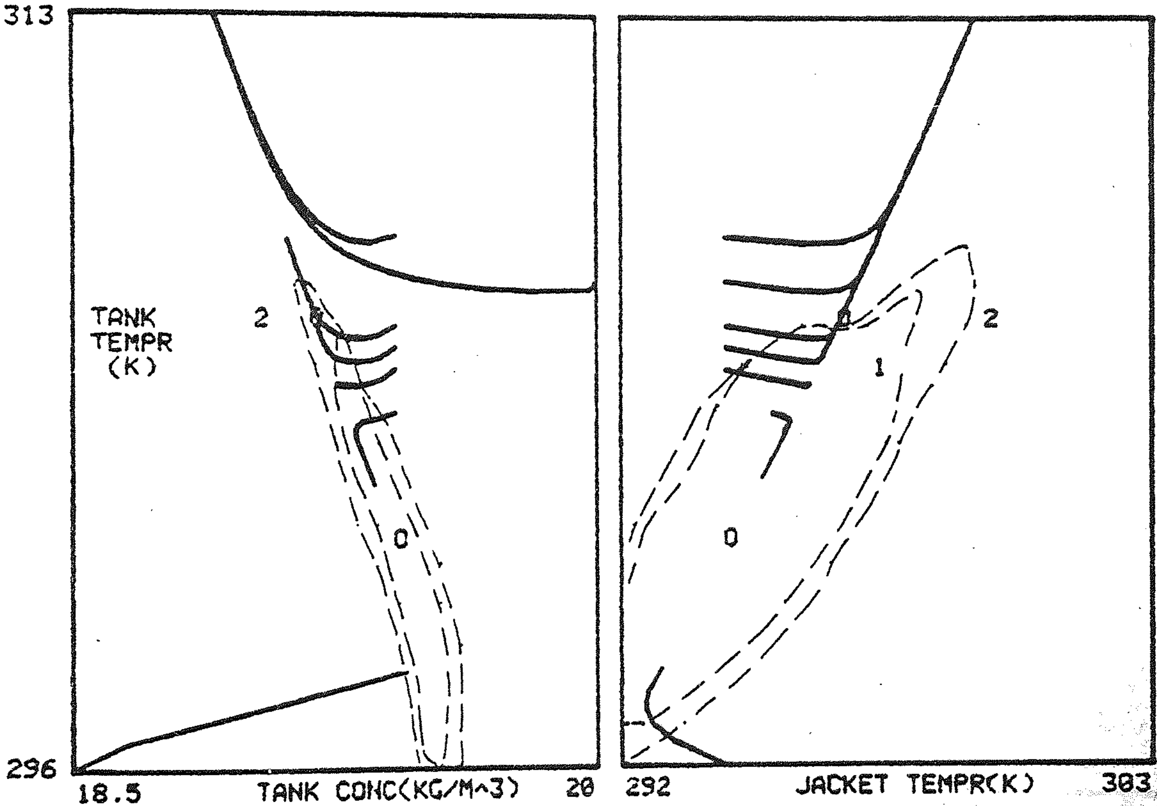
3.8.3 Comparison of Stability Region obtained by Both Methods

It can be seen from the figures that Krasovskii's theorem gives a highly conservative region of stability, due to the fact that a positive definite symmetric matrix is assumed as the Liapunov matrix. Plotting the trajectories of the system around the steady-state point by numerically integrating the model equations gives a true picture of its behaviour. The Liapunov contours obtained point towards the unstable operating point because one of the eigenvectors of matrix A coincides with the line joining the stable and unstable points.



0 = Stable/unstable operating points
1 = Liapunov contour of RAS

FIG.3.6 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=-1
(OPEN LOOP)

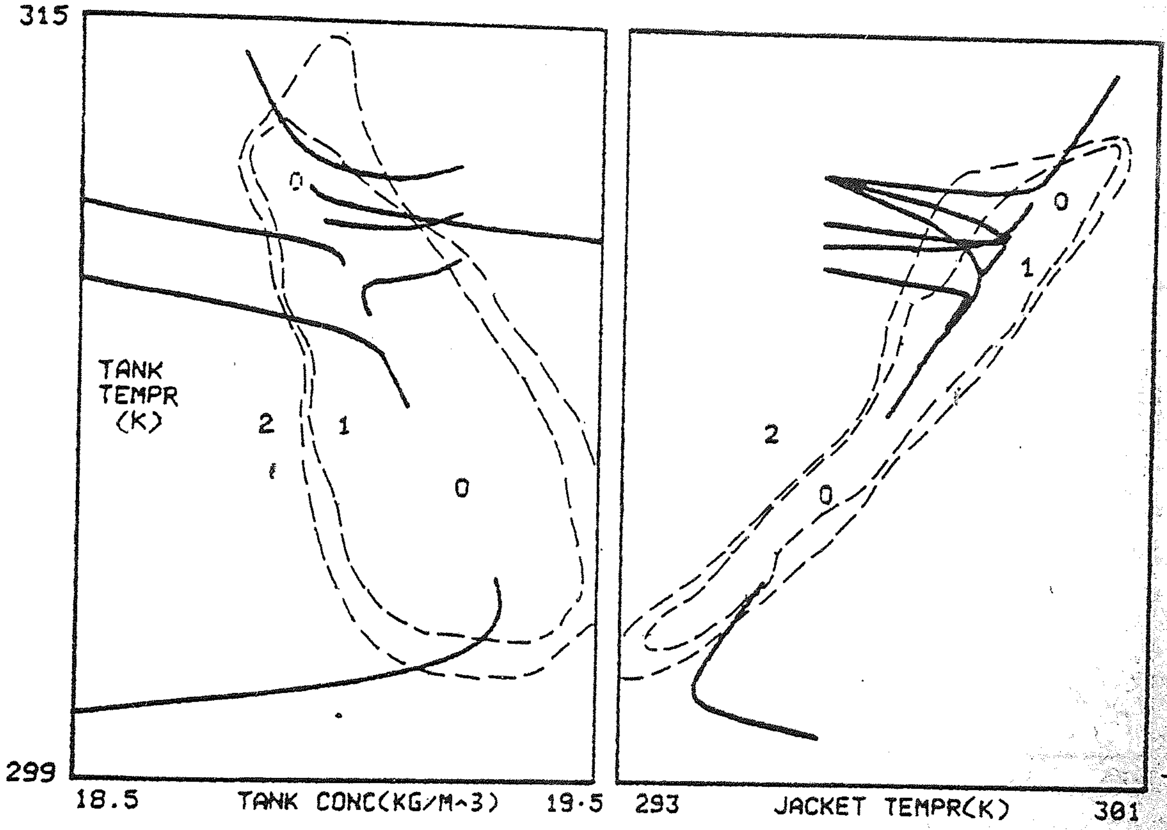


0 = Stable/unstable operating points

1 = Liapunov contour of RAS

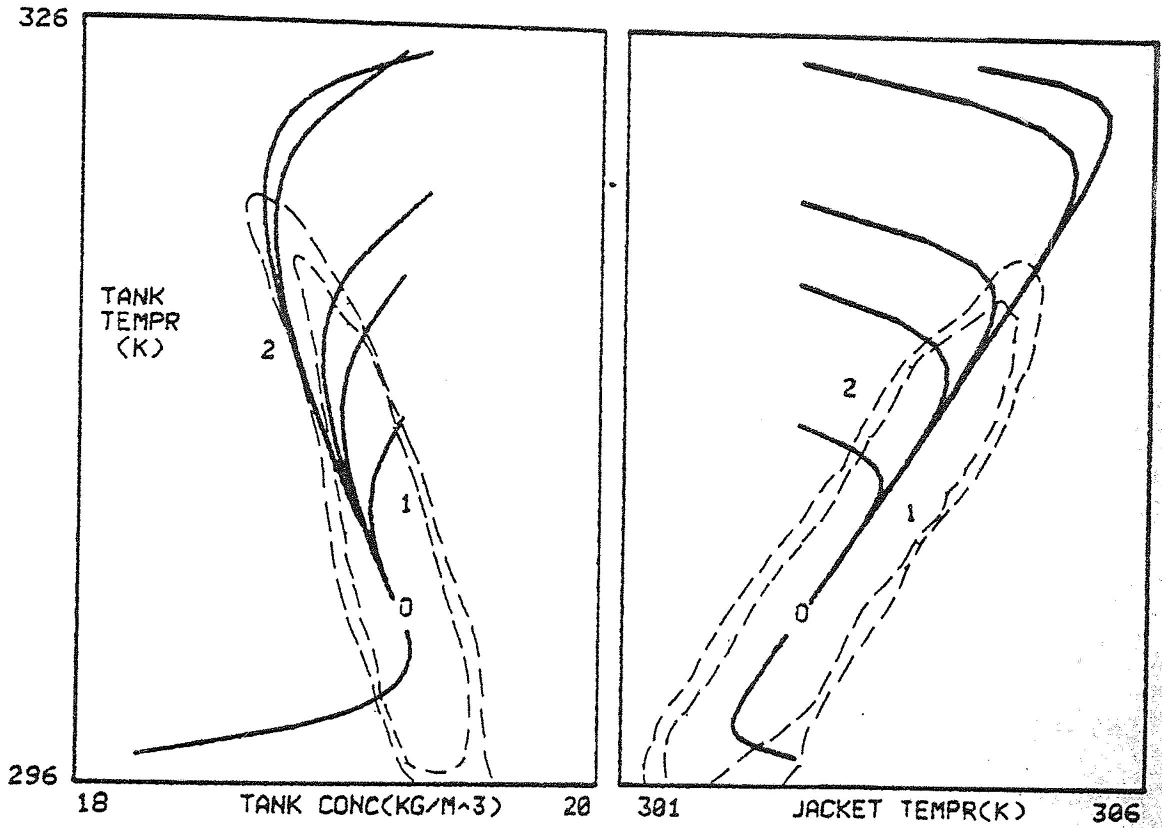
2 = Liapunov contour of SR

FIG.3.7 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=0
(OPEN LOOP)



0 = Stable/unstable operating points
1 = Liapunov contour of RAS
2 = Liapunov contour of SR

FIG.3.8 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=1 (OPEN LOOP)



0 = Stable/unstable operating points
1 = Liapunov contour of RAS
2 = Liapunov contour of SR

FIG.3.9 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=2 (OPEN LOOP)

Another important drawback of the former technique is that, a given system of differential equations may possess many Liapunov functions, each differing from the others in a non trivial manner. To each of these Liapunov functions there will be a corresponding RAS, which will, in general, be different. The fact that a particular point is not included in the region of stability for a particular Liapunov function does not necessarily indicate that the trajectories through that point fail to go to the origin.

It can be seen that both the techniques indicate that the stability region of the second order system is largest and that of the zero order the smallest; the -1 order system has a stability region slightly larger than that of first order system. In spite of the drawbacks, stability analysis by Krasovskii's theorem is superior to numerical integration because of the ease with which it can be programmed and it gives a very quick idea about the system behaviour. This technique is also useful for higher dimensional systems where phase-space techniques become meaningless. The conservative estimation of the stable region by this technique can also be used when designing reactor systems and gives a certain margin of safety.

3.9 EFFECT OF CONTROL

Incorporating a controller changes the system behaviour around the stable and unstable operating points. Various types of controller configurations affect the system in various ways. Controllers can be used to stabilise an operating point, to increase the stability region or to improve the transient behaviour of the system. In the sections below the effects of controllers on the eigenvalues, stability and transient behaviour of the system are described.

3.9.1 Effect on eigenvalues of the Characteristic Matrix

The effect of proportional type control of tank temperature of the form

$$\bar{F}_c = K_c Y \qquad (3.27)$$

on the eigenvalues of the characteristic matrix is tabulated in Table (3.6). Control stabilises inherently unstable operating points, which means that simple proportional controllers can be used to operate the system at inherently unstable points with ease. However, increase in controller gain induces oscillations, as is well known. The eigenvalues change their properties at different values of controller gains for various reaction orders.

A controller of the type

$$\bar{F}_c = K_c Z \qquad (3.28)$$

seem to have a different effect on the eigenvalues of the system. The eigenvalues for this type of control strategy are given in Table (3.7).

3.9.2 Effect on Stability of the System

From equations (3.12)-(3.18) it can be seen that

TABLE 3.6 NATURE OF EIGENVALUES AS A FUNCTION OF PROPORTIONAL GAIN FOR CONTROLLER OF THE TYPE IN EQUATION (3.27)

$K_c = K_2 \times 10^{-6}$

Reaction order	Type of operating point	Nature of eigenvalues
-1	U	un $\xrightarrow{K_2 = 4450}$ sn $\xrightarrow{8850}$ sf
	S	sn $\xrightarrow{1300}$ sf
0	U	un $\xrightarrow{3000}$ s node $\xrightarrow{9000}$ sf
	S	sn $\xrightarrow{10000}$ sf
1	S	sn $\xrightarrow{3500}$ sf
	U	un $\xrightarrow{2000}$ sn $\xrightarrow{4000}$ sf
2	S	sn $\xrightarrow{1400}$ sf

un = unstable node
sn = stable node
uf = unstable focus
sf = stable focus

TABLE 3.7 NATURE OF EIGENVALUES AS A FUNCTION OF PROPORTIONAL GAIN FOR CONTROLLER OF THE TYPE IN EQUATION (3.28)

$K_c = K_2 \times 10^{-6}$

Reaction order	Type of operating point	Nature of eigenvalues
-1	S	sn (up to K_2 = 47,000)
	U	un (up to K_2 = 20,000)
0	S	sn (up to K_2 = 30,000)
	U	un (up to K_2 = 13,000)
1	S	sn (up to K_2 = 13,000)
	U	un $\xrightarrow{11,000}$ sn
2	S	sn $\xrightarrow{4,050}$ sf

control affects only equations (3.15), (3.17) and (3.18). It can also be seen that equation (3.15) reduces the stability region to the maximum extent. Hence the study should involve strengthening equation (3.15) in order to increase RAS. Equations (3.15) and (3.18) can be strengthened if

$$J_{23} + J_{32} = 0$$

$$\text{or } \tau_3 + \frac{1}{V_c} \frac{d\bar{F}_c}{dY} (\gamma_{OSS} - \gamma_{SS} - \Xi) = 0 \qquad (3.29)$$

where $\tau_3 = 1/_{\tau_O} + 1/_{\tau_I}$

Various types of controller configuration can be tried to satisfy equation (3.29).

If a controller of the type described in equations (3.27) is considered, then equation (3.29) becomes

$$K_c = - \frac{V_c \tau_3}{(\gamma_{OSS} - \gamma_{SS} - \Xi)} \qquad (3.30)$$

Equation (3.30) gives a value for the proportional gain in terms of the system parameters and operating points in order to improve the RAS. If values are substituted in equation (3.30), neglecting Ξ then

$$K_c = 4.1435 \times 10^{-3}$$

and the controller gain given above will increase the RAS to its maximum value.

A controller of the type described in equation (3.28) cannot appreciably improve RAS because $\frac{d\bar{F}_c}{dY} = 0$ and hence equation (3.29) will yield no result. Equation (3.18) can be written as

$$-4\, J_{22}\, \{\tau_2 + \frac{\bar{F}_c}{V_c} + \frac{K_c}{V_c}(\gamma_{SS} + Z - \gamma_{OSS})\} > \tau_3^{\;2}$$

which on rearranging gives

$$K_c > \frac{V_c \tau_3^2 / \{-4J_{22}\}}{\{\gamma_{SS} + 2\,Z - \gamma_{OSS}\}} - \frac{V_c\, \tau_2}{\{\gamma_{SS} + 2Z - \gamma_{OSS}\}} \qquad (3.31)$$

an inequality condition, a lower limit for gain which is not a constant but a function of X, Y and Z.

Integral action incorporated into equation (3.27) gives

$$\bar{F}_c = K_c\, Y + \frac{1}{T_I} \int Y\, dt \qquad (3.32)$$

Substituting this into equation (3.29) and rearranging gives

$$K_c = \frac{-V_c\, \tau_3}{(\gamma_{OSS} - \gamma_{SS} - Z)} - \frac{Y}{(T_I\, dY/_{dt})} \qquad (3.33)$$

The first part on the right hand side of equation (3.33) is the same as equation (3.30) with an approximate numerical value of 4.1435×10^{-3}. Normally when Y is greater than zero (i.e. tank temperature greater than the S.S. value) then dY/dt should be less than zero in order to have stable behaviour. Then the second part of equation (3.33) $(-Y/(T_I\; dY/_{dt}))$ is greater than zero, thereby indicating that the gain should be greater for a P+I controller than for P controller for the same stability behaviour.

If derivative action is introduced to make

$$\bar{F}_c = K_c Y + T_D \frac{dY}{dt} \tag{3.34}$$

then equation (3.29) becomes

$$K_c = \frac{-V_c (\tau_3)}{(\gamma_{OSS} - \gamma_{SS} - Z)} - T_D J_{22} \tag{3.35}$$

Since $-J_{22}$ is greater than zero, as per equation (3.16), equation (3.35) shows that the gain value obtained for P+D controller should be greater than the gain obtained for a P controller for the same stability behaviour. From equations (3.33) and (3.35) it can be seen that the addition of integral or derivative action to proportional controller does not improve the stability of the system. If a controller of the form

$$\bar{F}_c = f(Y) \tag{3.36}$$

is assumed, where coolant flow is some function of Y then substituting into equation (3.29) gives

$$\tau_3 + \frac{1}{V_c} \frac{d\{f(Y)\}}{dY} (\gamma_{OSS} - \gamma_{SS} - Z) = 0 \tag{3.37}$$

or $$\int d\{f(Y)\} = -\tau_3 V_c \int \frac{dY}{(\gamma_{OSS} - \gamma_{SS} - Z)}$$

If Y is assumed to be independent of Z then

$$\bar{F}_c = \frac{-\tau_3 V_c Y}{(\gamma_{OSS} - \gamma_{SS} - Z)} \tag{3.38}$$

an equation similar to (3.27)with a value of K_c given in equation (3.30).

If the coolant flowrate is assumed to be a function of jacket temperature, Z

$$\bar{F}_c = f\ (Z) \tag{3.39}$$

then from equation (3.17)

$$-\tau_2 - \frac{\bar{F}_c}{V_c} + \frac{1}{\bar{V}_c}\frac{d\bar{F}_c}{dZ}\ (\gamma_{OSS} - \gamma_{SS} - Z) < 0$$

on integrating the equation for values of $Z > (\gamma_{OSS} - \gamma_{SS})$, it gives:

$$\bar{F}_c > \frac{V_c \tau_2 (-Z)}{(\gamma_{SS} - \gamma_{OSS} + Z)} \tag{3.40a}$$

and integration for values of $Z < (\gamma_{OSS} - \gamma_{SS})$ gives

$$\bar{F}_c < \frac{V_c \tau_2 (-Z)}{(\gamma_{SS} - \gamma_{OSS} + Z)} \tag{3.40b}$$

These equations simply specify an upper or lower limit to coolant flowrate.

If coolant flow is assumed to be both a function of Y and Z of the form

$$\bar{F}_c = f\ (Y, Z) \tag{3.41}$$

then simultaneously satisfying equation (3.29) and (3.17) will increase the stability region, i.e. to make

$$\frac{d\bar{F}_c}{dZ}\ (\gamma_{OSS} - \gamma_{SS} - Z) < 0 \tag{3.42}$$

and

$$\tau_3 + \frac{1}{V_c} \frac{d\bar{F}_c}{dY} (\gamma_{OSS} - \gamma_{SS} - Z) = 0 \tag{3.43}$$

Equation (3.42) is true if for values of $Z > (\gamma_{OSS} - \gamma_{SS})$, $\frac{d\bar{F}_c}{dZ}$ is > 0, ie when Z increases $\bar{F}_c$ increases and vice versa. Equation (3.43) can be expressed as

$$\bar{F}_c = \tau_3 V_c \int \frac{dY/dt}{(\gamma_{SS} - \gamma_{OSS} + Z)} dt$$

The term inside the integral has to be integrated numerically if this type of control strategy has to be applied to the system. The equations (3.13) to (3.18) are plotted in Fig. (3.10) for proportional control of the tank temperature.

The analysis carried out in this subsection is based on equations (3.13)-(3.18) which assumes a unit matrix as the Liapunov matrix. If some positive definite symmetric matrix is considered as Liapunov matrix then equations (3.21)-(3.26) have to be analysed in the same manner as above. It can be seen from these equations, unlike the previous case, conditions S_2, S_3, S_4, S_5 and S_6 are dependent on the control strategy chosen (equations (3.21)-(3.26)). Strengthening these conditions increases the stability region as mentioned before.

If S_7 is made equal to zero then condition S_4 is strengthened and S_5 (equation (3.25)) becomes

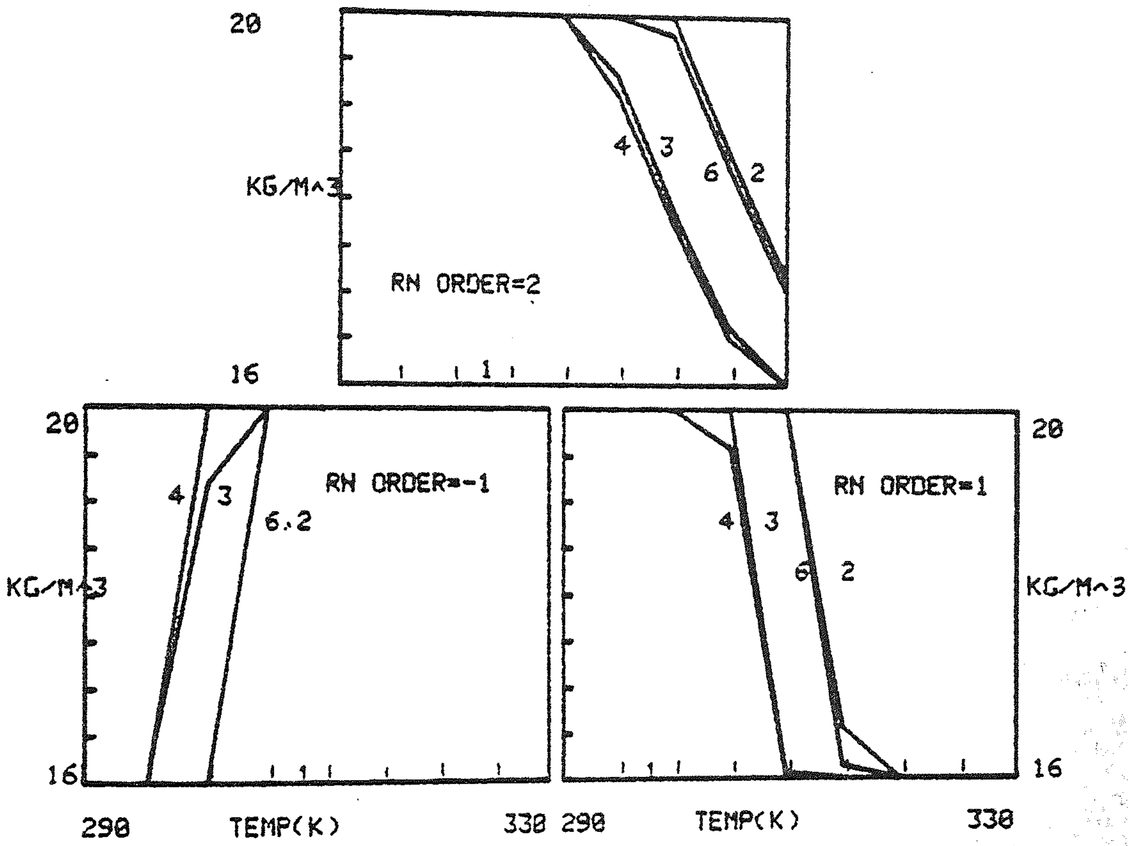


FIG.3.10 SEPARATRICES 1 TO 6 FOR VARIOUS REACTION ORDERS UNDER CONTROL OF THE TYPE GIVEN IN EQN.(3.27) (REFER TABLE(3.6) FOR GAIN VALUES) (A= I)

$$S_5 = S_1S_2S_3 - S_1S_9{}^2 - S_2S_8{}^2 > 0 \tag{3.44}$$

and if S_9 is made equal to zero then condition S_6 is strengthened and S_5 becomes

$$S_5 = S_1S_2S_3 - S_3S_7{}^2 - S_2S_8{}^2 > 0 \tag{3.45}$$

So if $(-S_3S_7{}^2) > (-S_1S_9{}^2)$ then S_9 can be made equal to zero or if the reverse is true then S_7 can be made equal to zero. If S_7 is made equal to zero then the equation for $\bar{F}_c$ is

$$\frac{A_{13}(\gamma_{OSS}-\gamma_{SS} - Z)}{V_c} \bar{F}_c = \{A_{12}(\tau_1 + \frac{1}{\tau}) - A_{13}/\tau_I\}Y$$

$$+ \quad \{(A_{11}-A_{12}) K_1(X + \alpha_{SS})^n e^{-Q/Y+\beta_{SS}}\} + \{(A_{12}-A_{22}) K_1 n$$

$$(X+\alpha_{SS})^{n-1}\} \int e^{-Q/(Y+\beta_{SS})} dY + K_{int}.$$

where K_{int} is the constant of integration. An approximate analytical solution for the integral can be obtained by expanding the term $e^{\frac{-Q}{(Y+\beta_{SS})}}$ by Maclauren's series and integrating.

If $\bar{F}_c$ is assumed to be a function of Z alone then S_3, S_5 and S_6 are affected because of the presence of term J_{33}. Condition S_6 requires

$$S_3 >= S_9{}^2 / S_2$$

while condition S_5 specifies

$$S_3 > \{S_1S_9{}^2 + S_2S_8{}^2 + 2\,S_7{}^2\} / S_4$$

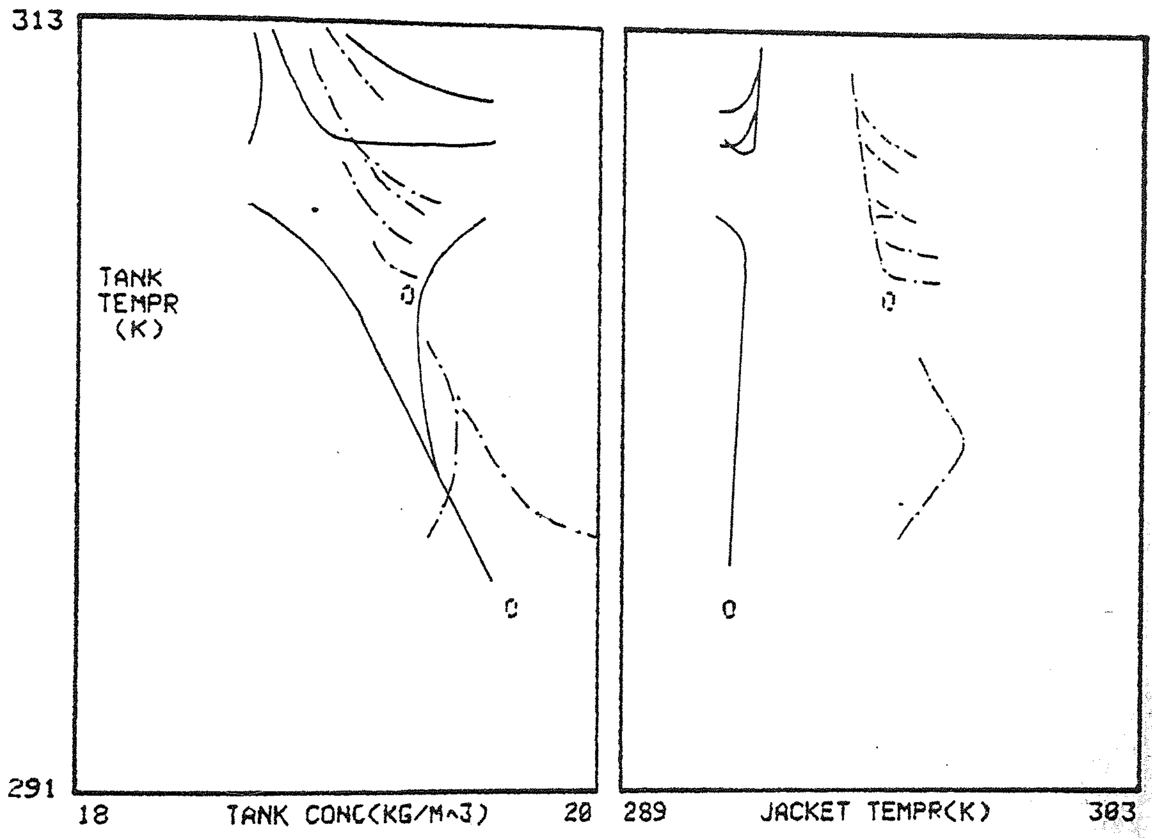
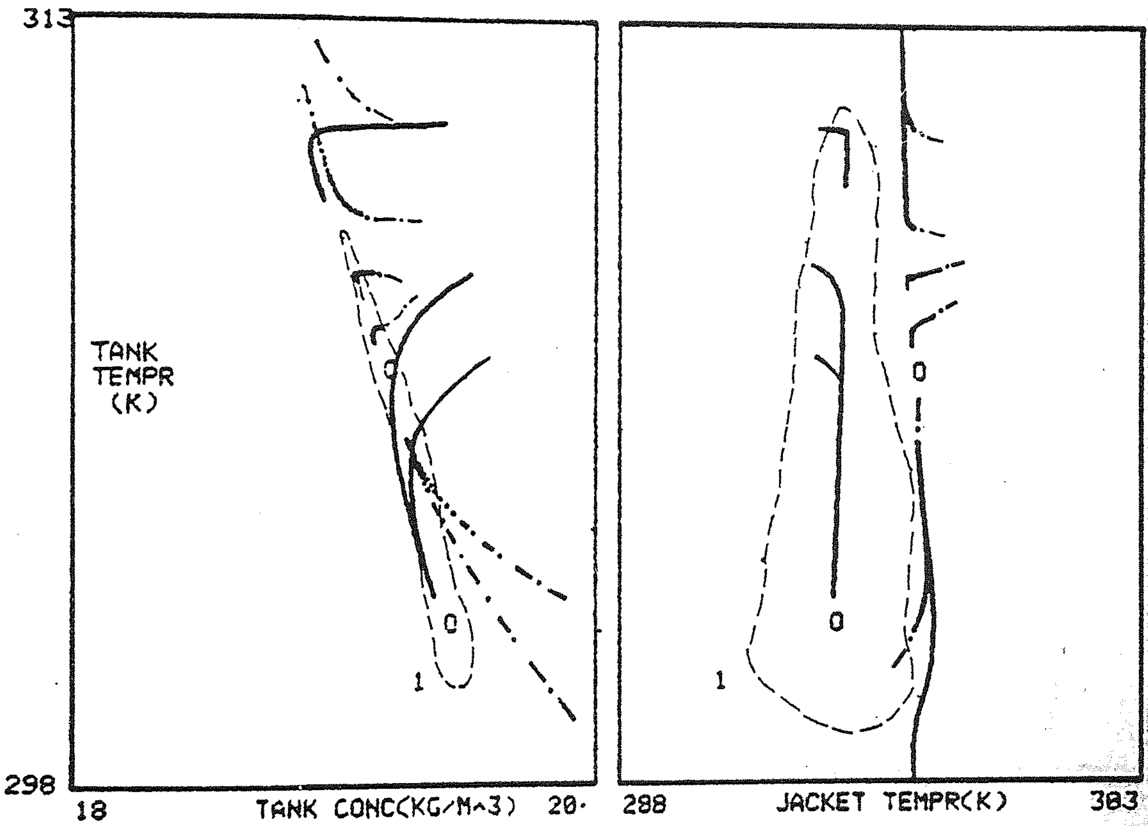


FIG.3.11 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=-1 FOR CONTROL OF THE TYPE GIVEN IN EQN.(3.27) (K_c=0.00445)

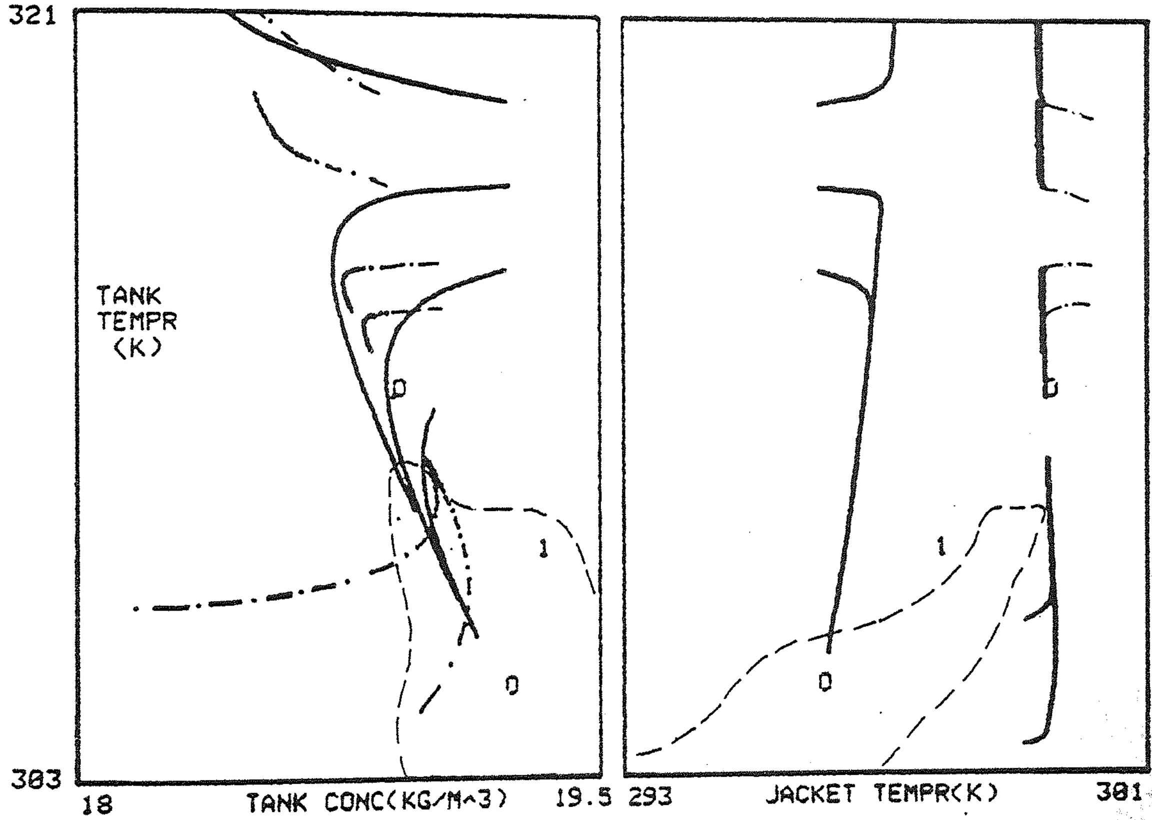


0 = Open loop stable /unstable operating points

1 = Liapunov contour of RAS

K_L=0.00425; volume=0.884x10^{-5}

FIG.3.12 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=0 FOR CONTROL OF THE TYPE GIVEN IN EQN.(3.27) (K_c=0.003)



0 = Open loop stable/unstable operating points
1 = Liapunov contour of RAS
K_L=0.012; volume=0.24×10^{-4}

FIG.3.13 PHASE-SPACE OF THE C.S.T.R. SYSTEM FOR REACTION ORDER=1 FOR CONTROL OF THE TYPE GIVEN IN EQN.(3.27) (K_c=0.002)

3.9.3 Effect on Dynamic Behaviour

The analysis carried out assuming a positive definite symmetric matrix as the Liapunov matrix is cumbersome and complicated. However, an accurate picture of the system can be obtained by numerically integrating the state equations for various reaction orders and control strategies. The computer program described in the previous section is used to study the transient behaviour for proportional type control of tank temperature and the results plotted in Figs. (3.11)-(3.13) for various reaction orders. It can be seen that the unstable point is stabilised by the introduction of this control, while oscillations are induced around the stable operating point. Although the numerical solution procedure is time consuming, it gives the exact behaviour of the system around the equilibrium points, but will be very tedious for higher order systems. The effects of other control strategies on the system behaviour described in this sub-section are not plotted but they were tried out experimentally on the reactor.

3.10 INTERACTION AND DECOUPLING

The system under consideration is an interacting multivariable one. The problem gets complicated because of the superimposition of interactions on external disturbances. There is however a fundamental difference between the effect of external disturbances and the effect of coupling coefficients. External disturbances do not affect the stability of the system as a whole, whereas the coupling coefficients, or in the general case the coupling operators, have a substantial influence on system stability.

Non-interaction is said to be achieved if the controlled variation of one of the variables does not influence the other variables. The three state variables, under consideration, can be decoupled to achieve

$$\frac{dX}{dt} = - D_1 X$$

$$\frac{dY}{dt} = - D_2 Y$$

$$\frac{dZ}{dt} = - D_3 Z$$

where $D_i^{'}$s are constants, with the help of three control parameters. In the present study only one state variable (i.e. Y) is decoupled, since only the coolant flowrate can be used as the manipulative variable.

If the load disturbances are assumed to enter the system through feed and coolant temperatures then equations (3.10)and (3.11) can be rewritten as

$$\frac{dY}{dt} = - \tau_1 Y + \frac{\beta_o}{\tau} + \frac{Z}{\tau_o} + R(X,Y) \tag{3.46}$$

$$\frac{dZ}{dt} = - \tau_2 Z + Y/_{\tau_I} + \frac{\gamma_o}{\tau_c} + \frac{\bar{F}_c}{V_c}(\gamma_o - \gamma_{SS} - Z + \gamma_{OSS}) \tag{3.47}$$

Decoupling of state variable Y is said to be achieved if it is possible to write an equation of the form

$$\frac{dY}{dt} = - DY \tag{3.48}$$

where D is a constant

An algebric equation for the coolant flowrate can be obtained by rearranging equation (3.47) to yield

$$\bar{F}_c = \{\dot{Z} + \tau_2 Z - Y/\tau_I - \gamma_o/\tau_c\} \frac{V_c}{\{\gamma_{OSS} + \gamma_o - \gamma_{SS} - Z\}} \quad (3.49)$$

where Z is given by solving equations (3.46) and (3.48) together. Thus

$$Z = (-DY + \tau_1 Y + \beta_o/\tau - R\,(X,Y))\,\tau_o \quad (3.50)$$

The constant D, otherwise known as the exponential decay constant, determines the speed of response. The larger the value of D, the faster will be the response, and the larger will be the coolant rate. As the pump capacity fixes an upper limit to the cooling water flowrate it is possible only to achieve piecewise decoupling, i.e. a condition in which D is modified so that the coolant rate is within the maximum allowable value.

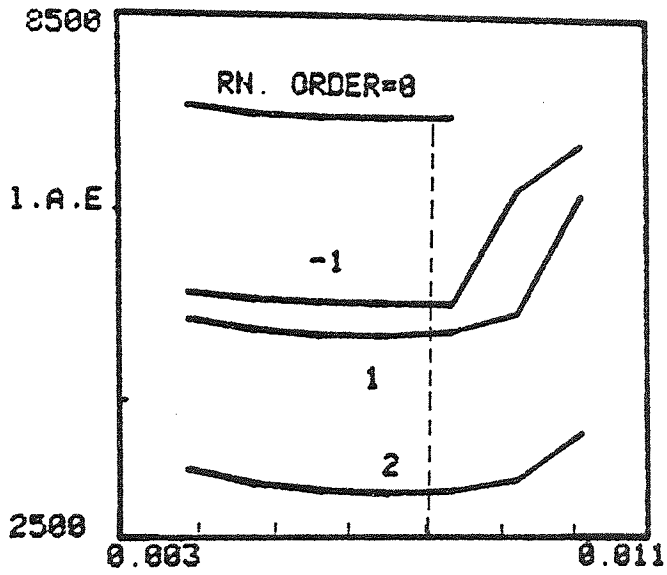
The piecewise decoupling procedure consists of the following steps

a) Take a large value for D ($=D_{max}$)

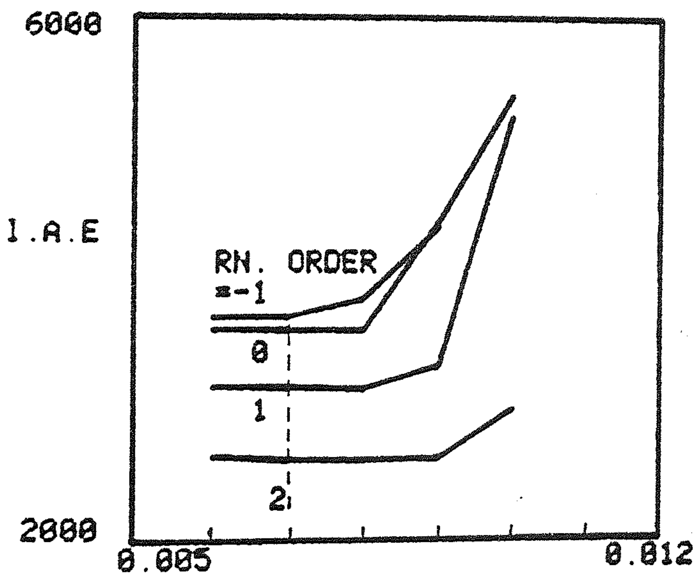
b) Solve equations (3.49) and (3.50) for $\bar{F}_c$

c) Check whether $\bar{F}_c \leq F_{cUL} - F_{cSS}$ and $\bar{F}_c \geq -F_{cSS}$

If so, set that value of coolant flowrate; otherwise reduce D by 10% and go to step b).



A)FOR CONDITIONS IN TABLE(3.1 & 2)



B)FOR CONDITIONS IN TABLE(3.3)

FIG.3.14 D_{max} versus IAE FOR VARIOUS REACTION ORDERS AND TWO DIFFERENT OPERATING CONDITIONS

This iterative procedure requires a digital computer as the controller. When perturbations are large the value of D will be small so as to maintain the coolant flowrate below the maximum value and as perturbations die down the value of D reaches the D_{max} value. An optimum value for D_{max} determines the minimum settling time for the system. The effect of D_{max} on the integral of the absolute error (IAE) can be determined theoretically by simulating the system for various D_{max} values and same starting conditions. A plot of IAE versus D_{max} for various orders is shown in Fig. (3.14). It is seen that the error is a minimum for $D_{max} = 0.007$. A large D_{max} value increases the speed at which perturbations die down, while too large a value also induces oscillations thereby increasing the settling time. It is also seen from Fig. (3.14 a) and (b) that irrespective of operating conditions or reaction orders the minimum IAE is for a D_{max} value of 0.007. The behaviour of the system for various reaction orders under the action of this control is shown in Figs. (3.15)-(3.18). The same computer program described in sub-section (3.8.2) is used to simulate the system response for various starting conditions. It can be seen that the stability region is increased enormously and the operating point is a stable node thereby improving the transient response.

The tank temperature and hence the tank concentration is made invariant from load changes in feed or coolant inlet temperatures by this control scheme. Theoretical studies carried out show that overshoot is negligible for step in feed temperature of the order of 3K and there are no oscillations on the system response. For larger load changes the coolant flowrate reaches the upper limit and hence perfect decoupling is not achieved.

$\dot{Z}$ in equation (3.49) can be calculated by numerical differentiation or by differentiating equation (3.50) to arrive at an analytical solution. It was found that the latter method gave a better system performance than the former.

3.10.1 Effect of Decoupling Type Control on Stability

The effect of this control on the stability of the C.S.T.R. can be analysed in the same manner as described in section (3.8). Control affects most of the elements of the Jacobian matrix to give

$$J_{21}, J_{23} = 0$$

$$J_{22} = -D$$

$$J_{31} = \frac{d\bar{F}_c}{dY} \frac{(\gamma_{OSS} + \gamma_O - \gamma_{SS} - Z)}{V_c}$$

$$J_{32} = {}^1/_{\tau_I} + \frac{d\bar{F}_c}{dY} \frac{(\gamma_{OSS} + \gamma_O - \gamma_{SS} - Z)}{V_c}$$

$$J_{33} = -\tau_2 + \frac{d\bar{F}_c}{dZ\, V_c} (\gamma_{OSS} + \gamma_O - \gamma_{SS} - Z) - \frac{\bar{F}_c}{V_c}$$

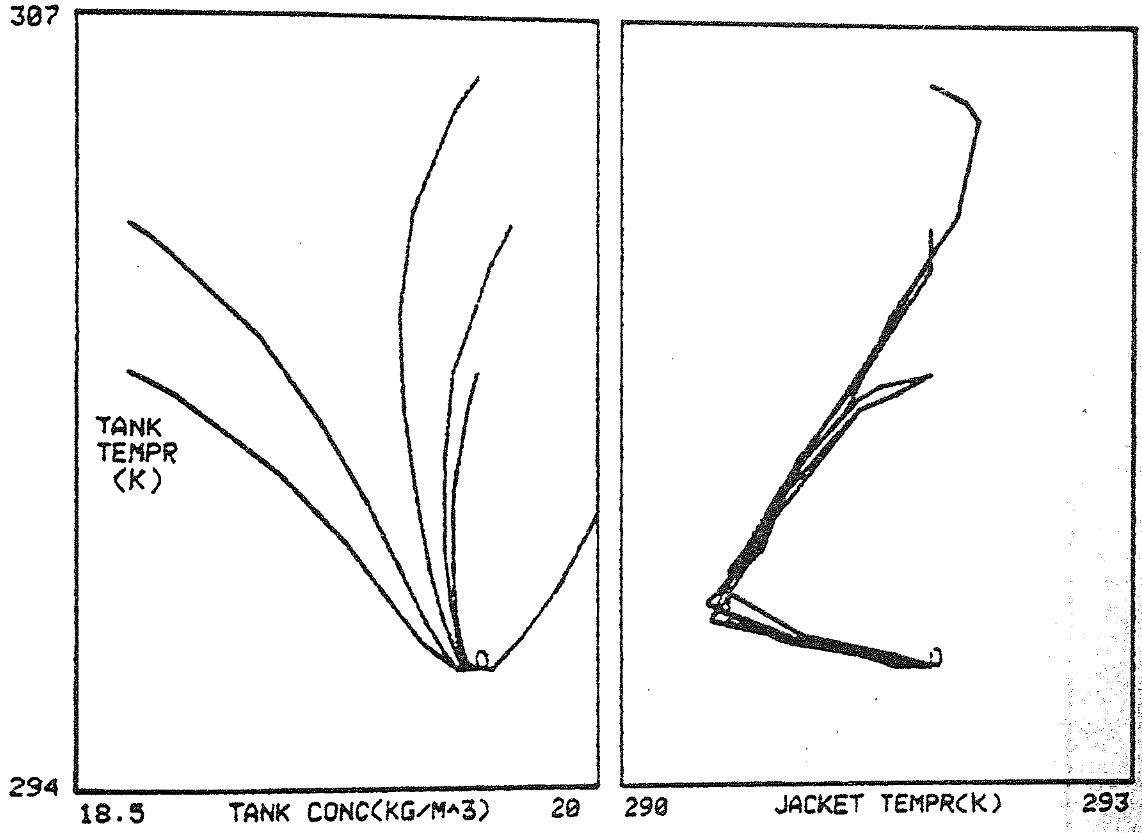
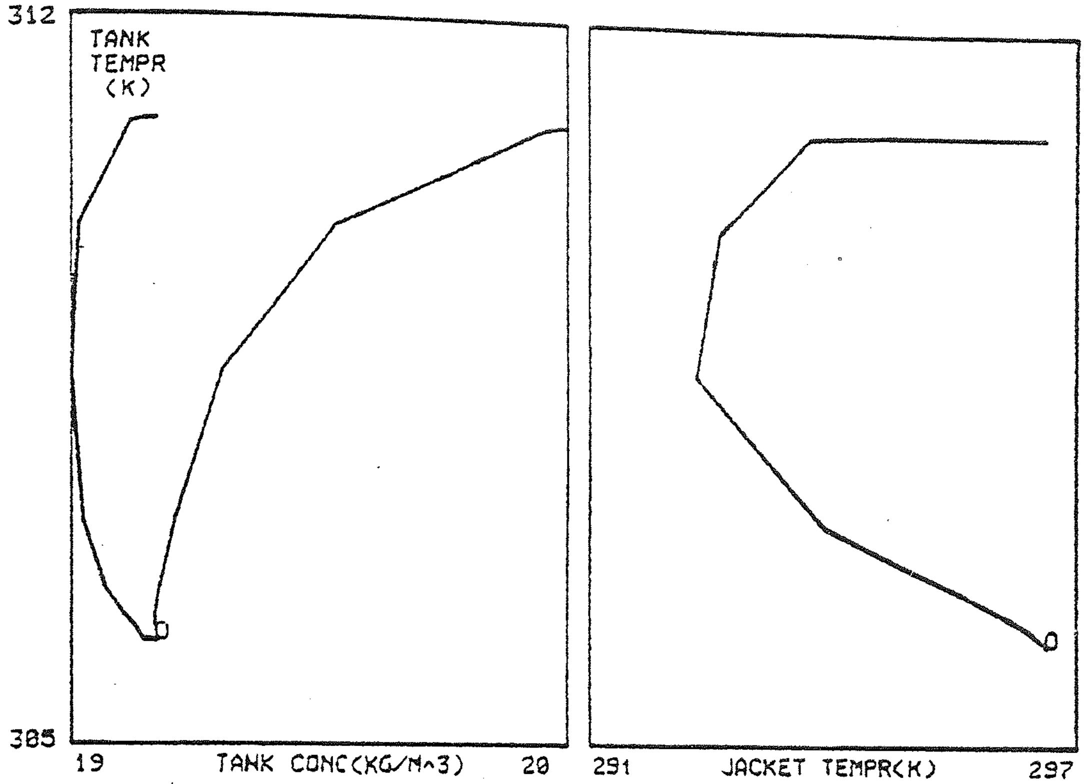
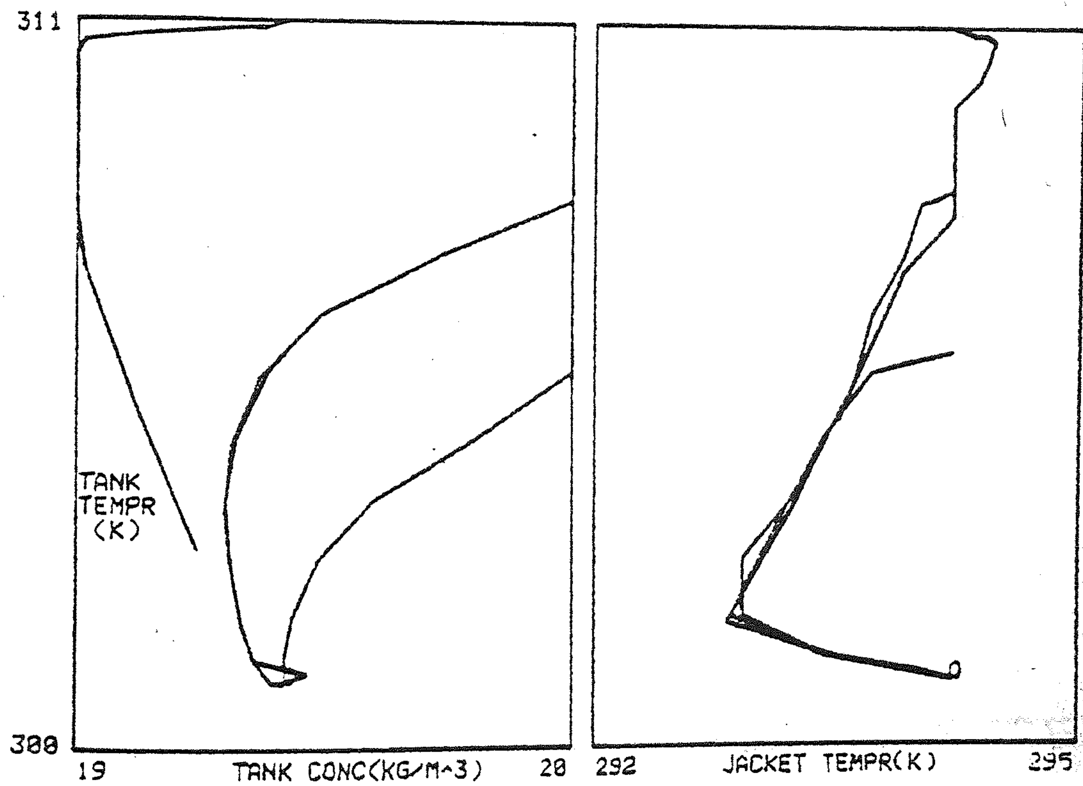


FIG.3.15 DECOUPLING TYPE CONTROL OF THE C.S.T.R. FOR REACTION ORDER= -1 (AT OPEN LOOP STABLE POINT)

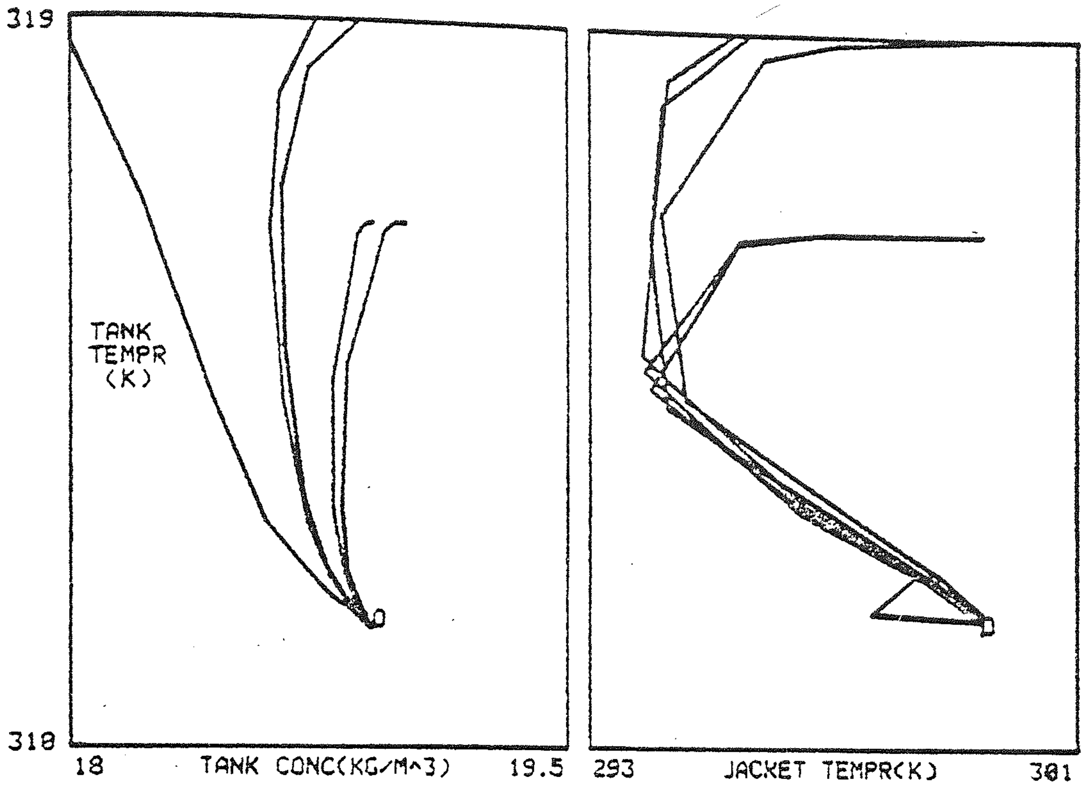


A) AT OPEN LOOP UNSTABLE POINT

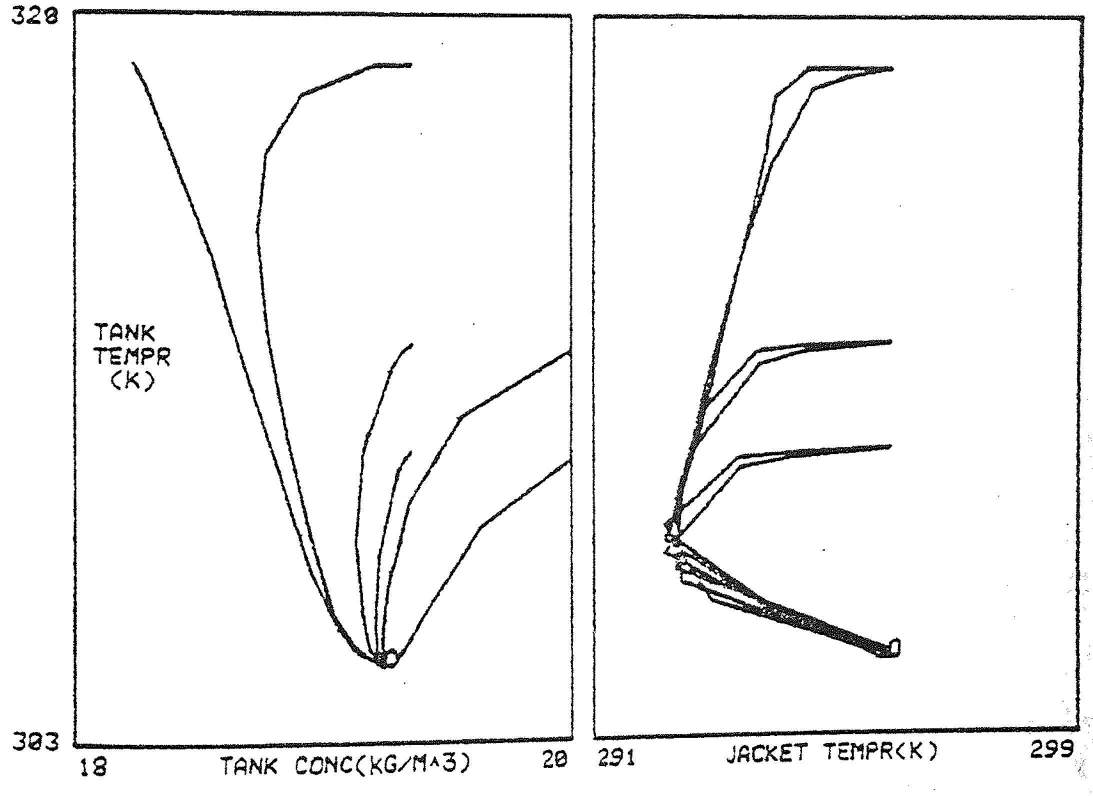


B) AT OPEN LOOP STABLE POINT

FIG.3.16 DECOUPLING CONTROL OF THE C.S.T.R. FOR REACTION ORDER= 0



A) AT OPEN LOOP UNSTABLE POINT



B) AT OPEN LOOP STABLE POINT

FIG.3.17 DECOUPLING TYPE CONTROL OF THE C.S.T.R. FOR REACTION ORDER= 1

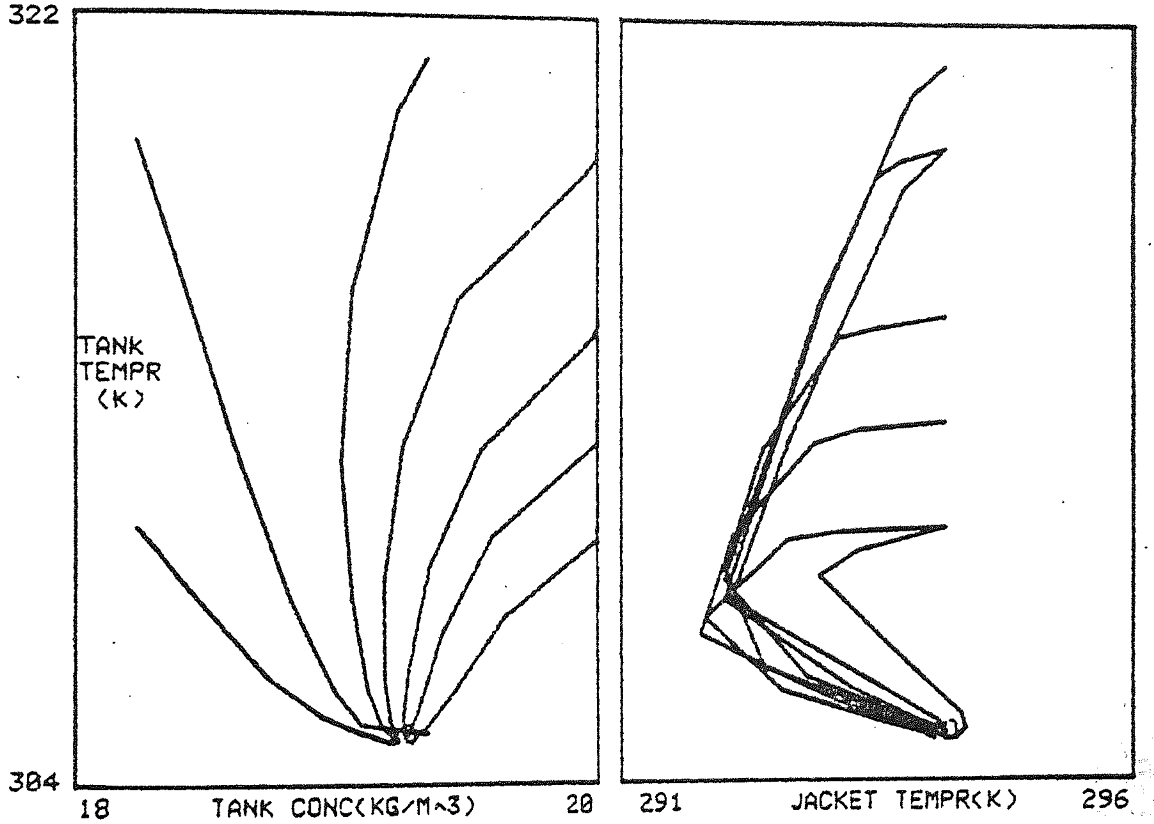


FIG.3.18 DECOUPLING TYPE CONTROL OF THE C.S.T.R. FOR REACTION ORDER= 2(AT OPEN LOOP STABLE POINT)

If these values are substituted into equations (3.13)-(3.18) then the separatrices become

$$S_1 = -2\ J_{11}$$

$$S_2 = -4\ J_{11}\ D - J_{12}^{\ 2}$$

$$S_3 = S_1 S_6 + 2\ J_{33}\ J_{12}^{\ 2} - 2\ J_{31} J_{12} J_{32} - 2\ J_{31}^{\ 2}\ D$$

$$S_4 = 2D$$

$$S_6 = -4\ J_{33} D - J_{32}^{\ 2}$$

It can be seen that conditions S_2, S_4, S_6 and hence S_3 are strengthened while S_1 remains unchanged. The larger the value of D, the stronger will be some of the separatrices.

3.11 INVARIANCE CONTROL

The principle of invariance, when applied to multi-variable control systems, will give the calculated relationships permitting selection of parameters of the system, so that one or more of its generalised coordinates will be independent of one or several disturbing influences applied to the system. Invariance of state variable is said to be achieved if

$$X = 0 \text{ and } \frac{dX}{dt} = 0 \qquad (3.51)$$

for zero initial conditions. Substituting these values into equations (3.9), (3.46) and (3.47) the following relationships are obtained

$$Y = 0 \text{ and } {dY}/{dt} = 0 \qquad (3.52)$$

$$\Xi = -\beta_o \tau_o / \tau$$

since β_o is a constant

$$\frac{d\Xi}{dt} = 0 \quad \text{and} \tag{3.53}$$

$$\bar{F}_c = \frac{\{\gamma_o/_{\tau_c} + \beta_o(\tau_o/_\tau)\tau_2\}V_c}{\{\gamma_{SS}-\gamma_{OSS}-\gamma_o-\beta_o\tau_o/_\tau\}} \tag{3.54}$$

$\bar{F}_c$ is a function of the operating parameters and step disturbances entering the system. When numerical values are taken from Tables (3.1) and (3.2) and substituted into equation (3.54) and, taking into account the upper limit on coolant flowrate, the inequality relationship:

$$5.88\ \bar{T}_{CO} + 3.49\ \bar{T}_O \leq T_{CSS}-T_{COSS} \tag{3.55}$$

is obtained. It can be seen (Fig (3.19)) from the plot of this equation, for the invariance of state variable X and Y that the load changes should be within the shaded portion of the graph. It can also be seen that step disturbances in feed temperature have a much more serious effect than steps in coolant temperature.
If disturbances entering the system are only due to a step in coolant temperature than equation (3.54) simplifies to

$$\bar{F}_c = \frac{\gamma_o\ V_c/_{\tau_c}}{(\gamma_{SS}-\gamma_{OSS}-\gamma_o)} \tag{3.56}$$

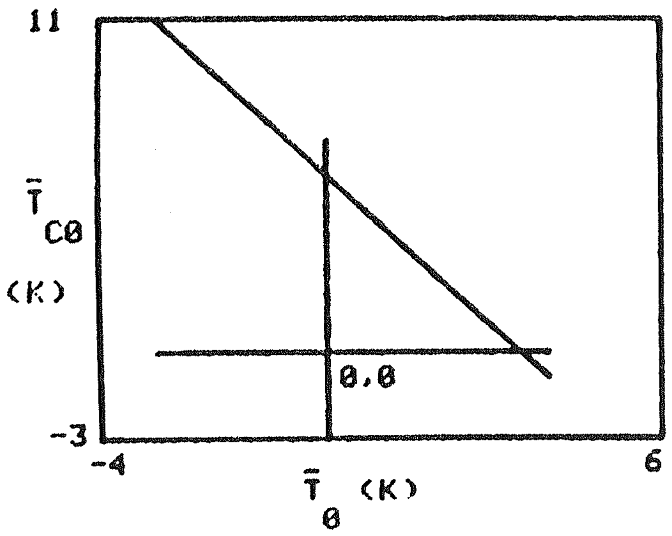
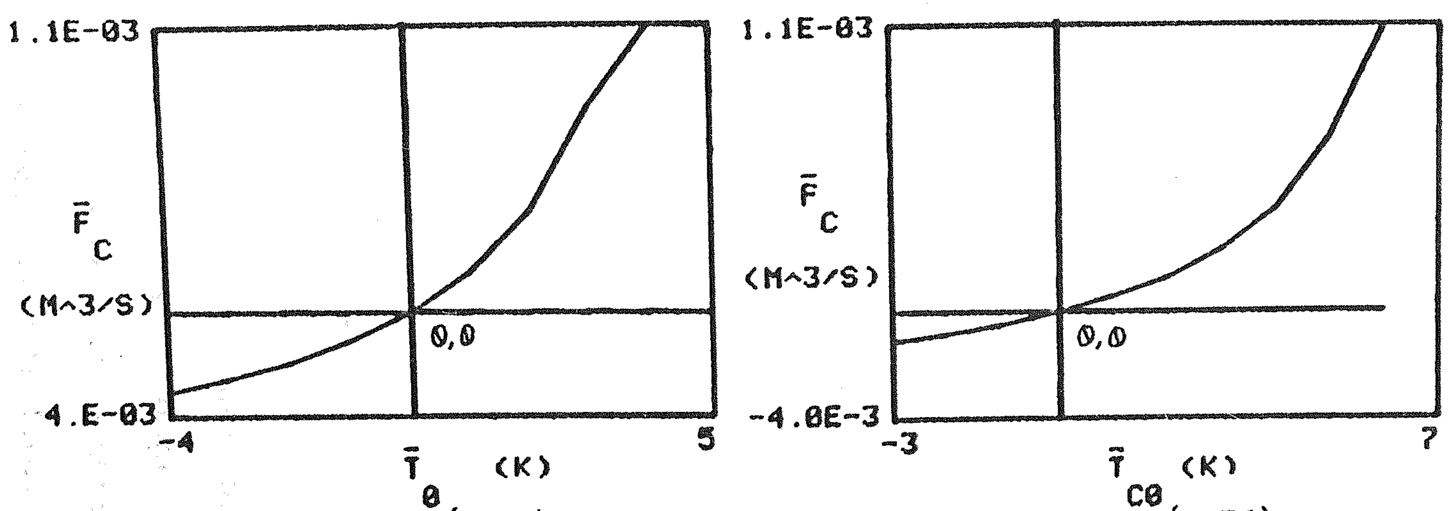


FIG.3.19 REGION OF INVARIANCE FOR STEP IN FEED AND COOLANT TEMPERATURES



A) EQUATION(3.57)

B) EQUATION(3.56)

FIG.3.20 EFFECT OF STEP CHANGES IN COOLANT AND FEED TEMPERATURES ON COOLANT FLOWRATE and $Z = 0$. This means that the invariance of the complete system (i.e. for all three state variables) is achieved when $\beta_o = 0$.

From equation (3.54) it can be seen that the control strategy is similar to feed-forward control, though it is derived from the state equations. The physical characteristics of the reactor and the operating points also affect the manipulated variable.

If disturbances are entering the system only through a step in tank inlet temperature then an equation similar to equation (3.56) is obtained

$$\bar{F}_c = \frac{\beta_o \frac{\tau_o}{\tau} \tau_2 V_c}{(\gamma_{SS} - \gamma_{OSS} - \beta_o \tau_o/\tau)} \qquad (3.57)$$

Equations (3.56) and (3.57) are plotted to find the effect of γ_o and β_o on $\bar{F}_c$ in Fig.(3.20). It can be seen that there is a discontinuity and at that point $\bar{F}_c$ reaches infinity. The discontinuity occurs when

in equation (3.56), $\gamma_o = (\gamma_{SS} - \gamma_{OSS})$

and in equation (3.57) $\beta_o = (\gamma_{SS} - \gamma_{OSS}) \frac{\tau}{\tau_o}$

Though the studies carried out so far have been on invariance control for steps in feed and coolant temperature, similar control equations can be obtained if the load change enters through a step in feed flowrate. Then equations (3.9) and (3.46) will be

$$\dot{X} = -\frac{X}{\tau} + \frac{\bar{F}}{V}(1 - X) - R(X, Y) \quad (3.58)$$

$$\dot{Y} = -\tau_1 Y - \frac{\bar{F}}{V}(\beta_{OSS} + \beta_O - \beta_{SS} - Y) + R(X, Y) + Z/\tau_o + \beta_O/\tau \quad (3.59)$$

where $\bar{F}$ denotes a perturbation value in feed flowrate. Invariance in X, in this case will not mean invariance in Y. For invariance in X, from equation (3.58)

$$Y = \frac{-Q}{\ln K_3} - \beta_{SS}$$

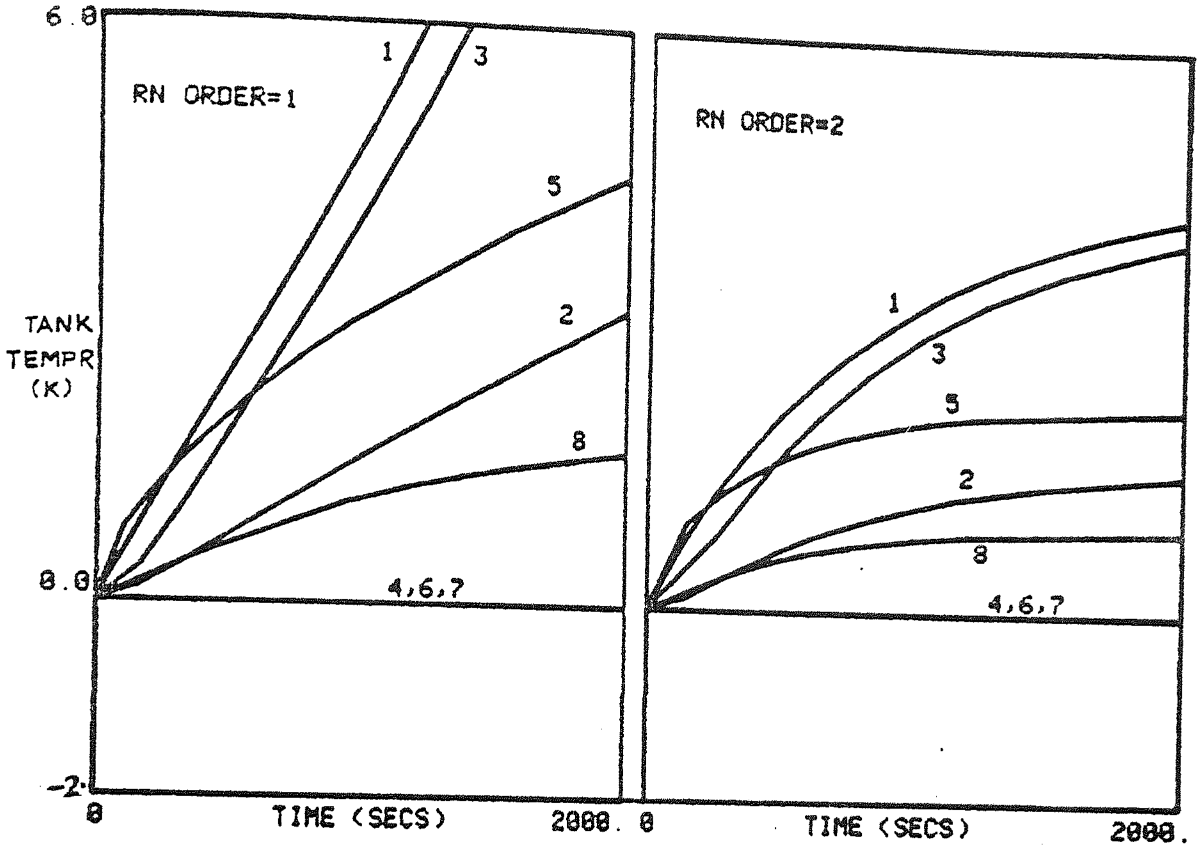
where $K_3 = \frac{\bar{F}}{V K_1 \alpha_{SS}^n} + e^{-Q/\beta_{SS}}$. The equation for Z and hence $\bar{F}_c$ can be obtained from equations (3.59) and (3.47) respectively. The attainment of invariance mainly depends on the following conditions

a) the mathematical model adequately described the system behaviour

b) the theoretically derived controller equations can be accurately executed

c) the control system is allowable by satisfaction of the dual channel condition.

The behaviour of the system for reaction orders one and two under the action of this control is plotted in Fig. (3.21). The superiority of this type of control can be easily seen when, perturbation value of tank temperature ($\bar{T}$) remains zero for some values of disturbance.



1 = Step of 2K in tank inlet temperature (uncontrolled)
2 = Step of 2K in jacket inlet temperature (uncontrolled)
3 = Step of 5K in jacket inlet temperature (uncontrolled)
4 = Step of 2K in tank inlet temperature (Invariance control)
5 = Step of 5K in tank inlet temperature (Invariance control)
6 = Step of 2K in jacket inlet temperature (Invariance control)
7 = Step of 5K in jacket inlet temperature (Invariance control)
8 = Step of 7K in Jacket inlet temperature (Invariance control)

FIG.3.21 INVARIANCE CONTROL FOR VARIOUS LOAD CHANGES

For step load disturbances in feed temperature, the equations for decoupling type control are the same as those for invariance control at t=o. As time increases the two schemes diverge, since there is a feedback loop in the former, while the latter is pure feed-forward control. A more detailed comparison study of these two control schemes with conventional ones is carried out in Appendix 7.

3.12 LIMIT-CYCLES

The limit-cycle behaviour, which is characteristic of a nonlinear system, has been extensively studied for two dimensional systems using Poincare-Bendixon's theorem. The system in phase-space will exhibit a closed curve. The oscillations about the operating point may not always be uniform due to the presence of nonlinearities, thereby exhibiting an average of the performance different from that at stable operation.

The existence of a limit-cycle is studied for a controller of the type

$$\bar{F}_c = - K_c X \qquad (3.60)$$

For the generation of limit-cycles the theory of Bifurcation states that if a system of differential equations contains a variable parameter its solution (trajectories in the phase-plane) also varies; and for some critical or bifurcation values of this parameter, if the characteristics of the equilibrium point changes (stable to unstable or vice versa) then, a limit-cycle is also generated (stable or unstable). The limit-cycle can be classified as a soft or hard type depending on whether or not it contracts to the origin for a particular value of the parameter.

3.12.1 Behaviour of Eigenvalues as Gain is increased

The behaviour of eigenvalues of the characteristic matrix for different gain values is shown in Table (3.8). The elements of the characteristic matrix are obtained from equation (3.12) where, in this particular case

$$J_{31} = -\frac{F_c}{V_c} (\gamma_{OSS} - \gamma_{SS} - \bar{z}) \tag{3.61}$$

It is seen from the table that as the gain value is increased the system ultimately becomes unstable, except for the first case. As stated by the theory of Bifurcation, a stable limit-cycle must be generated when the system becomes unstable from a stable configuration and similarly unstable limit-cycle must be generated when the system becomes stable. The existence of stable limit-cycles for this system can be verified by the second method of Liapunov.

3.12.2 Existence of limit-cycles

The direct method of Liapunov can be used for verifying the existence of stable limit-cycle for three or higher dimensional systems. When an unstable equilibrium point can be shown to have a closed region surrounding it within which $\dot{V}_L$, the time derivative of the Liapunov function V_L is negative, and all regions above and below it are positive then, there should be a closed curve inside this region towards which all

TABLE 3.8 BEHAVIOUR OF THE SYSTEM FOR VARIOUS GAIN VALUES FOR CONTROLLER OF TYPE IN EQUATION (3.60)

$K_c = K_2 \times 10^{-6}$

Reaction order	Nature of operating points	Behaviour of the system
-1	S	sn $\xrightarrow{K_2=1800}$ sf
-1	U	un $\xrightarrow{2300}$ sn $\xrightarrow{2400}$ sf $\xrightarrow{8960}$ uf
0	S	sn $\xrightarrow{1500}$ sf $\xrightarrow{47690}$ uf
0	U	un $\xrightarrow{1500}$ sn $\xrightarrow{1800}$ sf $\xrightarrow{14090}$ uf
1	S	sn $\xrightarrow{1000}$ sf $\xrightarrow{36210}$ uf
1	U	un $\xrightarrow{900}$ sn $\xrightarrow{1200}$ sf $\xrightarrow{10500}$ uf
2	S	sn $\xrightarrow{450}$ sf $\xrightarrow{65840}$ uf

trajectories converge. Since $\dot{V}_L$ is negative inside this region all trajectories converge, and as the equilibrium point is unstable, trajectories near the origin move towards this region. This argument does not hold good if a singular point is present inside the closed region. Again, as mentioned in the previous section, choosing a suitable positive definite symmetric Liapunov matrix constitutes the most important step in this technique. The A matrix is calculated from the relationship given below:

$$J^T A + A J = -I \qquad (3.62)$$

The Jacobian is calculated at the bifurcation value of the gain. The computer program to determine the stability region is given in Appendix (1.4) and the corresponding flowchart in Appendix (2.2).

The program determines the smallest value of $\dot{V}_L$ for various Liapunov values (K_L) and hence a closed region surrounding the equilibrium point within which $\dot{V}_L$ is negative. Table (3.9) gives the results from the program run for various reaction orders. From the table it can be seen that all the systems have a stable limit-cycle, and the limit-cycle expands as the gain is increased. These two facts are verified in the next subsection by simulating the system under these conditions. Reaction order -1 does not seem to possess a limit-cycle around its stable operating point. The other interesting observations made during the course of this study are

TABLE 3.9 REGION WITHIN WHICH $\dot{V}_L < 0$ FOR DIFFERENT REACTION ORDERS AND GAIN VALUES. $K_c = K_2 \times 10^{-6}$

Reaction order	Nature of Open Loop SS point	Gain K_2	Region where $\dot{V}_L<0$		Gain K_2	Region where $\dot{V}_L<0$	
			Minimum K_L	Maximum K_L		Minimum K_L	Maximum K_L
-1	U	9000	0.31×10^{-2}	0.33×10^{-2}	10000	0.34×10^{-2}	0.39×10^{-2}
0	U	15000	0.55×10^{-2}	0.158×10^{-1}	20000	0.115×10^{-1}	0.158×10^{-1}
0	S	48000	0.84×10^{-2}	0.92×10^{-2}	50000	0.89×10^{-2}	0.9×10^{-2}
1	U	12000	0.45×10^{-2}	0.1×10^{-1}	15000	0.12×10^{-2}	0.11×10^{-1}
1	S	36000	0.6×10^{-2}	0.172×10^{-1}	40000	0.72×10^{-2}	0.172×10^{-1}
2	S	66000	0.4×10^{-3}	0.6×10^{-3}	75000	0.5×10^{-3}	0.8×10^{-3}

1) Inherently unstable operating points do not possess a limit-cycle but stable limit-cycles appear only when the operating points become unstable from stable conditions.

2) Stable points become unstable by throwing out stable limit-cycles and the reverse happens with unstable points.

3) The stable and unstable limit-cycles and equilibrium point occur alternately.

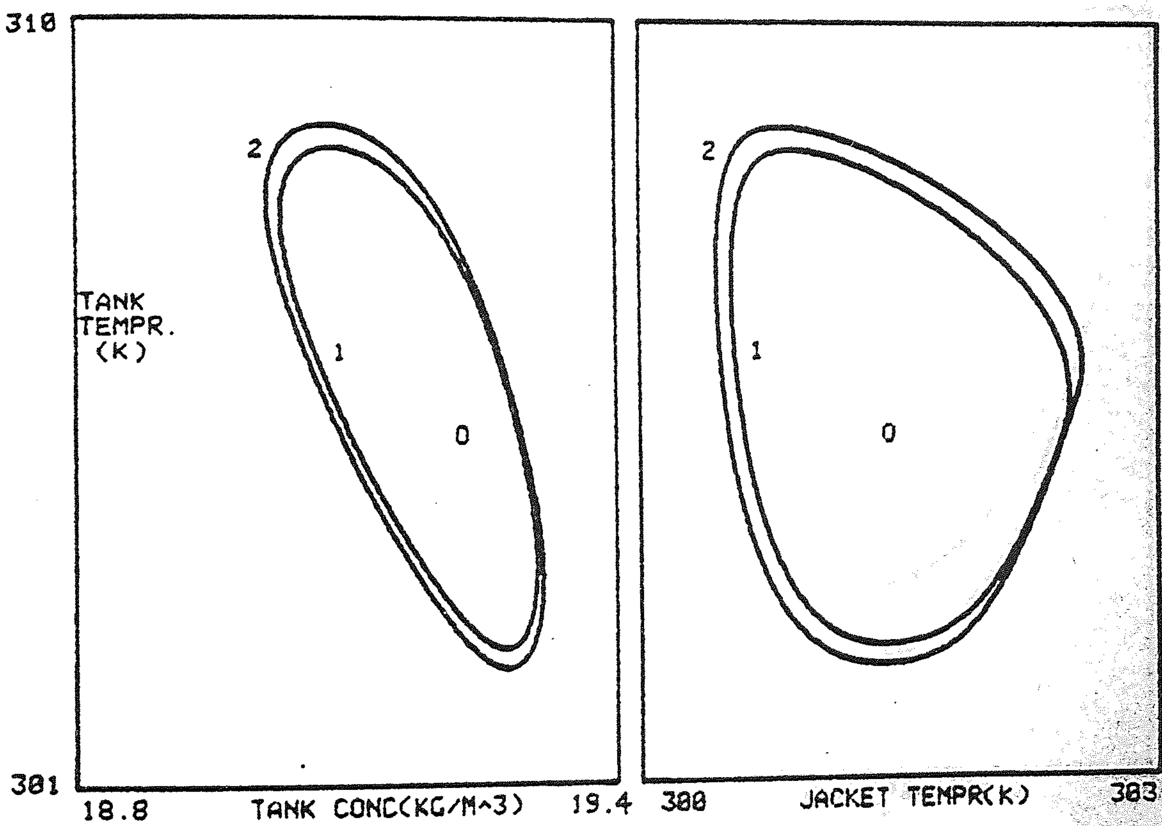
4) Sometimes a stable and an unstable limit-cycle merge together and the reverse action can also take place.

3.12.3 Effect of Reaction order on limit-cycles

The existence of limit-cycles is verified by solving the dynamic equations (3.9)-(3.11) and (3.60) for the gain values specified in Table (3.8) and are plotted in Figs. (3.22)-(3.27). The limit-cycle forms a closed curve in the phase-space and its shape is not perfectly elliptical due to the presence of nonlinearities and the limits on coolant flowrate. The time period of oscillation and the amplitude increases as gain is increased. The amplitude of oscillations is larger around the open loop unstable operating point than the stable point. The amplitude is largest for reaction order one. Table (3.10) gives the amplitude for different reaction orders. As expected -1 order does not possess a limit-cycle around its stable operating point.

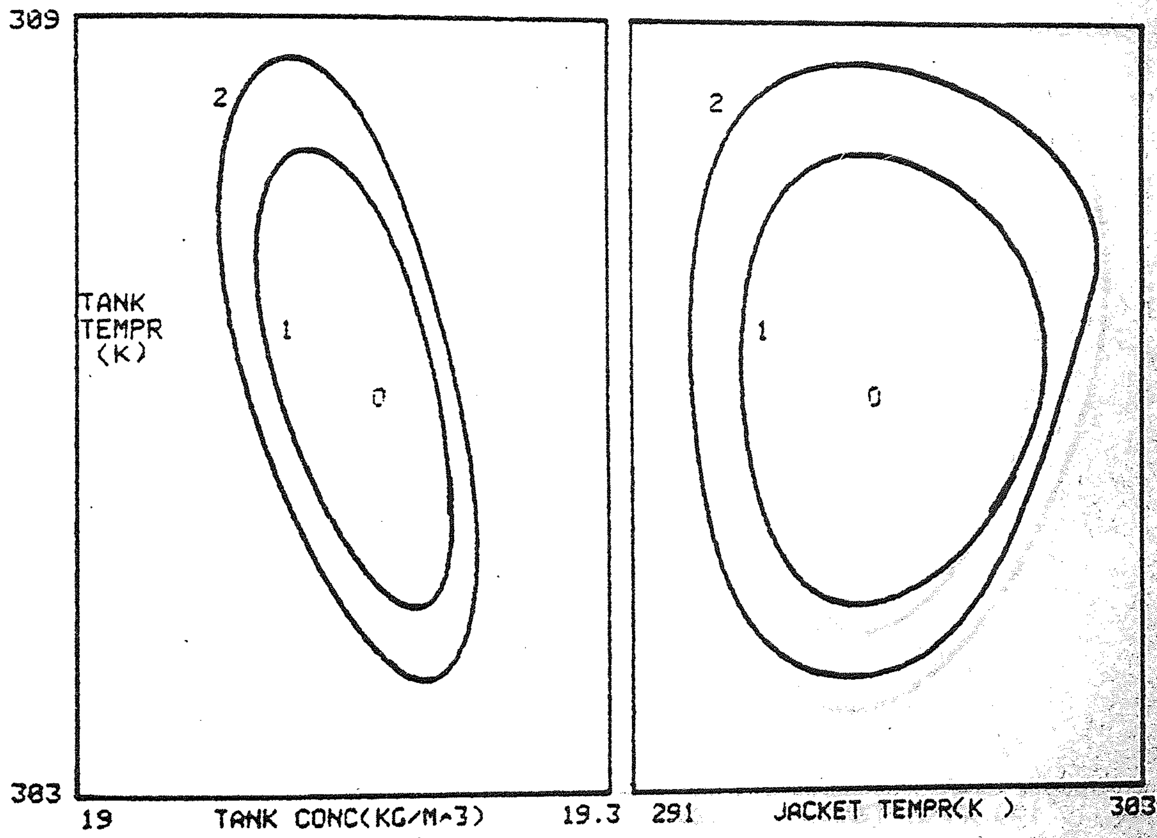
3.12.4 Harmonic Contents of Oscillation

The fundamental harmonics (sine and cosine terms)



0 = Open loop unstable operating point
1 = for gain(K_c)=0.009
2 = =0.010

FIG.3.22 LIMIT-CYCLE FOR REACTION ORDER= -1

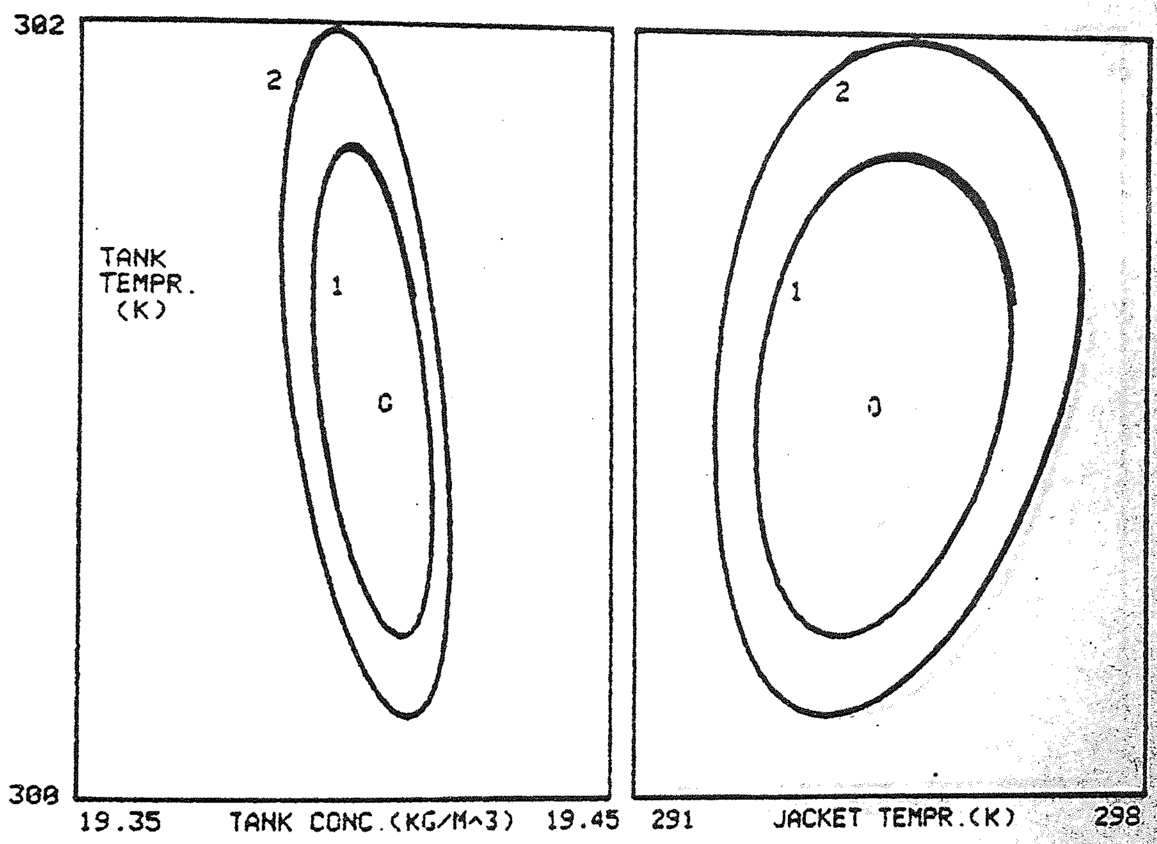


0 = Open loop unstable operating point

1 = for gain(K_c)=0.015

2 = =0.020

FIG.3.23 LIMIT-CYCLE FOR REACTION ORDER= 0

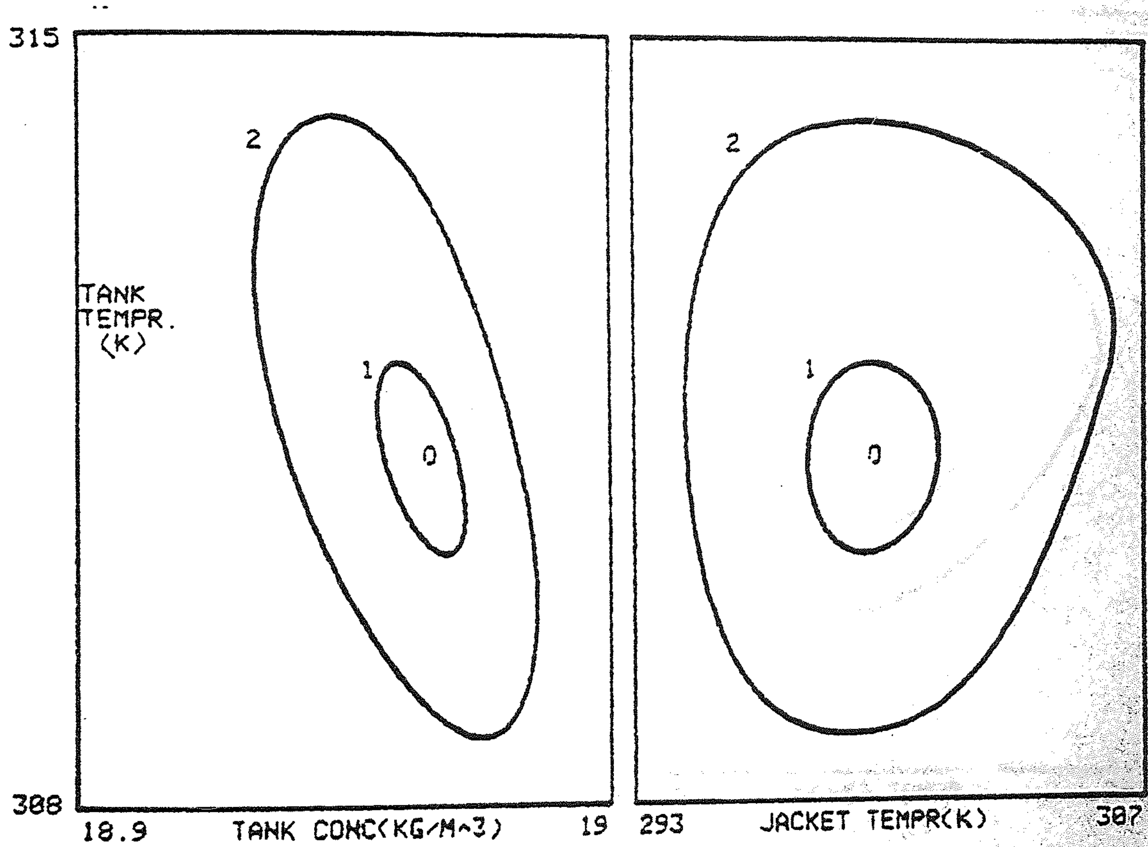


0 = Open loop stable operating point

1 = for gain(K_c)=0.048

2 = =0.050

FIG.3.24 LIMIT-CYCLE FOR REACTION ORDER= 0

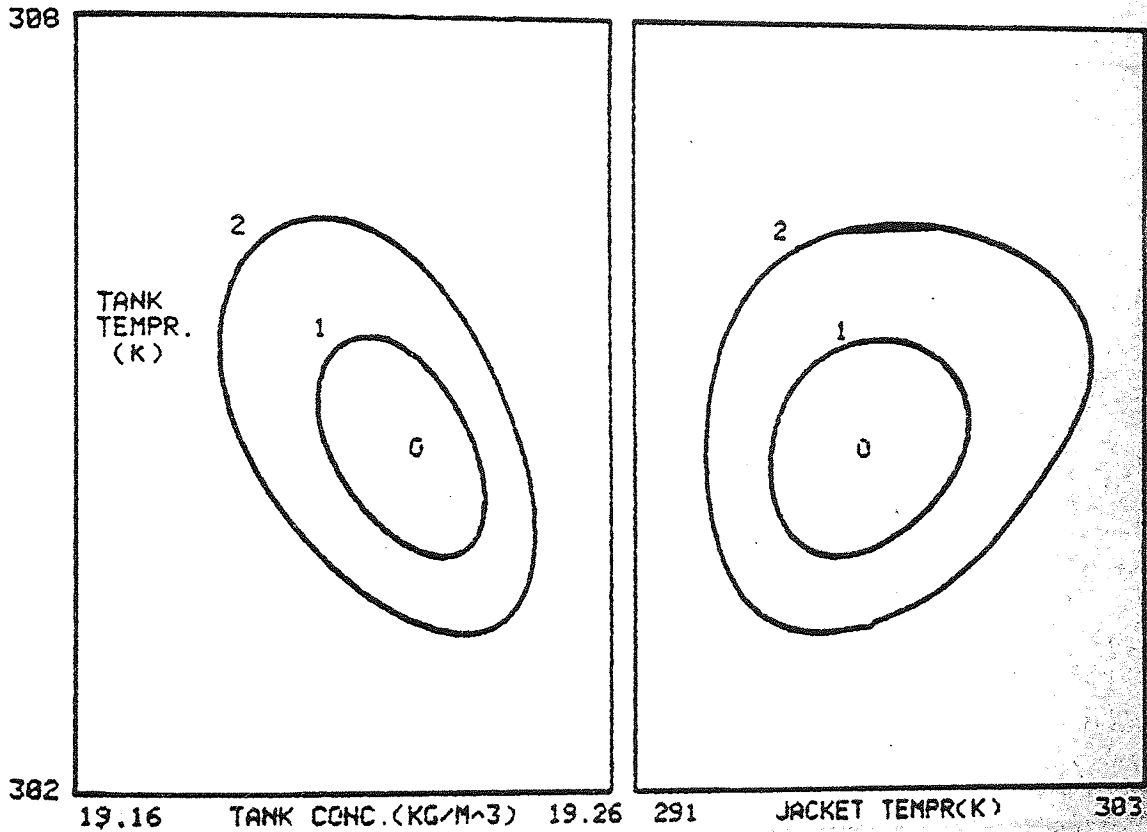


0 = Open loop unstable operating point

1 = for gain(K_c)=0.012

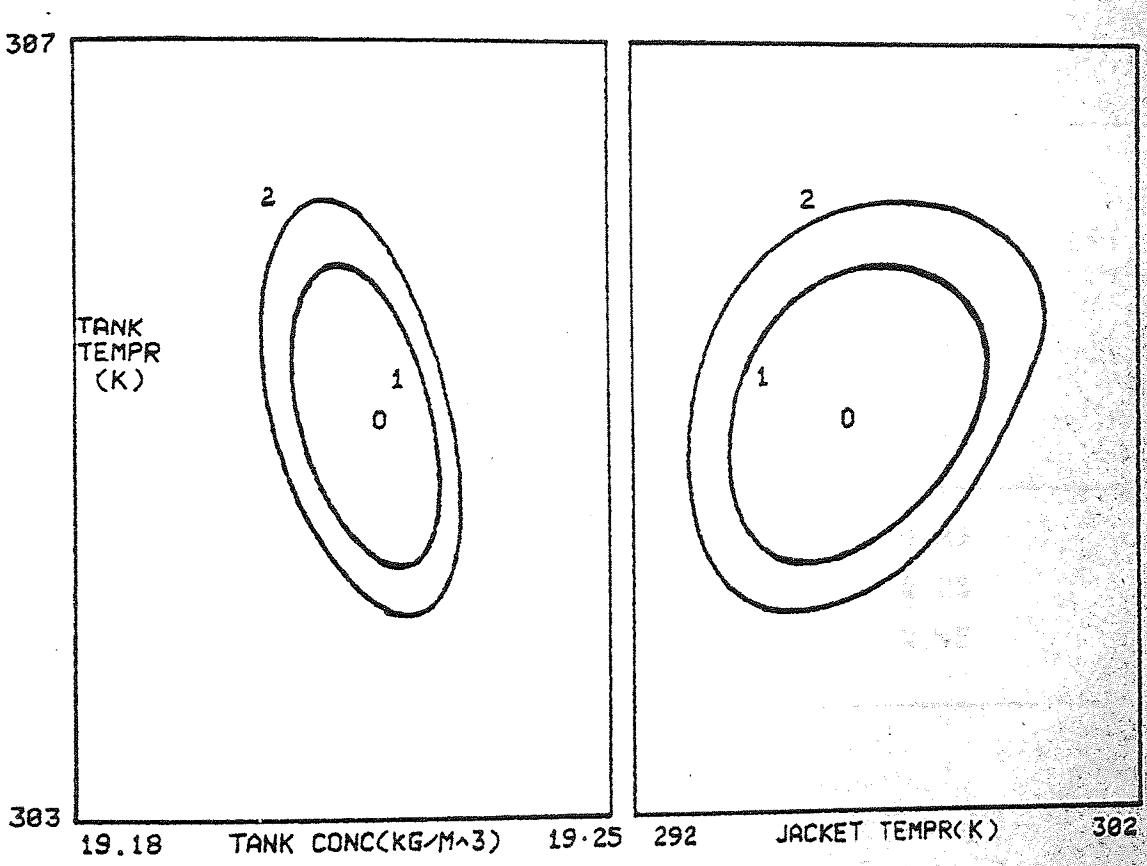
2 = =0.015

FIG.3.25 LIMIT-CYCLE FOR REACTION ORDER= 1



0 = Open loop stable operating point
1 = for gain(K_c)=0.036
2 = =0.040

FIG.3.26 LIMIT-CYCLE FOR REACTION ORDER= 1



0 = Open loop stable operating point

1 = for gain(K_c)=0.066

2 = =0.075

FIG.3.27 LIMIT-CYCLE FOR REACTION ORDER= 2

TABLE 3.10 AMPLITUDE OF OSCILLATION FOR DIFFERENT REACTION ORDERS

Order of Reaction	Nature of Operating Point	Amplitude of Oscillation in Temperature Axis (K)
2	S	1.1
1	S	1.9
0	S	0.875
1	U	2.85
0	U	2.25
-1	U	2.45

in the periodic behaviour can be obtained by approximating the state variables to

$$C = X_o + X_1 \cos wt + X_2 \sin wt \tag{3.63}$$

$$T = Y_o + Y_1 \cos wt + Y_2 \sin wt \tag{3.64}$$

$$T_c = Z_o + Z_1 \cos wt + Z_2 \sin wt \tag{3.65}$$

The constants X_o, X_1 etc. determine the effect of each harmonic on the overall system behaviour. These values can be calculated by substituting equations (3.63)-(3.65) into the state equations and solving the system of simultaneous equations obtained on simplification and neglecting the higher harmonics by the harmonic balance method. The other method, which is more accurate, is to fit equations (3.63)-(3.65) into the system response obtained by actually solving the equations. The values of the constant for various orders and gain values are given in Table (3.11).

The effect of gain on time average values (X_o, Y_o and Z_o) can be seen from the table. While X_o remains fairly constant Y_o increases and Z_o decreases, except for first order reaction, as gain is increased. The amplitude of the oscillations increases as gain is increased. When Table (3.2) is compared with (3.11) it can be seen that conversion is slightly more for -1 and 0 order systems at the open loop unstable point under the limit-cycling conditions than under open loop.

TABLE 3.11 HARMONIC CONTENTS OF LIMIT-CYCLES FOR VARIOUS ORDERS AND GAIN VALUES

Reaction order	Gain K_2	Time period (s)	X_0 (kg/m^3)	X_1 (kg/m^3)	X_2 (kg/m^3)	Y_0 (K)	Y_1 (K)	Y_2 (K)	Z_0 (K)	Z_1 (K)	Z_2 (K)
-1U	9000	1900	19.17	-0.12	.027	304.87	1.49	-1.56	295.76	-3.04	-1.74
	10000	1920	19.149	-0.1	-.125	305.69	3.01	0.84	294.681	-1.2	-4.4
OU	15000	1370	19.149	.0571	.00068	306.07	-.86	1.81	300.11	3.62	2.664
	20000	1450	19.147	-.0413	-.0546	306.38	2.35	-.18	295.53	-.25	-2.98
OS	48000	1070	19.405	0.006981	-.01056	301.12	.301	.543	294.65	1.78	-.918
	50000	1070	19.4	0.008879	.0148	301.18	-.87	.062	293.94	-.358	3.27
1U	12000	1350	18.99	0.0188	-.018	311.14	.141	.838	299.77	1.86	-.461
	15000	1380	18.98	-.0386	.06	311.25	-1.2	-2.43	300.77	-5.5	.44
1S	36000	960	19.224	0.011	.0113	304.53	-.8	.15	296.56	.0787	2.37
	40000	1236	19.225	-.00346	-.033	304.63	1.57	.245	296.8	2.45	-3.83
2S	66000	930	19.22	0.001357	.0102	305.25	-.714	-.26	296.19	-1.51	2.53
	75000	935	19.216	0.003593	.01365	305.26	-.993	-2	295.92	-1.56	3.8

3.13 Conclusions

The theoretical study carried out so far provided the following information for experimental work.

a) the reaction rate parameters and flowrate values that should be used so that the operating temperatures are within the range of instruments and heat of reaction generation capacity already available on the plant.

b) the effect of day to day changes in the temperature of water on system behaviour, so as to interpret the experimental results.

c) optimum gain or constant values to be used for various control strategies that are to be tried out on the plant.

d) the maximum allowable load disturbances that are permitted on the plant.

e) ways and effects of stabilising inherently unstable equilibrium points or generation of stable limit-cycles around them.

The theoretical studies also provided the following information about the effect of reaction order on the dynamics of a C.S.T.R. for the given set of reaction rate parameters

(1) as reaction order increases the difference between unstable and stable operating temperature also increases and hence an increase in the stability region.

(2) The stability region of first order seems to be similar to -1 order system.

(3) A lower proportional gain value is required to stabilise a first order unstable operating point than a

zero order unstable point.

(4) All orders have limit-cycles around their steady-state and unsteady-state points except for -1 order at the steady-state point.

(5) The time period and amplitude of oscillations change depending upon the reaction order and limit-cycles around unstable operating points generally have larger amplitudes than around stable points.

Though the dynamics of the valve and measuring elements, and the effect of sampling rate were not considered while carrying out this work, these effects have to be incorporated while simulating the dynamic behaviour of the complete plant for comparing it with experimental results.

CHAPTER 4

APPARATUS AND COMPUTER SYSTEM

4.1 INTRODUCTION

The complete partially simulated system consists of two interconnected parts, viz the plant items and the computer with its peripherals. The plant and the Honeywell 316 computer, are linked by a Honeywell Analogue Digital Input Output system (HADIOS). The measurements from the plant are amplified, conditioned and transmitted to the computer, where appropriate calculations for the partial simulation are carried out. The signals for control action and heat generation simulation are calculated and sent out from the computer. Water is used for the reactant as well as for the coolant medium.

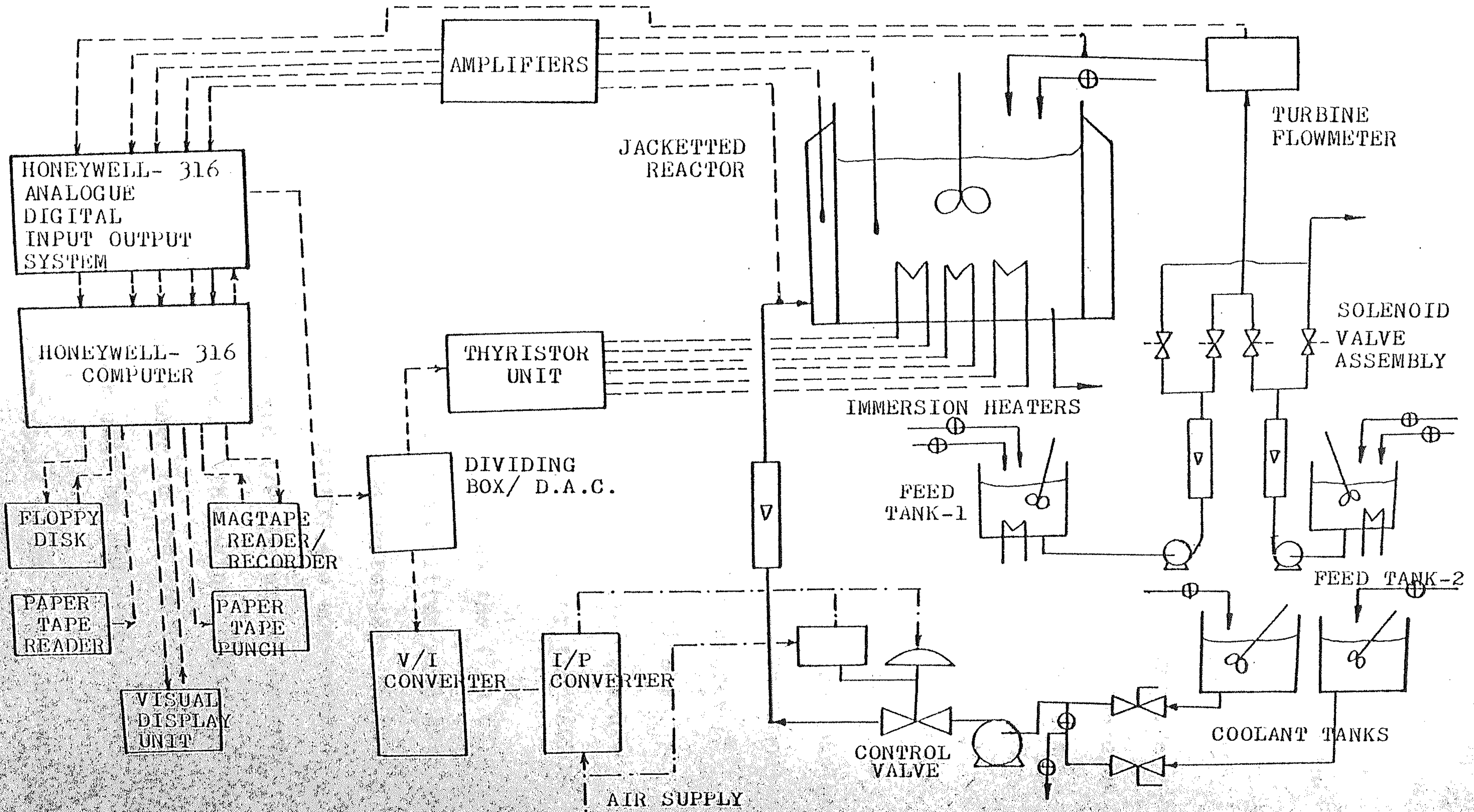
The schematic diagram of the experimental arrangement is shown in Fig. (4.1).

4.2 APPARATUS DESCRIPTION

A detailed description of the experimental arrangement and various instruments is given in the thesis by H. Farabi[15].

The essential experimental plant item is a copper jacketted cylindrical vessel of 0.285 m diameter and 0.4 m height. The liquid volume in the tank is $0.0173m^3$ and is maintained constant by an overflow pipe. The cooling jacket surrounds the vessel and the cooling water level is maintained constant by a large outlet at the side. The jacket volume is $0.008532m^3$. Stirrers inside

FIG.4.1 SCHEMATIC DIAGRAM OF THE PLANT AND THE COMPUTER SYSTEM



the reactor and jacket ensure complete mixing. Three 3 kW immersion heaters are provided at the bottom of the vessel for simulation of the reaction heat release. A thyristor unit controls the amount of energy sent to the heaters. The thyristor unit, which consists of two thyristors in inverse parallel arrangement, sends current pulses to the immersion heaters when they are triggered and the amount of energy received depends upon the trigger angle. The trigger angle is manipulated by the signals from the computer.

Comark thermocouples are fitted inside the tank and the jacket, and also at the feed and coolant inlets for monitoring purposes. The signals from the thermocouples are amplified five-fold before being sent to the computer. The sensitivity of the thermocouples is 0.1 degree C. A turbine flowmeter is fitted in the feed line to measure the flowrate of the feed. The meter outputs pulses to the counter, which are measured by the HADIOS.

A diaphragm control valve regulates the flow of coolant to the jacket. The valve is fitted with a valve positioner to reduce time delay and hysteresis. The analog output signals from the HADIOS are converted to pressure signals by the V/I and I/P converters before they are applied to the valve. The output signals from the computer are directed either to the control valve assembly or to the thyristor unit by the dividing box.

The feed to the reactor could be switched between two feed tanks by the help of an assembly of four

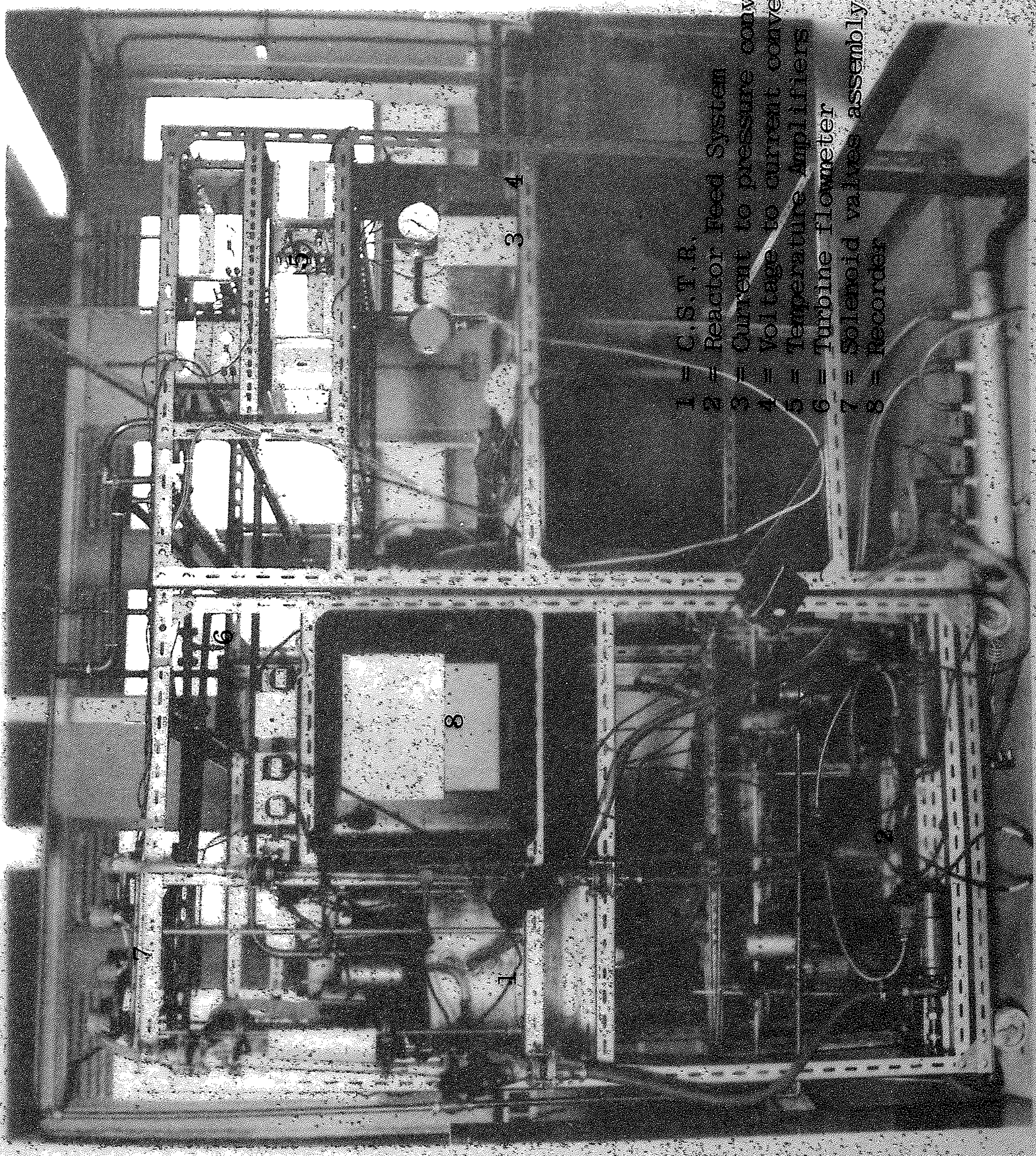
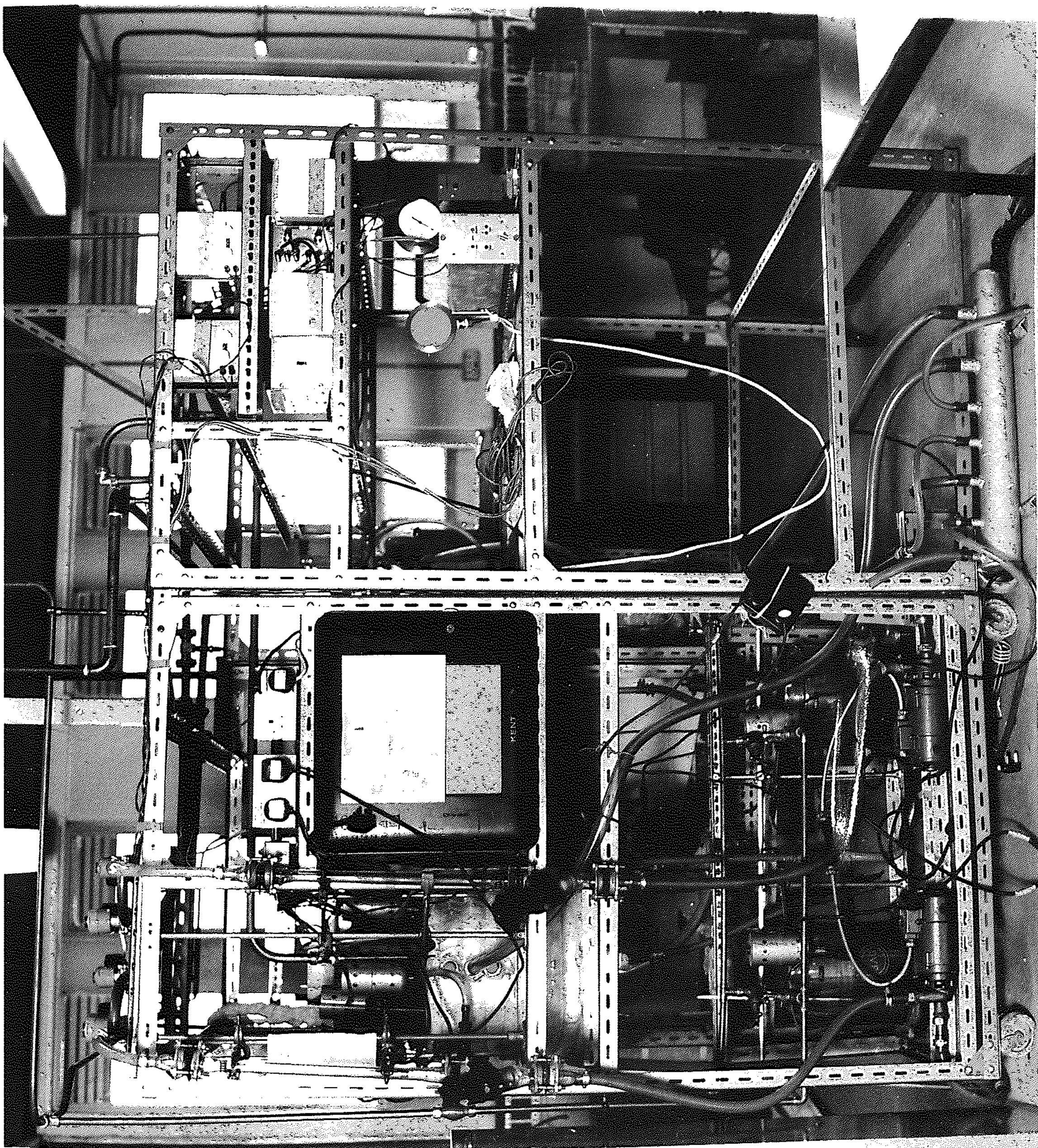


FIG. 4.2 EXPERIMENTAL ARRANGEMENT (FRONT VIEW)



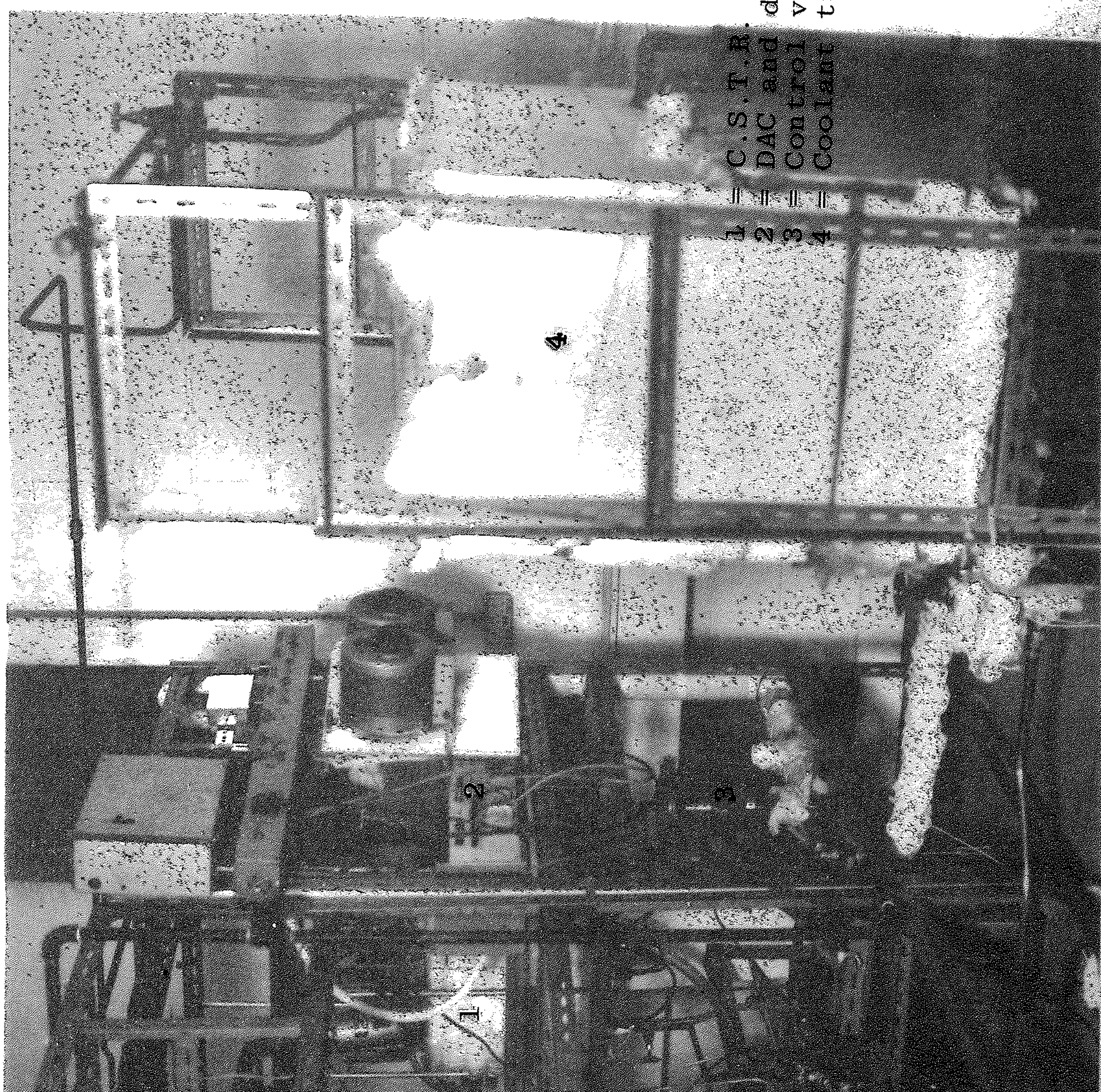
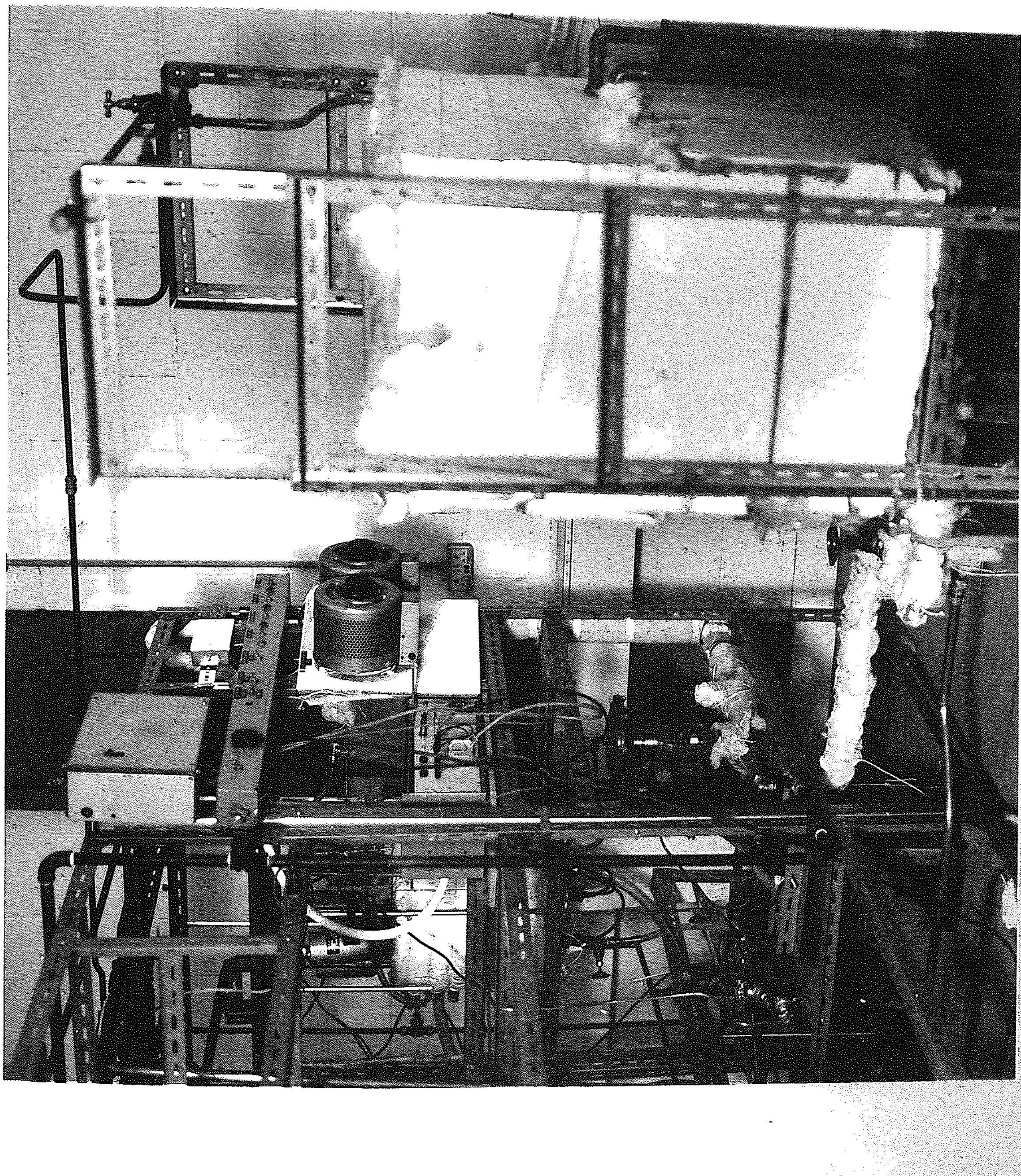


FIG. 4.3 EXPERIMENTAL ARRANGEMENT (REAR VIEW)



solenoid valves. Two tanks are provided for the jacket feed and the coolant can be switched from one tank to another manually. The feed and coolant flowrates can be monitored by rotameters, and any necessary adjustment made manually to the feed flowrate and to the coolant when on open loop.

No major changes were made on the equipment constructed by the previous research student. The coolant piping assembly was tidied up so as to reduce the time delay in the cooling water line from 30 secs to 2 secs. An extra hot water line was provided to the reactor mainly for use during start up. The amplifiers were modified and rewired so as to reduce noise and drift in the signals. Provisions were made to measure the coolant temperatures in the coolant supply tanks accurately and also to keep the coolant supply tanks well mixed.

4.3 LIMITATIONS OF INSTRUMENTS

Although the thermocouples can accept temperatures in the range 0-100°C, because of the immersion heater capacity of 9 kW the operating temperature range is restricted to 0-55°C, with an accuracy of 0.02°C. Error is introduced into the measurements due to A/D conversion.

The feed rate can be manipulated between 0-8.33 x $10^{-5} m^3/s$ and the coolant flowrate between 0-1.5 x $10^{-4} m^3/s$. The accuracy in manipulating coolant flow depends on the D/A converter. Even when the diaphragm valve is fully closed there is a leakage of coolant into the jacket at the rate of $8 \times 10^{-6} m^3/s$. Since the feed and coolant water are taken from an overhead storage tank, the inlet temperatures to the reactor and jacket vary from day to day. Provisions are there to heat these tanks if required, but there are no facilities for cooling them.

4.4 CALIBRATION

The various instruments and plant items were calibrated to connect the process parameter values to the corresponding signal (analog or counter). The calibration graphs for the turbine flowmeter, control valve and immersion heaters are given in Appendix(5 - Sections1-3) and the calibration equations in Appendix(5.7).

4.4.1 THERMOCOUPLES

The amplified signal from a thermocouple is in the form of an analog signal in the range 0-5V and is converted by the A/D converter to a number in the range 0-1023. So the digital signals received by the computer are directly correlated to the temperatures in a linear fashion.

4.4.2 TURBINE FLOWMETER

The flowmeter outputs pulses which are stored in counter A. The contents of the counter during one sample interval determines the counter rate. Since a rotameter is provided in the feed line the counter rate is directly calibrated to the feed flowrate by a set of linear equations.

4.4.3 IMMERSION HEATERS

The immersion heaters are controlled by a thyristor assembly. The power output by the heaters is inversely proportional to the trigger angle which in turn is manipulated by digital signals from the computer. Once the average supply voltage and the resistance of the heating elements were known, the trigger angle was plotted against power output since they are related by:

$$\text{Power} = \frac{V_S^{\,2}}{\pi R_L} (\pi - \alpha + \tfrac{1}{2} \operatorname{Sin} 2\alpha) \qquad (4.1)$$

The digital signal output by the computer is related to the trigger angle as

$$D_S = \alpha_1 \; 32767/\pi \qquad (4.2)$$

where $\alpha_1 = \pi - \alpha$

4.4.4 CONTROL VALVE

The digital signals from the computer in the range 0-32767 are converted to analog signals in the range 0-10 volts by the D/A converter. This voltage signal is converted to current in the range 0-20 mA DC. by a V/I converter and then to a pressure signal in the range 0-14 psig by a I/P converter. The coolant flow through the valve is directly correlated to the analog voltage signal. Since the control pressure acts on the top of diaphragm the coolant flowrate is inversely proportional to the HADIOS voltage output.

FIG. 4.4 HONEYWELL 316 COMPUTER AND ITS PERIPHERALS

4.5 THE HONEYWELL 316 AND THE HADIOS DATA ACQUISITION SYSTEM

The computer data acquisition system hardware consists of the following units

(i) A Honeywell 316 digital computer and associated peripherals.

(ii) A Honeywell analog digital input output system (HADIOS).

(iii) A remote signal conditioning box.

4.5.1 HONEYWELL 316 COMPUTER[46,47] AND ITS PERIPHERALS

The Honeywell 316 is a computer designed for real time systems application involving on-line control, data logging, data formatting, process monitoring and message switching. The general characteristics of the system include fully parallel organization, indexing, multilevel indirect addressing, powerful I/O system, a comprehensive 72 command instruction repertoire, and straight-forward logic for easy system interface and field expansion. The memory cycle time is 1.6 μS with a memory size of 16384 16 bits word. Programs written in Fortran, BASIC-16 or DAP-16 (assembly language) can be run on this machine, with provisions for mixed language segments.

The computer can support

(i) a Tektronic 4010-1 visual display unit (VDU)

or an ASR 33/35 teletype.

(ii) a high speed paper tape reader operating at 200 characters per second.

(iii) a high speed paper tape punch operating at 75 characters per second.

(iv) a magnetic tape cassette unit for input and output at 375 bytes per second.

(v) a floppy disk storage system.

4.5.2 HONEYWELL ANALOG DIGITAL INPUT OUTPUT SYSTEM[48]

HADIOS is a modular subsystem allowing a maximum number of mixed inputs and outputs to be interfaced to a computer with maximum efficiency. The HADIOS data highway has fifteen dedicated address lines and each device on the highway is allocated one or more of these. The device or subinterfaces can be analog or digital and input or output. The standard subinterfaces included in the HADIOS system are as follows:

(i) High level analog inputs:
This subinterface provides a maximum of thirty two separate analog signals in the range 0-5V being converted to a decimal number in the range 0-1023.

(ii) High speed counter input:
This subinterface can obtain the current contents of the counter which will be in the range of $0\text{-}255_{10}$. This subinterface can be operated in either the non-interrupt or the interrupt mode. In the interrupt mode an interrupt is generated when the counter is half full (127_{10}).

(iii) Digital output:

This subinterface consists of sixteen parallel output lines. Signals to sixteen analog channels can be sent by the digital to analog converter which makes use of twelve of the sixteen bits for data and the other four for selecting the analog channel. The analog output range is 0-10V corresponding to a digital range of $0\text{-}32767_{10}$ transmitted from the computer.

These subinterfaces can operate when control signals, initiated by programmable command, from the computer to the HADIOS are being output.

In this particular research four analog input channels are used to receive signals from the thermocouples, and one counter input for the turbine flowmeter. One digital output subinterface is used to send signals either to the thyristor unit or to the control valve.

4.5.3 REMOTE SIGNAL CONDITIONING BOX

This unit directs the signal from the HADIOS to the two analog output channels depending upon the control signal. The digital signal is also converted to the corresponding analog voltage by this unit. This unit is placed very near to the equipment to reduce noise and losses during transmission.

CHAPTER 5

ON-LINE SUPPORTING SOFTWARE

5.1 INTRODUCTION

A complete chapter has been devoted to the software used for on-line computing since its development formed the most important step in the experimental work. In mathematical computing, one is concerned solely with the solution of the problem, be it by analysis or simulation. This is also an element of on-line computing, but an equally important aspect is programming for a pattern of behaviour. The on-line programmer, is very intimately concerned with the manner of execution of his program. He is programming for a system in which the computer is only a part. The most important aspect of on-line computing that is not present in off-line work is control, signal processing, and the identification and modelling of the system.

The most important consideration a programmer should give for on-line computing is timing. He may be faced with the situation where there is an upperbound to the available time. An example of this is the case where it is essential to perform certain calculations between successive samples of a signal, yet maintain the highest possible sampling speed. Another important consideration the programmer must give is the ease with which he can change certain segments of his program and run it as quickly as possible. So the executive which controls the whole program must be written in a language which does not need compilation. Hence the executive program for the present work is written in BASIC, a language which needs a core resident interpreter. The main drawback of this programming language is its slow execution speed. So the segments which are well defined and free from errors can be written in a higher level language like FORTRAN or assembly language DAP 16 (H316 dependent language), and can be accessed from the executive.

The present package consists of nine subroutines written in FORTRAN and DAP 16 and accessed from the BASIC main program. These subroutines perform various tasks like input and output signals, simulation, plotting and other house-keeping tasks for the smooth execution of the program. The software also makes use of the back-up mass storage, mainly the floppy disk unit for storing program segments. The calling sequence and the listing of various subroutines are given in Appendix (4-sections 1-5).

5.2 HADIOS EXECUTIVE ROUTINES

The first five subroutines form the HADIOS executive and can be used to scan various analog channels and output signals to various devices in the plant.

The first two routines form the scanning sequence. The various analog and counter channels are scanned and their contents passed on to the BASIC program. These routines make use of the hardware clock. The scanning rate and number of samples per scan is modified by the user.

Subroutines 3,4 and 5 can be used to send digital output to various specified devices. While the first two routines can send output signals only at the beginning of a clock interrupt, subroutine 5 can change the values in between two clock interrupts.

The existing HADIOS EXEC 02 was modified so that the subroutine address table and modified error reporting segment were loaded at absolute location 37110_8. A listing of HADIOS subroutines is available in Webb's thesis[50].

A/D conversion is generally nonlinear because the quantization prevents it from being additive or homogeneous. This nonlinearity is difficult to deal with and it is generally tackled by treating it as a noise. In digital computation all arithmetic and conversion operations introduce high frequency noise while drift in source signals produces low frequency noise. Since the scanning routines are not provided with a software filter, smoothing of data is performed at the BASIC level.

5.3 INTEGRATION/SIMULATION ROUTINE

This routine performs the simulation of concentration given the operating conditions and reaction parameters by integration of the mass balance equation using the Fourth order Runge-kutta fixed step method. The step length and the initial condition for concentration are input data. The step is divided into fifty intervals internally and the numerical integration performed at each interval. The subroutine can also be used to integrate another differential equation, which is incorporated in the BASIC program. This facility is required if integral action is introduced into the control law.

5.4 TETRONIX GRAPHIC LIBRARY

The Tetronix extended graphic subroutines are combined together to form a single FORTRAN subroutine in order to reduce the total number of routines accessed from the BASIC level.

5.5 HOUSE-KEEPING SUBROUTINES

Two more subroutines are available which can do the following tasks

i) send output data either to the visual display unit

or to the paper tape punch.

ii) HALT the computer for programmer intervention.

iii) Punch a portion of blank tape so as to separate two sets of data for identification purposes.

iv) calculate the actual time elapsed to execute a set of BASIC program statements.

While the first three tasks are carried out by subroutine 8, the last one is performed by subroutine 9. Setting of sense switch 4 through software diverts output to the paper tape punch. Since subroutine 9 makes use of the hardware clock, this routine should not be run in conjunction with the HADIOS executive routines.

5.6 OVERLAY ROUTINE

This subroutine transfers a specified segment from floppy disk to computer core overwritting the segment already present. The addition of this subroutine, which can be called from the BASIC level, has increased the computer size to an unlimited extent. This subroutine is core resident and resides at the top of the memory.

For the present work the remaining subroutines were divided into two segments, one consisting of the entire Tetronix graphic library (segment 1) and the other consisting of the HADIOS executive, integrator and clock routines (segment 2). When graphical functions had to be performed segment 1 was copied onto core and if scanning or outputing of signal had to be carried out segment 2 was written onto the core. Although this copying of segments everytime increased the sampling time by 2.4 seconds it increased the core size by another 3K. If graphic functions are not required segment 1 could be completely omitted and segment 2 made core resident. Interrupts during the transfer operation cannot be handled by this routine.

Dummy maths library routines for converting real to integer and vice versa (C $·21 and C $ 12) are written so that, similar facilities available in the BASIC interpreter could be made use of instead of loading a duplicate version with the overlay routine. Segments should be transferred to disk from core prior to use by A $ D14, as the overlay routine is similar to it.

5.7 LOADING PROCEDURE

As there is very little base sector available in the BASIC interpreter, all the loading should be carried out so that each sector has its own cross sector referencing information at the top and no segments cross sector boundaries. The maths library routines must be grouped using utility program OBJCHOP so that each routine could be loaded separately at a suitable starting address. The force load and program break facilities have to be used whenever it is required.

5.7.1 INITIAL VERSION OF THE PACKAGE

In this version all the subroutines and libraries were loaded together starting from the location 20740_8 and moving upwards. Since all the subroutines were core resident there was no need for the overlay routine. The main drawback of this type of configuration was that there was no scope for development as very little free space was available. The simulator was numbered subroutine 6.

5.7.2 FINAL VERSION OF THE PACKAGE

In this version the overlay facilities were introduced making use of the floppy disk unit. As mentioned before the subroutine for transferring segments from disk to core is core resident with the BASIC interpreter. The I/O mod, subroutines address table and the modified error reporting segment are also made core resident. Segments 1 and 2 are loaded separately into core and copied onto disk using A$ D14. Both the segments were loaded from location 22000_8 upwards so that subroutine 7 when segment 1 is in the core is the Tetronix graphics library and when segment 2 is in the core is the simulator routine.

Segment 2 is much smaller than 1 at present but can be extended, if required, up to location 37107_8. Care should be taken not to overwrite the common block of segment 1 by segment 2. The memory map of the core resident portion and the two transferrable segments are given in Appendix (4.8).

5.8 CHANGES IN BASIC INTERPRETER

The basic interpreter is modified so as to include a new command which has many uses. The RUN command always clears the tables, thereby erasing all variable values and starts the program execution from the beginning. This particular action may sometimes be unwelcome when the programmer wishes to run a segment of his program making use of the values obtained from a previous segment or to start the program execution from an intermediate point instead of from the beginning, after the program has terminated due to an error. To include such an option, a new BASIC command START is included which is equivalent to RUN in the old version, while RUN m, where m is a statement number, can be used to run a program from the statement number specified without clearing the table. The command CLEAR is removed to accommodate the command START.

The importance of the change is made obvious in the next section which describes the BASIC program executive used for on-line experimental work.

5.9 ON-LINE BASIC PROGRAM

The program is divided into two main sections, the steady-state and the unsteady-state sections. The second section can be run only after the execution of the first which supplies the steady-state operating conditions. The reaction parameters corresponding to the order under investigation and the appropriate control equations must be loaded prior to the start of the program.

In the steady-state section, the user inputs steady-state feed and coolant flowrates. The computer scans and obtains the inlet temperatures from the plant and then plots the theoretical heat generation and removal curves (equations (3.5) and (3.6)). The scanning is performed and the experimental tank temperature is plotted on the same graph to find its deviation from the theoretical value. The user can manipulate variables until the two coincide to the required accuracy. Once the user is satisfied that the system has reached the steady-state, he can start the transient response studies by entering the second section after applying suitable load disturbances. In this section the following jobs are performed

i) scanning of channels and calculating various temperatures.

ii) calculating instantaneous concentration by numerical integration of the mass balance equation.

iii) calculating the heat generation and sending appropriate signals to the immersion heaters.

iv) calculating coolant flowrate depending upon the control strategy chosen and sending signals to the diaphragm control valve.

v) punching out values on the paper tape punch.

vi) plotting tank temperature and concentration, jacket temperature and flowrate.

vii) repeating all the steps until the simulation time is reached.

Facilities are available for re-running this section of the program with different conditions or continuing the present study further. The listing and flow chart of the BASIC program are given in Appendices (1.6) and (2.4) respectively. Polynomial equations have been formulated connecting process variables like feed and coolant flowrates and heat liberated against appropriate analog signals and counter pulses for the turbine flowmeter, control valve and immersion heaters respectively. (Refer Appendix (5.7)).

If the program stopped somewhere within section 2 due to error, then it could be re-run, if necessary, from the beginning of section 2, instead of from the beginning of section 1 with the modified RUN command discussed earlier.

5.9.1 EXECUTION TIME

A few segments of the BASIC program could have been written in FORTRAN in the form of subroutines for faster execution, but because the program was in the development stage it was much easier to modify and re-run in BASIC language.

The total sampling time during the execution of the second section, for any type of control strategy, except decoupling type control, was 11 seconds. The times taken for executing various sections of the program are listed below

i)	scanning, averaging and calculating temperatures	= 2 secs
ii)	simulation	= 4.3 secs
iii)	scaling and plotting, transmitting output signals to various devices	= 2.0 secs
iv)	transferring segments 1 and 2 to core from disk	= 2.4 secs

It is seen that simulation takes 40% of the computer time and so the user must strike a balance between accuracy of numerical integration and the maintenance of a high sampling rate. The difficulties that arise in not having a large number of steps between each time interval can be seen in chapter 8 when theoretical results are compared with experimental values.

5.10 CONCLUSIONS

The importance of on-line programming and the various aspects of it are described in this chapter. The subroutines and the program used for the simulation and control of the reactor system are described in detail. It is also shown how the present software could be increased further for larger control systems. The most important consideration in developing a software package is striking a balance between sampling rate and accuracy. It is considered that a reasonable attempt has been made to develop a software package which is able to provide easy and efficient use of the hardware facilities available.

CHAPTER 6

EXPERIMENTAL STUDIES

6.1 INTRODUCTION

Experiments on the plant were performed to study the effect of reaction order, control scheme and various operating parameters like feed and coolant temperatures, and flowrates on the stability and dynamic behaviour of the reactor. While the reaction heat generation and concentration were simulated by the computer depending upon the reaction order under investigation, the feed, coolant, tank and jacket temperatures were measured directly from the plant.

The following studies were made on the system

(i) Effect of reaction orders on the general stability of the open and closed loop systems.

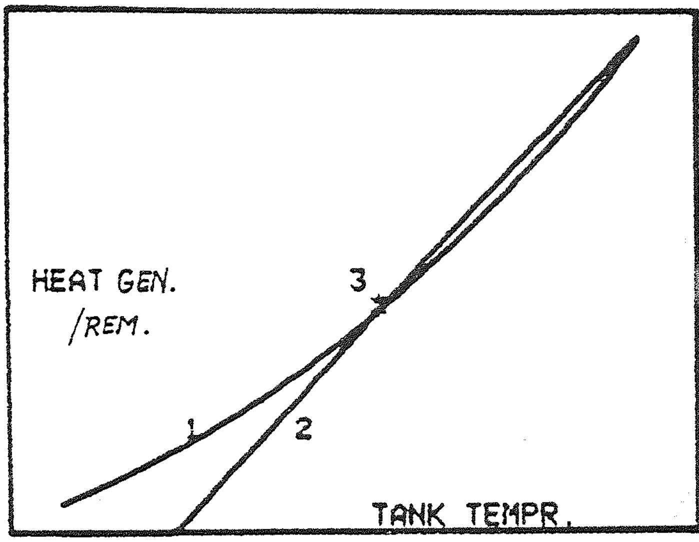
(ii) Effect of control on stability and transient behaviour of the system, in moving from an initial condition to its equilibrium point.

The strategies employed were feedback and decoupling type control

(iii) Control at the open loop unstable operating points using feedback and decoupling type control

(iv) Effect of feedback and invariance type control around a stable operating point for load disturbances in the form of steps in feed and coolant temperatures

(v) Generation of limit-cycles by positive feedback at open loop stable and unstable points and the effect of reaction order on these oscillations.




```
 F=     58·3333   FC=     45
T0=     16.9726 TC0=     16.7234 T=    31.863 TC=    23.3851
U*AREA= ·390441E-01 KCAL/S/C
HEAT INP(W): 4674.62              HEAT OUT(W): 4688.77
C = .19361E-01 GM/CC
 THEO. OP.TEMP :
   31·3735 S.S
MEASURED TANK FLOW RATE IN CC/S : 59·91
```

1 = Theoretical heat generation

2 = Theoretical heat removal

3 = Experimental tank temperature

FIG.6.1 TYPICAL COMPUTER OUTPUT AT THE END OF STEADY-STATE SECTION

6.2 STEADY-STATE BEHAVIOUR

For each experiment the system was first driven to a steady-state before starting the transient response studies. Given the operating conditions, the theoretical steady-state operating points were calculated and compared with the experimental values. By suitable modifications the experimental steady-state temperature was made to coincide with the theoretical value. The unstable operating point, if it existed, was also calculated by the computer.

The steady-state conditions for a given reaction order depended on the flowrates and temperatures of the feed and coolant. Since the day to day temperature of water used for experimental work changed, the operating conditions also changed appreciably. It was found that if the inlet water temperatures exceeded $18^{o}C$ it was not possible to get an operating temperature within the range of present equipment. Generally when the inlet temperatures were high, the feed and coolant flowrates had to be high in order to have a steady-state operating point. Fig. (6.1) gives a typical output from the computer at the end of the steady-state section. The plant thus had to be run for some time in order to confirm that it had reached its steady-state value.

Driving the system to the steady-state point can be considered as a start up problem. The various techniques tried to start the reactor from cold conditions were

(i) reduction of the feed flowrate to zero and subsequent manual adjustment of it.

(ii) similar manipulation of coolant flow.

(iii) sending hot water into the tank.

(iv) applying large signals to the immersion heaters.

6.3 TRANSIENT RESPONSE STUDIES

At the steady-state operating conditions disturbance was applied to the system manually in the following ways

(i) step in feed temperature by solenoid valves.

(ii) step in jacket temperature by shut off valves.

(iii) perturbation in tank or jacket temperature by the addition of hot water.

(iv) perturbation in tank concentration by feeding the disturbance value into the computer program.

The system behaviour was studied until the end of simulation time. The state variables tank temperature and concentration and jacket flowrate and temperature were plotted while the values were also punched out for later use. The response studies could be continued further or new disturbances could be introduced at the end of the simulation time.

The calculations had to be kept at a minimum during the transient section in order to maintain a high sampling rate. As mentioned in the previous chapter the normal sampling time was 11 seconds but was higher for decoupling type control, which involved iteration for the calculation of coolant flowrate.

For the present set of reaction rate parameters chosen, if the tank temperature exceeded 50^{o}C the required heat generation exceeded the 9 kW capacity of the immersion heaters. So if the tank temperature increased to beyond 50^{o}C the experiment was terminated and the system was assumed to be unstable for those set of conditions.

6.4 STABILITY ANALYSIS

The only way in which the RAS could be determined experimentally was to observe the behaviour of the system from different initial conditions. If the starting points in the phase space were outside the region of stability, then the tank and jacket temperatures would increase indefinitely. If the system had multiple operating points, one stable and the next higher one unstable then if the starting conditions were below the unstable point the system would be stable and above it would be unstable.

The effect of control on the stability was determined by carrying out similar experiments for different control schemes. Unstable operating points were stabilised by a feedback controller. For these experiments the system was first driven to the stable point and then moved to the unstable point by the use of feedback control.

6.5 EFFECT OF REACTION ORDER

Integer reaction orders ranging from -1 to 2 were simulated. Different activation energies were chosen for the different orders of reaction in order to keep the operating temperature within the limits of the instruments, while the heat of reaction, frequency factor and inlet concentration were maintained constant. The concentration of reactant in the tank at the steady-state condition was calculated from the steady-state mass balance equation depending upon the reaction order. Although a general algorithm could have been developed for calculating the steady-state concentration from the material balance equation for any reaction order, the actual concentration equations were stored in the computer so as to reduce the computation time during execution of steady-state phase.

The concentration equation for the reaction orders under consideration are given below

n=2

$$C_{SS} = \frac{F - (F^2 + 4FC_oK_4)^{\frac{1}{2}}}{-2K_4} \quad (6.1)$$

n=1

$$C_{SS} = \frac{C_o}{1 + K_4/F} \quad (6.2)$$

n=o

$$C_{SS} = C_o - K_4/F \quad (6.3)$$

n= -1

$$C_{SS} = C_o/_2 + (F^2C_o{}^2 - 4FK_4)^{\frac{1}{2}}/F \quad (6.4)$$

where $K_4 = k_o \ V \ e^{-E/RT_{SS}}$

6.6 CONTROLLER EQUATIONS

Various types of control strategies were tried on the system. Apart from the simple feedback controller, complicated schemes for decoupling state variables and maintaining the controlled variables within the limits of stability were considered. The various types of control scheme tried were

(i) proportional feedback control of

a) tank temperature (equation(3.27))

b) jacket temperature (equation(3.28))

c) tank concentration (for generation of limit-cycle -(equation(3.60))

(ii) Decoupling type control of tank temperature (equations(3.49)and(3.50))

(iii) Invariance type control for

a) step in tank inlet temperature (equation(3.57))

b) step in jacket inlet temperature (equation(3.56))

c) steps in both tank and jacket inlet temperatures (equation(3.54))

(iv) controller equation obtained from stability conditions with a view to strengthen RAS (equation (3.38)).

The controller equations were similar to the ones given in Chapter 3. Sometimes a comparison of controllers was also made for the same set of operating conditions.

6.7 LIMIT-CYCLES

Although the existence and the parameter conditions required for the generation of self sustained oscillations could be derived theoretically, during experimentation limit-cycles were generated by modifying the gain value by trial and error. So the gains chosen for experimental runs could not be termed as the bifurcation values. Longer simulation times were required in order to confirm that the oscillations were constant and self sustaining. Limit-cycles were generated not only at the open loop stable operating point but also at the open loop unstable points. The harmonic components of the oscillations were obtained theoretically from the system response.

6.8 PARAMETER VALUES CHOSEN

The parameter values chosen for experimental purposes were similar to those of the total simulation studies and are given in Appendix (5.6). The heat transfer coefficient was calculated at the steady-state condition during experimental runs and used for later calculations.

The exponential decay constant for decoupling type control was the optimum value determined in the theoretical studies, while controller gains for other schemes were chosen arbitrarily. Similarly the gains for limit-cycle studies and for stabilising unstable operating points were chosen by trial and error procedure.

CHAPTER 7

TOTAL SIMULATION OF THE PLANT

7.1 INTRODUCTION

The complete experimental arrangement not only consists of the jacketted reactor but also various time lags and transfer functions arising from thermocouples, the control valve and other electrical and pneumatic components. The effect of sampling (with zero order hold) was also considered since some time is taken up by the computer in processing the signals received from the plant. For verifying the experimental results with theoretical simulation the mathematical model equations of the plant should not only have the material and energy balance equations for the reactor and jacket but also first order transfer functions for the four thermocouples and one control valve together with samplers with zero order hold before the signals enter the computer. The block diagram of the entire plant is given in Fig. (7.1).

7.2 MODEL EQUATIONS OF THE PLANT

The model equations of the entire plant are given below

Mass balance in the reactor

$$F(C_o - C) - k_o V C^n e^{-E/RT^*} = V \frac{dC}{dt} \qquad (7.1)$$

Energy balance in the reactor

$$F\rho C_p (T_o - T) - UA\,(T - T_c) + \Delta H\, k_o V C^n e^{-E/RT^*} = V \rho C_p \frac{dT}{dt} \qquad (7.2)$$

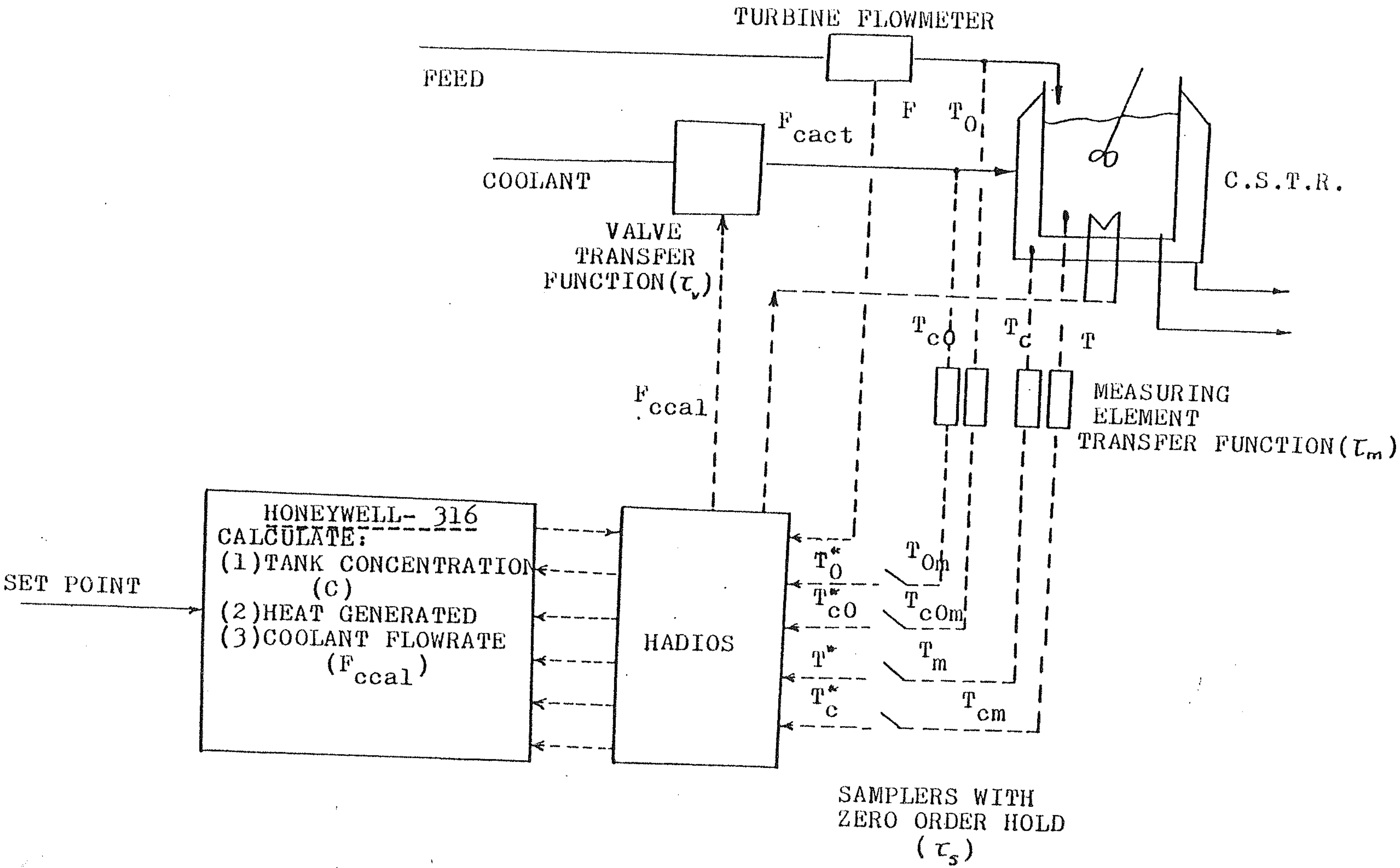


FIG.7.1 BLOCK DIAGRAM OF THE PLANT

Energy balance in the jacket

$$F_{C\,act}\,\rho_c\,C_{pc}(T_{co}-T_c) + UA(T-T_c) = V_c\rho_c C_{pc}\frac{dT_c}{dt} \quad (7.3)$$

Equations for measuring elements

$$\tau_m \frac{dT_{om}}{dt} + T_{om} = T_o \quad (7.4)$$

$$\tau_m \frac{dT_m}{dt} + T_m = T \quad (7.5)$$

$$\tau_m \frac{dT_{com}}{dt} + T_{com} = T_{co} \quad (7.6)$$

$$\tau_m \frac{dT_{cm}}{dt} + T_{cm} = T_c \quad (7.7)$$

Equation for valve

$$\tau_v \frac{dF_{cact}}{dt} + F_{cact} = F_{ccal} \quad (7.8)$$

Samplers

T_o^* = sampler (T_{om}, τ_s) (7.9)

T^* = sampler (T_m, τ_s) (7.10)

T_{co}^* = sampler (T_{com}, τ_s) (7.11)

T_c^* = sampler (T_{cm}, τ_s) (7.12)

F_{ccal} = Output value from the computer; calculated depending upon the control strategy (7.13)

This set of thirteen equations represents the plant almost exactly. Equation (7.1) is similar to equation (3.1) except that the effect of sampling on tank temperature is considered here. Similarly the control equation (equation (7.13)) will involve only the sampled temperature values and not the original ones. At steady state, equations (7.1) to (7.3) will be equivalent to equations (3.1) to (3.3) and the other equations can be ignored.

7.3. ASSUMPTIONS IN FORMULATING THE MODEL EQUATIONS

There are a few assumptions in formulating the model which are either verified through experiments or by visual observations. Some of the assumptions are

(i) Heat losses to the surroundings are negligible.

(ii) The tank and jacket are well mixed vessels.
This was verified for several typical operating conditions by residence time studies. These were carried out by comparing the response of these vessels with the response of a single continuous stirred tank for a step in inlet temperature. The response curves are included in Appendix (5 - sections 4-5).

(iii) The transfer functions are first order in nature. The time constants of the measuring element and valve are given in Appendix (5.6). The dynamics of the V/I and I/P converters are combined with the valve.

(iv) the time delay due to immersion heaters is neglected

(v) Sampling time during a run is constant. This is true except for decoupling type control, where the coolant rate is calculated by an iterative procedure.

(vi) The heat transfer coefficient does not vary with coolant flowrate. This is true because the jacket is a well mixed tank.

(vii) Liquid volumes inside the reactor and jacket are constant and do not vary with flowrate. This is generally true because large diameter outlet pipes have been provided for maintaining the liquid volumes.

(viii) All noise and errors entering the system are neglected. Errors are introduced during A/D and D/A conversions and other numerical computations which cannot be measured. Similarly noise enters the system due to drifts in electronic components. These errors and noises could have been simulated as random noise but they have been completely neglected in the present study.

Even when the control valve is fully closed there is some leakage into the jacket which should be considered in the total simulation studies. Since the feed flowrate is assumed constant during an experimental run, the effect of sampling on the determination of feed rate is neglected.

7.4 SOLUTION PROCEDURE

A computer program is written in SLAM for the ICL 1904S to simulate the complete plant using the equations (7.1) to (7.13). The differential equations are numerically integrated by the Runge-Kutta fixed step method. The communication interval is divided into 200 steps so that integrations are performed every 0.1 of a second. Various controller equations are also included in the program. The listing of the program is given in Appendix (1.5) and the corresponding flow chart in

Appendix (2.3).

7.5 COMPARISON OF EXPERIMENT WITH TOTAL SIMULATION

The total simulation program was run for each set of operating conditions obtained from the experimental run. The results of simulation were punched out on paper tape for reading into H-316. Since the tape was of even parity it had to be converted to one with no parity, by a tape conversion program. The listing of the tape conversion program is given in Appendix (4.6).

The converted data tape was read in and plotted with the experimental results for comparison purposes. The BASIC program which plots these two tapes is given in Appendix (1.7). If limit-cycle studies had been carried out, then the harmonic contents of the oscillation could also have been found from the response of the system and the approximate response plotted with the other two results.

CHAPTER 8

RESULTS AND DISCUSSION

8.1 INTRODUCTION

More than 180 experiments were carried out on the reactor system for the four reaction orders under consideration but due to limitations on space the results of only 92 experiments are reproduced here. Initially the system was driven to the steady-state; Table (8.1) gives the steady-state operating conditions for the different experiments. The theoretical steady-state and unsteady-state temperatures given in the table were calculated by the computer. Table (8.2) gives the various control schemes and disturbances introduced for the different experimental runs. The disturbances were either load changes or perturbations (different initial conditions) in state variables. The plots of different experimental runs for various control schemes and reaction orders are given in Appendix (6.1). The graphs for comparison of experimental results with total simulation are given in Appendix (6.2). Only half of the number of comparison graphs are reproduced, again due to limitation on space. More experiments were carried out on reaction order one than any other order. The following sections describe the various studies carried out on the reactor system.

8.2 OPERATING POINTS

It can be seen from Table (8.1) that the experimental steady-state temperature and the theoretical value coincide generally within 0.5K. For experiments concerning operations at the open loop unstable point the system is driven to the steady-state point and then moved to the theoretical unstable point by a suitable control scheme. The operating points depend on the reaction order as well as inlet conditions. The operating temperatures generally vary from 295 to 315 K.

8.2.1 Effect of Reaction Order

It can be seen that for second order reaction the system unstable point is absent because it is outside the ranges of the thermocouples. All other reaction systems possess a stable and an unstable point. The stable and unstable operating temperatures for the first order system are higher than those of the zero order system as verified by theory. The operating temperatures of the -1 order system are either slightly less or similar to those of the zero order system, though theory predicted that the operating temperatures of -1 order should be less than that of the zero order system for the same inlet conditions.

8.2.2 Effect of Inlet Parameters

The day to day changes in inlet tank and jacket temperatures had made it necessary to use different feed and coolant flowrates thereby changing the operating points. The feed temperature varied from 284 to 291 K (feed and coolant temperatures chosen for theoretical studies were 288 K), while the coolant temperature was in the range 280-291 K.

Increase in tank or jacket inlet temperatures increased tank outlet temperature. When experiment 42 is compared to 43 it can be seen that an increase of 4.5 K in coolant temperature has increased the steady-state temperature by 6K. Similar effects can be seen in experiments 55 and 58. An increase in feed temperature by 1K (experiments 48 and 50) increased the steady-state tank temperature by 2.4 K. Increase in feed flowrate also decreases the operating temperature, as can be seen between experiments 22 and 24.

8.3 Open Loop Stability Region

The system behaviour is studied from different starting conditions to determine the region of stability around the operating point. The stability region depended on the reaction order under consideration as well as the inlet conditions.

The second order system is the most stable of all the four systems. Even for very large disturbances in the state variables the system returns to steady-state (experiments 1 and 2).

1,0 and -1 order systems exhibit a stable region, within which the paths converge to the steady-state and all paths outside the region diverge away from it. For the first order system, experiment 14 shows a stable behaviour while 16 an unstable behaviour. In experiment 15 the tank temperature deviation remains constant (the fall in it is very slow), which could be termed as meta-stable behaviour. It could be noted that although in experiment 15 the system is meta-stable for a tank temperature deviation of 10 K, it is unstable in experiment 16 for a deviation of 8 K, since the perturbation is above the unstable point. The difference between unstable and stable steady-state tank temperatures is 5.5 K in experiment 16, while it is 10 K in experiment 15. For zero order reaction experiment 48 shows a stable behaviour while 49 an unstable one. Similarly for the -1 order system experiment 71 shows a stable behaviour while 69 an unstable behaviour. Experiment 70 exhibits a meta-stable behaviour.

The effect of a step in feed temperature was also studied on the system behaviour. For a step of 2.5 K the second order system (experiment 3) reaches a new steady-state temperature, an increase of 4.7 K whereas the tank temperature increases without reaching a steady-state for the other three reaction orders. Experiments 17, 52 and 72 give the behaviour of 1, 0 and -1 order systems respectively.

8.4 CLOSED LOOP STABILITY BEHAVIOUR

The stability behaviour of the closed loop system was studied with the following control strategies

(i) proportional control of tank temperature

(ii) proportional control of jacket temperature

(iii) control law obtained by the application of Krasovskii's theorem (equation (3.38)).

(iv) decoupling type control.

A detailed study of the last scheme is described in section 8.6.

The first scheme involves a simple proportional feedback loop for the control of tank temperature. This scheme increases RAS for all reaction orders. This strategy is not studied for reaction order 2 because the open loop system is stable within the limits of the instruments. Experiments 18-20 show the behaviour for a first order system. Experiment 20 shows that the system becomes unstable for small gain values and large disturbances. Similar experiments were conducted for zero order (experiments 50,51) and -1 order system (experiments 73, 74 and 75). Even meta-stable behaviour similar to open loop conditions was observed in experiments 75 and 51.

When jacket temperature is used as the controlled variable then larger gain values were required. Oscillations were induced in jacket temperature and flowrates. Experiments 21 and 22 were run for the first order system and experiment 76 for the -1 order system. Experiment 21 shows a meta-stable behaviour, with a very slow decrease in perturbations.

The third strategy in which the coolant flowrate is calculated from equation (3.38) is found to be superior to the other two schemes in improving RAS. The region is increased enormously and the perturbations die down very quickly. The fall is generally asymptotic in nature. Experiments 5, 23, 54 and 77 show the behaviour for reaction order 2, 1, 0 and -1 respectively.

The system behaviour is also studied with proportional control of tank temperature for a step in feed temperature in experiments 24, 25, 53 and 78. As expected, offset is introduced in tank temperature although the system is stabilised. This study is carried out mainly for comparing it with decoupling and invariance type control schemes.

8.5 OPERATING THE SYSTEM AT THE OPEN LOOP UNSTABLE POINT

The reactor system was operated at the inherently unstable point by using feedback control or decoupling type control. The feedback control schemes involved proportional control of tank or jacket temperature. Since the second order system does not possess an unstable point no studies were carried out on this reaction system. The studies using decoupling type control are described in Section 8.6.

8.5.1 Proportional Control of Tank Temperature

Experiment 28 shows that the gain value is not sufficient for stabilising the unstable point. The unstable operating point of the first order system is stabilised in experiments 29 and 30. Although the operating point is stabilised the stability region is small. The operating point is a stable node and as the gain is increased further it becomes a stable focus.

Experiments 57 and 58 give the behaviour of the zero order system and 79 and 80 the behaviour of the -1 order system. Although offset in experiment 58 is less than in 57 the operating point is not fully stabilised in both these cases. Experiment 80 shows that the unstable operating point of the -1 order is stabilised although the response is slow.

8.5.2 Proportional Control of Jacket Temperature

In this strategy the gain values have to be higher than those of the previous scheme. Oscillations are observed in jacket temperature and flowrate, since they are directly coupled by the control equation. Experiments 59 and 60 show the behaviour for zero order reaction. The operating point is not stabilised even for very large gain as there is an offset observed in both cases. Experiment 81 and 82 give the behaviour of the -1 order system. The unstable operating point is stabilised in experiment 82.

From the studies carried out on stabilising the open loop unstable point by these two control schemes it is seen that the first strategy has many advantages over the second.

8.6 CONTROL FOR DECOUPLING TANK TEMPERATURE

Many experiments were carried out on this control strategy for all the four reaction orders under consideration. The system behaviour seems to be generally independent of reaction order. The following sections describe the various studies carried out on the reactor system with this control strategy.

8.6.1 On Region of Stability

It is seen that stability region around the stable point increases enormously and the transient responses indicate that the operating point remains a stable node despite large coolant flowrates, unlike feedback control schemes, where the operating point may become a focus as the gain is increased. Initially coolant flowrate is high and oscillatory, but falls suddenly as perturbations die down. The initial oscillations are due to its sensitivity to the state variables.

Experiments 6, 7, 8 and 9 show the behaviour of the second order system for different initial conditions. The fall in temperature is generally asymptotic in nature. Experiment 9 shows that tank temperature remains independent of perturbations even in tank concentration. Experiments 32, 33, 34 and 35 show the behaviour for a first order system. Experiment 35 shows an increase in the stability region larger than any other strategy studied so far. Experiments 62, 63 and 64 give the system performance for zero order reaction while 85, 86 and 87 give it for -1 order system.

8.6.2 For Step In Feed Temperature

This strategy also decouples the tank temperature and hence tank concentration from a step in feed temperature. Experiments were carried out for different reaction orders for step in feed temperature. It is seen that there are no oscillations and the overshoot is generally very small. Experiment 13 gives the response of a second order system for a step of 4.75 K in feed temperature. Experiments 39, 40, 67, 68, 89 and 90 give the response of first, zero and -1 order systems for a step in feed temperature. For a step of 4.5 K (experiment 39) the overshoot is around 1 K. The exponential decay constant value, D, is generally small since the step change is persistent. In experiment 67 the step change was removed at 2200 seconds so there is an undershoot before the system goes back to steady-state. In experiment 90 there is a small negative offset in tank temperature, which may be due to errors either in arriving at the steady-state operating temperature or in the heat transfer coefficient.

8.6.3 Operation at Open Loop Unstable Operating Point

This control strategy was also tested in stabilising the open loop unstable operating point. This scheme was found to be definitely superior to the other methods described in the previous section. The unstable operating point is stabilised and the response is fast and smooth with no oscillations. Experiment 31 shows that the unstable operating point for the first order is stabilised by this scheme. Similar experiments were carried out on zero order (experiment 61) and -1 order system (experiment 83 and 84). In experiment 84 the deviation in temperature is of the order of 11 K in the positive direction, which shows the creation of a large asymptotic stable region around the open loop unstable point.

8.6.4 Effect of D_{max}

The system behaviour is studied for various D_{max} values ranging from 0.002 to 0.016 and different reaction orders. A small D_{max} value reduces the speed at which tank temperature dies down but the fall is asymptotic. Larger values induce oscillations in all state variables and increase settling time. Experiments 12, 37, 65 and 91 show oscillation in jacket flowrate for reaction orders 2,1,0 and -1 respectively for large D_{max} values. These responses can also be compared with the corresponding response with optimum (0.007) D_{max} value (experiments 6, 35, 62 and 85). Experiments 38 and 88 show the system response similar to optimum response for a D_{max} value of 0.005.

8.7 INVARIANCE CONTROL

Invariance control studies were carried out only for a first order reaction system, since the control equation is independent of reaction order. Experiments 41 and 42 show the system behaviour for a step in feed temperature. Perturbations in tank temperature are very small when compared to similar behaviour under the action of feedback control (experiments 24 and 25). Experiments 43, 44 and 45 show that invariance of all the three state variables is achieved for a step in coolant temperature. This is true even for a step of magnitude 7 K. Oscillations in jacket flowrate are due to its sensitivity to the coolant inlet temperature when γ_o is very nearly equal to $(\gamma_{SS}-\gamma_{OSS})$ (note the denominator term in equation (3.56)). Experiments 46 and 47 show the system behaviour for steps in feed as well as coolant temperatures. In all the cases perfect invariance of the state variables tank temperature and concentration is achieved since the load changes are such that the coolant flowrate is within the limits.

8.8 LIMIT-CYCLES

A limit-cycle was generated at open loop stable and unstable operating points for the four reaction orders under consideration. Since reaction order two does not possess an open loop unstable point, a limit-cycle was generated only at the stable point. Long simulation times were necessary in order to confirm that the oscillations were persistent. The following subsections describe the various studies carried out in the generation of limit-cycles at the stable and the unstable operating points.

8.8.1 At Open Loop Stable Point

Experiments 4, 26 and 55 show the limit-cycle behaviour of 2,1 and 0 order systems at their respective steady-state operating points. Even for very large gain values, sustained nonlinear oscillations were not found at the steady-state operating point of the -1 order system. The gain of the second order system is higher than that of the other two orders. Oscillations in jacket temperature are highly nonlinear because there are lower and higher limits on the coolant flowrate. Table (8.3 (a)) gives the amplitude of oscillation in tank and jacket temperatures for the three reaction orders under consideration. It shows that the amplitudes are largest for reaction order 2 and smallest for reaction order 1. The time average tank and jacket temperatures are determined by the harmonic balance method, which is described in subsection 8.3.3. The amplitude of oscillation of jacket temperature is larger than that of tank temperature, generally of the order of two in all cases.

8.8.2 At Open Loop Unstable Point

In these experiments the open loop unstable point is stabilised in the sense that all the trajectories inside the region enclosing the limit-cycle will remain within this region as time tends to infinity and some trajectories outside this region tend towards this region (since the limit-cycle is stable from both sides). Experiments 27, 56 and 92 show the limit-cycle behaviour of 1,0 and -1 order systems at their respective open loop unstable points. The gain of the zero order system is the largest of the three values under consideration. Amplitudes in tank and jacket temperatures are much larger than in the previous case. The amplitudes of the -1 order system are the least and that of zero order system are largest (refer to Table 8.3 (b)). The ratio of jacket to tank temperatures is around 1.75.

8.8.3 Harmonic Components of Nonlinear Oscillations

The harmonic contents of the nonlinear oscillations discussed above are determined by fitting the equations (3.63)-(3.65) into the system responses and calculating the constants. Table (8.4) gives the constants for different reaction orders. The accuracy of the determination of these constants can be seen when these approximate equations are plotted with the actual response. X_o, Y_o and Z_o give the time average concentration, tank and jacket tempeatures respectively. The cosine component in the jacket temperature (Z_1) is larger than the sine component (Z_2), whereas the sine component in the tank temperature (Y_2) is larger than the cosine component (Y_1). A comparison of X_o, Y_o and Z_o values with corresponding operating points gives the effect of nonlinear oscillations on the system performance. In all cases the conversion is reduced slightly due to oscillations. In certain cases the jacket temperature goes down by 1 K, while there is very little change in the tank temperature.

8.9 TOTAL SIMULATION VERSUS EXPERIMENTAL RESULTS

The experimental results are plotted with corresponding total simulation values for all cases in order to confirm their validity. Only half the number of these comparison graphs are reproduced here, again due to limitation on space. Graphs where the theoretical results fit exactly with the experimental results are omitted. It can be seen that generally the experimental tank concentration coincides with the total simulation.

This may be due to the fact that concentration is simulated in the experimental work. Deviation in experimental and theoretical concentration (Figs. (A.6.2. 10, 12, 31, 32, 33 and 34)) may be due to the fact that different step lengths are used in the integration techniques used. A step length of 0.1 seconds is used in the Runge-Kutta fixed step method in total simulation, while a step length of 0.2 seconds is used in experimental work. Another reason for deviation between theoretical and experimental results for decoupling type control may be due to the fact that the sampling time changes during an experimental run because of the iterations involved in the calculation of the cooling water flowrate for this particular control scheme. This change in sampling time is not incorporated in the total simulation studies.

Oscillations in jacket temperature are observed in experiments 22 and 60, while there are no oscillations in the corresponding total simulation runs (Figs. (A.6.2. 13, 30)). This may be due to the fact that the thermocouple inside the jacket may be near the coolant inlet so that sudden increase in flow may be affecting the temperature around the region immediately. Due to spurious oscillations in jacket temperature, the jacket flowrate also oscillates because the control is based on jacket temperature.

In limit-cycle experiments (Figs. (A.6.2. 3, 15, 16, 28, 29 and 47)), apart from plotting the total simulation results, the approximate responses obtained from equations

(3.63)-(3.65) are plotted with the experimental results. These approximate responses seem to fit the theoretical results very well because the constants of the equations were determined based on the theoretical response.

Large deviations in experimental and simulated tank temperature are observed in Figures (A.6.2.10, 12, and 15). Similarly large deviations in experimental and simulated jacket temperature are observed in Figures (A.6.2, 12, 15,16, 31, 32, 33 and 34). Deviations are observed only when there are sudden changes in temperature or during oscillations. This may be due to mixing effects of the jacket or the thermocouples may possess two time constants, one for increasing and another for decreasing temperatures. Noise and errors arising due to D/A and A/D conversions are not included in the total simulation model equations. Although the heaters extend through half of the vessel from the bottom, there may be temperature gradients along the height of the tank when large quantities of heat are output (when temperature and concentration perturbations are large positive numbers).

TABLE 8.1 STEADY STATE OPERATING CONDITIONS

Reaction Order = 2

Expt. No.	F (x 10^{-5} m^3/s)	F_c (x 10^{-5} m^3/s)	T_O(K)	T_{CO}(K)	Operating points (S)			Theoretical Temperature (K)
					T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	
1	4.583	3.75	287.16	283.77	302.99	19.219	293.37	302.76
2	3.75	3.33	283.41	282.58	301.4	19.117	292.00	301.61
3	3.75	3.0	283.9	282.58	303.85	19.029	294.05	303.9
4	3.958	3.333	285.99	280.27	302.5	19.12	291.78	302.5
5	3.958	3.417	285.14	281.07	302.2	19.133	291.37	302.54
6-10	4.583	3.333	286.61	280.91	301.18	19.272	291.37	300.91
11	4.33	3.333	286.3	281.44	303.49	19.13	292.827	303.1
12	4.33	3.333	286.09	280.68	301.6	19.196	291.3	302.09
13	4.33	3.5	287.94	282.43	307.37	18.993	295.19	307.74

TABLE 8.1 (contd.) STEADY STATE OPERATING CONDITIONS

Reaction Order = 1

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points(S or U) T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	Theoretical Temperature (K)
14	5	4.0	287.23	287.33	302.94	19.305	293.66	303.43 S 310.43 U
15	5	3.5	287.47	287.32	302.80	19.01	295.09	302.57 S 312.07 U
16	5	3.33	287.47	287.8	305	19.225	296.5	304.37 S 309.87 U
17	5.83	5.21	289.86	290.64	305.6	19.307	296.27	305.46 S 315.27 U
18,20	4.792	3.83	287	285.9	301.49	19.33	292.89	302.1 S 311.1 U
19	5.417	5.0	288.91	289.21	304.92	19.286	295.19	304.71 S 313.51 U
21	4.583	3.833	287.47	284.48	301.46	19.306	292.82	301.27 S 311.67 U

/continued

Continuation Sheet

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points S or U)			Theoretical Temperature (K)
					T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	
22	4.583	3.667	287.47	285.31	302.8	19.250	294.12	302.08 S 311.47 U
23	4.583	3.333	286.99	284.6	303.65	19.215	294.12	303.39 S 308.19 U
24	4.792	3.5	287.5	284.95	300.93	19.35	293.48	300.5 S 313.5 U
25	5.21	5.0	288.91	288.74	303.71	19.304	295.05	303.91 S 314.31 U
26	4.167	4.0	286.47	282.75	300.12	19.308	290.84	299.67 S 310.07 U
27	4.167	3.667	286.23	282.06	312.13	18.645	298.24	297.63 S 312.13 U
28	5	3.875	287.47	286.85	314.83	18.727	300.4	306.67 S 314.83 U

/continued

Continuation Sheet

Expt. No.	F $(\times 10^{-5}\ m^3/s)$	F_c $(\times 10^{-5} m^3/s)$	T_O(K)	T_{CO}(K)	Operating Points(S or U)			Theoretical Temperature (K)
					T_{SS}(K)	$C_{SS}(kg/m^3)$	T_{CSS}(K)	
29-30	4.792	3.6	286.99	286.37	312.39	18.888	300.1	301.99 S 312.39 U
31	3.6	3.5	286.09	280.82	306.9	18.92	295.03	301.99 S 306.99 U
32-38	3.6	3.33	285.33	280.91	299.4	19.24	290.3	299.43 S 304.5 U
39	4.167	3.33	283.51	280.91	293.17	19.52	287.1	292.1 S –
40	4.167	3.6	286.28	281.05	296.79	19.41	289.15	296.88 S 313.28 U
41	5.417	5.21	288.55	288.75	304.31	19.308	294.86	304.75 S 312.15 U
42	4.792	3.5	287.5	284.95	301.04	19.346	293.14	301.5 S 312.1 U

Continuation Sheet

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points(S or U)			Theoretical Temperature (K)
					T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	
43-45	4.792	3.6	287.61	280.4	295.6	19.54	287.7	295.3 S 320.5 U
46	5.417	3.6	288.85	288.91	303.57	19.335	296.34	304.05 S 314.05 U
47	5.417	3.5	288.78	289.0	304.13	19.315	296.9	304.58 S 313.18 U

Table 8.1 (contd.)

Reaction Order=0

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points (S or U)			Theoretical Temperature (K)	
					T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)		
48	4.792	4.0	289.79	282.29	300.07	19.422	290.827	299.79 305.19	S U
49	4.583	3.917	288.65	283.25	299.52	19.419	291	299.25 304.25	S U
50	4.792	4.0	288.77	282.66	297.67	19.512	289.736	297.37 307.17	S U
51	4.583	4.0	288.32	281.74	297.2	19.51	288.65	296.92 306.12	S U
52	4.792	3.167	286.47	286.65	296.22	19.56	291.71	296.67 306.67	S U
53	4.792	3.167	286.09	286.29	295.3	19.588	291.1	295.3 307.7	S U
54	4.583	3.747	287.89	284.49	298.64	19.4536	291.37	298.89 304.49	S U

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Continuation Sheet

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_C ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points (S or U) T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	Theoretical Temperature (K)	
55	4.583	4.0	287.61	283.07	296.656	19.525	289.19	296.41 306.61	S U
56	4.583	3.833	287.89	282.7	305.49	19.124	294.34	297.29 305.49	S U
57	4.583	3.833	288.89	282	304.1	19.203	293.29	299.29 304.1	S U
58	4.583	4.0	287.56	285.64	305.16	19.143	295.4	298.56 305.16	S U
59	4.458	3.333	287.89	284.03	304.49	19.158	295.19	298.49 304.49	S U
60	4.792	3.417	288.2	284.52	305.6	19.156	295.9	298.6 305.6	S U
61	4.583	3.708	288.46	282.33	304.46	19.1829	293.82	298.66 304.46	S U

/Continued

Continuation Sheet

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points (S or U) T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	Theoretical Temperature (K)	
62-64	4.583	3.708	288.51	282.29	298.87	19.445	290.09	298.91 304.11	S U
65	4.583	3.667	287.23	284.13	297.44	19.498	290.19	297.43 305.03	S U
66	4.583	3.833	288.2	284.54	298.87	19.445	291.75	298.82 305.02	S U
67	4.792	3.747	289.27	283.05	299.6	19.433	291.03	299.77 303.47	S U
68	4.792	3.5	288.86	282.76	298.5	19.482	290.65	298.86 305.26	S U

Table 8.1 (contd.)

Reaction Order=-1

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points(S or U) T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)	Theoretical Temperature (K)	
69	4.458	2.5	287.94	284.36	298.09	19.513	292.29	298.14 299.34	S U
70	4.167	2.75	287.59	283.76	296.38	19.55	290.91	296.38 300.18	S U
71	3.958	3.5	287.32	285.23	297.3	19.486	291.39	297.32 299.32	S U
72	3.958	3.333	286.47	286.42	295.55	19.559	291.25	295.87 300.47	S U
73	3.75	3.917	287.54	283.39	295.78	19.525	289.23	295.54 303.34	S U
74	3.958	3.75	288.08	283.02	295.73	19.552	289.09	296.08 300.68	S U
75	3.75	3.5	287.89	282.89	296.56	19.491	289.91	297.09 298.69	S U

/Continued

Continuation Sheet

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points (S or U)			Theoretical Temperature (K)	
					T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)		
76	4.167	3.333	288.29	283.76	296.56	19.543	290.28	297 299.99	S U
77	4.458	3.333	287.09	287.07	295.18	19.622	291.11	295.69 302.49	S U
78	4.167	3.333	286.85	286.65	296.06	19.563	291.57	296 301.25	S U
79	4.167	3.333	288	283.3	301.81	19.282	293.39	295.4 301.8	S U
80	3.75	3.5	287.13	284.13	298.93	19.374	292.02	296.73 298.93	S U
81	3.75	3.5	286.75	283.85	300.76	19.268	292.87	294.55 300.75	S U
82	3.75	3.333	286.8	283.99	300	19.314	292.72	295.2 300	S U

/Continued

Continuation Sheet

Expt. No.	F ($\times 10^{-5}$ m^3/s)	F_c ($\times 10^{-5}$ m^3/s)	T_O(K)	T_{CO}(K)	Operating Points (S or U)			Theoretical Temperature (K)	
					T_{SS}(K)	C_{SS}(kg/m^3)	T_{CSS}(K)		
83,84	4.36	3.333	287.65	285.71	301.86	19.313	294.52	296.26 301.86	S U
85-87	4.38	3.333	287.25	286.06	296	19.578	291.16	295.7 302.26	S U
88	4.41	3.167	287.47	286.1	295.73	19.6	291.23	296.07 302.07	S U
89	4.36	3.333	287.13	285.57	294.39	19.64	290.1	294.73 303.13	S U
90	4.05	3.333	286.83	285.23	294.95	19.592	290.1	295.3 301	S U
91	4.41	3.167	287.42	286.01	295.64	19.603	291.11	295.81 302.22	S U
92	6.455	3.833	291.2	291.7	304.0	19.4372	298.571	302 304.0	S U

TABLE 8.2 CONTROL SCHEMES AND LOAD CHANGES
(See Page No 170 for Key to Control Strategies)

Reaction Order=2

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
1	A.6.1.1	1	11.5	-	2	-	-	Stable, perturbations die down quickly
2	A.6.1.2	1	12.5	0.8	3.5	-	-	Stable, perturbations die down quickly
3	A.6.1.3	1	-	-	-	2.5	-	New SS temperature 4.7K above
4	A.6.1.4	9 K_2=90000	-	-	-	-	-	Limit-cycle (nonlinear oscillations)
5	A.6.1.5	4	11.5	0.837	6	-	-	Stable, perturbations die down quickly
6	A.6.1.6	8 D_{max}=0.007	14	0.22	4.7	-	-	Stable, perturbations die down quickly
7	A.6.1.7	"	-	-1	-	-	-	Tank temperature remains constant

Continued

Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
8	A.6.1.8	D^8_{max}=0.007	-5	-	-1.3	-	-	Stable
9	A.6.1.9	"	-	0.7	-	-	-	Stable
10	A.6.1.10	"	-	-	-	3	-	Tank temperature remains constant
11	A.6.1.11	D^8_{max}=0.005	10.5	0.82	4.5	-	-	Stable, behaviour similar to 6
12	A.6.1.12	D^8_{max}=0.015	12	0.803	5.2	-	-	Stable, oscillations in tank and jacket temperature
13	A.6.1.13	D^8_{max}=0.007	-	-	-	4.75	-	Small overshoot in tank temperature

Table 8.2 (contd.)

Reaction Order=1

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
14	A.6.1.14	1	7.5	-	1.0	-	-	Stable, perturbations die down fast
15	A.6.1.15	1	10.0	-	4.7	-	-	Metastable, perturbations remain constant
16	A.6.1.16	1	8.0	-	2.0	-	-	Unstable, all state variables move away from SS point
17	A.6.1.17	1	-	-	-	2.75	-	4K increase in tank temperature
18	A.6.1.18	2 K_2=500	13	-	5.0	-	-	Stable, perturbations die slowly
19	A.6.1.19	2 K_2=30000	10.5	-	2.5	-	-	Stable, oscillations due to large gain
20	A.6.1.20	2 K_2=500	14	-	5.5	-	-	Unstable

Continued

Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
21	A.6.1.21	3 $K_2=1000$	13.5	-	1.3	-	-	Metastable
22	A.6.1.22	3 $K_2=10000$	12.5	-	5.5	-	-	Stable, oscillations in jacket temperature and flowrate
23	A.6.1.23	4	12.5	-	3.5	-	-	Stable, fast response
24	A.6.1.24	2 $K_2=30000$	-	-	-	4.6	-	Offset in tank temperature
25	A.6.1.25	2 $K_2=50000$	-	-	-	3.5	-	Large oscillations and smaller offset
26	A.6.1.26	9 $K_2=16000$						Limit-cycle behaviour at SS point
27	A.6.1.27	9 $K_2=8600$						Limit-cycle behaviour at unstable point

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
28	A.6.1.28	$K_2^2=500$	-3.5	0.623	-3.2	-	-	The unstable point is not stabilised
29	A.6.1.29	$K_2^2=20000$	-6	-	-5.5	-	-	The unstable point is stabilised
30	A.6.1.30	$K_2^2=20000$	2.8	-	1.0	-	-	The unstable point is stabilised Further confirmation
31	A.6.1.31	$D_{max}^8=0.007$	-5.5	-0.17	-4	-	-	The unstable point is stabilised by this strategy
32	A.6.1.32	$D_{max}^8=0.007$	13	-1	6.5	-	-	Stable and fast response
33	A.6.1.33	"	-	-1	-	-	-	Tank temperature remains constant
34	A.6.1.34	"	-5.2	-5	-1.5	-	-	Stable

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
35	A.6.1.35	8 D_{max}=0.007	15.5	0.6	10.5	-	-	Stable
36	A.6.1.36	8 D_{max}=0.01	12	0.622	4	-	-	A bit of oscillation in jacket flow
37	A.6.1.37	8 D_{max}=0.015	12	0.622	4	-	-	Large oscillations in all state variables
38	A.6.1.38	8 D_{max}=0.005	11	0.646	4.8	-	-	Stable, smooth response
39	A.6.1.39	8 D_{max}=0.007	-	-	-	4.5	-	Largest offshoot is 1K
40	A.6.1.40	8 D_{max}=0.007	-	-	-	3.5	-	Small perturbation
41	A.6.1.41	6	-	-	-	3.4	-	Perturbation in tank temperature is very small

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
42	A.6.1.42	6	-	-	-	4.8	-	Perturbation in tank temperature is very small
43	A.6.1.43	7	-	-	-	-	7	Invariance in all three state variables
44	A.6.1.44	7	-	-	-	-	5	Invariance in all three state variables
45	A.6.1.45	7	-	-	-	-	2.5	Invariance in all three state variables
46	A.6.1.46	10	-	-	-	0.75	2.7	Invariance in tank temperature and concentration
47	A.6.1.47	10	-	-	-	2.0	2.1	Invariance in tank temperature and concentration

Table 8.2 (contd.)

Reaction Order=0

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
48	A.6.1.48	1	6.5	-	1.1	-	-	Stable
49	A.6.1.49	1	7.5	0.46	2	-	-	Unstable
50	A.6.1.50	2 K_2=500	10.5	-	3.5	-	-	Stable, perturbations die down fast
51	A.6.1.51	2 K_2=100	11.5	-	3	-	-	Metastable, perturbations remain constant
52	A.6.1.52	1	-	-	-	2.6	-	Tank temperature deviation is 3.7K
53	A.6.1.53	2 K_2=10000	-	-	-	3	-	Offset of 1.2K
54	A.6.1.54	4	13.7	-	6.2	-	-	Stable, fast response

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
55	A.6.1.55	9 K_2=60000	-	-	-	-	-	Limit-cycle at stable operating point
56	A.6.1.56	9 K_2=100000	-	-	-	-	-	Limit-cycle at unstable operating point
57	A.6.1.57	2 K_2=2000	-5	-	-3	-	-	Unstable operating point is not stabilised
58	A.6.1.58	2 K_2=3500	-6.5	-	-4	-	-	Unstable operating point is not stabilised but perturbation is less
59	A.6.1.59	3 K_2=15000	-6	-0.1	-2.5	-	-	Unstable operating point is not stabilised
60	A.6.1.60	3 K_2=30000	-6.4	-	-3.5	-	-	Unstable operating point is not stabilised
61	A.6.1.61	8 D_{max}=0.007	-6.0	.01	-3.5	-	-	Unstable operating point is stabilised, but response is slow

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
62	A.6.1.62	D^8_{max}=0.007	13.5	0.44	5.5	-	-	Stable, fast response
63	A.6.1.63	"	13.1	-0.6	7.1	-	-	Stable, fast response
64	A.6.1.64	"	-5.9	-0.6	-0.6	-	-	Stable, fast response
65	A.6.1.65	D^8_{max}=0.016	15.8	0.401	3.8	-	-	Stable oscillations in jacket flowrate
66	A.6.1.66	D^8_{max}=0.002	13.5	0.445	6.7	-	-	Stable, response is slow compared to experiment 62
67	A.6.1.67	D^8_{max}=0.007	-	-	-	4.2	-	An overshoot of + 1.0K
68	A.6.1.68	"	-	-	-	2.5	-	No offset

Table 8.2 (contd.)

Reaction Order=-1

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}'$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
69	A.6.1.69	1	4.8	-	0.5	-	-	Unstable
70	A.6.1.70	1	4.8	-	0.6	-	-	Metastable, perturbations remain constant
71	A.6.1.71	1	4.5	-	0.6	-	-	Stable, slow response
72	A.6.1.72	1	-	-	-	2.5	-	Unstable, 3.8K deviation in 1200 seconds
73	A.6.1.73	2 K_2=500	8	-	1.2	-	-	Stable, slow response
74	A.6.1.74	"	13	-	3	-	-	Unstable
75	A.6.1.75	2 K_2=2000	12.5	0.01	3.5	-	-	Metastable

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
76	A.6.1.76	3 $K_2=10000$	13.5	0.4	4.7	-	-	Stable, very slow fall in tank temperature
77	A.6.1.77	4	15	0.3	6.2	-	-	Stable, fast response
78	A.6.1.78	2 $K_2=30000$	-	-	-	2.6	-	Stable, very small offset
79	A.6.1.79	2 $K_2=2000$	-6.2	0.01	-3.7	-	-	Unstable operating point is not stabilised
80	A.6.1.80	2 $K_2=3500$	+9	-	1.0	-	-	Unstable point is stabilised, slow response
81	A.6.1.81	3 $K_2=8000$	-5.2	-	-2.5	-	-	Unstable point is not stabilised
82	A.6.1.82	3 $K_2=10000$	-4	-	-2.7	-	-	Unstable point is stabilised

Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{oo}$ (K)	
83	A.6.1.83	$D_{max}^{8}=0.007$	-5.4	-0.2	-3.2	-	-	Unstable operating point is stabilised. Fast response
84	A.6.1.84	"	11.2	-	3.0	-	-	Unstable operating point is stabilised.Fast response.Further confirmation.
85	A.6.1.85	"	12.5	0.4	4.2	-	-	Stable, fast response
86	A.6.1.86	"	0	0.43	0	-	-	Tank temperature remains constant
87	A.6.1.87	"	-2.8	-0.4	-	-	-	Stable
88	A.6.1.88	$D_{max}^{8}=0.005$	8.8	-	2.4	-	-	Stable, slower response when compared to experiment 84
89	A.6.1.89	$D_{max}^{8}=0.007$	-	-	-	3.6	-	No offset, an overshoot of 0.4K

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Continuation Sheet

Expt. No.	Figure No.	Control Strategy	Initial Perturbation			Load Changes		Comments
			$\bar{T}$ (K)	$\bar{C}$ (kg/m^3)	$\bar{T}_c$ (K)	$\bar{T}_o$ (K)	$\bar{T}_{co}$ (K)	
90	A.6.1.90	8 D_{max}=0.007	-	-	-	2.3	-	An offset of - 0.3K
91	A.6.1.91	8 D_{max}=0.011	10.2	-	3	-	-	Stable, fast response, oscillations in jacket flow
92	A.6.1.92	9 K_2=28000	-	-	-	-	-	Limit-cycle at unstable point

Control strategies

1 = uncontrolled
2 = proportional feedback control of tank temperature
3 = proportional feedback control of jacket temperature
4 = controller equation derived from stability conditions
6 = invariance control for step in feed temperature
7 = invariance control for step in coolant temperature
8 = decoupling type control of tank temperature
9 = proportional feedback control of tank concentration
10 = invariance control for steps in feed and coolant temperatures

TABLE 8.3 AMPLITUDE OF TANK AND JACKET TEMPERATURES FOR DIFFERENT REACTION ORDERS

Reaction order	Amplitude of Tank Temperature (K)	Amplitude of Jacket Temperature (K)
2	2.5	5.5
1	0.85	1.5
0	2	4.5

a) at open loop stable point

Reaction order	Amplitude of Tank Temperature (K)	Amplitude of Jacket Temperature (K)
1	4.2	6
0	5	8.5
-1	0.95	1.25

b) at open loop unstable point

TABLE 8.4 HARMONIC COMPONENTS OF THE LIMIT-CYCLES

Reaction order	Nature of op. pt.	Time period (S)	X_0 (kg/m^3)	X_1 (kg/m^3)	X_2 (kg/m^3)	Y_0 (K)	Y_1 (K)	Y_2 (K)	Z_0 (K)	Z_1 (K)	Z_2 (K)
2	S	1295.2	19.1248	-0.03467	.01557	302.38	.01054	-3.0311	290.5	-5.725	-2.094
1	S	1500	19.3082	.01148	.0058	300.087	-.5972	.2147	292.26	.993	1.143
0	S	1395	19.5199	-.02523	.00732	296.62	-.0203	-1.42	298.82	-3.08	-.7
1	U	1750	18.668	.1962	-.02812	312.71	-2.25	4.22	296.35	6.73	1.86
0	U	1800	19.194	-.0149	.1181	304.22	-3.58	-3.28	297.41	-5.7	-1.59
-1	U	1720	19.4338	-.00995	-.01757	304.23	0.796	.0232	298.73	.496	-1.694

CHAPTER 9

CONCLUSIONS AND RECOMMENDATIONS

Many conclusions are drawn from the theoretical, experimental and total simulation studies carried out so far on the C.S.T.R., and are summarised in the following sections. A few recommendations are also made for further studies.

9.1 CONCLUSIONS

9.1.1 On Theoretical Work

The theoretical work carried out initially helped to design the experiments. It also gave an idea about the operating ranges for various parameters. Much of this work was verified later through experiments. The conclusions drawn are listed below.

(i) Reaction order $|n|$ (absolute of n) is more stable than order $|n-1|$ for any inlet conditions. Generally reaction order 1 is more stable than -1 but for certain inlet conditions the reverse is true.

(ii) The region of asymptotic stability (RAS) depends on the reaction order to a large extent.

(iii) Although the algorithm for the determination of the RAS, using Krasovskii's theorem, can easily be programmed its limitations and conservativeness is brought out in the comparison graph.

(iv) Although qualitative stability analysis by Krasovskii's theorem has limitations, it can be used to design control schemes, which are much superior to conventional control schemes.

(v) The open loop unstable operating point is easily stabilised by simple proportional feedback control. Sometimes limit-cycle is also generated at this point by a suitable control scheme.

(vi) A control strategy which decouples tank temperature from other state variables (decoupling type control) is found to be superior to conventional controllers for increasing RAS, for step type disturbance in feed temperature or for stabilising open loop unstable points.

(vii) Invariance control is simple and found to be very effective for load disturbances in feed or coolant inlet temperatures.

(viii) Liapunov's method was tried for determining the existence of limit-cycles in three dimensional state space and found to be successful. There are no other methods reported so far for high dimensional systems. This method is also useful for the determination of the existence of multiple stable and unstable limit-cycles.

(ix) A method was devised to determine the harmonic components of the nonlinear oscillations and found to be very successful.

9.1.2 On Experimental and Total Simulation Studies

The partial simulation technique is confirmed as a powerful tool in studying the dynamics of a reactor. This technique embraces the advantages of total simulation and the realities involved in experimental work. It is seen that various exothermic chemical reactions are simulated in the reactor with ease. Different complicated control schemes are also applied to the system since a digital computer is used as the controller. The on-line software package developed as part of the study is found to be versatile and powerful. Other important conclusions drawn on the studies carried out are

(i) The operating points and RAS depend on the inlet conditions, and order of reaction. The later affects the system behaviour qualitatively.

(ii) The unstable operating point separates the state space into stable and unstable regions. So the difference between unstable and stable temperatures gives an idea about the stability region.

(iii) A simple proportional feedback controller increases RAS. A control scheme developed based on the second method of Liapunov is found to be better than feedback control schemes.

(iv) The open loop unstable point is easily stabilised with proportional feedback control or decoupling type control schemes. Using the latter scheme a system operating point can be switched from a stable to an unstable point in the shortest time without oscillation. Control of tank temperature was found to be superior to control of jacket temperature.

(v) Decoupling type control increases RAS for all reaction orders to a large extent.

(vi) Invariance control for load disturbances is definitely superior to feedback control schemes, although an additional feedback loop may reduce drifts.

(vii) Decoupling type control also makes tank temperature and concentration invariant to changes in feed temperature.

(viii) A limit-cycle is generated at stable and unstable operating points. The amplitude and time period of oscillation depends on reaction order and the nature of the operating point.

(ix) The harmonic components of the nonlinear oscillation determined are found to be very accurate, as seen in the comparison graphs. Only the first harmonics are found to be predominant.

(x) The time average conversion is found to be slightly less than steady-state conversion.

(xi) The model of the entire plant developed for total simulation studies consists of several differential equations and samplers. The transient behaviour of the reactor coincides well with the corresponding model response.

(xii) Limitations on coolant flowrate limits the largest disturbances and load changes that can be applied to the system without making it unstable.

9.2 RECOMMENDATIONS

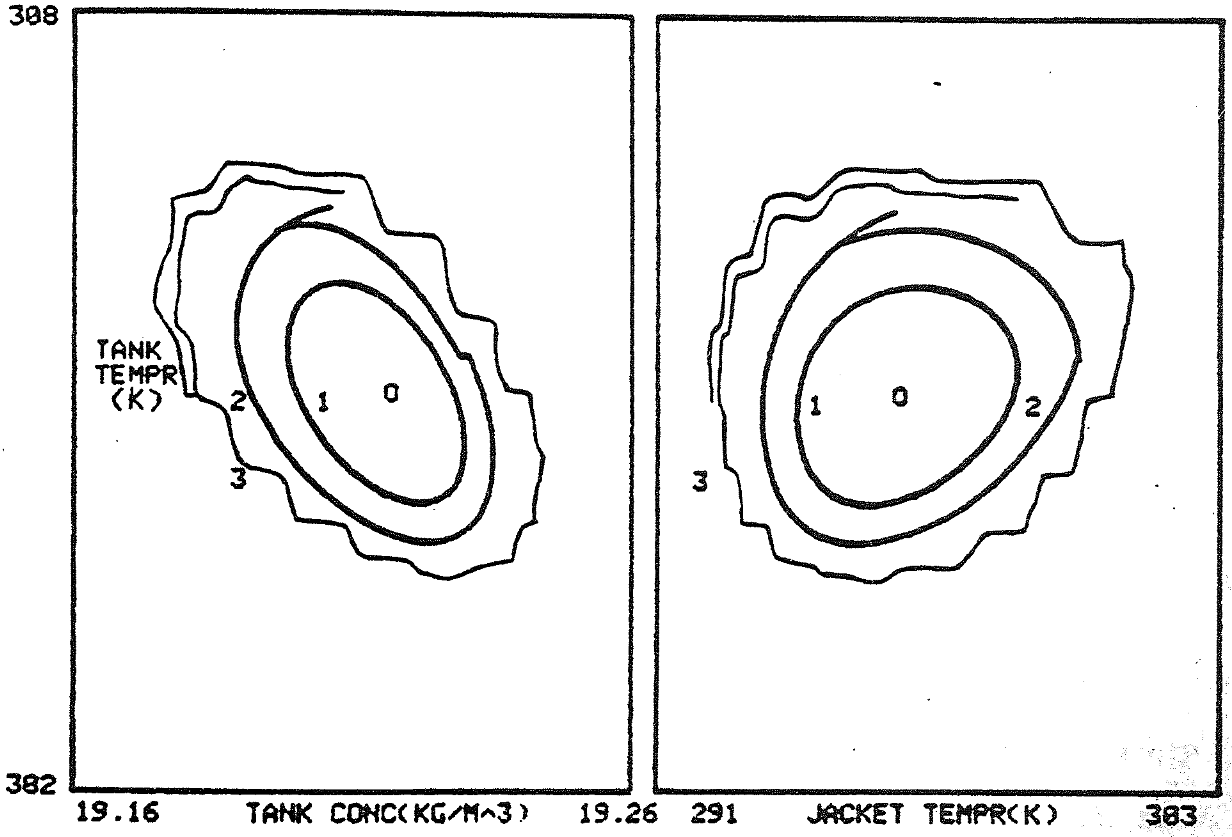
There is a large scope for further work on the reactor system by making a few modifications. Examples of these are

(i) The feed flowrate can also be used as a manipulative variable by adding a control valve to the feed line. With two manipulative variables tank temperature and concentration can be decoupled in the same way as described in the previous chapters. Invariance control for step in feed concentration can also be incorporated in the system.

(ii) The addition of another C.S.T.R. in series creates many stability problems. The effect of flow of coolant cocurrent or countercurrent to the feed on the stability can be studied.

(iii) As the equation generated for invariance control scheme is different from that of the conventional feed-forward control a comparative study of invariance and P + I + D and feed-forward control could usefully be carried out.

(iv) Sampling with zero order hold introduces time lags and hence instabilities. Thus if the sampling time is large, time lag may be large and the effect of this on limit-cycle offers an interesting study. A stable limit-cycle for low sampling time may become unstable as sampling time is increased. Fig. (9.1) shows the effect of sampling on the limit-cycle generated at the first order open loop stable operating point. The period of oscillation increases as the sampling time is increased and for a sampling time of 80 seconds is no longer a closed stable trajectory but slowly unwinds.



Gain (K_c) =0.036

0 = Open loop stable operating point

1 = Sampling time =0 secs. , Time period=960secs.

2 = =20 secs., =1160secs.

3 = =80 secs., =1300secs.

FIG.9.1 EFFECT OF SAMPLING TIME ON THE LIMIT-CYCLE GENERATED AT THE OPEN LOOP STABLE OPERATING POINT OF A FIRST ORDER SYSTEM

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APPENDICES

APPENDIX 1

LISTING OF COMPUTER PROGRAMS

A.1.1 PROGRAM FOR OBTAINING THE STABLE AND UNSTABLE OPERATING POINTS

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10   REM GENERALISED PROGRAM FOR OBTAINING SS VALUES AND
15   REM ROOTS OF LINEARISED SYSTEM FOR VARIOUS REACTION
17   REM ORDERS.
20   READ V,V1,C0,R,K,D,U
30   DATA 17300,8532,.001,.00198,2000,30,.037
40   PRINT"WHAT ARE THE INLET CONDITIONS";
50   INPUT F,F1,T0,T1,C1
60   FOR I=1 TO 9
70   O=I-5
80   PRINT "TYPE OF STUDY: 1=CALCULATE E,GIVEN OP. TEMPR."
90   PRINT TAB(15);"2=CALCULATE OP. TEMPR. GIVEN E"
91   INPUT I2
92   T9=V/F
94   T8=V1/F1
96   I0=U/(V*C0)
98   I1=U/(V1*C0)
100  I9=0
105  IF I2 >= 2 THEN 500
107  REM CALCULATE ACTIVATION ENERGY FOR THE GIVEN
108  REM OPERATING TEMPERATURE
110  PRINT"WHAT IS THE STEADY STATE TEMPERATURE DESIRED";
115  INPUT T2
190  PRINT"WHAT IS THE NEAREST E VALUE";
200  INPUT E
210  E=E+.005
220  Q=E*C0/(R*D*C1)
230  I9=I9+1
240  B1=T2*Z
250  C2=C1-.0001
260  C3=C2
270  X=K*C3 ** O*EXP(-Q/B1)
280  H0=F*(C1-C3)-X*V
290  H1=-F-O*X*V/C3
300  C2=C3-H0/H1
320  IF ABS((C2-C3)/C3)>.00001 THEN 260
330  T3=(U*T2+F1*C0*T1)/(U+F1*C0)
340  H0=F*C0*(T0-T2)-U*(T2-T3)+X*V*D
360  IF I9=1 AND H0<0 THEN 2470
400  IF H0*1000 > 1.E-08 THEN 210
405  Q=E/R
410  PRINT"REACTION ORDER=";O
420  PRINT"E=";E;"T1=";T2;"C1=";C3;"TC1=";T3
430  PRINT"HEAT IN KWS=";4.181*V*K*D*C3 ** O*EXP(-E/(R*T2))
440  GOTO 2000
445  REM CALCULATE OPERATING TEMPERATURE FOR GIVEN
447  REM ACTIVATION ENERGY
500  DIM B(9)
520  MAT READ B
530  DATA 21.99,19.605,17.22,14.83,12.444,10.06
535  DATA 7.67,5.285,2.9
610  Q=B(I)/R
620  T5=T0+1.5
630  T2=T5
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```
640  X=EXP(-Q/T2)
650  T3=(U*T2+F1*R*C0*T1)/(U+F1*R*C0)
660  C2=C1-.00001
670  C3=C2
680  H1=F*(C3-C1)+K*V*X*C3 ** U
690  H2=F+K*V*X*U*C3 ** (U-1)
700  IF H2=0 THEN 720
710  C2=C3-H1/H2
720  IF ABS(C3-C2)/C2 <= 0.0001 THEN 740
730  GOTO 670
740  Y=K*D*V*C3 ** U*X
750  H2=Y*Q/T2 ** 2-F*R*C0-U
760  H1=F*R*C0*(T0-T2)-U*(T2-T3)+Y
780  I2=.9
790  IF ABS(T5-T2)>.5 THEN 810
800  I2=.4
810  T5=T2-(H1/H2)*I2
820  IF ABS(T2-T5)/T5 <=.00001 THEN 410
830  GOTO 630
1995  REM CALCULATE EIGEN VALUES
2000  DIM A(3,3)
2010  A1=C3/C1
2020  B1=T2*Z
2030  Q=E*C0/(D*R*C1)
2040  A(1,3)=A(3,1)=0
2050  A(2,1)=K*C1 ** (U-1)*A1 ** (U-1)*U*EXP(-Q/B1)
2060  A(1,1)=-1/T9-A(2,1)
2070  A(1,2)=K*C1 ** (U-1)*A1 ** U*EXP(-Q/B1)
2080  A(1,2)=A(1,2)*Q/B1 **2
2090  A(2,2)=-(1/T9+I0)-A(1,2)
2100  A(2,3)=I0
2110  A(3,2)=I1
2120  A(3,3)=-(1/T8+I1)
2130  B5=-(A(1,1)+A(2,2)+(3,3))
2140  P7=A(2,2)*A(3,3)
2150  P8=A(2,3)*A(3,2)
2160  P9=A(1,2)*A(2,1)
2170  B6=A(1,1)*(A(2,2)+A(3,3))+P7-P8-P9
2180  B7=-(A(1,1)*(P7-P8)-A(3,3)*P9)
2190  R9=-B7/B6
2200  R8=R9
2210  H0=R8 ** 3+R8 ** 2*B5+R8*B6+B7
2220  H1=3*R8 ** 2+2*R8*B5+B6
2230  H2=6*R8+2*B5
2240  R9=R8-H0/H1-H1/2/H2
2250  IF ABS(H0)>1.E-07 THEN 2200
2260  B8=B5+R8
2270  B9=B6+R8*(B5+R8)
2280  R9=R8
2290  R8=0
2300  B6=B8 ** 2-4*B9
2310  IF B6>0 THEN 2340
2320  R8=1
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```
2330  B6=ABS(B6)
2340  B6=SQRT(B6)
2350  B5=-B8
2360  PRINT"THE ROOTS ARE"
2370  IF R8=1 THEN 2400
2380  PRINT R9,(B5+B6)/2,(B5-B6)/2
2390  GOTO 2410
2400  PRINT R9,B5/2;"+I";B6/2,B5/2;"-I";B6/2
2405  REM CALCULATE THE NEXT HIGHER OPER. TEMPR.
2410  IF I9<0 THEN 2450
2420  I9=-1
2430  T5=T1+2.5
2440  GOTO 630
2450  NEXT I
2460  END
2470  PRINT "GIVE A LOWER VALUE OF E"
2480  GOTO 190
2490  END
```

A.1.2 <u>PROGRAM TO DETERMINE THE SEPARATRICES</u>

```
      TRACE2
      MASTER SEPARATRIX
C   PROGRAM TO CALCULATE SEPARATRICES BASED ON
C   KRASOVSKII'S THEOREM
      INTEGER ORD
      REAL K,I0,I1,K8,KC
      DIMENSION A(3,3),EE(4),B(3,3)
      DATARH,RHC,CP,CPC,V,VC,R,K,DH/1.,1.,0.001,0.001,17300.
     1,8532.,0.00198,2000.,30./,U/0.037/
      DATAEE/14.83,12.445,10.06,7.67/
      READ(5,209)F,FC,T0,TC0,C0
      READ(5,2099)((B(I,J),J=1,3),I=1,3)
 2099 FORMAT(3E0.0)
      IJJ=0
  209 FORMAT(5F0.0)
  100 FORMAT(3F0.0)
      A(1,3),A(3,1)=0.
      ZZ=RH*CP/(DH*C0)
      TH=V/F
      I0=U/(RH*CP*V)
      I1=U/(RHC*CPC*VC)
      THC=VC/FC
      G0=TC0*ZZ
      WRITE(6,99)((B(I,J),I=1,3),J=1,3)
 99   FORMAT(10X,'[A]MATRIX:'/,3(3(5X,F9.4)/))
 200  FORMAT(5X,'ORDER OF REACTION=',I2)
 300  FORMAT(2X,'SEPARATRIX=',I2//20X,'TEMP',10X,'CONC')
 2888 READ(5,2099,END=9000)KC,XKC
      WRITE(6,1134)KC,XKC
 1134 FORMAT(20X,2E15.6)
      IJJ=IJJ+1
      X3=0
      DO1000IJK=1,4
C   CALCULATE SEPARATRICES FOR RN. ORDER=-1,1 & 2
      IF(IJK.EQ.2)GOTO1000
      ORD=IJK-2
      IF(IJJ.EQ.1)READ(5,100)TISS,CISS,TCISS
      Q=EE(IJK)*CP/(R*DH*C0)
      AISS=CISS/C0
      BISS=TISS*ZZ
      GISS=TCISS*ZZ
      WRITE(6,200)ORD
      DO2000IJX=1,5
      IF(IJX.EQ.1.AND.IJK.EQ.3)GOTO2000
      IJKX=IJX
      IF(IJX.GT.4)IJKX=IJX+1
      WRITE(6,300)IJKX
      DO3000IX=1,13
      T1=290.+(IX-1)*5.
      X2=(T1-TISS)*ZZ
      R1=EXP(-Q/(X2+BISS))
      C2=C0
      IRM=0
```

```
 1    C1=C2
      A(2,1)=K*ORD*C1**(ORD-1)*R1
      A(1,1)=-1/TH-A(2,1)
      A(1,2)=-K*C1**ORD*R1*Q/((BISS+X2)**2*C0)
      A(2,2)=-(1/TH+I0)-A(1,2)
      BB=VC/(G0-GISS-X3)
      DFCX3=XKC
      DFCX2=KC
      A(3,2)=I1+DFCX2/BB
      FCB=KC*X2+XKC*X3
      A(3,3)=-(1/THC+I1)-FCB/VC+DFCX3/BB
      A(2,3)=I0
      DF1=-K*ORD*(ORD-1)*R1*C1**(ORD-2)
      DF2=-A(2,1)*Q/(C0*(BISS+X2)**2)
      DF3=-DF1
      DF4=-DF2
      FN1=2*A(1,1)*B(1,1)+2*A(2,1)*B(1,2)
      FN2=2*A(2,2)*B(2,2)+2*(A(3,2)*B(2,3)+A(1,2)*
     1B(1,2))
      DFN1=2*DF1*B(1,1)+2*B(1,2)*DF3
      DFN2=2*DF4*B(2,2)+2*DF2*B(1,2)
      GOTO(10,20,30,30,202),IJX
C  SEPARATRIX 1
 10   FN=TH*K*R1*(B(1,1)-B(1,2))/B(1,1)
      IF(IJK.EQ.1)C1=SQRT(FN)
      IF(IJK.EQ.4)C1=-1/(2*FN)
      IF(IRM.EQ.1)GOTO 401
      GOTO70
C  SEPARATRIX 2
 20   FN=-(-(1/TH+I0)*B(2,2)+B(2,3)*A(2,3))/(B(1,2)
     1-B(2,2))*C1**ORD/A(1,2)
      IF(IJK.EQ.1)C1=1/FN
      IF(IJK.EQ.3)C1=FN
      IF(IJK.EQ.4.AND.FN.LT.0.)GOTO3000
      IF(IJK.EQ.4)C1=SQRT(FN)
      IF(IRM.EQ.1)GOTO 401
      GOTO70
C  SEPARATRIX 3
 30   XX=B(1,2)*(A(1,1)+A(2,2))+A(2,1)*B(2,2)+B(1,1)
     1*A(1,2)+B(1,3)*A(3,2)
      DXX=B(1,2)*(DF1+DF4)+DF3*B(2,2)+B(1,1)*DF2
      FN=FN1*FN2-XX**2
      DFN=DFN1*FN2+FN1*DFN2-2*XX*DXX
      IF(IJX.EQ.4)GOTO40
      GOTO50
C  SEPARATRIX 4
 40   YY=B(1,3)*(A(1,1)+A(3,3))+B(1,2)*A(2,3)+A(2,1)
     1*B(2,3)
      DYY=B(1,3)*DF1+DF3*B(2,3)
C  SEPARATRIX 6
202   ZZ=B(2,3)*(A(2,2)+A(3,3))+B(2,2)*A(2,3)+A(3,2)*
     1B(3,3)+A(1,2)*B(1,3)
      S3=-2*A(3,3)*B(3,3)-2*A(2,3)*B(2,3)
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      DZZ=B(2,3)*DF4+DF2*B(1,3)
      FN=S3*FN-2*XX*YY*ZZ+FN1*ZZ**2+FN2*YY**2
      DFN=S3*DFN-2*DXX*YY*ZZ-2*XX*DYY*ZZ-2*XX*YY*DZZ+
     1DFN2*YY**2+FN2*DYY*2*YY
     2+DFN1*ZZ**2+FN1*DZZ*2*ZZ
      IF(IJX.EQ.4)GOTO50
      FN=-S3*FN2-ZZ**2
      DFN=-ZZ*2*DZZ-1*S3*DFN2
   50 IF(IRM.EQ.1)GOTO 401
      IF(DFN.EQ.0)GOTO60
      C2=C1-FN/DFN
      C3=C1
      IF(C1.EQ.0.)C3=C2
      IF(C3.EQ.0.)GOTO60
      IF(ABS(C2-C1)/C3.GE.0.0005)GOTO1
   60 C1=C2
   70 WRITE(6,400)T1,C1
  400 FORMAT(19X,F6.2,8X,F9.7)
      C2=C1*1.1
      IRM=1
      GOTO 1
  401 IF(FN.GE.0.)WRITE(6,1012)
 1012 FORMAT(1H+,46X,'+')
      IF(FN.LT.0.)WRITE(6,1013)
 1013 FORMAT(1H+,46X,'-')
      ZZ=CP/(DH*C0)
 3000 CONTINUE
 2000 CONTINUE
 1000 CONTINUE
 2222 CONTINUE
      GOTO2888
 9000 CONTINUE
      STOP
      END
      FINISH
```

A.1.3 PROGRAM TO DETERMINE THE LARGEST RAS

```
C   PROGRAM TO DETERMINE THE LARGEST RAS USING
C   KRASOVSKII'S THEOREM
        SUBROUTINE MAXLIAP(XKA1,XDKA,XKA2,A,XK,VSUM1)
C   SUBROUTINE TO CALCULATE LARGEST LIAPUNOV VALUE
C   WITHIN WHICH -VDOT > 0
        REAL KA,KA1,KA2
        DIMENSION DF(3,3),X4(3),X3(3),A(3,3),X(3),FN(3)
        REAL ITHO,ITHI,KC
        INTEGER ORD
        COMMON/THREE/IOO4,IS,IST
        COMMON/SIX/A1,B1,A2,B2,C2,AAA,BBB,CCC,DDD,FN1
        COMMON/SEVEN/IPK,IPD,KA1,KA2,IFAIL,DKA
        COMMON/FIVE/TH,THC,CO,A1SS,B1SS,G1SS,ITHO,ITHI,K
       1,Q,ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
        VSUM1=0.
        KA1=XKA1
        KA2=XKA2
        DKA=XDKA
        IPK=0
   52   FORMAT(9X,'LIAP K',12X,'X1C',12X,'X2C',12X,'X3C',12X,
       1'OBJ',12X,'VOLUME')
        SINDEX=190.*178.
        NX=3
        KA=KA1
 1929   WRITE(2,300)
  300   FORMAT(/5X,' [A] MATRIX:')
        DO 4 I=1,NX
        WRITE(2,200)(A(I,J),J=1,NX)
    4   CONTINUE
        CALL SYLVES(NX,A,0),RWTURNS(9999)
  200   FORMAT(2X,3(E14.6,2X))
        WRITE(2,52)
   54   FORMAT(8X,'X1C',15X,'X2C',15X,'X3C',15X,'OBJ',15X,
       1'X3C',15X,'OBJ',15X,'X3C')
    7   WRITE(IOO4,50)KA
   50   FORMAT(/2X,'LIAPUNOV K=',E13.6)
        XK=KA
        WRITE(IOO4,54)
        X(1)=-0.003+.82
        SMIN=10.**70
        VSUM=0.
        DO 1002 IJ1=1,61
        M=IJ1/2
        INDEXI=2
        IF(M*2.EQ.IJ1)INDEXI=4
        IF(IJ1.EQ.1.OR.IJ1.EQ.61)INDEXI=1
        X(1)=X(1)+.003
        X1C=X(1)-A1SS
        XB=-0.015375
        DO 1003 IJ2=1,65
        XB=XB+.015375
        X(2)=XB/10.25
        M=IJ2/2
```

```
      INDEXJ=2
      IF(M*2.EQ.IJ2)INDEXJ=4
      IF(IJ2.EQ.1.OR.IJ2.EQ.65) INDEXJ=1
      INDEX=INDEXI*INDEXJ
      X2C=X(2)-(BISS-B0)
      YY=EXP(-Q/(BISS+X2C))
      FN1=-X1C/TH-((X1C+A1SS)**ORD*YY-XX)*CORD
      FN(1)=FN1
      X3(1)=X3(2)=X3(3)=0.
      IODEX=0
 1010 CALL VAR3(X1C,X2C,X3C,IODEX,KA,A),RETURNS(1005)
      X3(IODEX)=X3C
      IF(X3C.LT.XGG)X3(IODEX)=XGG
      IF(X3C.LT.XGG)GOTO 1010
      CALL JACOBIA(X1C,X2C,X3C,DF)
      FN(2)=A1+B1*X3C
      FN(3)=A2+B2*X3C+C2*X3C**2
  808 DSUMF=0.
      DO 802 L=1,NX
      DO 802 I=1,NX
      DO 802 J=1,NX
  802 DSUMF=DSUMF+FN(I)*FN(J)*DF(L,J)*((A(I,L)+A(L,I))*I5
      X4(1)=X1C
      X4(2)=X2C
      X4(3)=X3C
      DO 803 I=1,NX
      DO 803 J=1,NX
  803 DSUMF=DSUMF+(A(I,J)*X4(I)*FN(J)+A(I,J)*X4(J)*FN(I))/10.**7
      OBJ=-DSUMF
      WRITE(IO04,1006)X1C,X2C,X3C,OBJ
 1006 FORMAT(5X,4(E14.7,2X))
      IF(OBJ.LT.0..AND.IST.EQ.1)GOTO 1911
      IF(OBJ.LT.0..AND.IST.EQ.0)GOTO 1909
      IF(OBJ.GT.SMIN)GOTO 1010
      SMIN=OBJ
      X1MIN=X1C
      X2MIN=X2C
      X3MIN=X3C
      GOTO 1010
 1005 CONTINUE
      IF(X2C*KC.GT.120.)VSUM=VSUM-FLOAT(INDEX)*.18*
     1(X3(1)-X3(2))*(1./10.25-(BISS-B0)-120./KC)/SINDEX
C  VOLUME OF THE ELLIPSOIDAL REGION
      VSUM=VSUM+FLOAT(INDEX)*.18*(X3(1)-X3(2))/SINDEX
 1003 CONTINUE
 1002 CONTINUE
      IF(SMIN.GT.10.**69)GOTO 1009
 1919 WRITE(7,1007)KA,X1MIN,X2MIN,X3MIN,SMIN,VSUM
      VSUM1=VSUM
 1007 FORMAT(5X,6(E14.6,2X),5X)
      IPD=0
      IF(IST.EQ.1)GOTO 1910
 1911 CALL LIAPK(KA)
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```
      IF(IPD.LE.0)GOTO 7
      GOTO 9999
 1009 KA1=KA1+DKA
      WRITE(7,1007)KA
      KA=KA1
      GOTO 7
 1909 XK=KA-DKA
 1910 WRITE(2,1008)XK,VSUM1
 1008 FORMAT(5X,E14.6,64X,E14.6)
 9999 CONTINUE
      RETURN
      END
      SUBROUTINE LIAPK(KA)
C TO INCREASE LIAPUNOV VALUE
      COMMON/SEVEN/IJK,IPD,KA1,KA2,IFAIL,DKA
      REAL KA,XK(3),KA1,KA2
      IPD=-1
      KA=KA+DKA
      KA1=KA
      IF(KA.GE.KA2)IPD=1
      RETURN
      END
      SUBROUTINE SYLVES(N,B,INDEX),RETURNS(NA)
C  DETERMINE POSITIVE DEFINITNESS OF A SYMMETRIC MATRIX
      REAL C(3,3),DET,WKSPCE(3)
      DIMENSION B(3,3)
      DO 10 K=1,N
      IFAIO=0
      DO 1 I=1,K
      WKSPCE(I)=0.
      DO 1 J=1,K
    1 C(I,J)=B(I,J)
      IC=3
      CALL F03AAF(C,IC,K,DET,WKSPCE,IFAIO)
      IF(IFAIO.GT.0)GOTO 5
      IF(DET.LT.0)GOTO 2
   10 CONTINUE
      IF(INDEX.EQ.0)WRITE(2,400)
  400 FORMAT(/20X,' [A] MATRIX IS +VE DEFINITE')
      RETURN
    2 IF(INDEX.EQ.0)WRITE(2,100)
  100 FORMAT(/20X,' [A] MATRIX IS -VE DEFINITE')
      RETURN NA
    5 IF(INDEX.EQ.0)WRITE(2,500)
  500 FORMAT(/20X,' [A] MATRIX IS INDETERMINATE')
      RETURN NA
      END
      SUBROUTINE CONSTAN(KA1,DKA,KA2,XMULT1,IJK)
C REACTOR OPERATING PARAMETERS AND CONSTANTS
      INTEGER ORD
      REAL ITHO,ITHI,KA1,KA2,KC
      COMMON/EIGHT/A1US,B1US,G1US
      COMMON/THREE/IOO4,IS,IST
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```
      COMMON/FOUR/I6
      COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K,Q,
     1ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      DATA RH,RHC,CP,CPC,V,ZC,R,QK,DH/1.,1.,0.001,0.001,17300.,
     18532.,0.00198,2000.,30./,U/0.037/
      VC=ZC
   90 FORMAT(4I2)
      READ(1,90)ORD
      E=14.83
      IF(ORD.EQ.0)E=12.445
      IF(ORD.EQ.1)E=10.06
      IF(ORD.EQ.2)E=7.67
      READ(1,100)F,FC,T0,TC0,C0
  100 FORMAT(5F10.6)
      READ(1,200)T1SS,C1SS,TC1SS
      READ(1,200)T1US,C1US,TC1US
  200 FORMAT(3F11.7)
      READ(1,201)KC
      WRITE(2,150)ORD
  150 FORMAT(/20X,'ORDER OF REACTION :',I2)
      WRITE(2,151)F,FC,T0,TC0,C0
  151 FORMAT(/5X,'F=',F10.3,5X,'FC=',F10.3,5X,'T0=',
     1F10.3,5X,'TC0=',F10.3,5X,'C0=',F10.8)
      WRITE(2,152)T1SS,C1SS,TC1SS
  152 FORMAT(/5X,'T1SS:',F10.3,5X,'C1SS:',F10.3,5X,
     1'TC1SS:',F10.3)
      WRITE(2,185)KC
  185 FORMAT(/20X,' CONTROLLER GAIN=',1PE14.7)
  900 A1SS=C1SS/C0
      ZZ=RH*CP/(DH*C0)
      B1SS=ZZ*T1SS
      G1SS=ZZ*TC1SS
      G0=ZZ*TC0
      A1US=C1US/C0
      B1US=ZZ*T1US
      G1US=ZZ*TC1US
      B0=T0*ZZ
      K=ORD-1
      TH=V/F
      CORD=QK*C0**K
      ITHO=U/(RH*CP*V)
      ITHI=U/(RHC*CPC*VC)
      THC=VC/FC
      Q=E*RH*CP/(R*DH*C0)
      XX=EXP(-Q/B1SS)*A1SS**ORD
      XIO=1./TH+ITHO
      XII=1./THC+ITHI
      READ(1,201)KA1,DKA,KA2
  201 FORMAT(3E13.6)
      READ(1,90)IOO4,I5,I6,IST
      READ(1,201)XMULT1
      READ(1,90)IJK
      IF(I6.EQ.1)WRITE(2,186)
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  186 FORMAT(20X,'CONTROL ON TANK TEMPERATURE')
      IF(I6.EQ.2)WRITE(2,187)
  187 FORMAT(20X,'CONTROL ON TANK CONCENTRATION')
      IF(I5.EQ.1)WRITE(2,188)
  188 FORMAT(20X,'REAL TIME SYSTEM')
      IF(I5.EQ.-1)WRITE(2,189)
  189 FORMAT(20X,'INVERSE TIME SYSTEM')
      XKC=KC
      XGG=G0-G1SS
      IF(IST.EQ.0)WRITE(2,190)
  190 FORMAT(20X,'MAXIMISATION OF REGION OF ASY. STABILITY')
      IF(IST.EQ.1)WRITE(2,191)
  191 FORMAT(20X,'MAXIMISATION OF REGION OF STABILITY')
      RETURN
      END
      SUBROUTINE RUTH(N,A,INDEX),RETURNS(NA)
C  DETERMINE THE NATURE OF ROOTS OF JACOBIAN MATRIX
C BY RUTH'S CRITERION
      REAL II(3,3)
      COMMON/THREE/I004,I5,IST
      DIMENSION A(3,3),B(4,4),C(3,3),P(5)
      IF(I5.EQ.1)GOTO 6
      DO 7 I=1,N
      DO 7 J=1,N
    7 A(I,J)=-A(I,J)
    6 P(1)=1.
      DO 2 I=1,N
      DO 2 J=1,N
      B(I,J)=0.
      IF(I.EQ.J)B(I,J)=1.0
    2 CONTINUE
      DO 10 K=1,N
      DO 3 I=1,N
      DO 3 J=1,N
      SUM=0.
      DO 13 L=1,N
   13 SUM=A(I,L)*B(L,J)+SUM
    3 C(I,J)=SUM
      TR=0.
      DO 5 I=1,N
    5 TR=TR+C(I,I)
      P(K+1)=-TR/K
      DO 1 I=1,N
      DO 1 J=1,N
      II(I,J)=0.0
      IF(I.EQ.J) II(I,J)=P(K+1)
    1 CONTINUE
      DO 4 I=1,N
      DO 4 J=1,N
    4 B(I,J)=C(I,J)+II(I,J)
   10 CONTINUE
      K11=N+1
      DO 22 I=1,K11
```

```
      DO 22 J=1,K11
      IF((I.NE.K11.AND.J.NE.K11).AND.I5.EQ.-1)A(I,J)=-A(I,J)
   22 B(I,J)=0.0
      I=N/2
      M=(K11)/2
      IF(I*2.EQ.N) M=(N+2)/2
      K=0
      K12=M-1
      DO 21 I=1,M
      DO 21 J=1,2
      K=K+1
   21 B(J,I)=P(K)
      DO 23 J=3,K11
      DO 23 K=1,K12
   23 B(J,K)=B(J-2,K+1)-(B(J-2,1)*B(J-1,K+1))/B(J-1,1)
      DO 25 J=1,K11
      IF(B(J,1)) 24,25,25
   25 CONTINUE
      GO TO 26
   24 IF(INDEX.EQ.0)WRITE(2,200)

      RETURNNA
  200 FORMAT(/20X,'REAL PARTS OF THE ROOTS OF [J] MATRIX ARE +VE')
      RETURNNA
   26 DO 27 I=1,K11
      IF(B(I,1)) 24,28,27
   27 CONTINUE
      IF(INDEX.EQ.0)WRITE(2,300)
  300 FORMAT(/20X,'REAL PARTS OF THE ROOTS OF [J] MATRIX ARE -VE')
      RETURN
   28 IF(INDEX.EQ.0)WRITE(2,400)
  400 FORMAT(/20X,'PURE IMAGINARY ROOTS IN [J] MATRIX')
      RETURN
      END
      SUBROUTINE JACOBIA(X1C,X2C,X3C,DF)
C     CALCULATE JACOBIAN OF THE SYSTEM AT A GIVEN POINT
      INTEGER ORD
      REAL ITHO,ITHI,KC
      DIMENSION DF(3,3)
        COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K,Q,
     1 ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      DF(1,3)=0.
      DF(2,3)=ITHO
      CALL COOLANT(X1C,X2C,X3C,FCB,DFCX1,DFCX2,DFCX3)
      DF(3,1)=DFCX1*(XGG-X3C)/VC
         DF(3,2)=ITHI+DFCX2*(XGG-X3C)/VC
          DF(3,3)=-XII-FCB/VC+DFCX3*(XGG-X3C)/VC
      YY=EXP(-Q/(B1SS+X2C))
   40 DF(1,1)=-1./TH-YY *CORD*ORD*(X1C+A1SS)**K
      DF(1,2)=-(X1C+A1SS)**ORD*YY      *(Q/(X2C+B1SS)**2)   *CORD
      DF(2,1)=-DF(1,1)-1./TH
      DF(2,2)=-XIO-DF(1,2)
      RETURN
```

```
      END
      SUBROUTINE COOLANT(X1,X2,X3,FCB,DFCX1,DFCX2,DFCX3)
C DETERMINE COOLANT FLOWRATE
      INTEGER ORD
      REAL ITHO,ITHI,KC
      COMMON/FOUR/I6
      COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K,Q,
     1ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      DFCX3=0.
      IF(I6.EQ.2)GOTO 20
C     CONTROL      FCB=KC*X2C
   10 FCB=KC*X2
      DFCX1=0.
      DFCX2=KC
      RETURN
C     CONTROL     FCB=-KC*X1C
   20 FCB=-KC*X1
      DFCX1=-KC
      DFCX2=0.
      RETURN
      END
      SUBROUTINE VAR3(X1C,X2C,X3C,IODEX,KA,A),RETURNS(NA)
C CALCULATE X3(STATE VARIABLE CORRESPONDING TO
C  JACKET TEMPERATURE) GIVEN THE OTHER TWO VALUES
      INTEGER ORD
      REAL KC,ITHO,ITHI,KA,KA1,KA2
      DIMENSION A(3,3)
      COMMON/SIX/ A1,B1,A2,B2,C2,AAA,BBB,CCC,DDD,FN1
      COMMON/EIGHT/A1US,B1US,G1US
      COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K
     1,Q,ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      IODEX=IODEX+1
      IF(IODEX.NE.0)GOTO 100
      YY=EXP(-Q/(B1US+X2C))
      FN1=-X1C/TH-((X1C+A1US)**ORD*YY-A1US**ORD*EXP(-Q/B1US))*CORD
  100        IF(IODEX.GT.2)RETURN NA
      IF(IODEX.EQ.2)GOTO 1000
      A1=-X2C*XIO-FN1-X1C/TH
      B1=ITHO
      CALL COOLANT(X1C,X2C,X3C,FCB,DFCX1,DFCX2,DFCX3)
      A2=X2C*ITHI+FCB*XGG/VC
      B2=-XII-FCB/VC
      C2=0.0
      AAA=A(2,2)*B1**2+2*A(3,2)*B1*B2+A(3,3)*B2**2
      BBB=2*(A(2,1)*FN1*B1+B2*A(3,1)*FN1+A(2,2)*A1*B1+
     1A(3,2)*(A1*B2+A2*B1)+A(3,3)*A2*B2)
      CCC=2*A(2,1)*FN1*A1+A(2,2)*A1**2+2*A(3,1)*FN1*A2
     1+A(1,1)*FN1**2+2*A(3,2)*A1*A2+A(3,3)*A2**2 -KA
      AAA=AAA+A(3,3)/10.**7
      BBB=BBB+2.*(A(1,3)*X1C+A(2,3)*X2C)/10.**7
      CCC=CCC+(A(1,2)*X1C*X2C+A(1,1)*X1C**2+A(2,2)*X2C**2)/10.**7
      DDD=BBB**2-4*AAA*CCC
      IF(DDD.LT.0.) RETURN NA
```

```
      X3C=(-BBB+SQRT(DDD))/(2*AAA)
      RETURN
 1000 X3C=(-BBB-SQRT(DDD))/(2*AAA)
      RETURN
      END
      SUBROUTINE FUNCTIO(X1C,X2C,X3C,FN)
C   CALCULATE FUNCTION AT A GIVEN POINT
      DIMENSION DF(3,3),FN(3)
      INTEGER ORD
      REAL KC,ITHO,ITHI
        COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K
     1,Q,ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      YY=EXP(-Q/(B1SS+X2C))
      FN(1)=-X1C/TH-CORD*(YY*(A1SS+X1C)**ORD-XX)
      FN(2)=-XIO*X2C+X3C*ITHO-FN(1)-X1C/TH
       CALL COOLANT(X1C,X2C,X3C,FCB,DFCX1,DFCX2,DFCX3)
      FN(3)=-XII*X3C+X2C*ITHI+FCB*(XGG-X3C)/VC
      RETURN
      END
      SUBROUTINE SOLVEA(N,B,A,I)
C TO SOLVE [J]T [A]+[A] [J] =-[B]
      REAL P(9,9),A(3,3),B(3,3),AV(9,1),BV(9,1)
     1,WKSPCE(9),AA(9,9),BB(9,1),I(3,3)
      IEXIT=0
      IA=1
      IB=9
      P(1,1)=2*B(1,1)
      P(2,2)=B(1,1)+B(2,2)
      P(7,7)=P(3,3)=B(1,1)+B(3,3)
      P(4,4)=B(1,1)+B(2,2)
      P(5,5)=2*B(2,2)
      P(8,8)=P(6,6)=B(2,2)+B(3,3)
      BV(1,1)=I(1,1)
      BV(5,1)=I(2,2)
      BV(9,1)=I(3,3)

      BV(4,1)=BV(2,1)=I(1,2)
      BV(7,1)=BV(3,1)=I(1,3)
      BV(6,1)=BV(8,1)=I(2,3)
      P(9,9)=2.*B(3,3)
      P(1,5)=P(1,6)=P(1,8)=P(1,9)=
     1P(2,4)=P(2,6)=P(2,7)=P(2,9)=
     2P(3,4)=P(3,5)=P(3,7)=P(3,8)=
     3P(4,2)=P(4,3)=P(4,8)=P(4,9)=
     4P(5,1)=P(5,3)=P(5,7)=P(5,9)=
     5P(6,1)=P(6,2)=P(6,7)=P(6,8)=
     6P(7,2)=P(7,3)=P(7,5)=P(7,6)=
     7P(8,1)=P(8,3)=P(8,4)=P(8,6)=
     8P(9,1)=P(9,2)=P(9,4)=P(9,5)=0.0
      P(2,5)=P(3,6)=P(1,4)=P(1,2)=P(4,5)=P(7,8)=B(2,1)
      P(2,8)=P(3,9)=P(1,7)=P(1,3)=P(4,6)=P(7,9)=B(3,1)
      P(5,2)=P(5,4)=P(6,3)=P(4,1)=P(2,1)=P(8,7)=B(1,2)
      P(3,1)=P(8,2)=P(9,3)=P(7,1)=P(6,4)=P(9,7)=B(1,3)
```

```
      P(2,3)=P(4,7)=P(5,8)=P(6,9)=P(8,9)=P(5,6)=B(3,2)
      P(3,2)=P(6,5)=P(7,4)=P(8,5)=P(9,8)=P(9,6)=B(2,3)
      NI=9
      CALL F04AEF(P,IB,BV,IB,NI,IA,AV,IB,WKSPCE,AA,IB,
     1BB,IB,IEXIT)
      K=0
      DO 20 L=1,N
      DO 20 J=1,N
      K=K+1
   20 A(J,L)=AV(K,1)*10.**5
      RETURN
      END
      PROGRAM JFINLI(DATA1,OUTPUT,ERROR2,ERROR1,TAPE 1=DATA1,
     1TAPE 2=OUTPUT,TAPE 6=ERROR1,TAPE 7=ERROR2)
C  MASTER WHERE MAXIMISATION OF LIAPUNOV VOLUME IS
C  CARRIED OUT
      COMMON/EIGHT/A1US,B1US,G1US
      DIMENSION DF(3,3),AA(3,3),A(3,3),NT(6),DAA(6),B(3,3)
      CALL CONSTAN(XKA1,DKA,XKA2,XMULT1,IJK)
      CALL JACOBIA(0.,0.,0.,DF)
      X1C=X2C=X3C=0.0
      WRITE(2,201)
  201 FORMAT(20X,'JACOBIAN AT THE ORIGIN'/5X,'[J] MATRIX')
      DO 3I=1,3
      WRITE(2,200)(DF(I,J),J=1,3)
  200 FORMAT(2X,3(E15.8,3X))
    3 CONTINUE
      CALL RUTH(3,DF,0),RETURNS(9999)
  101 FORMAT(3I2)
      IF(IJK-1)999,998,1000
C  INPUT MATRIX B FOR CALCULATING MATRIX A IN
C  [J]T [A]+[A] [J] =-[B]
999       READ(1,100)((B(I,J),J=I,3),I=1,3)
        CALL SOLVEA(3,DF,A,B)
      CALL EIVECT(A)
      WRITE(2,1025)
      CALLMAXLIAP(XKA1,DKA,XKA2,A,XK,VOL)

  998 IF(IJK.EQ.1)READ(1,100)X1C,X2C,X3C,VOL
      READ(1,100)X1MIN,X1D,X2MIN,X2D,X3MIN,X3D
      READ(1,101)NX1,NX2,NX3
      DO 1026 I=1,3
      DO 1026 J=I,3
 1026 AA(I,J)=A(I,J)
C  MAXIMISE VOLUME FOR DIFFERENT [A] MATRIX VALUES
C  CALCULATED WITH DIFFERENT JACOBIAN MATRICES
      DO 887 I1=1,NX1
      X1=X1MIN+X1D*I1
      DO 887 I2=1,NX2
      X2=X2MIN+X2D*I2
      DO 887 I3=1,NX3
      X3=X3MIN+X3D*I3
      CALL JACOBIA(X1,X2,X3,DF)
```

```
      CALL SOLVEA(3,DF,A,B)
      WRITE(2,109)X1,X2,X3
      CALL MAXLIAP(XKA1,DKA,XKA2,A,XK,VSUM)
      IF(VSUM.LT.VOL)GOTO 887
      X1C=X1
      X2C=X2
      X3C=X3
      VOL=VSUM
      DO 1023 I=1,3
      DO 1023 J=I,3
 1023 AA(I,J)=A(I,J)
  887 CONTINUE
  109 FORMAT(10X,'MAXIMISATION CARRIED OUT AT:',3(E14.7,2X))
 1025 FORMAT(30X,'MATRIX [A] OBTAINED FROM JTA+AJ=-I')
  106       IF(IJK.NE.2)GOTO105
 1000 READ(1,100)((AA(I,J),J=I,3),I=1,3)
  100 FORMAT(6E13.6,I2)
      READ(1,100)VOL
  105 INK=INK1=0
      DO 1021 I=1,3
      DO 1021 J=I,3
      A(I,J)=AA(I,J)
 1021 A(J,I)=A(I,J)
      IDIR=1
C  MAXIMISE LIAPUNOV VOLUME BY MODIFYING THE ELEMENTS
OF [A] MATRIX
 1005 XMULT=XMULT1+1.
      INDEX=1
 1010 IMP=0
 1020 IF(INDEX.GT.3)GOTO 1022
      K=1
      J=INDEX
      A(K,J)=AA(K,J)*XMULT
      A(J,K)=A(K,J)
      GOTO 1024
 1022 J=INT(INDEX/2.+.89)
      K=2
      IF(INDEX.EQ.6)K=3
      A(K,J)=AA(K,J)*XMULT
      A(J,K)=A(K,J)
 1024 CALL MAXLIAP(XKA1,DKA,XKA2,A,XK,VSUM)
      IF(VSUM.GT.VOL)GOTO 1030
      IF(IMP.EQ.1)GOTO 1040
      IMP=1
      XMULT=1.-XMULT1
      IDIR=-1
      GOTO 1020
 1040 INDEX=INDEX+1
      A(K,J)=AA(K,J)
      A(J,K)=A(K,J)
      XMULT=1.+XMULT1
      IF(INDEX.LT.7)GOTO 1010
      IF(INK.EQ.0)GOTO 9000
```

```
      INK=0
      GOTO 1005
 1030 INK=1
      VOL=VSUM
      AA(K,J)=A(K,J)
      GOTO 1010
 9000 INK1=INK1+1
      IF(INK1.EQ.3)GOTO9001
      XMULT1=XMULT1/2.
      GOTO 1005
 9001 DO 800 I=1,3
      DO 800 J=I,3
      A(I,J)=AA(I,J)
  800 A(J,I)=A(I,J)
      XK=-1.E+05
      CALL MAXLIAP(XKA1,DKA,XKA2,A,XK,VSUM)
      CALL EIVECT(A)
      IN=-1
      CALL VAR3(A1US,B1US,X3C,IN,XK,A),RETURNS(300)
      IN=1
      CALL VAR3(A1US,B1US,X3C1,IN,XK,A),RETURNS(0300)
      WRITE(2,1002)XK,G1US,X3C,X3C1
 1002 FORMAT(2X,4(E13.6,2X))
  300 CONTINUE
 9999 CONTINUE
      STOP
      END
      SUBROUTINE EIVECT(A)
C   DETERMINE EIGEN VALUES/VECTORS OF MATRIX [A]
      DIMENSION A(3,3),R(3),V(3,3),E(3)
      IFAIL=0
      CALL F02ABF(A,3,3,R,V,3,E,IFAIL)
      IF(IFAIL.NE.0)WRITE(2,100)IFAIL
  100 FORMAT(20X,'IFAIL=',I2)
      WRITE(2,105)(R(I),I=1,3)
  105 FORMAT(5X,'EIGEN VALUES:',3(E14.7,3X)//5X,'EIGEN VECTORS:')
      DO 1000 I=1,3
      WRITE(2,110)(V(I,J),J=1,3)
  110 FORMAT(19X,3(E14.7,3X))
 1000 CONTINUE
      RETURN
      END
```

A.1.4 PROGRAM TO DETERMINE THE EXISTENCE OF LIMIT-CYCLES

```
C   PROGRAM TO DETERMINE THE EXISTENCE OF LIMITCYCLES
C   IN THREE DIMENSIONAL SPACE BY DIRECT METHOD OF LIAPUNOV
      SUBROUTINE MAXLIAP(XKA1,XDKA,XKA2)
C   SUBROUTINE TO DETERMINE THE REGION WITHIN WHICH
C   VDOT <0 FOR A SYSTEM WITH UNSTABLE ORIGIN(OPERATING POINT)
      REAL KA,KA1,KA2
      DIMENSION DF(3,3),X4(3),J1(3,3),X3(3)   ,A(3,3),X(3),FN(3)
      REAL ITHO,ITHI,KC
      INTEGER ORD
      COMMON/EIGHT/I7
      COMMON/THREE/IOO4,I5
      COMMON/SIX/A1,B1,A2,B2,C2,AAA,BBB,CCC,DDD,A,FN1
           COMMON/SEVEN/IPK,IPD,KA1,KA2,KA,IFAIL,DKA
        COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K
     1,Q,ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      KA1=XKA1
      KA2=XKA2
      DKA=XDKA
        IPK=0
   52 FORMAT(9X,'LIAP K',12X,'X1C',12X,'X2C',12X,'X3C',12X,'OBJ',
     112X,'VOLUME')
      SINDEX=190.*178.
           NX=3
    2      CALL JACOBIA(0.,0.,0., DF)
      ICHECK=0
 10         WRITE(2,100)
  100 FORMAT(/5X,'JACOBIAN MATRIX')
      KA=KA1
      DO 3 I=1,NX
      WRITE(2,200)(DF(I,J),J=1,NX)
  200 FORMAT(2X,6(E15.8,3X))
    3 CONTINUE
      CALL RUTH(NX,DF,0),RETURNS(8888)
 8888 DO 8887 I=1,3
      DO 8887 J=1,3
      J1(I,J)=0
      IF(I.EQ.J)J1(I,J)=-1
 8887 CONTINUE
      IF(I7.EQ.0)CALL SOLVEA(NX,DF,A,J1)
      IF(I7.EQ.1)READ(1,141)((A(I,J),J=I,3),I=1,3)
  141 FORMAT( 6E13.6)
      A(2,1)=A(1,2)
      A(3,1)=A(1,3)
      A(3,2)=A(2,3)
1929        WRITE(2,300)
  300 FORMAT(/5X,'[A] MATRIX:')
      DO 4 I=1,NX
      WRITE(2,200)(A(I,J),J=1,NX)
    4 CONTINUE
      CALL SYLVES(NX,A,0),RETURNS(6666)
      CALL EIVECT(A)
      WRITE(2,52)
   54 FORMAT(8X,'X1C',15X,'X2C',15X,'X3C',15X,'OBJ',15X,'X3C'
```

```
 1,15X,'OBJ',15X,'X3C')
  7 WRITE(IOO4,50)KA
 50 FORMAT(/2X,'LIAPUNOV K=',E13.6)
    WRITE(IOO4,54)
    X(1)=-0.003+.82
    SMIN=10.**70
    VSUM=0.
    DO 1002 IJ1=1,61
    M=IJ1/2
    INDEXI=2
    IF(M*2.EQ.IJ1) INDEXI=4
    IF(IJ1.EQ.1.OR.IJ1.EQ.61) INDEXI=1
    X(1)=X(1)+0.003
    X1C=X(1)-A1SS
    XB=-0.015375
    DO 1003 IJ2=1,65
    XB=XB+0.015375
    X(2)=XB/10.25
    M=IJ2/2
    INDEXJ=2
    IF(M*2.EQ.IJ2) INDEXJ=4
    IF(IJ2.EQ.1.OR.IJ2.EQ.65) INDEXJ=1
    INDEX=INDEXI*INDEXJ
    X2C=X(2)-(B1SS-B0)
              YY=EXP(-Q/(B1SS+X2C))
       FN1   =-X1C/TH-((X1C+A1SS)**ORD*YY-XX)*CORD
    FN(1)=FN1
    X3(1)=X3(2)=X3(3)=0.
    IODEX=0
1010 CALL VAR3(X1C,X2C,X3C,IODEX),RETURNS(1005)
    X3(IODEX)=X3C
    IF(X3C.LT.XGG)X3(IODEX)=XGG
    IF(X3C.LT.XGG) GOTO 1010
     CALL JACOBIA(X1C,X2C,X3C,DF)
    FN(2)=A1+B1*X3C
    FN(3)=A2+B2*X3C+C2*X3C**2
 808 DSUMF      =0.0
    DO 802 L=1,NX
    DO 802 I =1,NX
    DO 802 J=1,NX
 802 DSUMF=DSUMF+FN(I)*FN(J)*DF(L,J)*((A(I,L)+A(L,I)))*I5
    X4(1)=X1C
    X4(2)=X2C
    X4(3)=X3C
    DO 803 I=1,NX
    DO 803 J=1,NX
 803 DSUMF=DSUMF+(A(I,J)*X4(I)*FN(J)+A(I,J)*X4(J)*FN(I))/10.**10
    OBJ=-DSUMF
    WRITE(IOO4,1006)X1C,X2C,X3C,OBJ
1006 FORMAT(5X,4(E14.7,2X))
    IF(OBJ.LT.0.)GOTO 1909
    IF(OBJ.GT.SMIN)GOTO 1010
    SMIN=OBJ
```

```
      X1MIN=X1C
      X2MIN=X2C
      X3MIN=X3C
      GOTO 1010
 1005 CONTINUE
      IF(X2C*KC.GT.120.) VSUM=VSUM-FLOAT(INDEX)*.18*
     1(X3(1)-X3(2))*(1./10.25-(B1SS-B0)-120/KC)/SINDEX
      VSUM=VSUM+FLOAT(INDEX)*.18*(X3(1)-X3(2))/SINDEX
 1003 CONTINUE
 1002 CONTINUE
      IF(SMIN.GT.10.**69) GO TO 1009
1919        WRITE(2,1007)KA,X1MIN,X2MIN,X3MIN,SMIN,VSUM
 1007 FORMAT(5X,6(E14.6,2X),5X,)
      IPD=0
      CALL LIAPK
      IF(IPD.LE.0) GO TO7
      GO TO 9999
 1009 KA1=KA1+DKA
      WRITE(2,1007)KA
      KA=KA1
      GOTO 7
 1909 X1MIN=X1C
      X2MIN=X2C
      X3MIN=X3C
      SMIN=OBJ
      VSUM=0.
      GOTO 1919
 6666 A(1,1)=ABS(A(1,1))
      A(2,2)=ABS(A(2,2))
      A(3,3)=ABS(A(3,3))
      ICHECK=ICHECK+1
      IF(ICHECK.EQ.2)GOTO6667
      GOTO 1929
 6667 KC=KC*0.98
      WRITE(2,185)KC
  185 FORMAT(/20X,'CONTROLLER GAIN=',1PE14.7)
      GOTO 2
 9999 CONTINUE
      RETURN
      END
      SUBROUTINE CONSTAN(KA1,DKA,KA2)
C   INPUT REACTOR OPERATING PARAMETERS AND
C   CONSTANTS
      INTEGER ORD
      REAL ITHO,ITHI,KA1,KA2    ,KA ,KC
      COMMON/EIGHT/I7
      COMMON/THREE/IOO4,I5
      COMMON/FOUR/I6
        COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K,Q,
     1 ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      DATA RH,RHC,CP,CPC,V,ZC,R,QK ,DH/1.,1.,0.001,0.001,17300.,
     18532.,0.00198,2000.,30./,U/0.037/
      VC=ZC
```

```
 90 FORMAT(4I2)
    READ(1,90) ORD
      E=14.83
            IF(ORD.EQ.0) E=12.445
            IF(ORD.EQ.1) E=10.06
            IF(ORD.EQ.2) E= 7.670
    READ(1,100) F,FC,T0,TC0,C0
100 FORMAT(5F10.6)
    READ(1,200)T1SS,C1SS,TC1SS
200 FORMAT(3F11.7)
    READ(1,201)KC
    WRITE(2,150) ORD
150 FORMAT(/20X,'ORDER OF REACTIONS :',I2)
     WRITE(2,151)F,FC,T0,TC0,C0
151   FORMAT(/5X,'F=',F10.3,5X,'FC=',F10.3,5X,'T0=',F10.3,5X,
   1  'TC0=',F10.3,5X,'C0=',F10.8)
      WRITE(2,152)T1SS,C1SS,TC1SS
152    FORMAT(/5X,'T1SS:',F10.3,5X,'C1SS:',F10.8,5X,'TC1SS:',
   1  F10.3)
    WRITE(2,185) KC
185 FORMAT(/20X,' CONTROLLER GAIN =',1PE14.7)
900 A1SS=C1SS/C0
    ZZ=RH*CP/(DH*C0)
    B1SS=ZZ*T1SS
    G1SS=ZZ*TC1SS
     G0=TC0*ZZ
    B0=T0*ZZ
    K=ORD-1
    TH=V/F
    CORD=QK*C0**K
    ITHO=U/(RH*CP*V)
    ITHI=U/(RHC*CPC*VC)
    THC=VC/FC
    Q=E*RH*CP/(R*DH*C0)
    XX=EXP(-Q/B1SS)*A1SS**ORD
    XIO=1./TH+ITHO
    XII=1./THC+ITHI
    READ(1,201) KA1,DKA,KA2
201 FORMAT(3E13.6)
    READ(1,90)IOO4,I5,I6,I7
    IF(I6.EQ.1)WRITE(2,186)
186 FORMAT(20X,'CONTROL ON TANK TEMPERATURE')
    IF(I6.EQ.2)WRITE(2,187)
187 FORMAT(20X,'CONTROL ON TANK CONCENTRATION')
    IF(I5.EQ.1)WRITE(2,188)
188 FORMAT(20X,'REAL TIME SYSTEM')
    IF(I5.EQ.-1)WRITE(2,189)
189 FORMAT(20X,'INVERSE TIME SYSTEM')
    XKC=KC
    XGG=G0-G1SS
    RETURN
    END
    SUBROUTINE VAR3(X1C,X2C,X3C,IODEX),RETURNS(NA)
```

```
C   TO CALCULATE X3 GIVEN THE OTHER TWO VALUES
      INTEGER ORD
      REAL KC,ITHO,ITHI,KA,KA1,KA2
      DIMENSION A(3,3)
      COMMON/SIX/ A1,B1,A2,B2,C2,AAA,BBB,CCC,DDD,A,FN1
      COMMON/SEVEN/IPK,IPD,KA1,KA2,KA,IFAIL,DKA
      COMMON/FIVE/TH,THC,C0,A1SS,B1SS,G1SS,ITHO,ITHI,K
     1,Q,ZZ,ORD,CORD,G0,B0,VC,KC,XX,XIO,XII,XGG
      IODEX=IODEX+1
      IF(IODEX.GT.2)RETURN NA
      IF(IODEX.EQ.2)GOTO 1000
      A1=-X2C*XIO-FN1-X1C/TH
      B1=ITHO
      CALL COOLANT(X1C,X2C,X3C,FCB,DFCX1,DFCX2,DFCX3)
      A2=X2C*ITHI+FCB*XGG/VC
      B2=-XII-FCB/VC
      C2=0.0
      AAA=A(2,2)*B1**2+2*A(3,2)*B1*B2+A(3,3)*B2**2
      BBB=2*(A(2,1)*FN1*B1+B2*A(3,1)*FN1+A(2,2)*A1*B1+
     1A(3,2)*(A1*B2+A2*B1)+A(3,3)*A2*B2)
      CCC=2*A(2,1)*FN1*A1+A(2,2)*A1**2+2*A(3,1)*FN1*A2
     1+A(1,1)*FN1**2+2*A(3,2)*A1*A2+A(3,3)*A2**2 -KA
      AAA=AAA+A(3,3)/10.**10
      BBB=BBB+2.*(A(1,3)*X1C+A(2,3)*X2C)/10.**10
      CCC=CCC+(A(1,2)*X1C*X2C+A(1,1)*X1C**2+A(2,2)*X2C**2)/10.**10
      DDD=BBB**2-4*AAA*CCC
      IF(DDD.LT.0.) RETURN NA
      X3C=(-BBB+SQRT(DDD))/(2*AAA)
      RETURN
 1000 X3C=(-BBB-SQRT(DDD))/(2*AAA)
      RETURN
      END
      PROGRAM JFINLI(DATA0,OUTPUT,DATA,ERRORS,TAPE 1=DATA0,
     1TAPE 2=OUTPUT,TAPE 6=ERRORS)
      CALL CONSTAN(XKA1,DKA,XKA2)
      CALL MAXLIAP(XKA1,DKA,XKA2)
      STOP
      END
```

A.1.5 PROGRAM FOR THE SIMULATION OF THE COMPLETE EXPERIMENTAL ARRANGEMENT

```
   FORTRAN(CP)
  OPTIONSERRMSG,DEBUG1,SLIST
  PROGDESC
  LIST(LP)
  PROGRAM(SLAM)
  INPUT 1=CR0
  INPUT 3=TR0
  INPUT 5=CR1
  OUTPUT2=LP0
  OUTPUT6=LP1
  COMPRESSINTEGER ANDLOGICAL
  COMPACT
  END
  MASTER REACT
C   TOTAL SIMULATION OF THE COMPLETE PLANT
C   SLAM SOURCE PROGRAM
  INTEGER ORD
  REAL K,KC,I1,I0
  DATAV/17300./,VC/8532./,R/.00198/,K/2000./,
 1CP/0.001/,CPC/0.001/,RH/1.0/,RHC/1.0/,I/0/
 2,DH/30./
C  REACTOR OPERATING PARAMETERS
  A1SS=C1SS/C0
  TH=V/F
  THC=VC/FC
  Q=E*RH*CP/(R*DH*C0)
  ZZ=RH*CP/(DH*C0)
  I0=U/(V*RH*CP)
  I1=U/(VC*CPC*RHC)
  BST=BSTT*ZZ
  B1SS=T1SS*ZZ
  G1SS=TC1SS*ZZ
  B0=B00*ZZ
  G0=TC0*ZZ
  G0S=G00*ZZ
  XKN=K*C0**(ORD-1)
  RR2=EXP(-Q/(B1SS+X2S))*(X1+A1SS)**ORD
  RR1=EXP(-Q/B1SS)*A1SS**ORD
  DC1=-X1/TH-XKN*(RR2-RR1)
C  VALVE TRANSFER FUNCTION
  TVA=2.
  DFCBA=(FCB-FCBA)/TVA
  FCBA=INTGRL(DFCBA,0.0)
C  MEASURING ELEMENTS TRANSFER FUNCTION
  TME=19.
  DX2B=(X2-X2B)/TME
  X2B=INTGRL(DX2B,BST)
  DX4B=(X3-X4B)/TME
  X4B=INTGRL(DX4B,BGT)
  NO SORT(X2S,X4S=X2B,X4B)
C  SAMPLERS FOR TANK & JACKET TEMPERATURES WITH
C  ZERO ORDER HOLD
  IF(ABS(TIME-TIMEX).LT.1.E-05)X4S=X4B
```

```
      IF(ABS(TIME-TIMEX).LT.1.E-05)X2S=X2B
      IF(KEEP.NE.1.OR.(INT(TIME/TSA+.0001).
     1LE.ITIM))GOTO 1223
      ITIM=ITIM+1
      X2S=X2B
      X4S=X4B
 1223 CONTINUE
      END
      NO SORT(FCB,AX=X1,X2S,X4S,DC1)
C  CONTROL STRATEGIES BLOCK
      AX=0.
      GOTO(10,20,30,40,50,60,70,90,100),INDEX
      WRITE(2,99)
   99 FORMAT(20X,'*****ERROR IN INDEX******')
      STOP
C       UNCONTROLLED SYSTEM
   10 FCB=0.
      GOTO 80
C     PROP CONTROL OF TANK TEMPERATURE
   20 FCB=KC*X2S
      GOTO 80
C     PROP CONTROL OF JACKET TEMPERATURE
   30 FCB=KC*X4S
      GOTO 80
C    FN. OF  X2S
   40 FCB=(I0+I1)*VC*X2S/(G1SS-G0+X4S)
      GOTO 80
C    INVARIANCE FOR STEP IN TANK FEED TEMPERATURE
   50 FCB=B0*(I1+1/THC)*VC/(I0*TH*(G1SS-G0-
     1B0/(TH*I0)))
      GO TO 80
C    INVARIANCE FOR STEP IN JACKET FEED TEMPERATURE
   60 FCB=G0S*VC/(THC*(G1SS-G0-G0S))
      GOTO 80
C    INVARIANCE FOR STEP IN
C    TANK & JACKET INLET TEMPERATURES
   70 A11=B0/(TH*I0)
      FCB=(G0S/THC+A11*(I1+1/THC))*VC
     1/(G1SS-G0-G0S-A11)
      GOTO 80
C      NONINTERACTING CONTROL
   90  AX=KC
 1001 TDT1=-AX*X2S
      TX3=(TDT1+(1/TH+I0)*X2-XKN*(RR2-RR1))/I0
     1-B0/(TH*I0)
      IF(TX3/ZZ.LT.-8..OR.TX3/ZZ.GT.10.)GOTO1002
      TDTC1=-AX*TDT1/I0+(1/TH+I0)*TDT1/I0-XKN*(
     1ORD*(A1SS+X1)**(ORD-1)*DC1*EXP(-Q/(B1SS+X2S))+
     2RR2*Q*TDT1/(B1SS+X2S)**2)/I0
      FCB=(-TDTC1+X2*I1-(1/THC+I1)*TX3+G0S/THC)*VC/
     1(TX3+G1SS-G0-G0S)
      IF(FCB.GT.(8.-FC).AND.FCB.LT.(150.-FC))GOTO1000
 1002 AX=AX/1.1
```

```
      IF(AX.LT.1.E-06)GOTO 1003
      GO TO 1001
 1003 FCB=150.-FC
 1000 CONTINUE
      GOTO 80
C     LIMIT CYCLE
  100 FCB=-KC*X1
   80 IF(FCB.LT.(-FC+8.))FCB=-FC+8.
      IF(FCB.GT.(150.-FC))FCB=150.-FC
      END
      NOSORT(E=ORD)
C  ACTIVATION ENERGY
      E=14.83
      IF(ORD.EQ.0)E=12.445
      IF(ORD.EQ.1)E=10.060
      IF(ORD.EQ.2)E=7.670
      END
      TC1=X4S/ZZ
      TERMINATE(TIME.GT.FTIM.OR.T1.GT.30.)
C  REACTOR MASS AND ENERGY BALANCE
      X1=INTGRL(DC1,BCT)
      BCT=BCTT/C0
      BBST=BST
      X2=INTGRL(DT1,BBST)
      BBGT=BGT
      X3=INTGRL(DTC1,BBGT)
      DT1=-X2/TH+B0/TH-(X2-X3)*I0-DC1-X1/TH
      DTC1=-X3/THC+(X2-X3)*I1+(FCBA)*(G0-X3-G1SS+G0S)
     1/VC+G0S/THS
      T1=X2S/ZZ
      NOSORT(ORD,F,FC,T0,TC0,C0,T1SS,C1SS,TC1SS,
     1INDEX,IOD,KC,U,G00,BSTT,B00,BCTT,BGTT,FTIM,
     2ISTEP,TIME=I)
C  INPUT AND OUTPUT.INPUT FLOW RATE IN CC/S,
C  TEMPR. IN K & CONCN. IN GMS/CC
      I=I+1
      ITIM=0
      JJ=0
      IF(I.GT.1)GOTO98
      INPUT ORD
      INPUT F,FC,T0,TC0,C0
      INPUT T1SS,C1SS,TC1SS,U
      TITLE'DYNAMIC BEHAVIOUR OF A CSTR FOR REACT. ORDER',IL
      OUTECIORD
      OUTECIF,FC,T0,TC0,C0
      OUTECIT1SS,C1SS,TC1SS,U
   98 INPUT INDEX,KC,BSTT,BCTT,BGTT,B00,G00,
     1TIMEX,FTIM,ISTEP,TSA
      TIME=TIMEX
      OUTPUT 'INDEX=',INDEX
      CALL HEAD(INDEX)
      IF(INDEX.EQ.2.OR.INDEX.EQ.3)WRITE(2,113)KC
  113 FORMAT(10X,'KC=',E13.5)
```

```
      IF(B00.GT.1.E-09)WRITE(2,111)B00
      IF(G00.GT.1.E-09)WRITE(2,112)G00
  111 FORMAT(10X,'STEP IN TANK INLET TEMPERATURE:',F6.2)
  112 FORMAT(10X,'STEP IN JACKET INLET TEMPE.:',F6.2)
  811 CONTINUE
      END
      OUTHD'TIME',12S,'T1',12S,'C1',12S,'TC1',12S,
     1'FCB'
      NO SORT(=TIME,T1,C1,TC1,FCBA,AX)
      IF(I006.NE.1)GOTO 114
      OUTECI TIME,T1,C1,TC1,FCBA
      IF(INDEX.EQ.8)WRITE(2,115)AX
      IF(INDEX.EQ.9)CALL MINMAX(JJ,T1,TIME,CINT)
  115 FORMAT(1H+,68X,1PG13.5)
  114 CONTINUE
      END
      C1=X1*C0
      BGT=BGTT*ZZ
C  INTEGRATION PARAMETERS
      INTINF
      ALG:RKFS
      INDVAR:TIME
      CI:CINT=20
      STEPS:ISTEP
      END
      REPEAT
      END
      SUBROUTINE MINMAX(I,TC1,TIME,CI)
C  SUBROUTINE TO FIND AMPLITUDE DURING
C LIMIT CYCLE STUDIES
      DIMENSION XMAX(3)
      I=I+1
      T=TIME-CI
      XMAX(I)=TC1
      IF(I.LT.3) RETURN
      IF(XMAX(2).GE.XMAX(3).AND.XMAX(2).GE.XMAX(1))
     1WRITE(6,1010)XMAX(2),T
 1010 FORMAT(5X,'T1=',E14.7,' AT TIME=',E9.2,'SECS')
      IF(XMAX(2).LE.XMAX(3).AND.XMAX(2).LE.XMAX(1))
     1WRITE(6,1010)XMAX(2),T
      XMAX(1)=XMAX(2)
      XMAX(2)=XMAX(3)
      I=2
      RETURN
      END
      SUBROUTINE HEAD(IND)
C SUBROUTINE TO WRITE TITLE
      GOTO(1,2,3,4,5,6,7,8,9),IND
    1 WRITE(2,100)
  100 FORMAT(10X,'UNCONTROLLED SYSTEM')
      RETURN
    2 WRITE(2,101)
  101 FORMAT(10X,'PROPORTIONAL CONTROL OF TANK TEMPERATURE')
```

```
      RETURN
    3 WRITE(2,102)
  102 FORMAT(10X,'PROPORTIONAL CONTROL OF JACKET TEMPERATURE')
      RETURN
    4 WRITE(2,103)
  103 FORMAT(10X,'COOLANT RATE FUNCTION OF TANK TEMPERATURE')
      RETURN
    5 WRITE(2,104)
  104 FORMAT(10X,'INVARIANCE CONTROL FOR STEP IN '
     1,'FEED TEMPERATURE')
      RETURN
    6 WRITE(2,105)
  105 FORMAT(10X,'INVARIANCE CONTROL FOR '
     1,'STEP IN COOLANT TEMPERATURE')
      RETURN
    7 WRITE(2,106)
  106 FORMAT(10X,'INVARIANCE CONTROL FOR STEP'
     1,'IN FEED AND COOLANT'/20X,'TEMPERATURES')
      RETURN
    8 WRITE(2,107)
  107 FORMAT(10X,'NONINTERACTING TYPE CONTROL')
      RETURN
    9 WRITE(2,108)
  108 FORMAT(10X,'LIMIT CYCLE STUDIES')
      RETURN
      END
      FINISH
```

A.1.6 BASIC PROGRAM FOR ON-LINE WORK

A.1.6.1 EXECUTIVE PROGRAM

```
10  DIM A(13),B(120): REM   INITIALISATION:I6,I7=0
11  INPUT B(120):A(0)=1:A(1)=3:A(2)=2:A(3)=30:A(4)=33:A(5)=2
12  A(6)=1:A(7),A(8),A(9),A(10),A(11)=0:A(12),A(13)=1
13  GOSUB 902:I9,I8=0:J6=4
20  PRINT "INPUT TANK FLOW RATE IN LTR/MIN";: INPUT F1
21  PRINT "INPUT JACKET FLOW RATE IN LTR/MIN";: INPUT F2
24  REM   TRANSFER SEGM2 TO CORE FROM DISK: GOSUB 1600
25  F5=F2*1000/60:B(90)=0:D=0
27  REM   SET JACKET FLOW: GOSUB 1000: GOSUB 9005:U=.37E-01
65  REM   SCAN & PLOT THEORETICAL HEAT GN. & REM.: GOSUB 6500
66  FOR J7=1,J6: GOSUB 1600: GOSUB 9000:I6=1
67  REM   SET IMMERSION HEATERS: GOSUB 2000
68  REM   HEAT TRANSFER COEFFICIENT:U=F5*(T3-T2)*.1E-02/(T1-T3)
70  REM   TRANSFER SEGM1 FROM DISK TO CORE: GOSUB 1550
72  REM   PLOT MEASURED VALUES: GOSUB 6900
75  IF J7<>J6 THEN 110
95  C(0)=1:C(5)=1:C(6)=45:B(15)=3: GOSUB 5900
96  C(7)=4:B(15)=5: GOSUB 5900
97  REM  OUTPUT S.S. VALUES TO THE SCREEN: GOSUB 9100
98  I6=0: GOSUB 3000: GOSUB 6025
110  NEXT J7: GOSUB 9500:B(15)=6: GOSUB 5900: GOSUB 1600
111  INPUT I7: ON I7+1 GOTO 65,20,129,131,800
129  REM  SCAN AND PRINT WITHOUT PLOTTING:I6=0: FOR J7=1,10
130  GOSUB 9005: GOSUB 9100: GOSUB 2000: NEXT J7: GOTO 111
131  REM           THIS LINE IS USED BY CONTROL SUBROUTINES
132  J6=3:H9=2*A(0)*(A(2)-1):H2=6.5:H=H9+H2
133  REM  STORE S.S. VALUES:S1=C1:S2=T1+273.1:S3=T3+273.1
147  PRINT "TYPE OF CONTROL";: INPUT K1
148  IF K1<>2 THEN  IF K1<>3 THEN  IF K1<>9 THEN 600
150  PRINT "INPUT P. AND I. VALUES";: INPUT K2,K3: GOTO 600
151  PRINT : PRINT "EXPT. NO:";B(120): PRINT "RN. ORDER:";O1
152  PRINT "F(L/M):";F1,"FC(L/M):";F2: PRINT "T0:";T0,"TC0:";
153  PRINT T2: PRINT "S.S. VALUES";S1;S2;S3: GOSUB 6025
154  PRINT "CONTROL STRATEGY";K1: GOSUB 902
155  I7=1: CALL (8,I7,B(91)):B(92)=4:T=-H:B(19)=0:I2=3
157  REM  START OF TRANSIENT RESPONSE STUDIES
160  I6=1:T=T+H: GOSUB 9005:B(120)=0: CALL (9,B(120),H2)
180  GOSUB 699: GOSUB 7000: IF (F5+F3)<0 THEN F3=-F5
185  IF (F5+F3)>150 THEN F3=150-F5
200  REM  JACKET FLOW RATE:F2=(F5+F3)*60/1000
205  GOSUB 1000: GOSUB 2000: IF (B(89)-T)>.1E-02 THEN 160
217  IF B(90)=1 THEN 220
218  B(89)=0:B(90)=1: GOTO 155
220  B(18)=1: GOSUB 4000:B(120)=1: CALL (9,B(120),H2)
222  H2=H2*20/1000:H=H2+H9: IF T<Z(0)-.1E-02 THEN 160
223  REM  END OF TRANSIENT RESPONSE STUDIES
249  B(90)=0:I7=1: CALL (8,I7,B(90)): GOSUB 9500
250  INPUT B(90):B(89)=0
251  ON B(90) GOTO 155,253,147,255
253  B(90)=0: GOTO 155
255  END : REM  END OF MASTER SEGMENT
```

```
500  REM  OUTPUT STATE VARIABLES TO PAPER TAPE: GOSUB 900
502  PRINT T0;",";T1;",";C1: PRINT T2;",";T3;",";(F3+F5)
510  GOSUB 902: RETURN
511  REM
600  PRINT "TIME FROM WHICH GRAPHS TO BE PLOTTED";
601  INPUT B(89): PRINT "INPUT SIMULATION TIME";
602  INPUT Z(0):A9=INT(Z(0)/100+.1E-02-1)
603  PRINT "INPUT MIN,MAX & NO OF DIV. IN T1 GRAPH";
604  INPUT B(1),B(2),B(9):B(9)=B(9)-1
605  PRINT "INPUT MIN,MAX & NO OF DIV. IN TC1 GRAPH";
606  INPUT B(3),B(4),B(10):B(10)=B(10)-1
607  PRINT "INPUT MIN,MAX & NO OF DIV. IN C1 GRAPH";
608  INPUT B(5),B(6),B(11):B(11)=B(11)-1
609  GOSUB 900: IF B(90)=3 THEN 154
612  GOTO 151
698  REM
699  REM  CONC. SIMULATOR:X1=(C1-S1)/C0
700  X2=(T1+273.1-S2)/600:X3=(T3+273.1-S3)/600
701  IF B(90)=1 THEN 705
702  IF T<>0 THEN 705
703  PRINT "INPUT INITIAL CON. DEV.";: INPUT X1:X1=X1/C0
705  CALL (7,O1,F6,E,C0,S2,S1,X1,X2,J3,F3,F4,H,J4,J5)
706  C1=X1*C0+S1: RETURN
800  PRINT "INPUT TEMPR. AT WHICH CONTROL IS DESIRED";
801  INPUT T1:I6=1: GOSUB 3000
802  T3=(U*T1+F2*T2/60)/(F2/60+U):I7=3: GOTO 131
899  REM
900  REM         SET SNSW4 ON:B(91)=1: GOTO 904
902  REM         RESET SNSW4:B(91)=0
904  I7=0: CALL (8,I7,B(91)): RETURN
906  REM
1000  REM          ROUTINE TO SET JACKET FLOW RATE
1002  IF F2<=2.3 THEN O1=-1.41542*F2+9.54589
1004  IF F2>=7.5 THEN O1=-.583999*F2+7.21557
1006  IF F2>2.3 THEN  IF F2<=5 THEN O1=-.825452*F2+8.13453
1008  IF F2>5 THEN  IF F2<7.5 THEN O1=-.493939*F2+6.46235
1010  O1=O1*.32767E05/10:N=8
1012  REM          SEND SIGNAL TO CHANNEL 2: GOSUB 9000
1014  RETURN
1016  REM
1500  REM  TO TRANSFER SEGM1 FROM DISK TO CORE:B(119)=.15323E05
1502  B(115)=1:B(116)=1:B(117)=1:B(118)=9216:I7=1
1504  CALL (6,B(115),B(116),B(117),B(118),B(119),F7)
1506  IF F7=0 THEN  RETURN
1510  PRINT "ERROR NO";F7;"TRANSFERRING SEGM";I7: STOP
1550  REM    TO TRANSFER PART OF SEGM1 FROM DISK TO CORE
1552  B(119)=.12286E05: GOTO 1502
1600  REM       TO TRANSFER SEGM2 FROM DISK TO CORE:I7=2
1602  B(115)=1:B(116)=7:B(117)=1:B(118)=9216
1604  B(119)=.12286E05: GOTO 1504
```

```
2000  REM    SUBROUTINE TO SET IMMERSION HEATERS: DIM Z(3)
2001  GOSUB 3000
2002  IF H2>500 THEN 2006
2004  Z(1)=-.153234E-05:Z(2)=.197036E-02:Z(3)=.340653
2005  GOTO 2050
2006  IF H2<2400 THEN 2010
2008  Z(1)=.675824E-06:Z(2)=-.296997E-02:Z(3)=5.20372
2009  GOTO 2050
2010  Z(1)=0:Z(2)=.50393E-03:Z(3)=.738165
2050  Q1=Z(1)*H2↑2+Z(2)*H2+Z(3)
2052  Q1=Q1*.32767E05/3.1415:N=4
2054  REM         SEND SIGNALS TO CHANNEL 1: GOSUB 9000
2056  RETURN
2058  REM
3000  REM   REACTION KINETICS ROUTINE
3002  REM   **REACTION PARAMETERS** C0=.02,DH=30,K=2000
3004  REM   V=17300,VC=8532
3012  F6=F1*1000/60:J8=F6:C0=.2E-01
3015  J9=2000*.173E05*EXP(-E/(.198E-02*(T1+273.1)))
3021  H4=(U*T1+F2*T2/60)/(F2/60+U)
3022  H4=4.18**(F6*(T1-T0)+1000*U*(T1-H4)
3023  REM  HEAT REMOVAL
3024  H3=4.18*1000*(F1*(T1-T0)+F2*(T3-T2))/60
3025  REM  HEAT GEN.:H1=30*C1↑O1*J9*4.18*1000:H2=H1/3
3027  IF I6=1 THEN  RETURN
3030  PRINT "HEAT INP(W):";H1,"HEAT OUT(W):";H3
3035  PRINT "C1=";C1;"GM/CC": RETURN
3040  REM
4000  REM  ROUTINE FOR PLOTTING & OUTPUT TRANSIENT RESPONSE
4002  B(19)=B(19)+1:B(92)=B(92)+1
4004  IF B(92)>2.2 THEN  GOSUB 500
4010  Y1=30:Y2=45:B(7)=0:B(8)=150:B(12)=3
4020  IF B(18)<>1 THEN 4025
4022  J1=Y1+(Y2-Y1)*(T1-B(1))/(B(2)-B(1)): GOTO 4070
4025  IF B(18)<>2 THEN 4035
4030  J1=Y1+(Y2-Y1)*(T3-B(3))/(B(4)-B(3))
4035  IF B(18)<>3 THEN 4045
4040  J1=Y1+(Y2-Y1)*(C1-B(5))/(B(6)-B(5))
4045  IF B(18)<>4 THEN 4070
4050  J1=Y1+(Y2-Y1)*((F5+F3)-B(7))/(B(8)-B(7))
4070  GOSUB 5000:B(18)=B(18)+1: IF B(18)<4.2 THEN 4020
4080  GOSUB 1600: RETURN
```

```
5000  REM  PLOTTER ROUTINE: DIM C(7)
5002  B(16)=0:B(17)=1500:B(15)=1
5015  C(1)=0:C(4)=0: IF B(18)>1.1 THEN 5030
5017  IF B(19)>1.1 THEN 5030
5020  C(2)=3700:C(4)=6+2*(Y2-Y1): GOSUB 5900
5022  B(15)=2: GOSUB 5900
5030  IF B(18)>1 THEN 5032
5031  P1=400:P2=5:Y4=B(2):Y6=B(1): GOTO 5050
5032  IF B(18)>2 THEN 5037
5035  P1=1950:P2=5:Y4=B(4):Y6=B(3): GOTO 5050
5037  IF B(18)>3 THEN 5042
5040  P1=400:P2=6+Y2-Y1:Y4=B(6):Y6=B(5): GOTO 5050
5042  P1=1950:P2=6+Y2-Y1:Y4=B(8):Y6=B(7)
5050  IF B(19)>1.1 THEN 5100
5055  GOSUB 5800
5100  C(0)=3:C(5)=T*1500/Z(0)+P1:C(6)=J1-Y1+P2
5102  IF B(19)<1.1 THEN 5115
5110  B(15)=3:C(0)=1:C(5)=B(101+(B(18)-1)*2)
5111  C(6)=B(102+(B(18)-1)*2): GOSUB 5900
5112  C(0)=3:C(5)=T*1500/Z(0)+P1:C(6)=J1-Y1+P2: GOSUB 5900
5115  B(101+(B(18)-1)*2)=C(5):B(102+(B(18)-1)*2)=C(6)
5116  IF T<Z(0)-.1E-01 THEN 5200
5117  C(5)=P1-260: IF B(18)=4 THEN C(5)=P1+1450
5118  IF B(18)=2 THEN C(5)=P1+1400
5119  IF B(18)=3 THEN C(5)=P1-400
5120  C(6)=Y2-Y1+P2-1: GOSUB 5505: PRINT Y4:C(5)=P1-295
5125  C(6)=(Y2+Y1)/2-Y1+P2: IF B(18)>2 THEN 5130
5127  C(5)=P1-225: IF B(18)=2 THEN C(5)=P1+1540
5128  GOSUB 5505: PRINT "DEG":C(6)=C(6)-2: GOSUB 5505
5129  PRINT " C":C(5)=P1-260
5130  IF B(18)<>3 THEN 5135
5132  C(5)=P1-295: GOSUB 5505: PRINT "GM/CC"
5135  IF B(18)<>4 THEN 5142
5137  C(5)=P1+1550: GOSUB 5505: PRINT "CC/S":C(5)=P1+1380
5142  C(6)=P2: IF B(18)=3 THEN C(5)=P1-400
5143  IF B(18)=2 THEN C(5)=P1+1400
5144  GOSUB 5505: PRINT Y6: FOR Q1=1,A9
5145  C(5)=P1+Q1*100*1500/Z(0): GOSUB 5520: NEXT Q1
5157  C(6)=P2-2:C(5)=P1: IF B(18)>2 THEN 5170
5160  GOSUB 5505: PRINT "0":C(5)=P1+450: GOSUB 5505
5165  PRINT "TIME(SECS)":C(5)=P1+1280: GOSUB 5505
5170  PRINT Z(0): GOSUB 5300: IF B(18)<4 THEN 5200
5182  GOSUB 5500: PRINT "TANK TEMPERATURE": GOSUB 5500
5184  PRINT "JACKET TEMPERATURE": GOSUB 5500
5187  PRINT "TANK CONCENTRATION": GOSUB 5500
5189  PRINT "JACKET FLOW RATE":B(15)=6: GOSUB 5900: PRINT
5195  PRINT : PRINT : PRINT : PRINT : PRINT : RETURN
5200  RETURN
```

```
5300  B(15)=3:C(0)=1:C(5)=P1+B(16)
5305  FOR I3=1,B(8+B(18)):C(6)=P2+I3*(Y2-Y1)/(B(8+B(18))+1)
5307  GOSUB 5400: NEXT I3: RETURN
5400  GOSUB 5900:C(0)=3:C(5)=P1+B(16)+30: GOSUB 5900
5410  C(0)=1:C(5)=P1+B(16): RETURN
5500  B(15)=4:C(7)=0: GOSUB 5900
5502  REM
5505  REM  OUTPUT CHARACTERS ON SCREEN:B(15)=3:C(0)=1
5507  GOSUB 5900:B(15)=5:C(7)=2: GOSUB 5900: RETURN
5520  REM
5800  REM  DRAW WINDOWS:C(0)=1:B(15)=3:C(5)=P1:C(6)=P2
5801  GOSUB 5900:C(0)=3:C(5)=B(17)+P1: GOSUB 5900
5802  C(6)=Y2-Y1+P2: GOSUB 5900:C(5)=B(16)+P1
5804  GOSUB 5900:C(6)=P2: GOSUB 5900: RETURN
5806  REM
5900  CALL (7,B(15),C(0)): RETURN
5902  REM
6000  REM  ROUTINE TO CALCULATE THEORETICAL HEAT
6002  REM  GENERATION & REMOVAL:B(116)=T1:I6=1
6004  T1=T0+4:B(12)=0: FOR I5=1,60:T1=T1+.4: GOSUB 3000
6007  GOSUB 6800: IF I5=1 THEN 6018
6015  IF SGN(H1-H4)=SGN(H5) THEN 6018
6016  B(12)=B(12)+1:H5=H1-H4:B(B(12)+12)=T1
6017  B(B(12)+16)=-1: IF H5<0 THEN B(B(12)+16)=1
6018  H5=H1-H4: NEXT I5:T1=B(116):I6=0: RETURN
6020  REM
6022  REM  ROUTINE TO PRINT THEOR. OP. POINTS
6025  PRINT " THEO. OP TEMP.:": IF B(13)=0 THEN  RETURN
6027  FOR I5=1,B(12): PRINT B(12+I5);
6028  IF B(16+I5)<>1 THEN  PRINT "U.S."
6032  IF B(16+I5)=1 THEN  PRINT "S.S."
6035  NEXT I5: RETURN
6500  REM  PLOT HEAT GENERATION AND REMOVAL CURVES: GOSUB 1500
6501  C(1)=0:C(4)=100:B(15)=1:C(2)=100:C(3)=0: GOSUB 5900
6502  B(15)=2: GOSUB 5900:P1,P2,B(17),Y1=50:Y2=100
6503  B(16)=0: GOSUB 5800: GOSUB 6000: RETURN
6505  REM
6700  C(5)=(B(92)-(T0+4))*50/30+50:C(6)=(B(91)-1800)*50/8000+50
6702  GOSUB 5900: RETURN
```

```
6800  B(19)=B(19)+1: IF H4<1800 THEN H4=1800
6802  IF B(19)=1 THEN 6808
6804  FOR Q1=1,2:C(0)=1:B(92)=T1-.4:B(91)=B(88+Q1): GOSUB 6700
6806  B(92)=T1:C(0)=3:B(91)=H1: IF Q1=2 THEN B(91)=H4
6807  GOSUB 6700: NEXT Q1
6808  B(89)=H1:B(90)=H4: RETURN
6810  REM
6900  REM  PLOT EXPTL. S.S. VALUES:B(92)=T1:B(91)=H1:C(0)=1
6902  B(15)=3: GOSUB 6700:B(15)=5: GOSUB 5900: PRINT "*"
6904  B(19)=0: RETURN
6906  REM
7000  REM   CONTROL SUBROUTINE
8999  REM
9000  REM  SEND DIGITAL OUTPUT TO ANALOG CHANNELS
9002  CALL (5,D,N,Q1):N=0: CALL (5,D,N,Q1): RETURN
9004  REM
9005  REM  SCANNING ROUTINE:B(119)=0
9007  CALL (1,A(0),B(0)): CALL (2):B(119)=B(119)+1
9010  IF B(119)=2 THEN 9050
9040  B(115)=B(33):B(116)=B(30):B(117)=B(32)
9042  B(118)=B(31): GOTO 9007
9050  T0=(B(33)+B(115))*97/2046:T1=(B(30)+B(116))*95/2046
9052  T2=(B(32)+B(117))*94/2046:T3=(B(31)+B(118))*94/2046
9054  RETURN
9100  PRINT "F=";F6,"FC=";F5
9101  PRINT "T0=";T0;"TC0=";T2;"T1=";T1;"TC1=";T3
9102  U=F5*(T3-T2)*.1E-02/(T1+-T3)
9104  REM
9500  REM  CALCULATE TANK FLOW RATE
9502  Q1=((127-A(7))*B(50)+B(49))/A(0)
9504  F7=Q1*.296448E-01+.678044
9505  IF F7>3.5 THEN F7=Q1*.340529E-01+.325588
9508  PRINT "MEASURED TANK FLOW RATE IN CC/S";
9510  PRINT F7*1000/60: RETURN
```

A.1.6.2 <u>REACTION ORDERS</u>

```
3005  REM  **ORDER=-1**:O1=-1:E=14.83
3019  IF J6<>3 THEN C1=SQR((J8*C0)↑2-4*J8*J9)
3020  IF J6<>3 THEN C1=C0/2+C1/(2*J8)
```

```
3005  REM  ORDER=0**:O1=0:E=12.445
3020  IF J6<>3 THEN C1=C0-J9/J8
```

```
3005  REM  **ORDER=1**:O1=1:E=10.06
3020  IF J6<>3 THEN C1=J8*C0/(J8+J9)
```

```
3005  REM  **ORDER=2**:O1=2:E=7.67
3019  IF J6<>3 THEN C1=SQR(J8↑2+4*J8*C0*J9)
3020  IF J6<>3 THEN C1=(-J8+C1)/(2*J9)
```

A.1.6.3 VARIOUS CONTROLLER EQUATIONS

```
131   S5=T2+273.1:S4=T0+273.1
7002  IF K1>4 THEN 7005
7003  ON K1 GOTO 7015,7025,7035,7045
7005  ON K1-5 GOTO 7055,7065,7085,7095,7105
7014  REM
7015  REM  UNCONTROLLED SYSTEM:F3,F4=0: RETURN
7022  REM
7025  REM  PROPORTIONAL CONTROL ON TANK TEMP.
7027  F3=K2*X2:F4=0: RETURN
7030  REM
7034  REM  PROPORTIONAL CONTROL ON JACKET TEMP.
7035  X3=(T3-S3+273.1)/600:F3=K2*X3:F4=0: RETURN
7037  REM
7043  REM  COOLANT RATE FUNCTION OF TANK TEMPR.
7045  S4=S3+T3-S3+273.1-S5:F3=(8530/.173E05+1)*U
7050  F3=F3*(T1+273.1-S2)/(S4*.1E-02):F4=0: RETURN
7052  REM
7063  REM  INVARIANCE FOR STEP IN TANK FEED TEMPR.
7065  S6=T0+273.1-S4:F3=S5-S3+.1E-02*S6*F6/U:F4=0
7070  F3=-S6*F6*.1E-02*(1000+F5/U)/F3: IF S6<0 THEN  RETURN
7072  IF (F3+F5)>0 THEN  RETURN
7073  REM
7074  REM  INVARIANCE FOR STEP IN JACKET FEED TEMPR.
7075  S4=273.1+T2-S5:F3=S3-S5-S4:F3=S4*F5/F3
7077  IF S4<0 THEN  RETURN
7078  IF (F3+F5)>0 THEN  RETURN
7079  F3=150-F5: RETURN
7081  REM
7093  REM  LIMIT CYCLE STUDIES
7095  X1=(C1-S1)/C0:F3=-K2*X1:F4=0: RETURN
7097  REM
7103  REM  INVARIANCE FOR CHANGES IN TANK & JACKET
7104  REM  INLET TEMPR.
7105  S6=(T0+273.1-S4):F3=S6*F6*(1+F5*.1E-02/U)
7110  S7=T2+273.1-S5:F3=S7*F5+F3:F4=0
7111  F3=F3/(S3-S5-S7-S6*F6*.1E-02/U): RETURN
```

A.1.6.4 DECOUPLING TYPE CONTROL OF TANK TEMPERATURE

```
131   B(37)=.173E05/F6:B(39)=2000*C0↑(O1-1):S4=T0+273.1
134   S5=(T2+273.1)/600:B(38)=U/17.3:B(40)=(F5+U*1000)/8532
135   B(36)=(S1/C0)↑O1*EXP(-E/(.198E-02*S2))
7084  REM
7085  REM  DECOUPLING TYPE CONTROL
7086  REM  INITIALISATION: GOSUB 7200
7088  REM  ITERATION:B(49)=B(43)*B(50)+B(44)
7089  IF (B(49)-(S5-S3/600))*(8-B(49)/600)<0 THEN 7093
7090  GOSUB 7300: IF (F3+F5)*(150-F3-F5)>0 THEN  RETURN
7093  B(50)=B(50)/1.1: IF B(50)>.1E-04 THEN 7088
7097  F3=150-F5: RETURN
7100  REM
7200  B(41)=(X1+S1/C0)↑O1*EXP(-E/(.198E-02*(X2*600+S2)))
7202  B(42)=-X1/B(37)-B(39)*(B(41)-B(36)):B(50)=.7E-02
7203  B(43)=-X2/B(38)
7204  B(44)=((1/B(37)+B(38))*X2-B(39)*(B(41)-B(36)))/B(38)
7205  B(44)=B(44)-(T0+273.1-S4)/(600*B(37)*B(38))
7206  B(45)=(1.188*(X2+S2/600)↑2)*B(38)
7207  B(45)=-X2*(1/B(37)+B(38))/B(38)+X2*B(41)*B(39)*E/B(45)
7208  B(46)=-O1*B(42)*B(41)*B(39)/(B(38)*(S1/C0+X1))
7210  B(48)=X2*U/8.532: RETURN
7212  REM
7298  REM  CALCULATION OF COOLANT FLOW RATE
7300  B(47)=-B(50)↑2*B(43)+B(45)*B(50)+B(46)
7305  F3=(-B(47)+B(48)-B(40)*B(49))*8532/(B(49)+S3/600-S5)
7307  RETURN
```

A.1.7 PROGRAM FOR PLOTTING EXPERIMENTAL AND TOTAL SIMULATION RESULTS

```
5  B(29),B(19),C3=0
10  DIM A(13),B(120)
11  REM  GET SCALES FOR THE PLOTS: GOSUB 600
19  REM  OPERATING POINTS
20  READ S1,S2,S3: DATA 32.39,.19124E-01,21.24
159  REM  READ RESULTS FROM TOTAL SIMULATION PROGRAM
160  I6=1: INPUT T,T1,C1,T3:J3=1:F5=0
162  T1=T1+S1:C1=C1+S2:T3=T3+S3
219  REM  PLOT SIMULATION VALUES
220  B(18)=1: GOSUB 4000: IF T<Z0-2 THEN 160
221  REM  PLOT CURVE FIT: GOSUB 8999:B(19)=.1E08
222  REM READ EXPTL. VALUES & PLOT: INPUT T: INPUT N8,T1,C1
223  INPUT N8,T3,N8:B(18)=1: GOSUB 7000
225  IF T<Z0-2 THEN 222
226  REM  EXIT FROM GRAPHICS: GOSUB 5182
235  REM  END OF MASTER: END
237  REM
600  PRINT "INPUT SIMULATION TIME";: INPUT Z0
601  PRINT "INPUT MIN,MAX & NO OF DIV. IN T1 GRAPH";
602  INPUT B(1),B(2),B(9):B(9)=B(9)-1
603  B(9)=B(9)-1
604  PRINT "INPUT MIN,MAX & NO OF DIV. IN TC1 GRAPH";
605  INPUT B(3),B(4),B(10):B(10)=B(10)-1
606  PRINT "INPUT MIN MAX & NO DIV. IN C1 GRAPH";
607  INPUT B(5),B(6),B(11):B(11)=B(11)-1
608  A9=INT(Z0/100+.1E-02-1): RETURN
611  INPUT B(5),B(6),B(11):B(11)=B(11)-1: RETURN
612  REM
4000  REM  PLOTTING ROUTINE:B(19)=B(19)+1
4001  REM  FIND TIME PERIOD OF OSCILLATION: GOSUB 4950
4002  IF B(19)=5 THEN 4004
4003  IF B(19)<>30 THEN  IF B(19)<>55 THEN 4010
4004  B(29)=B(29)+1:B(29+B(29))=T:B(32+B(29))=C1
4005  B(35+B(29))=T1:B(38+B(29))=T3
4010  Y1=30:Y2=45:B(7)=0:B(8)=150:B(12)=3
4020  IF B(18)<>1 THEN 4024
4022  J1=Y1+(Y2-Y1)*(T1-B(1))/(B(2)-B(1))
4024  IF B(18)<>2 THEN 4035
4030  J1=Y1+(Y2-Y1)*(T3-B(3))/(B(4)-B(3))
4035  IF B(18)<>3 THEN 4045
4040  J1=Y1+(Y2-Y1)*(C1-B(5))/(B(6)-B(5))
4045  IF B(19)>.9E06 THEN 7002
4070  GOSUB 5000:B(18)=B(18)+1: IF B(18)<3.2 THEN 4020
4080  RETURN
```

```
4949  REM   TIME PERIOD OF OSCILLATION
4950  IF B(19)=1 THEN C2=T1
4951  IF B(19)=2 THEN B(28)=SGN(T1-C2)
4952  IF B(28)<0 THEN 4955
4953  IF T1>C2 THEN  IF C3<C2 THEN W=2*3.141/T
4954  GOTO 4956
4955  IF T1<C2 THEN  IF C3>C2 THEN W=2*3.141/T
4956  C3=T1: RETURN
4958  REM
5000  DIM C(7):B(16)=0:B(17)=1500:B(15)=1
5015  C(1)=0:C(4)=0: IF B(18)>1.1 THEN 5030
5017  IF B(19)>1.1 THEN 5030
5020  C(2)=3700:C(4)=6+2*(Y2-Y1): GOSUB 5900
5021  B(15)=2: GOSUB 5900
5030  IF B(18)>1 THEN 5032
5031  P1=400:P2=5:Y4=B(2):Y6=B(1): GOTO 5050
5032  IF B(18)>2 THEN 5040
5035  P1=1950:P2=5:Y4=B(4):Y6=B(3): GOTO 5050
5040  P1=1200:P2=6+Y2-Y1:Y4=B(6):Y6=B(5): GOTO 5050
5050  IF B(19)>1.1 THEN 5100
5051  C(0)=1:B(15)=3:C(5)=P1:C(6)=P2: GOSUB 5900
5052  C(0)=3:C(5)=B(17)+P1: GOSUB 5900
5055  C(6)=Y2-Y1+P2: GOSUB 5900:C(5)=B(16)+P1
5056  GOSUB 5900:C(6)=P2: GOSUB 5900
5100  C(0)=3:C(5)=T*1500/Z0+P1:C(6)=J1-Y1+P2
5101  IF B(19)<1.1 THEN 5115
5110  B(15)=3:C(0)=1:C(5)=B(101+(B(18)-1)*2)
5111  C(6)=B(102+(B(18)-1)*2): GOSUB 5900
5112  C(0)=3:C(5)=T*1500/Z0+P1:C(6)=J1-Y1+P2: GOSUB 5900
5115  B(101+(B(18)-1)*2)=C(5):B(102+(B(18)-1)*2)=C(6)
5116  IF T<Z0-2 THEN 5200
5117  C(5)=P1-260: IF B(18)=4 THEN C(5)=P1+1450
5118  IF B(18)=2 THEN C(5)=P1+1400
5119  IF B(18)=3 THEN C(5)=P1-500
5120  C(6)=Y2-Y1+P2-1: GOSUB 5505: PRINT Y4:C(5)=P1-295
5125  C(6)=(Y2+Y1)/2-Y1+P2: IF B(18)>2 THEN 5130
5127  C(5)=P1-225: IF B(18)=2 THEN C(5)=P1+1540
5128  GOSUB 5505: PRINT "DEG":C(6)=C(6)-2
5129  GOSUB 5505: PRINT " C":C(5)=P1-260
5130  IF B(18)<>3 THEN 5135
5132  C(5)=P1-295: GOSUB 5505: PRINT "GM/CC"
5135  IF B(18)<>4 THEN 5142
5137  C(5)=P1+1550: GOSUB 5505: PRINT "CC/S":C(5)=P1+1380
```

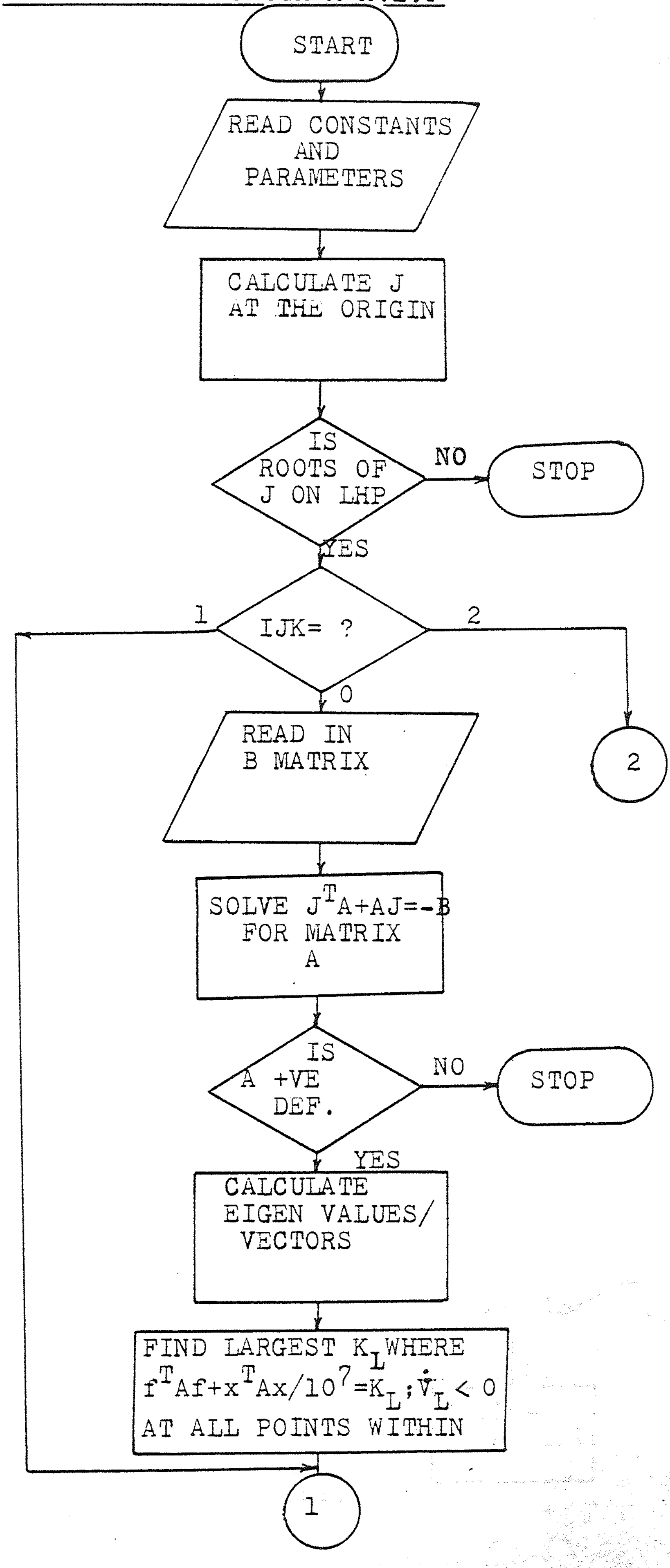
```
5142 C(6)=P2: IF B(18)=3 THEN C(5)=P1-500
5143 IF B(18)=2 THEN C(5)=P1+1400
5144 GOSUB 5505: PRINT Y6
5145 FOR Q1=1,A9:C(5)=P1+Q1*100*1500/Z0: GOSUB 5520
5157 NEXT Q1:C(6)=P2-2:C(5)=P1: IF B(18)>2 THEN 5170
5160 GOSUB 5505: PRINT "0":C(5)=P1+450: GOSUB 5505
5165 PRINT "TIME(SECS)":C(5)=P1+1280: GOSUB 5505: PRINT Z0
5170 GOSUB 5300: RETURN
5172 REM
5182 GOSUB 5500: PRINT "TANK TEMPERATURE"
5183 GOSUB 5500: PRINT "JACKET TEMPERATURE"
5187 GOSUB 5500: PRINT "TANK CONCENTRATION"
5195 B(15)=6: GOSUB 5900: PRINT : PRINT : PRINT
5200 RETURN
5300 B(15)=3:C(0)=1:C(5)=P1+B(16)
5305 FOR I3=1,B(8+B(18)):C(6)=P2+I3*(Y2-Y1)/(B(8+B(18))+1)
5306 GOSUB 5400: NEXT I3: RETURN
5400 GOSUB 5900:C(0)=3:C(5)=P1+B(16)+30: GOSUB 5900
5410 C(0)=1:C(5)=P1+B(16): RETURN
5500 B(15)=4:C(7)=0: GOSUB 5900
5505 B(15)=3:C(0)=1: GOSUB 5900:B(15)=5:C(7)=2
5506 GOSUB 5900: RETURN
5520 GOSUB 5505: PRINT "!": RETURN
5522 REM
5900 CALL (7,B(15),C(0)): RETURN
5902 REM
5999 REM  PLOT CURVE FIT
6000 FOR T=0,Z0,.2/W
6001 X=X0+X1*COS(W*T)+X2*SIN(W*T):B(19)=.2E11
6002 Y=B(65)+B(66)*COS(W*T)+B(67)*SIN(W*T)
6003 Z=B(68)+Z1*COS(W*T)+Z2*SIN(W*T):T1=Y:C1=X:T3=Z
6004 GOSUB 7000: NEXT T
6006 REM
7000 REM  PLOT EXPTL. VALUES
7001 FOR Q1=1,3:B(18)=Q1:- GOTO 4010
7002 IF B(18)<>1 THEN 7012
7005 P1=400:P2=5:Y4=B(2):Y6=B(1)
7010 GOTO 7050
7012 IF B(18)<>2 THEN 7020
7015 P1=1950:P2=5:Y4=B(4):Y6=B(3): GOTO 7050
7020 IF B(18)<>3 THEN 7050
7022 P1=1200:P2=6+Y2-Y1:Y4=B(6):Y6=B(5)
7050 C(5)=T*1500/Z0+P1:C(6)=J1-Y1+P2
7052 IF B(19)>.1E11 THEN 7055
7053 GOSUB 5505: PRINT "O": GOTO 7057
7055 GOSUB 5505: PRINT "1"
7057 NEXT Q1: RETURN
```

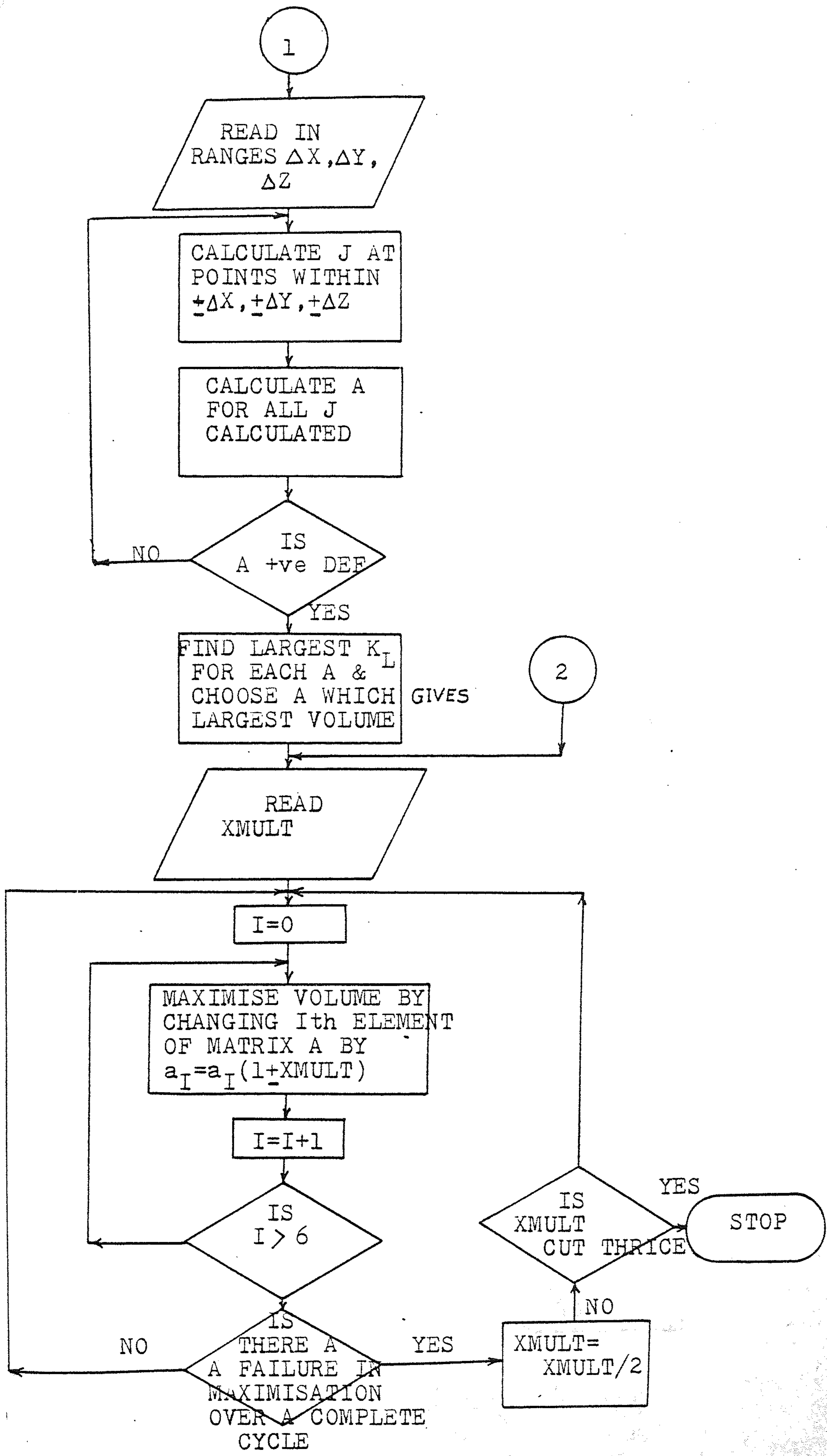
```
8999  REM  OBTAIN THE HARMONICS OF THE OSCILLATIONS
9000  FOR I=1,3:B(51+(I-1)*3)=COS(W*B(29+I))
9002  B(52+(I-1)*3)=SIN(W*B(29+I)): NEXT I
9005  FOR I=1,3:B(50)=B(33+(I-1)*3):B(53)=B(34+(I-1)*3)
9006  B(56)=B(35+(I-1)*3)
9009  B(59)=B(50)-B(53):B(60)=B(51)-B(54):B(61)=B(52)-B(55)
9011  B(62)=B(50)-B(56):B(63)=B(51)-B(57):B(64)=B(52)-B(58)
9013  B(66)=B(60)*B(64)-B(63)*B(61)
9014  B(66)=(B(59)*B(64)-B(62)*B(61))/B(66)
9015  B(67)=(B(59)-B(66)*B(60))/B(61):B(65)=B(66)*B(51)
9016  B(65)=B(50)-B(65)-B(67)*B(52): IF I<>1 THEN 9020
9018  IF I<>1 THEN 9020
9019  X0=B(65):X1=B(66):X2=B(67)
9020  IF I<>2 THEN 9025
9022  Y0=B(65):Y1=B(66):Y2=B(67)
9025  IF I<>3 THEN 9050
9027  B(68)=B(65):Z1=B(66):Z2=B(67)
9050  NEXT I:I=0:B(65)=1: REM  SEND VALUES TO PAPER TAPE
9051  CALL (8,I,B(65)): PRINT "X VAL";X0;X1;X2
9052  PRINT "Y VAL";Y0;Y1;Y2: PRINT "Z VAL";B(68);Z1;Z2
9053  B(65)=0: CALL (8,I,B(65)):B(65)=Y0:B(66)=Y1:B(67)=Y2
9054  GOSUB 6000: RETURN
```

APPENDIX 2

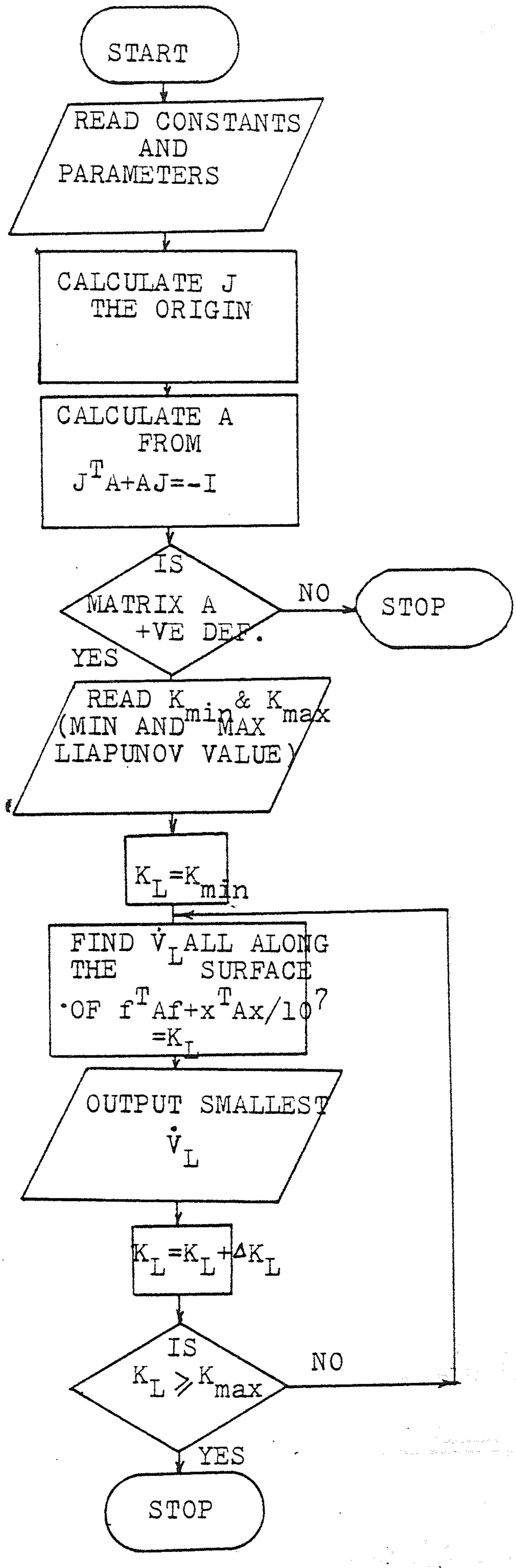
FLOW CHART OF COMPUTER PROGRAMS

A.2.1 FLOW CHART OF PROGRAM A.1.3

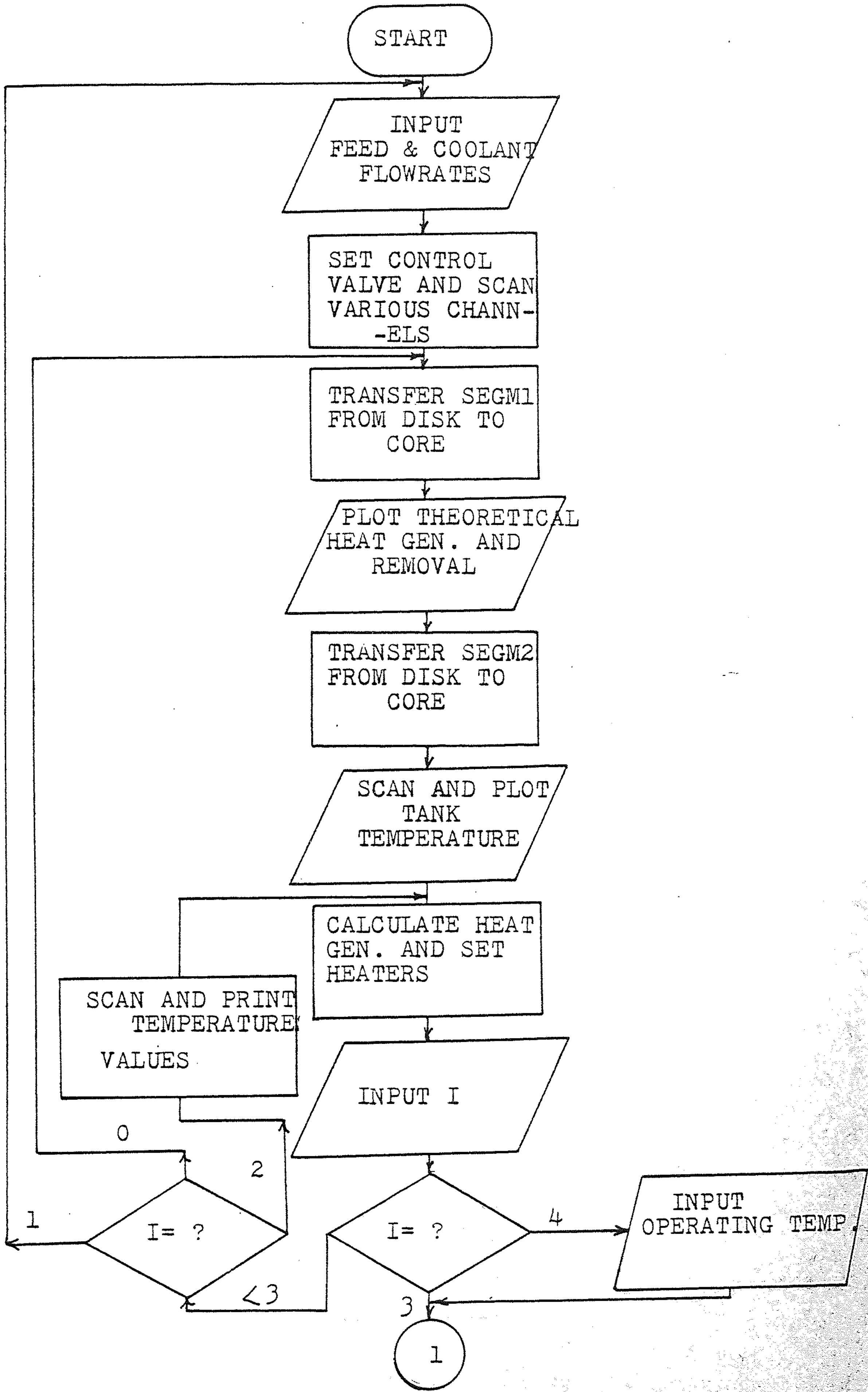


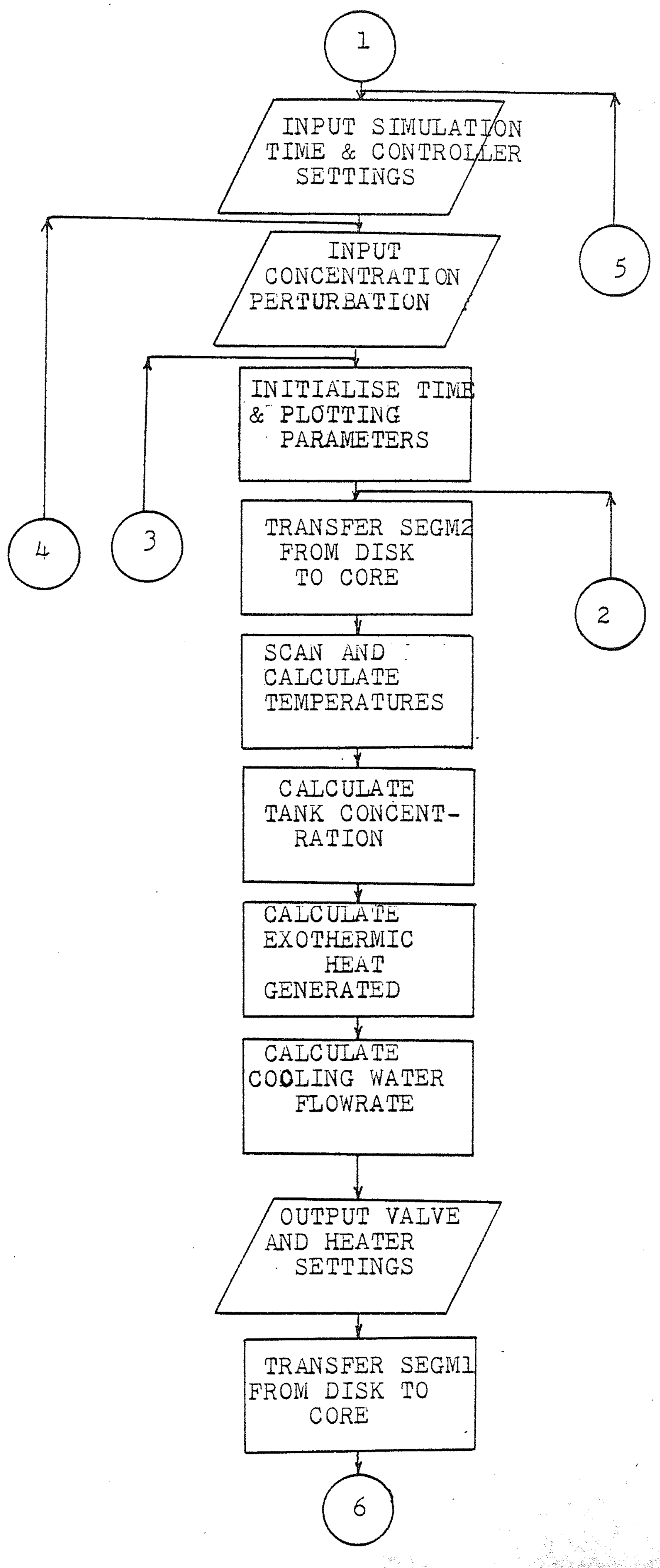

1
READ IN RANGES ΔX, ΔY, ΔZ
CALCULATE J AT POINTS WITHIN ±ΔX, ±ΔY, ±ΔZ
CALCULATE A FOR ALL J CALCULATED
IS A +ve DEF
NO
YES
FIND LARGEST K_L FOR EACH A & CHOOSE A WHICH GIVES LARGEST VOLUME
2
READ XMULT
I=0
MAXIMISE VOLUME BY CHANGING Ith ELEMENT OF MATRIX A BY a_I=a_I(1±XMULT)
I=I+1
IS I > 6
IS THERE A FAILURE IN MAXIMISATION OVER A COMPLETE CYCLE
NO
YES
XMULT= XMULT/2
NO
IS XMULT CUT THRICE
YES
STOP

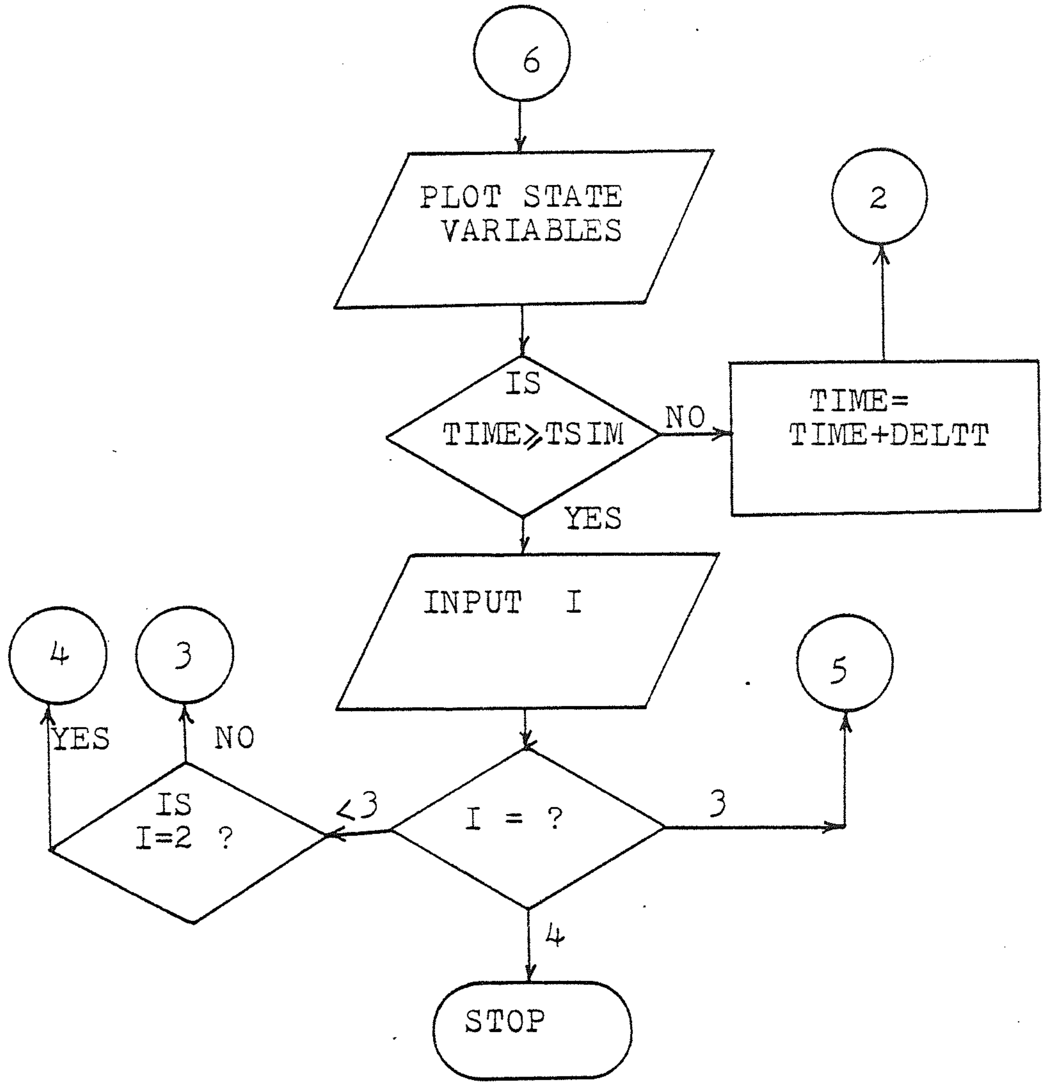
A.2.2 FLOW CHART OF PROGRAM A.1.4



A.2.3 FLOW CHART OF PROGRAM A.1.6




1
INPUT SIMULATION TIME & CONTROLLER SETTINGS
5
INPUT CONCENTRATION PERTURBATION
INITIALISE TIME & PLOTTING PARAMETERS
4
3
TRANSFER SEGM2 FROM DISK TO CORE
2
SCAN AND CALCULATE TEMPERATURES
CALCULATE TANK CONCENTRATION
CALCULATE EXOTHERMIC HEAT GENERATED
CALCULATE COOLING WATER FLOWRATE
OUTPUT VALVE AND HEATER SETTINGS
TRANSFER SEGM1 FROM DISK TO CORE
6


6
PLOT STATE VARIABLES
2
IS TIME≥TSIM
NO
TIME= TIME+DELTT
YES
INPUT I
4
3
5
YES
NO
IS I=2 ?
<3
I = ?
3
4
STOP

APPENDIX 3

THEOREMS AND TECHNIQUES USED IN PROGRAMMING

APPENDIX 3

THEOREMS AND TECHNIQUES USED IN PROGRAMMING

A.3.1 Routh's Criterion for Matrix J[52]

The necessary and sufficient condition that the eigenvalues of the matrix J are on the left half of plane is that the n^{th} order polynomial formed

$$a_o S^n + a_1 S^{n-1} + \dots \qquad a_n = 0$$

satisfies the Routh-Hurwitz criteria namely

$$a_o, a_1 > 0$$

$$\begin{vmatrix} a_1 & a_3 \\ a_o & a_2 \end{vmatrix} > 0$$

$$\begin{vmatrix} a_1 & a_3 & a_5 \\ a_o & a_2 & a_4 \\ o & a_1 & a_3 \end{vmatrix} > 0 \quad \text{etc.}$$

The constants $a_o, a_1, \dots a_n$ can be directly obtained from the matrix J by the following rule

$$P_1 = {}^{a_1}/_{a_o} = -Tr(J) \qquad \text{(Trace of Jacobian)}$$

$$P_k = {}^{a_k}/_{a_o} = -\frac{1}{k}\,Tr(JG_{k-1}) \quad k = 2, \dots n$$

$$G_1 = J + P_1 I_n$$

$$G_k = JG_{k-1} + P_k I_n \qquad k = 2 \dots (n-1)$$

A.3.2 Solution of $J^T A + AJ = -B$ for Matrix A

The left hand side of the equation can be expanded to arrive at a matrix equation of the form

$$\{P\}\ \{A_c\} = \{B_c\}$$

where A_c and B_c are (9x1) column vectors and P a (9x9) matrix if A is a (3x3) matrix. The elements of A_c and B_c are formed from matrix A and B respectively. This equation is solved for A_c by the Gauss Jordan elimination method. If matrix B is symmetric then A will also be symmetric.

A.3.3 Volume of Ellipsoid

The volume of the Liapunov contour is given by

$$\text{Volume} = \int_{X=-\alpha_{SS}}^{X=1-\alpha_{SS}} \int_{Y=-(\beta_{SS}-\beta_O)}^{Y=Y_{upper}} (f_2(X,Y,K_L)-f_1(X,Y,K_L))\, dX\, dY$$

The upper limit on Y, Y_{upper} is arbitrarily chosen. The functions f_1 and f_2 are obtained by manipulating the Liapunov equation

$$f^T A f + x^T A x/10^7 = K_L$$

The volume is numerically evaluated by the extended Simpson's rule

$$\text{Volume} = \frac{(b-a)^2}{(\Sigma w_1)(\Sigma w_j)} \sum_{j=1}^{m} \sum_{i=1}^{n} (f_2-f_1)$$

where n and m are the number of steps in the X and Y directions. w_i and w_j are the weighting factors. b and a are the upper and lower bounds on the variables X and Y. The boundary is made square, if necessary, by change of variable.

For 6 divisions in the i direction and 4 divisions in the j direction, the product $w_i w_j$ is given in the following table.

j \ i						
1	2	4	2	4	2	1
2	4	8	4	8	4	2
4	8	16	8	16	8	4
2	4	8	4	8	4	2
1	2	4	2	4	2	1

A.3.4 Logical Search Technique for Determining the Largest Liapunov Volume

The search method involves two parts. They are (i) calculate the Jacobian at different places in the state space and hence a A matrix according to procedure given in Appendix (3.2). Determine the A matrix which gives the largest Liapunov volume and then

(ii) change the elements of this matrix A to maximise on the volume. The elements of the matrix are changed one at a time as

$$A_{ij} = A_{ij} \pm K\, A_{ij}$$

Initially a large multiplication factor (K) is used and if the maximisation fails, the factor is reduced by half and the process continued. This halving procedure is carried out thrice before it is stopped.

A.3.5 Sylvester's Theorem

A matrix is said to be positive definite if the determinants formed by the principal diagnol elements are greater than zero.

For matrix A to be positive definite the following conditions have to be satisfied.

$$A_{11} > 0$$

$$\begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} > 0$$

$$|A| > 0$$

APPENDIX 4

ON-LINE SOFTWARE PACKAGE

APPENDIX 4

ON LINE SOFTWARE PACKAGE

The listing and calling procedure of various FORTRAN and DAP16 subroutines loaded with the BASIC interpreter to form the ONLINE SIMULATION PACKAGE are described in detail.

A.4.1 CALLING PROCEDURE OF SUBROUTINES 1 to 9

Subroutines 1 and 2 together from the scanning routines.

Subroutine 1

CALL (1,A(O), B(O)

A and B are dimensioned 12 and 120 respectively in the program

Inputs -	A(O)	= scanning interval, secs
	A(1)	= Device required
		= 1 Analog inputs
		= 2 Counter 1
		= 4 Counter 2
		= 8 Counter 3
		= 16 Digital input A
		= 32 Digital input B
		= 64 Digital output A
		= 128 Digital output B
	A(2)	= number of scans required including the initial scan
	A(3)	= first analog channel to be scanned
	A(4)	= last analog channel to be scanned

	A(5)	= number of samples of each analog channels per scan
	A(6)	= counter 1 scan type =0 no counter interrupt =1 enable counter interrupt
	A(7)	= counter 1 preset value
	A(8) & A(9)	= counter 2 scan and preset values
	A(10)& A(11)	= counter 3 scan and preset values
	A(12)	= digital output A mode = 0 from 16 bit array at BASIC level = 1 from subroutines 3,4 or 5 = 2 from user supplied
	A(13)	= digital output B mode
<u>Outputs</u> -	B(0)-B(47)	= analog input channels
	B(48)	= counter 1 interrupt time
	B(49)	= counter 1 contents at scanning time
	B(50)	= number of interrupts by the counter 1 during last scanning interval
	B(51),B(52) & B(53)	= Counter 2
	B(54),B(55) & B(56)	= Counter 3
	B(57)toB(72)	= value read on bits 1 to 16 of digital input A

B(73)toB(88) = digital input B

B(89)toB(104) = values output on digital output A

B(105)toB(120) = for digital output B

Subroutine 2

CALL (2)

A call to this routine discontinues clock and counter interrupt when all scans requested have been done.

Subroutine 3

CALL (3,D,N,X)

to send digital signals to various devices during scanning

D = 0 digital output A

= 1 digital output B

N = analog output channel

= 4 for thyristor unit

= 8 valve drive

x = digital signal to be output

$0 \leq x \leq 32767$

Subroutine 4

A special subroutine which can control up to eight valve drives, which is not used for the present work.

Subroutine 5

CALL (5,D,N,x)

the arguments in this routine are the same as those of subroutine 3. Subroutine 5, when called, sends signals to the devices immediately while, subroutine 3 sends only at the beginning of each scan.

Subroutine 6

This routine transfers segments from disk to core. The segments should have been stored in disk previously by the program A$\not{S}$D14.

CALL (6,U,T,S,B1,B2,E)

U = disk unit number

T = Track number

S = sector number

B1= starting address on core, a decimal number

B2= Last address on core, a decimal number

E = error on return

= o normal exit

Subroutine 7

There are two routines available with the same number because of the overlaying facility. If segment 1 is in core, then the Tetronix graph library can be assessed by a call to subroutine 7, whereas a similar call when segment 2 is in core can be used to access the simulator and integrator routine.

Tetronix graphic package

Various plotting facilities can be performed by a call to this routine

CALL (7,N,A(O))

where A is dimensioned 7

N = 1 Enter graphic mode

= 2 set the windows

= 3 perform the graphic functions like draw, move etc.

= 4 to invoke cursor facilities

= 5 output alphanumeric characters on screen

= 6 leave the graphics mode.

A(O) = perform graphics when N = 3

= 1 dark move

= 2 move and draw the point

= 3 draw a line connecting the initial and the final point

for these three cases the absolute value of x and y coordinates are given for plotting (A(5) and A(6)).

A(O) = 4, 5 and 6 perform similar operations if Δx Δy are given.

A(1) = minimum value of x value

A(2) = range of x

A(3),A(4) = minimum value and range of y

A(5),A(6) = x and y value to be plotted

A(7) = to output text on the screen or to invoke the cursor facility.

Simulator and Integrator

This routine numerically integrates the mass balance equation by the Fourth order Runge-kutta fixed step method to obtain the instantaneous concentration. This routine can also be used to integrate the error when Integral action is incorporated in the control scheme.

CALL (7,O,F,E,CO,S2,S1,X1,X2,INDEX,FCB,DFCB,H, IRP,IJK)

Inputs

O = reaction order

F = feed flowrate, cm^3/s

E = activation energy, kcal/mol/K

CO = inlet concentration, gm/cm^3

S2 = steady state temperature, K

S1 = steady state concentration, gms/cm^3

X2 = state variable corresponding to tank temperature

= (T -S2)/600

X1 = state variable corresponding to tank concentration = $(C - S1)/C_o$

(initial condition for integration)

DFCB = error to be integrated, calculated in the BASIC program

INDEX = 1, no error integration is to be performed

≠1, error DFCB is to be integrated and output in FCB

H = step length for integration, s

IRP = > 0 ≤ 4 if integration is not completed from one step to next step interval

IJK = house keeping variable

= 1 initially

<u>Output</u>

X1 = present value corresponding to X2

FCB = integrated value of DFCB

IJK = 51 integration is completed.

IRP = 10 integration is completed.

Subroutine 8

This routine is used to access sense switch 4 through software or to perform other housekeeping tasks

CALL (8,I,J)

I = 0 set or reset SNSW4

J = 0 reset SNSW4

J = 1 set SNSW4, so output will be directed to paper tape punch

I ≠ 0 to perform other tasks

J = 0 output few frames of blank tape (punch leader)

J = 1 HALT the computer until START button is pressed

Subroutine 9

To obtain CPU time for executing a set of BASIC program commands.

CALL (9,I,T)

Input I = 0 start the clock

I = 1 stop the clock

Output On exit when I = 1, the time elapsed in seconds is given by = T* 20/1000.

A.4.2 LISTING OF SUBROUTINE 6 AND OTHER ASSOCIATED ROUTINES

A.4.2.1 SUBROUTINE DTOC

```
C     SUBROUTINE TO TRANSFER FROM DISK TO CORE
      SUBROUTINE DTOC(UNIT,TR1,SE1,BUFF1,BUFF2,ERR)
      IUNIT=UNIT
      I1=TR1
      I2=SE1
      IBUF1=BUFF1
      IBUF2=BUFF2
   70 K=IBUF2-IBUF1+1
      IF(K.GT.64)K=64
C     CALL THE  DISK TRANSFER ROUTINE
      DO 30 II=1,20
      CALL RWSC(IUNIT,I1,I2,IBUF1,K,IER)
      IF(IER.EQ.0)GOTO50
      IF(II.EQ.10)CALL A$DO3(IUNIT)
   30 CONTINUE
   50 IF(K.LT.64.OR.IER.NE.0)GOTO90
      I2=I2+3
      IF(I2.LE.26)GOTO80
      I2=I2-26
      IF(I2.EQ.1)I1=I1+1
   80 IBUF1=IBUF1+64
      GOTO70
   90 ERR=IER
      CALL A$DO3(IUNIT)
      RETURN
      END
```

A.4.2.2 SUBROUTINE RWSC

```
                                     SUBR   RWSC
                                     REL
          000130           OPMD      EQU    '130
          001030           DSKO      EQU    '1030
          000230           OPCD      EQU    '230
          000530           DEMK      EQU    '530
          000030           IPMD      EQU    '030
          000130           DFMK      EQU    '130
          000530           IPLA      EQU    '530
          001030           DSKI      EQU    '1030
          000330           OPDA      EQU    '330
          000430           STAT      EQU    '430
00000     0 00 00000       COLT      ***
00001     077777           STT       OCT    77777
00002     0 00 00000       DERR      ***
00003     001000           SCCD      OCT    '1000
00004     0 00 00000       TEMP      ***
00005     0 00 00000       SBUF      ***
00006     0 000000         RWSC      DAC    **
00007     0 10 00000                 CALL   F$AT
00010     000006                     DEC    6
00011     0 000000         UNIT      DAC    **
00012     0 000000         TRAK      DAC    **
00013     0 000000         SECT      DAC    **
00014     0 000000         BUFF      DAC    **
00015     0 000000         SECL      DAC    **
00016     0 000000         ERR       DAC    **
00017     14 0130                    OCP    OPMD
00020    -0 02 00015                 LDA*   SECL
00021     140407                     TCA
00022     0 04 00000                 STA    COLT
00023    -0 02 00014 L               LDA*   BUFF
00024     0 04 00005 S0              STA    SBUF
00025     0 02 00115                 LDA    ='37777
00026     0 07 00005                 SUB    SBUF
00027     140407                     TCA
00030     0 04 00005                 STA    SBUF
00031     140040                     CRA
00032     0 04 00002                 STA    DERR
00033    -0 02 00011 S1              LDA*   UNIT
```

```
00034   0406 76                 ARR    2
00035  -0 06 00013              ADD*   SECT
00036   0 06 00003              ADD    SCCD
00037   74 1030                 OTA    DSKO
00040   0 01 00037              JMP    *-1
00041   14 0230                 OCP    OPCD
00042  -0 02 00011   S2         LDA*   UNIT
00043   0406 76                 ARR    2
00044  -0 06 00012              ADD*   TRAK
00045   0 04 00004              STA    TEMP
00046   0 02 00114              LDA    =1
00047   0406 73                 ARR    5
00050   0 06 00004              ADD    TEMP
00051   74 1030                 OTA    DSKO
00052   0 01 00051              JMP    *-1
00053   14 0230                 OCP    OPCD
00054   0 35 00005              LDX    SBLF
00055   14 0030                 OCP    IFMD
00056   34 0130      S4         SKS    DFMK
00057   0 01 00075              JMP    DEST
00060   14 0530                 OCP    IPDA
00061   54 1030                 INA    DSKI
00062   0 01 00061              JMP    *-1
00063  -0 04 00001              STA*   STT
00064   140040                  CRA
00065   0 12 00000   S6         IRS    0
00066   101000                  NOP
00067   0 12 00000              IRS    COUT
00070   0 01 00056              JMP    S4
00071   34 0530                 SKS    DEMK
00072   0 01 00071              JMP    *-1
00073   14 0030                 OCP    IFMD
00074   0 01 00101              JMP    D2
00075   34 0530      DEST       SKS    DEMK
00076   0 01 00056              JMP    S4
00077   0 02 00113   D1         LDA    ='100
00100   0 04 00002              STA    DERR
00101   14 0030      D2         OCP    IFMD
00102   14 0430                 OCP    STAT
00103   54 1030                 INA    DSKI
00104   0 01 00103              JMP    *-1
00105   0 03 00112              ANA    ='37000
00106   0 06 00002              ADD    DERR
00107   0404 72                 LGR    6
00110  -0 04 00016              STA*   ERR
00111  -0 01 00006              JMP*   RWSC
00112   037000                  END
00113   000100
00114   000001
```

A.4.2.3 SUBROUTINE A$DO3

```
                                   SUBR   A$DO3,ADO3
                                   REL
00000    0 000000        ADO3      DAC    **
00001    0 10 00000                CALL   F$AT
00002    000001                    DEC    1
00003    0 000000        LD        DAC    **
00004   -0 02 00003                LDA*   LD
00005    0406 76                   ARR    2
00006    0 03 00014                ANA    CMD
00007    14 0130                   OCP    OPMD
00010    74 1030                   OTA    DSKO
00011    0 01 00010                JMP    *-1
00012    14 0230                   OCP    OPCD
00013   -0 01 00000                JMP*   ADO3
         000130          OPMD      EQU    '130
         001030          DSKO      EQU    '1030
00014    034400          CMD       VFD    2,0,3,7,2,0,1,1,1,0,7,0
         000230          OPCD      EQU    '230
                                   END
```

A.4.2.4 SUBROUTINES C$12,C$21

```
                                   SUBR   C$12
                                   REL
00000    0 000000        C$12      DAC    **
00001    0 10 06247                JST    C12              CONVERT INT
00002   -0 01 00000                JMP*   C$12
         006247          C12       EQU    '6247
                                   SUBR   C$21
00003    0 000000        C$21      DAC    **
00004    0 10 06260                JST    C21              CONVERT REAL
00005    0 01 00007                JMP    ERR
00006   -0 01 00003                JMP*   C$21
         006260          C21       EQU    '6260
00007    0 10 05243      ERR       JST    BER              ERROR REPORT
00010    151311                    BCI    1,RI
         005243          BER       EQU    '5243
                                   END
```

A.4.3 LISTINGS OF SUBROUTINES 7

A.4.3.1 SUBROUTINE GRAPH

```
C   GRAPH
          SUBROUTINE GRAPH(XN,A)
          DIMENSION A(8)
          IX=IFIX(XN+.2)
          GO TO(10,15,20,30,40,50),IX
   10     CALL INITT(0)
          RETURN
   15     CALL VWINDO(A(2),A(3),A(4),A(5))
          RETURN
   20     IF=IFIX(A(1)+.1)
          GO TO(1,2,3,4,5,6),IF
    1     CALL MOVEA(A(6),A(7))
          RETURN
    2     CALL POINTA(A(6),A(7))
          RETURN
    3     CALL DRAWA(A(6),A(7))
          RETURN
    4     CALL MOVER(A(6),A(7))
          RETURN
    5     CALL POINTR(A(6),A(7))
          RETURN
    6     CALL DRAWR(A(6),A(7))
          RETURN
   30     IC=IFIX(A(8)+.2)
          CALL VCURSR(IC,A(6),A(7))
          A(8)=FLOAT(IC)
          RETURN
   40     IC=IFIX(A(8)+.2)
          CALL ANCHO(IC)
          RETURN
   50     IX=A(6)
          IY=A(7)
          CALL FINITT(IX,IY)
          RETURN
          END
```

A.4.3.2 SUBROUTINE SIMULATOR/INTEGRATOR

```
C    SUBROUTINE SOLVE
      SUBROUTINE CNTRL(OR,F,E,C0,T1SS,C1SS,X1,X2,XIND,FCB,
     1DFCB,DELT,XRP,XJK)
      INTEGER ORD
      DIMENSION XK(4,2)
      INDEX=IFIX(XIND+0.1)
      TH=17300./F
      ZZ=1./(30000.*C0)
      ORD=IFIX(OR+0.1)
      Q=E/(59.4*C0)
      Z1SS=C1SS/C0
      B1SS=T1SS*ZZ
  215 XRP=XRP+1.01
      IRP=IFIX(XRP)
  210 DC1=-X1/TH-2000.*C0**(ORD-1)*((X1+Z1SS)**ORD*EXP(-Q/(
     1B1SS+X2))-Z1SS**ORD*EXP(-Q/B1SS))
      IF(IRP.EQ.1) XX=X1
      XK(IRP,1)=DC1*DELT/50.
      YY=FLOAT(IFIX(FLOAT(IRP)/2.+0.9))*.5
      X1=X1+XK(IRP,1)*YY
      IF(INDEX.EQ.1.AND.IRP.NE.4) GO TO 215
      IF(INDEX.EQ.1.AND.IRP.EQ.4) GO TO 220
      IF(IRP.EQ.1) XXK=FCB
      XK(IRP,2)=DFCB*DELT/50.
      FCB=FCB+XK(IRP,2)*YY
  205 IF(IRP.NE.4) RETURN
  220 XRP=0.
      XJK=XJK+1.001
      IJK=IFIX(XJK)
      X1=XX+(XK(1,1)+2.*(XK(2,1)+XK(3,1))+XK(4,1))/6.
      IF(INDEX.GT.1) FCB=XXK+(XK(1,2)+2.*(XK(2,2)+XK(3,2))
     1+XK(4,2))/6.
      IF(IJK.LE.50.AND.INDEX.EQ.1) GO TO 215
      IF(IJK.LE.50.AND.INDEX.GT.1) RETURN
      XRP=-10.
      RETURN
      END
```

A.4.4 LISTING OF SUBROUTINE 8

A.4.4.1 SUBROUTINE SU89

```
                                  SUBR   SU89
00000    0 000000         SU89   DAC    **
00001    0 10 00025              JST    VAL
00002    101040                  SNZ
00003    0 01 00014              JMP    SU8                    JMP TO SN4 ROUT
00004    0 10 00025              JST    VAL
00005    101040                  SNZ
00006    0 01 00012              JMP    PLD1                   JMP TO PUNCH
00007    000000                  HLT                           PAUSE
00010    0 12 00000       PLD2   IRS    SU89
00011   -0 01 00000              JMP*   SU89                   RETURN
00012    0 10 05432       PLD1   JST    PLD                    PUNCH LEADER
00013    0 01 00010              JMP    PLD2
         005432           PLD    EQU    '5432
00014    0 10 00025       SU8    JST    VAL                    SNSW4 ROUTINE
00015    101040                  SNZ
00016    0 01 00021              JMP    *+3
00017   -0 12 00024              IRS*   PFLG
00020    0 01 00023              JMP    *+3
00021    140040                  CRA
00022   -0 04 00024              STA*   PFLG
00023    0 01 00010              JMP    PLD2
00024    0 000000         PFLG   XAC    PFLG
00025    0 000000         VAL    DAC    **                     ARGUMENT ROUTIN
00026   -0 02 00000              LDA*   SU89
00027    0 04 00033              STA    TEMP
00030   -0 02 00033              LDA*   TEMP
00031    0 12 00000              IRS    SU89
00032   -0 01 00025              JMP*   VAL
00033    000000           TEMP   BSZ    1
                                 END
```

A.4.4.2 I/O MOD

```
                            *    I/Ø MOD FOR S/R 8
                                 REL
                                 ENT    IOMOD,AA
                                 ENT    FFLG
00000    101004        AA        SS3
00001    0 01 00004              JMP    *+3
00002    140040                  CRA
00003    0 04 00105              STA    '105
00004    0 02 00406              LDA    '406
00005   -0 01 00006              JMP*   *+1
00006    004143                  OCT    4143
00007    0 12 00105    BB        IRS    '105
00010    140040                  CRA
00011    0 04 00106              STA    '106
00012   -0 10 00014              JST*   *+2
00013   -0 01 00015              JMP*   *+2
00014    003065                  OCT    3065
00015    004575                  OCT    4575
00016    0 02 00036    CC        LDA    FFLG
00017    100040                  SZE
00020    0 01 00023              JMP    *+3
00021    101002                  SS4
00022    0 01 00025              JMP    *+3
00023    14 0002                 OCP    2
00024    0 12 00106              IRS    '106
00025   -0 10 00027              JST*   *+2
00026   -0 01 00030              JMP*   *+2
00027    003047                  OCT    3047
00030    004212                  OCT    4212
00031    0 12 00105    DD        IRS    '105
00032    140040                  CRA
00033    0 04 00106              STA    '106
00034   -0 01 00035              JMP*   *+1
00035    005245                  OCT    5245
00036    000000        FFLG      BSZ    1
                                 ABS
         000727        BASE      EQU    '727
                                 ORG    BASE
00727    0 000000                DAC    AA
00730    0 000007                DAC    BB
00731    0 000016                DAC    CC
00732    0 000031                DAC    DD
                                 ORG    '4142
04142   -0 01 00727              JMP*   BASE
                                 ORG    '4574
04574   -0 01 00730              JMP*   BASE+1
                                 ORG    '4211
04211   -0 01 00731              JMP*   BASE+2
                                 ORG    '5244
05244   -0 01 00732              JMP*   BASE+3
                                 END
```

A.4.5 LISTING OF SUBROUTINE 9

```
                                   SUBR   ITIM
                                   REL
00000    0 000000       ITIM   DAC    **
00001   -0 02 00000            LDA*   ITIM
00002    0 04 00020            STA    DMY
00003    0 12 00000            IRS    ITIM
00004   -0 02 00020            LDA*   DMY
00005    101040                SNZ
00006    0 01 00021            JMP    TER
00007   -0 02 00000            LDA*   ITIM
00010    0 04 00016            STA    DMY1
00011    0 02 00061            LDA    TIM
00012    0 07 00027            SUB    CONS
00013    14 0220               OCP    '220
00014   -0 10 00675            JST*   C$12
00015   -0 10 00654            JST*   H$22
00016    0 000000       DMY1   DAC    **
00017    0 01 00024            JMP    OUT
00020    000000         DMY    BSZ    1
         000061         TIM    EQU    '61
         000675         C$12   EQU    '675
         000654         H$22   EQU    '654
00021    0 02 00027     TER    LDA    CONS
00022    0 04 00061            STA    TIM
00023    14 0020               OCP    '20
00024    0 12 00000     OUT    IRS    ITIM
00025    0 12 00000            IRS    ITIM
00026   -0 01 00000            JMP*   ITIM
00027    100010         CONS   DEC    -32760
                               END
```

A.4.6 LISTING OF TAPE CONVERSION PROGRAM

```
                                      ABS
                                      ORG    '20000
20000    0 10 20023   STRT  JST    INP
20001    100040                     SZE
20002    0 01 20005               JMP    NEXT
20003    0 10 20031               JST    OUT
20004    0 01 20000               JMP    STRT
20005    0 03 20046   NEXT  ANA    ='177
20006    0 04 20022               STA    CHAR
20007    0 05 20045               ERA    =4
20010    101040                     SNZ
20011    000000                     HLT
20012    0 02 20022               LDA    CHAR
20013    0 05 20044               ERA    ='12
20014    101040                     SNZ
20015    0 10 20036               JST    CR
20016    0 02 20022               LDA    CHAR
20017    0 05 20043               ERA    ='200
20020    0 10 20031               JST    OUT
20021    0 01 20000               JMP    STRT
20022    000000         CHAR  BSZ    1
20023    0 000000       INP   DAC    **
20024    14 0001                    OCP    1
20025    54 1001                    INA    '1001
20026    0 01 20025               JMP    *-1
20027    14 0101                    OCP    '101
20030   -0 01 20023               JMP*   INP
20031    0 000000       OUT   DAC    **
20032    14 0002                    OCP    2
20033    74 0002                    OTA    2
20034    0 01 20033               JMP    *-1
20035   -0 01 20031               JMP*   OUT
20036    0 000000       CR    DAC    **
20037    0 02 20042               LDA    ='215
20040    0 10 20031               JST    OUT
20041   -0 01 20036               JMP*   CR
20042    000215                     END
20043    000200
20044    000012
20045    000004
20046    000177
```

A.4.7 MODIFICATIONS IN THE BASIC INTERPRETER

LOCATION		CONTENTS
{'1036}	=	'1054
{'1037}	=	'1100
{'2130}	=	'151724 (ST)
{'2131}	=	'140722 (AR)
{'2132}	=	'152000 (TV)

i) Command START is equivalent to RUN in the old version

ii) Command RUN in this version does not clear tables

iii) Command CLEAR in the old version is removed.

{'7367}	=	'22000 highest octal address available for user program and tables
{ '522}	=	'27606 starting location of subroutine 5
{ '523}	=	'37204 starting location of subroutine 6
{ '524}	=	'22000 starting location of subroutine 7
{ '525}	=	'37150 starting location of subroutine 8
{ '526}	=	'27740 starting location of subroutine 9

A.4.8 MEMORY MAP

A.4.8.1 MEMORY MAP OF GRAPHICS ROUTINES (SEGMENT 1)

```
*LOW    22000
*START  21777
*HIGH   34446
*NAMES  11104
*COMN   35441
*BASE   34457
*BASE   33641
*BASE   32631
*BASE   30760
*BASE   31373
*BASE   26635
*BASE   27175
*BASE   25314
*BASE   23712
*BASE   24652
*BASE   22711
GRAPH   22000
INITT   22402
FINITT  22552
WINDO   22566
MOVEA   22626
POINTA  23000
DRAWA   23030
MOVER   23074
POINTR  23122
DRAWR   23150
MOVABS  23176
VCURSR  23216
DCURSR  23244
ANCHO   23342
ANMODE  23376
NEWLIN  23420
CARTN   23426
LINEF   23466
NEWPAG  23512
SVSTAT  23556
RESTAT  24000
LVLCHT  24142
VECMOD  24176
V2ST    24250
PNTMOD  24456
MODCHK  24514
REL2AB  24542
XYCNVT  25000
```

TKDASH	26000
REVCOT	27000
IOWAIT	27106
CLIPT	30000
WINCOT	31000
PCLIPT	31116
TOUTPT	31316
TINPUT	31334
EXP	32000
SQRTX	32340
SQRT	32340
ABS	32454
MOD	32466
FLOAT	32514
INT	32524
IDINT	32524
IFIX	32524
E$21	32534
M$11X	33000
M$11	33000
D$11X	33060
D$11	33060
M$22X	33130
M$22	33130
D$22X	33311
D$22	33311
C$12	33550
C$21	33602
S$22	34000
A$22	34006
N$22	34230
REAL	34242
L$22	34242
H$22	34252
F$ER	34270
F$HT	34300
F$AT	34336
ARG$	34420
AC1	34440
AC2	34441
AC3	34442
AC4	34443
AC5	34444
SAVE	35441
TKTRNX	35631

A.4.8.2 MEMORY MAP OF SIMULATOR (SEGMENT 2)

*LOW	22000
*START	21777
*HIGH	25500
*NAMES	12561
*COMN	37777
*BASE	23750
*BASE	24743
*BASE	22762
CNTRL	22000
N$22	23000
REAL	23012
L$22	23012
H$22	23022
R$ER	23040
R$HT	23050
C$12	23106
S$22	23140
A$22	23146
R$AT	23370
ARG$	23454
M$22X	24000
M$22	24000
L$22X	24161
D$22	24161
EXP	25000
FLOAT	25340
INT	25350
IDINT	25350
IFIX	25350
E$21	25360
C$21	25440
AC1	25472
AC2	25473
AC3	25474
AC4	25475
AC5	25476

A.4.8.3 MEMORY MAP OF HADIOS ROUTINES (SEGMENT 2)

*LOW	00551
*START	00551
*HIGH	37137
*NAMES	12762
*COMN	37777
*BASE	37140
*BASE	27723
*BASE	26666
HADIOS	26000
IFLG	26477
F$AT	26670
MYSR	27603**
SUBS	27606
ITIM	27740
ERCL	37126

A.4.8.4 MEMORY MAP OF DISK TRANSFER ROUTINES(CORE RESIDENT)

*LOW	00727
*START	37150
*HIGH	37771
*NAMES	12716
*COMN	37777
*BASE	37776
SUB9	37150
DTOC	37204
C$12	37420
C$21	37423
RWSC	37440
A$DO3	37550
REAL	37566
L$22	37566
H$22	37576
L$33	37614
F$AT	37630
ARG$	37712
IOMOD	37732
PFLG	37770

APPENDIX 5

CALIBRATION, R.T.D. STUDIES AND PARAMETER VALUES

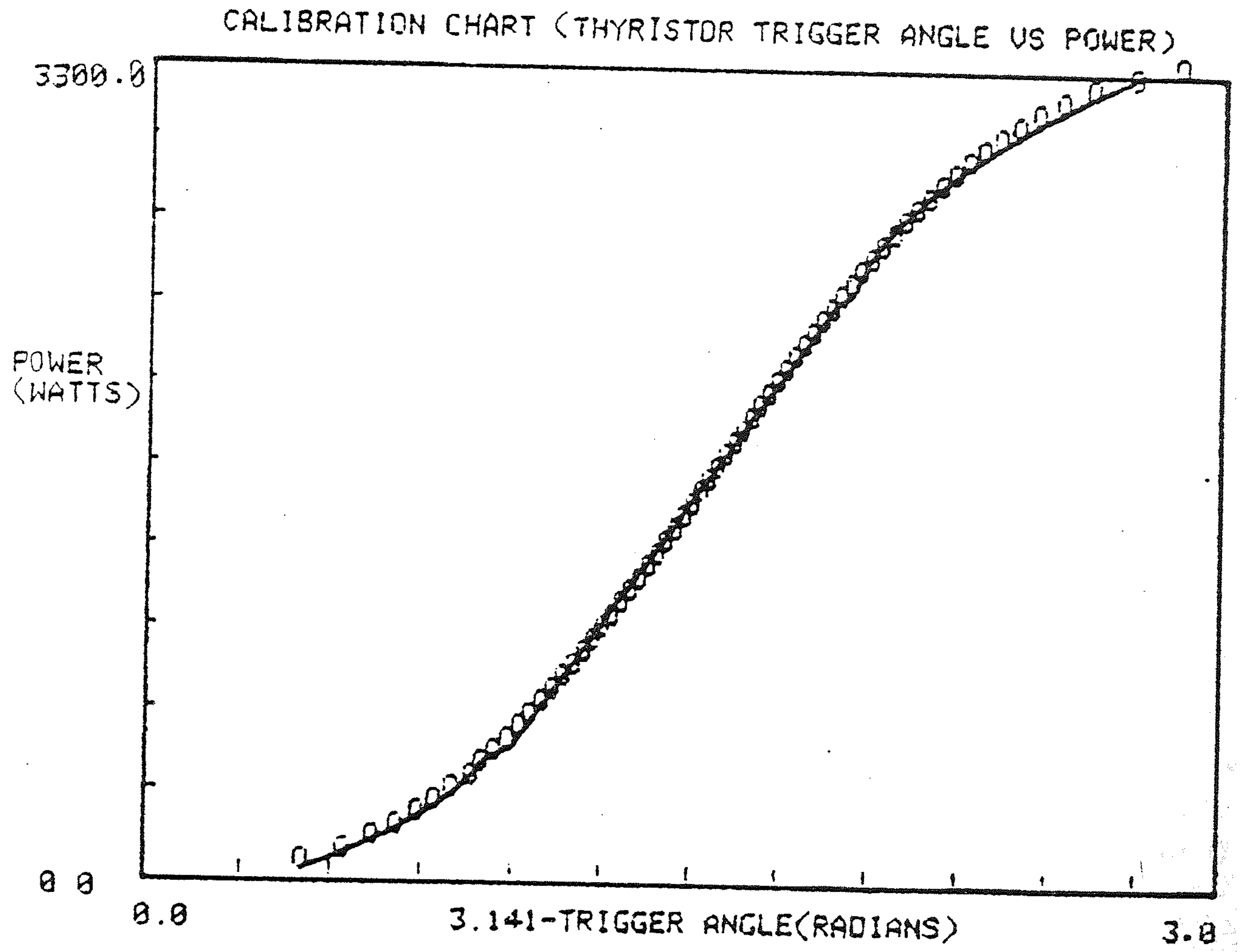


FIG.A.5.1 IMMERSION HEATERS CALIBRATION FIGURE

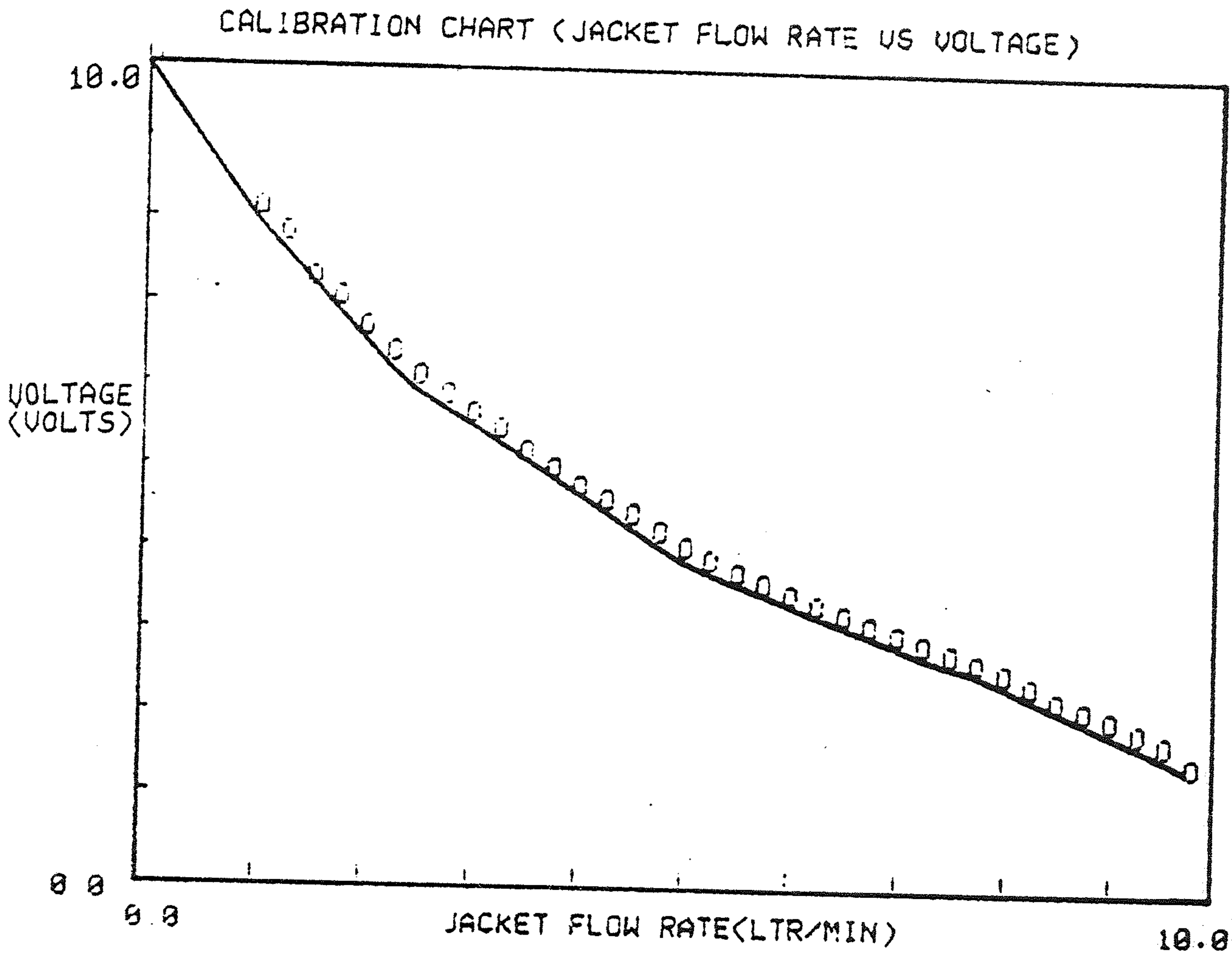


FIG.A.5.2 CONTROL VALVE CALIBRATION FIGURE

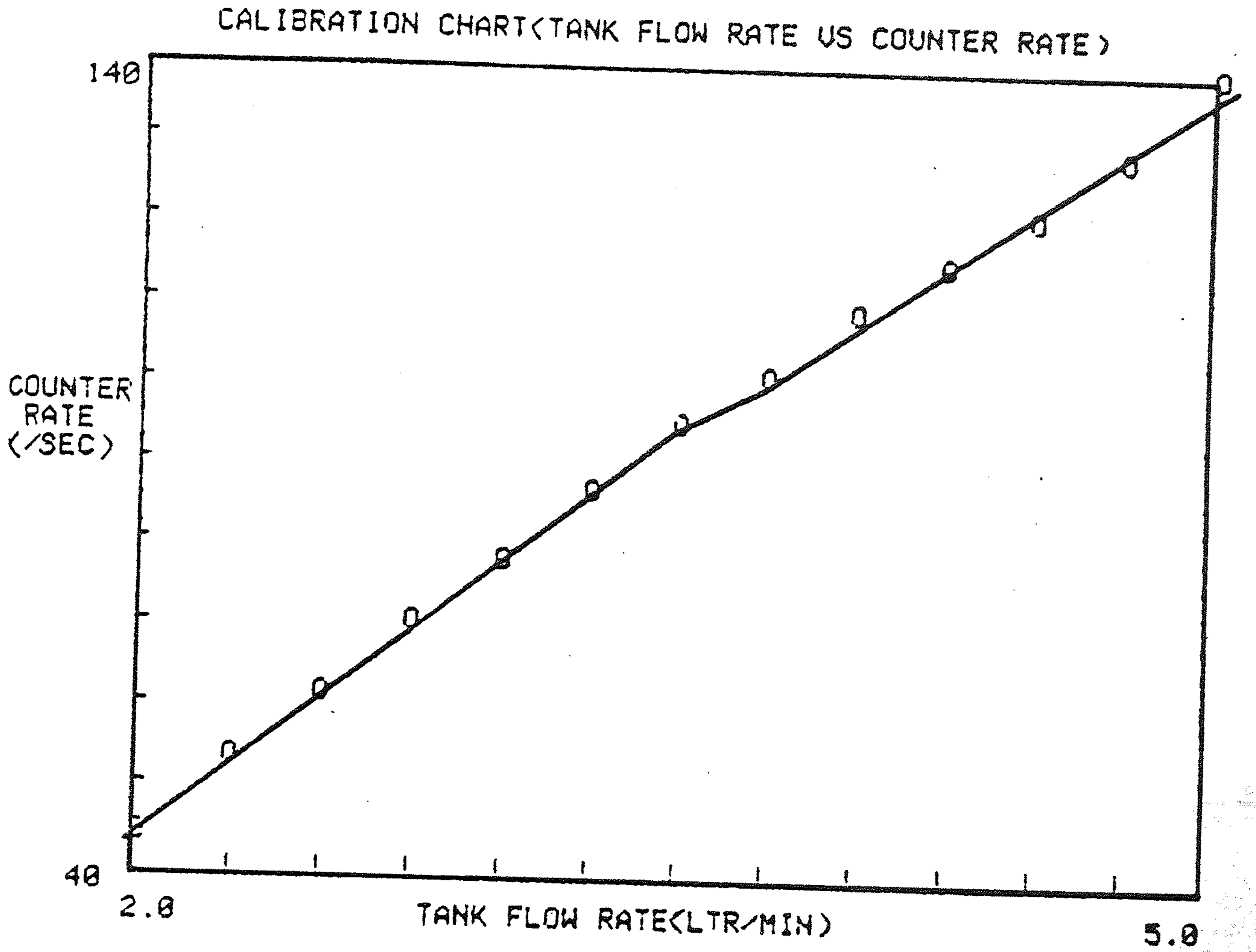
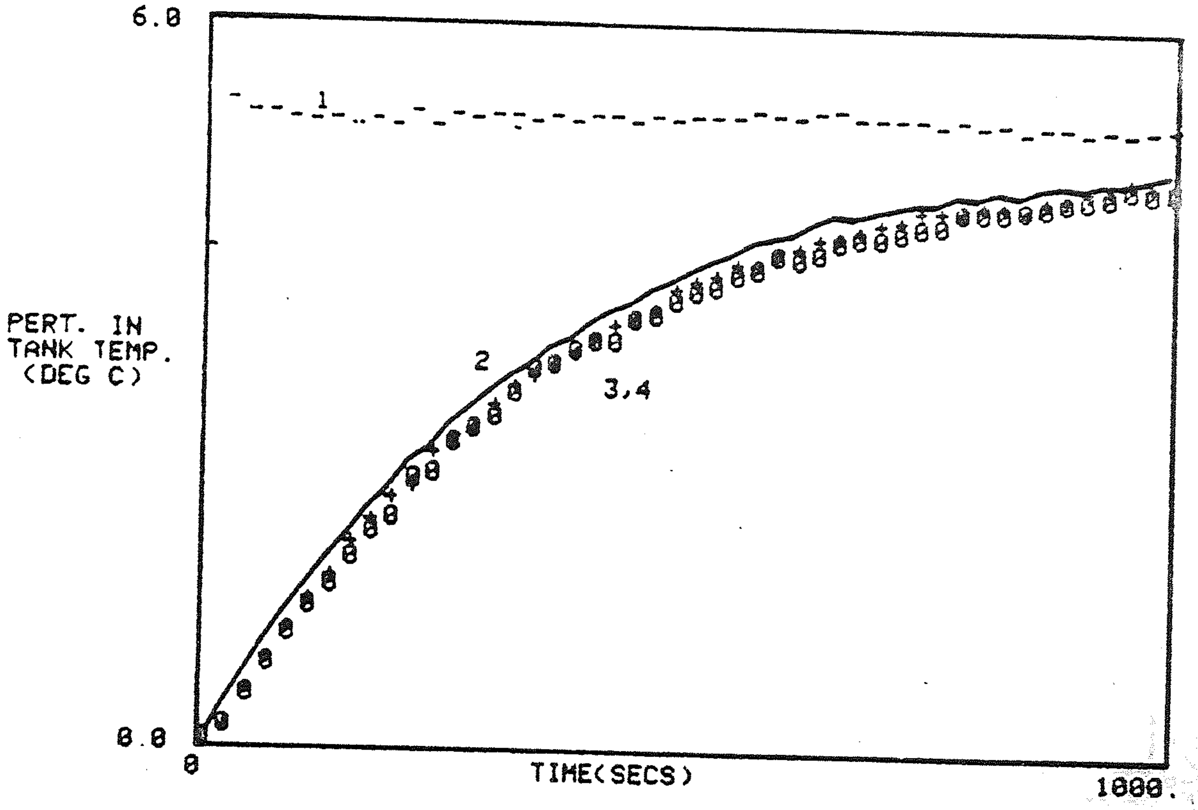


FIG.A.5.3 TURBINE FLOWMETER CALIBRATION FIGURE

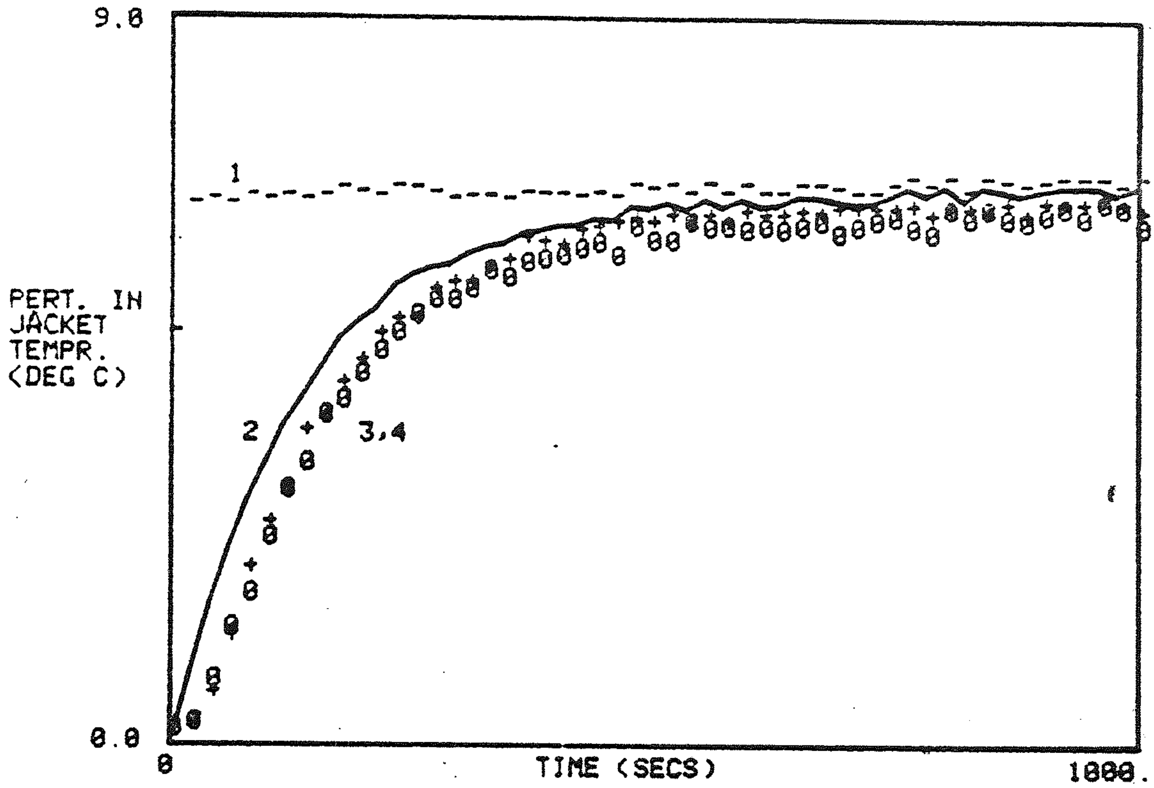


1 = Step change in feed temperature

2 = Model response of a single continuous stirred vessel

3,4 = Actual response of the tank

FIG.A.5.4 RTD STUDIES IN TANK FOR STEP IN FEED TEMPERATURE



1 = Step change in coolant temperature

2 = Model response of a single continuous stirred vessel

3,4 = Actual response of the jacket

FIG.A.5.5 RTD STUDIES IN JACKET FOR STEP IN COOLANT TEMPERATURE

A.5.6 PARAMETER VALUES CHOSEN

A.5.6.1 FOR TOTAL SIMULATION/THEORETICAL STUDIES

V	=	17.3×10^{-3} m^3
V_c	=	8.532×10^{-3} m^3
ρ, ρ_c	=	1000 kg/m^3
C_p, C_{pc}	=	4.1868 kJ/kg K
UA	=	0.1549 kJ/s K
τ_m	=	19 s
τ_v	=	2 s
τ_s	=	11-15 s

n	E (kJ/kg mole K)	k_o
-4	92067.73	2×10^{18} kg^5/m^{15} s
-3	82061.28	2×10^{15} kg^4/m^{12} s
-2	72012.96	2×10^{12} kg^3/m^9 s
3	22127.24	2×10^{-3} m^6/kg^2 s
4	12141.72	2×10^{-6} m^9/kg^3 s

A.5.6.2 FOR TOTAL SIMULATION/EXPERIMENTS

ΔH	=	-125604 kJ/kg
C_o	=	20 kg/m^3
R	=	8.28986 kJ/kg mole K
F_{cUL}	=	1.5×10^{-4} m^3/s

n	E (kJ/kg mole K)	k_o
-1	62090.24	2×10^9 kg^2/m^6 s
0	52104.73	2×10^6 kg/m^3 s
1	42119.21	2000 s^{-1}
2	32112.76	2 m^3/kg s

A.5.7 CALIBRATION EQUATIONS

TURBINE FLOWMETER

$$F = Q_1 \times 0.49408 \times 10^{-6} + 11.30073 \times 10^{-6}$$

If $F > 5.833 \times 10^{-5}$ $F = Q_1 \times 0.56748 \times 10^{-6} + 5.42647 \times 10^{-6}$

CONTROL VALVE

If $F_c <= 3.833 \times 10^{-5}$ $V_S = -84925.2 \times F_c + 9.54589$

If $F_c >= 12.5 \times 10^{-5}$ $V_S = -35039.94 \times F_c + 7.21557$

If $F_c > 3.833 \times 10^{-5}$ and $<= 8.33 \times 10^{-5}$

$$V_S = -49527.12 \times F_c + 8.13453$$

If $F_c > 8.33 \times 10^{-5}$ and $< 12.5 \times 10^{-5}$

$$V_S = -29636.34 \times F_c + 6.46235$$

IMMERSION HEATERS

$$\alpha_1 = Z_1H^2 + Z_2H + Z_3$$

If $H < 500$ $Z_1 = -0.153234 \times 10^{-5}$

$Z_2 = .197036 \times 10^{-2}$

$Z_3 = .340653$

If $H > 2400$ $Z_1 = .675824 \times 10^{-6}$

$Z_2 = -.296997 \times 10^{-2}$

$Z_3 = 5.20372$

If $H > 500$ and < 2400 $Z_1 = 0$

$Z_2 = .50393 \times 10^{-3}$

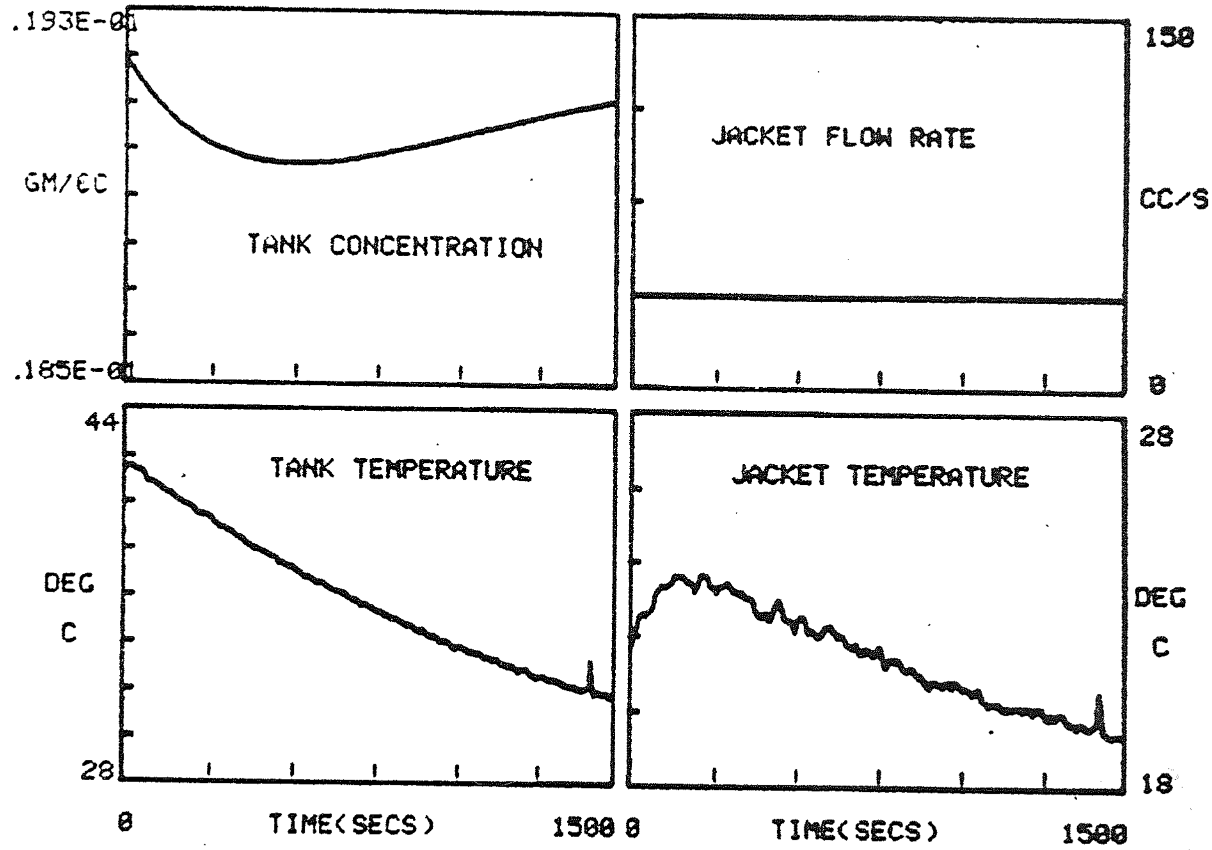
$Z_3 = .738165$

APPENDIX 6

EXPERIMENTAL AND TOTAL SIMULATION GRAPHS

(REFER TABLES (8.1) AND (8.2) FOR OPERATING CONDITIONS)

A.6.1 EXPERIMENTAL RESULTS



Reaction order = 2
Open loop studies
Initial perturbations in state variables

FIG.A.6.1.1 EXPERIMENT NO:1

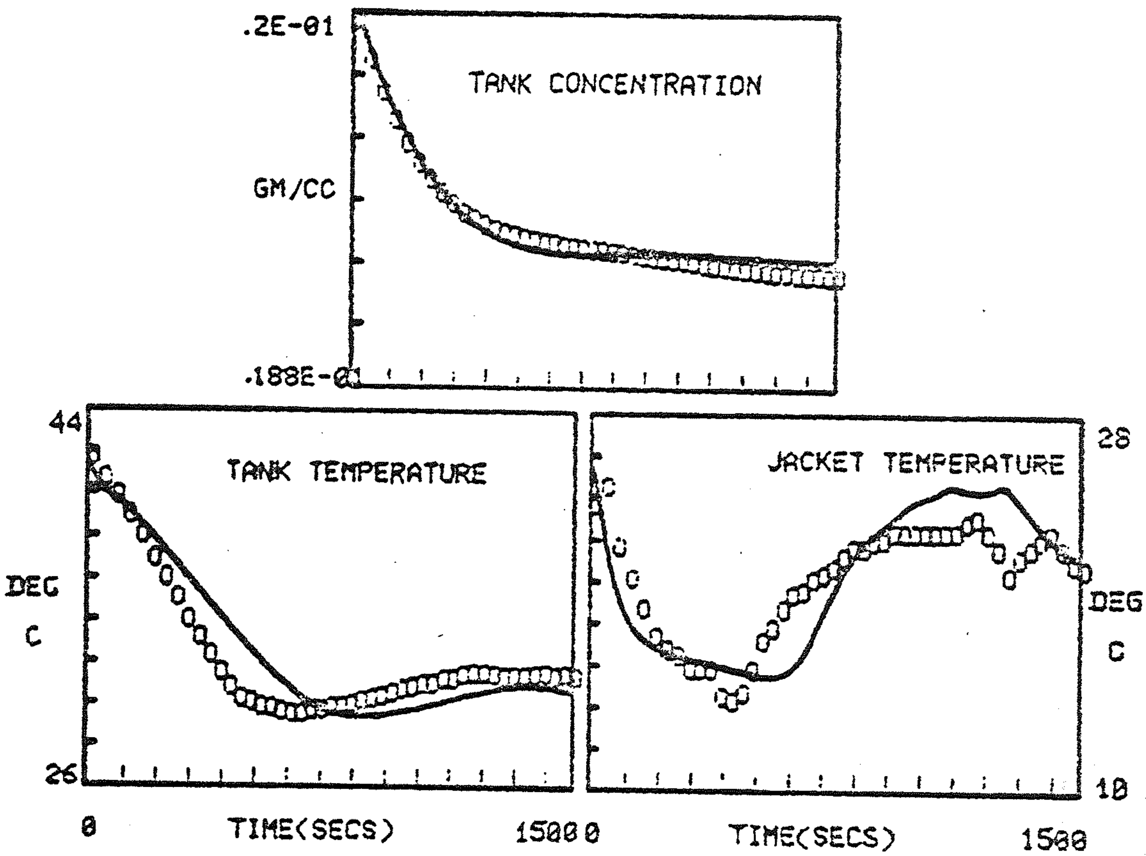


FIG.A.6.2.9 EXPERIMENT NO:12

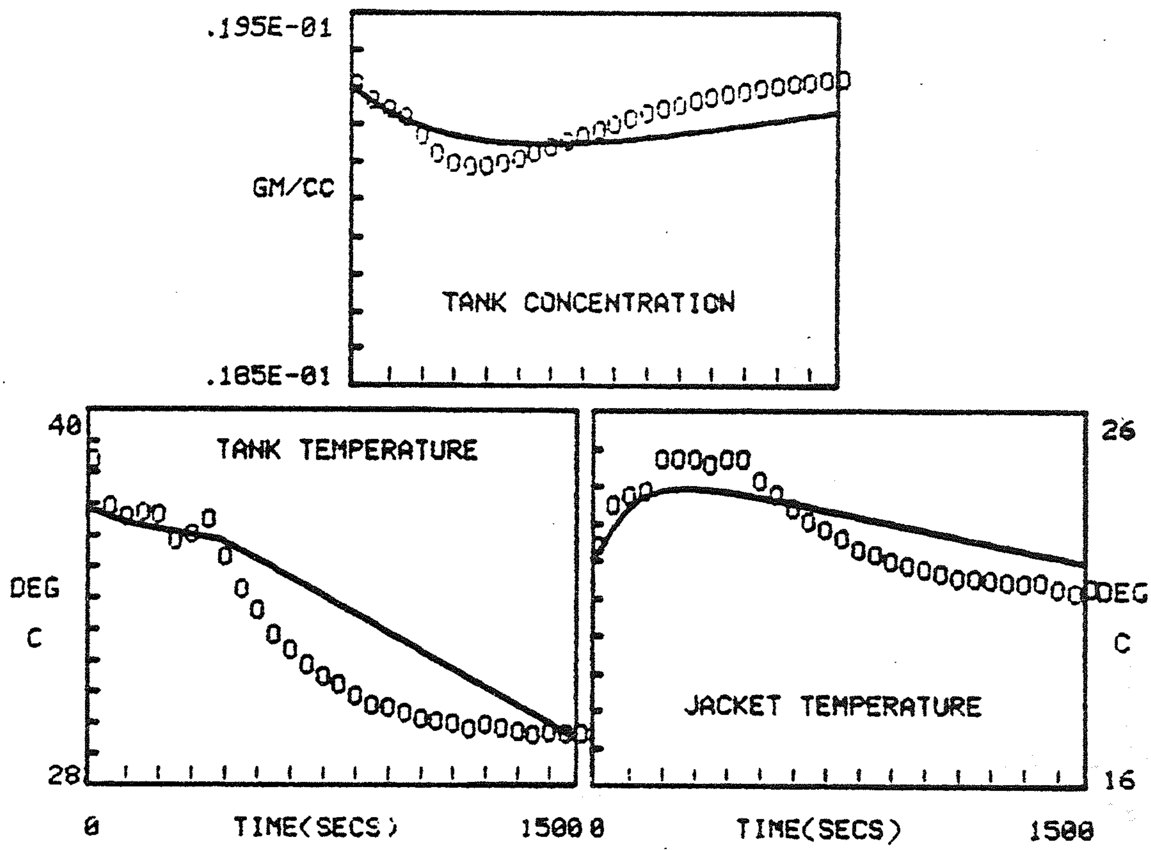


FIG.A.6.2.10 EXPERIMENT NO:14

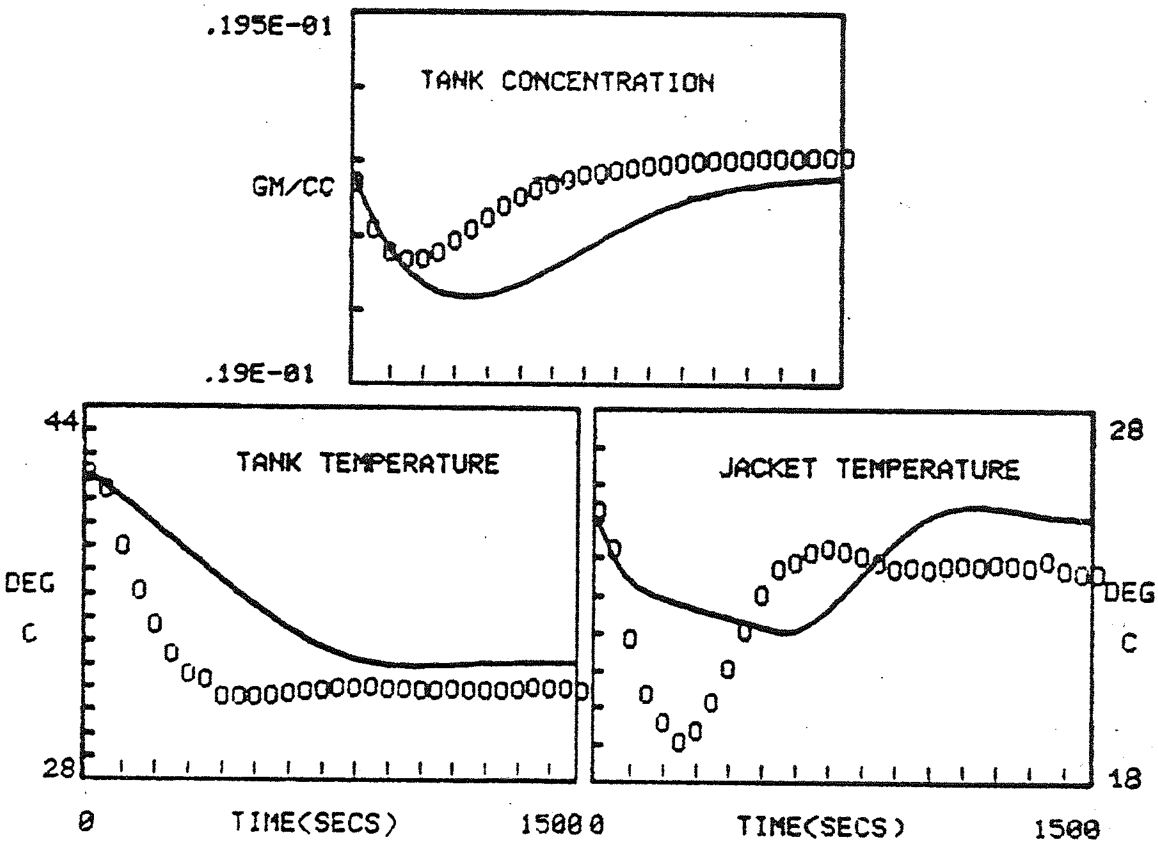


FIG.A.6.2.11 EXPERIMENT NO:19

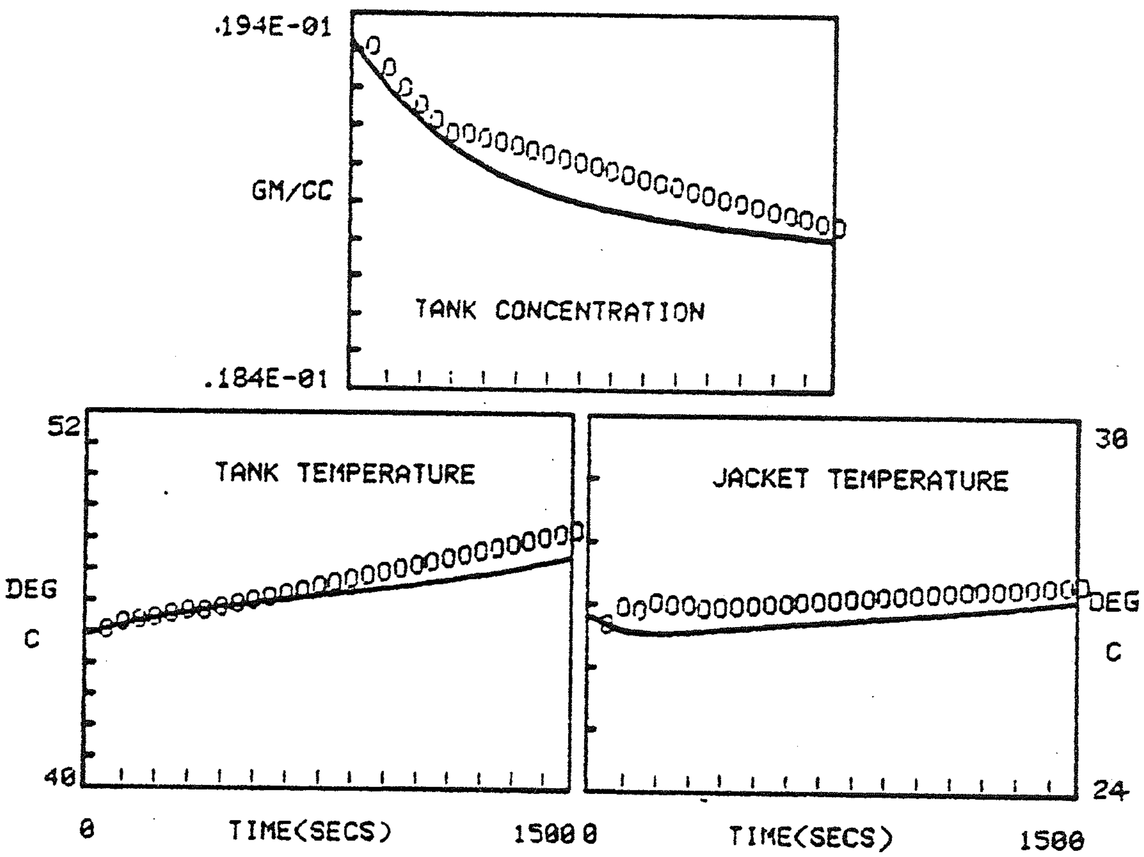


FIG.A.6.2.12 EXPERIMENT NO:20

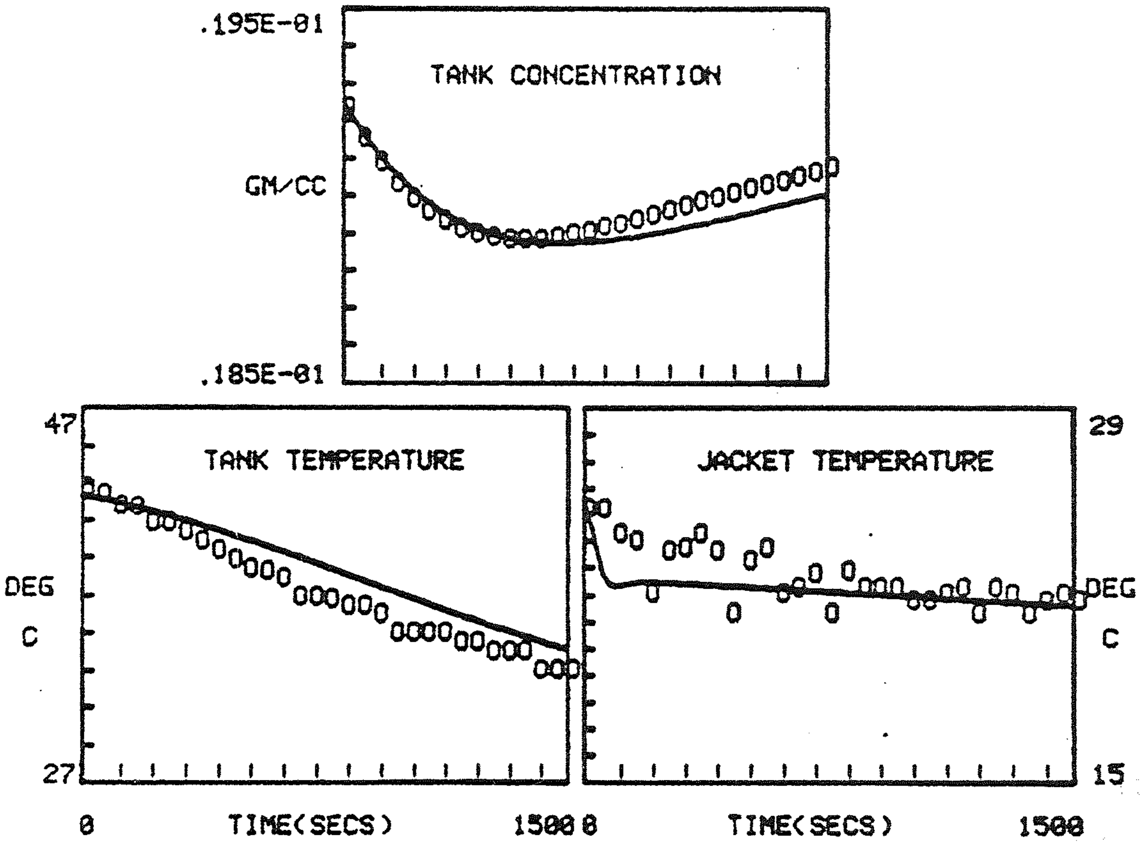


FIG.A.6.2.13 EXPERIMENT NO:22

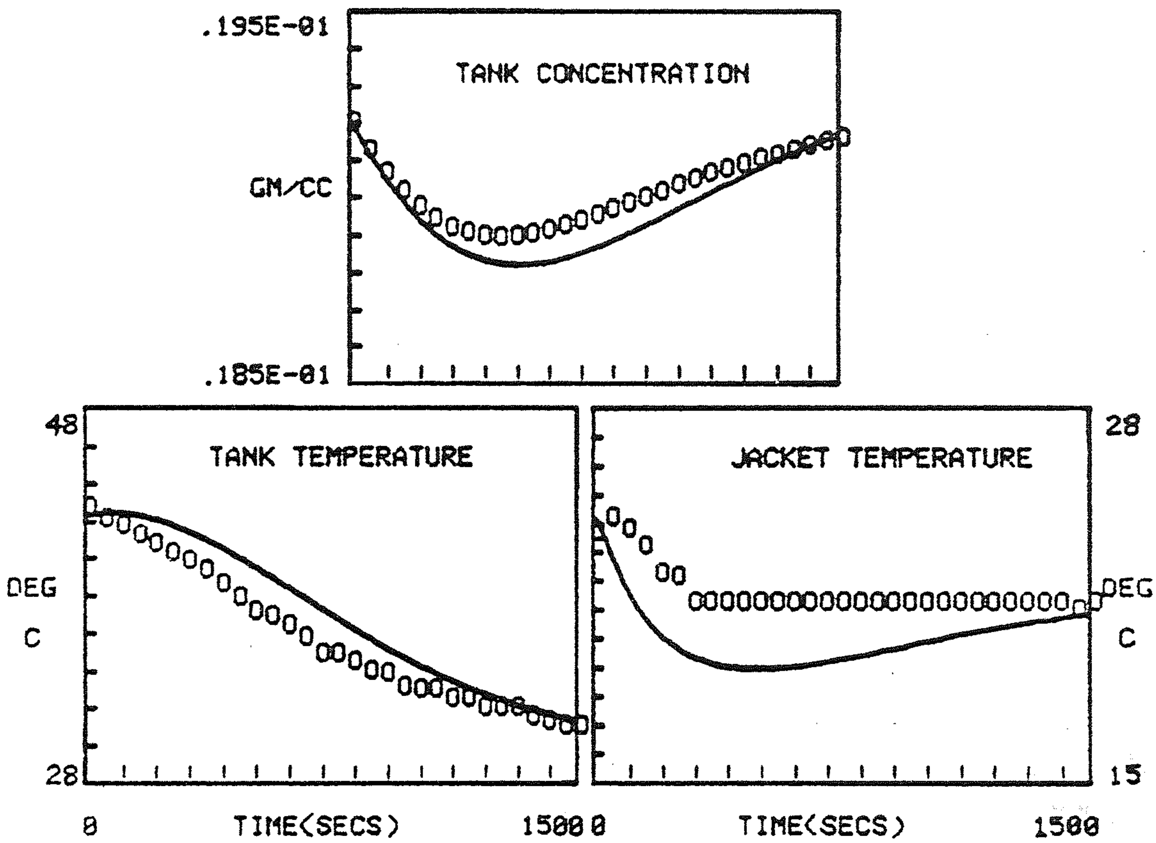


FIG.A.6.2.14 EXPERIMENT NO:23

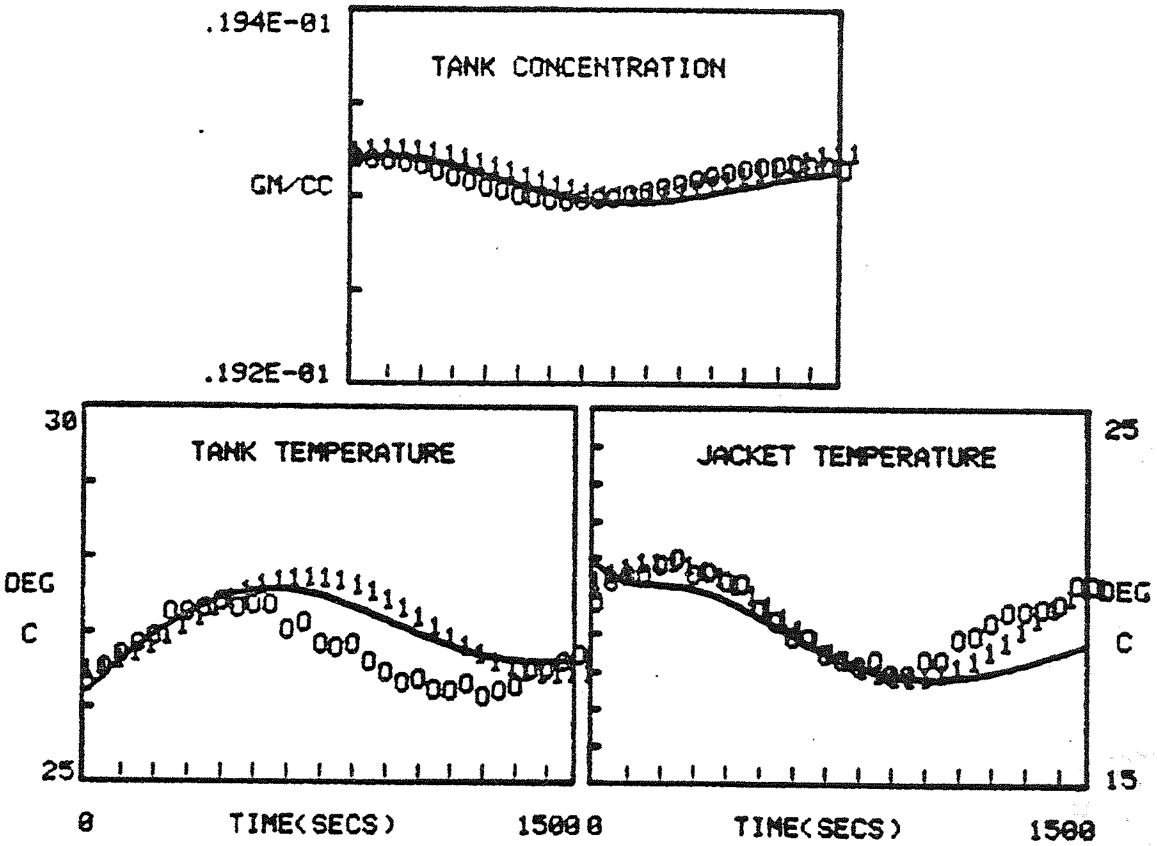


FIG.A.6.2.15 EXPERIMENT NO:26

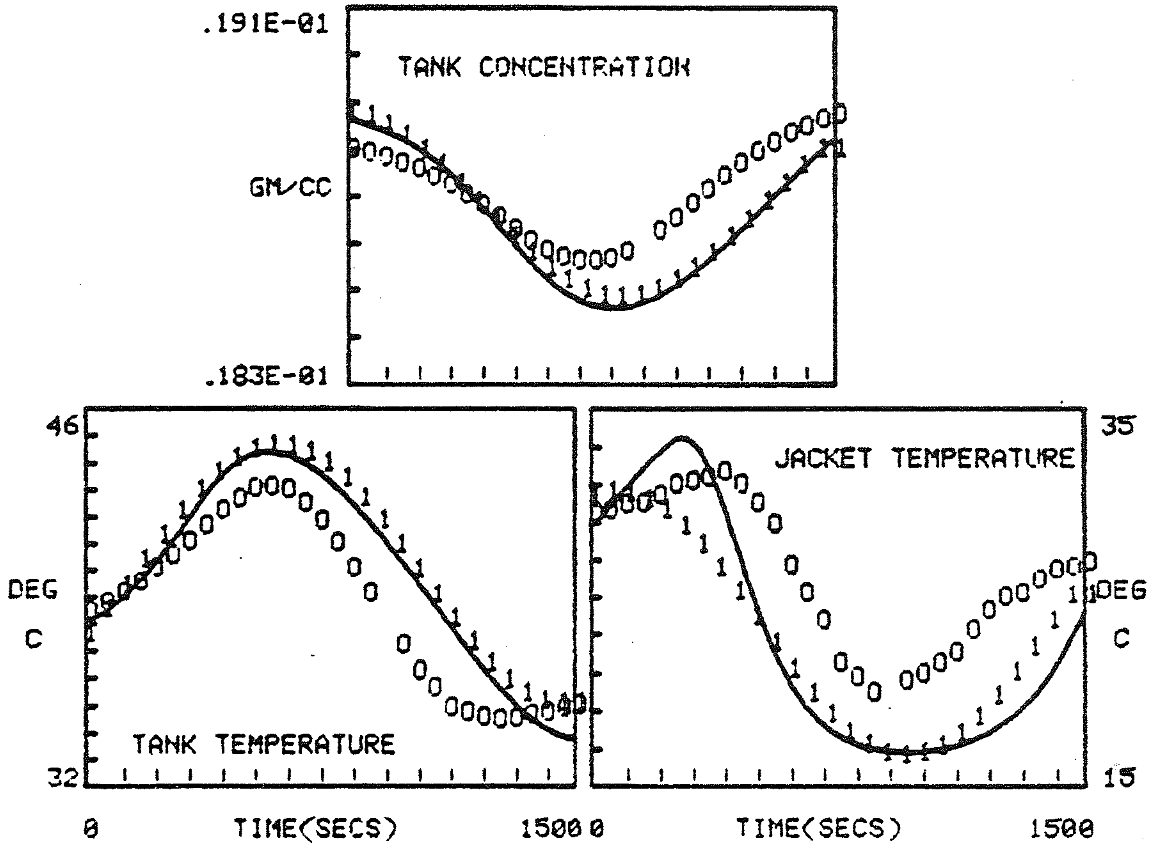


FIG.A.6.2.16 EXPERIMENT NO:27

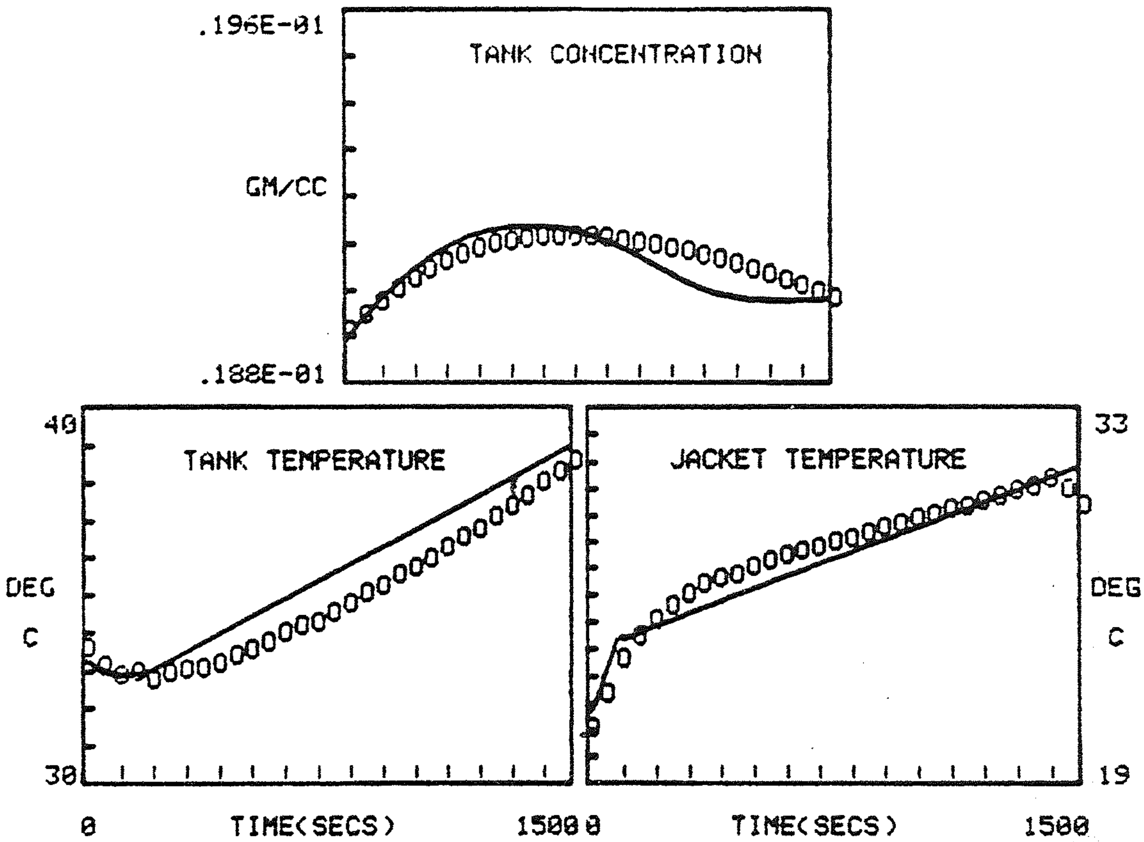


FIG.A.6.2.17 EXPERIMENT NO:29

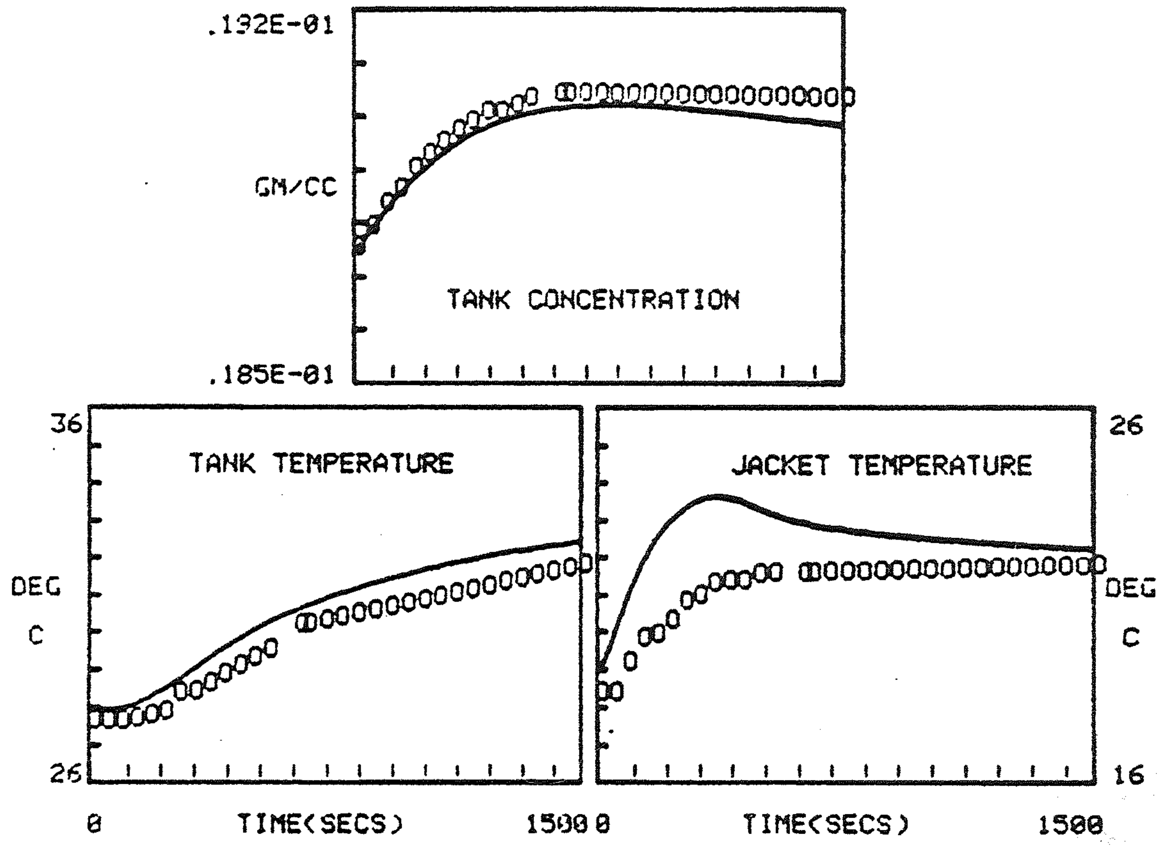


FIG.A.6.2.18 EXPERIMENT NO:31

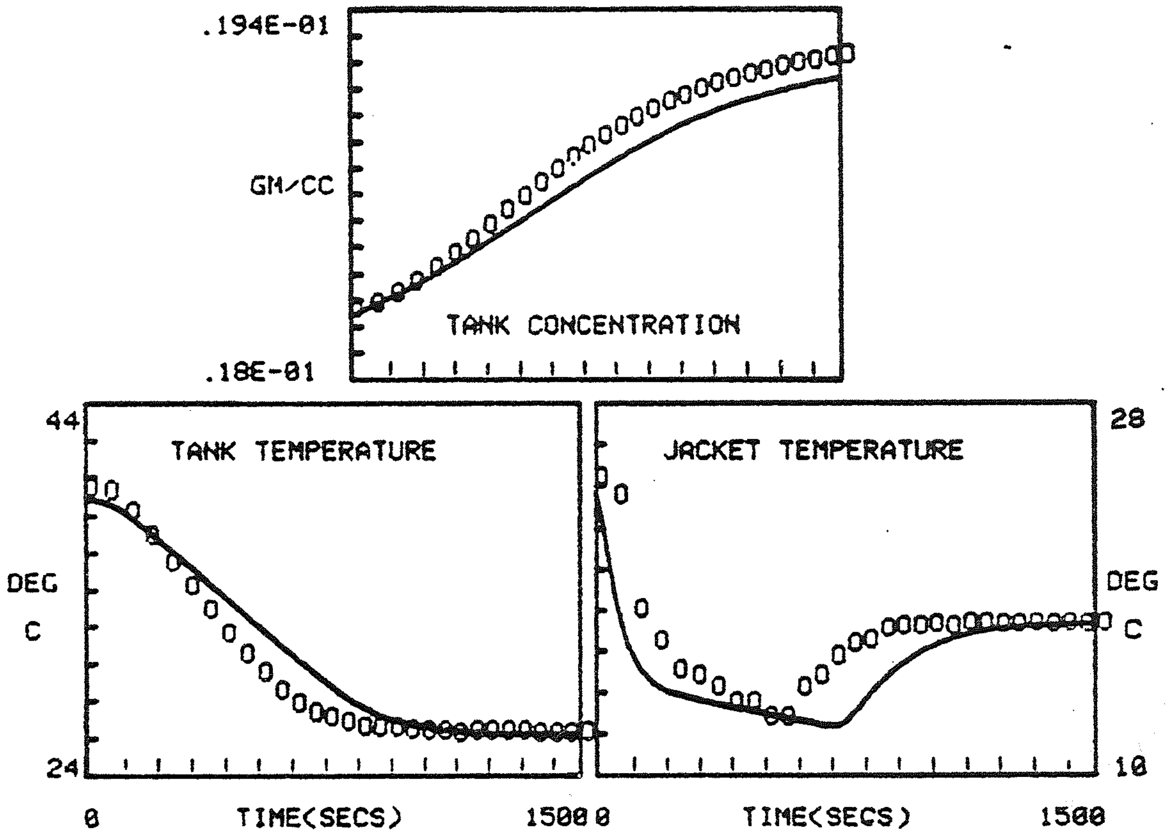


FIG.A.6.2.19 EXPERIMENT NO:32

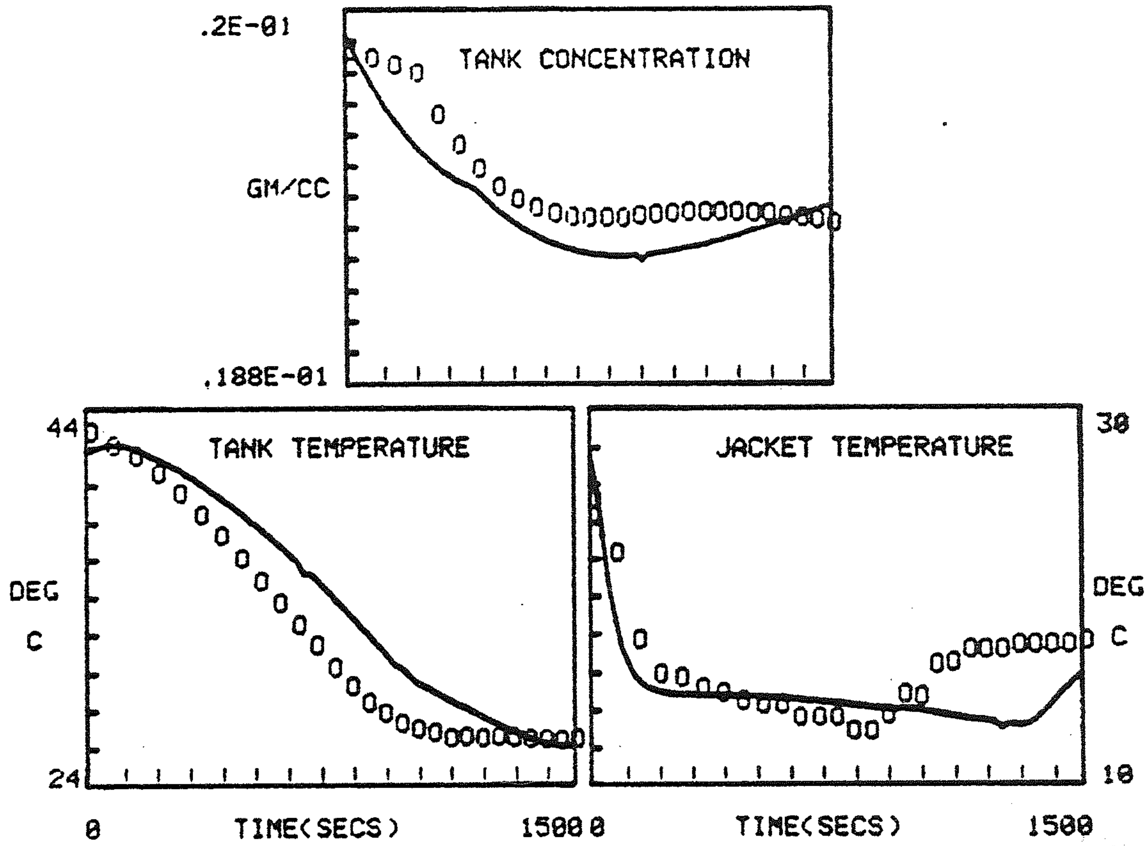


FIG.A.6.2.20 EXPERIMENT NO:35

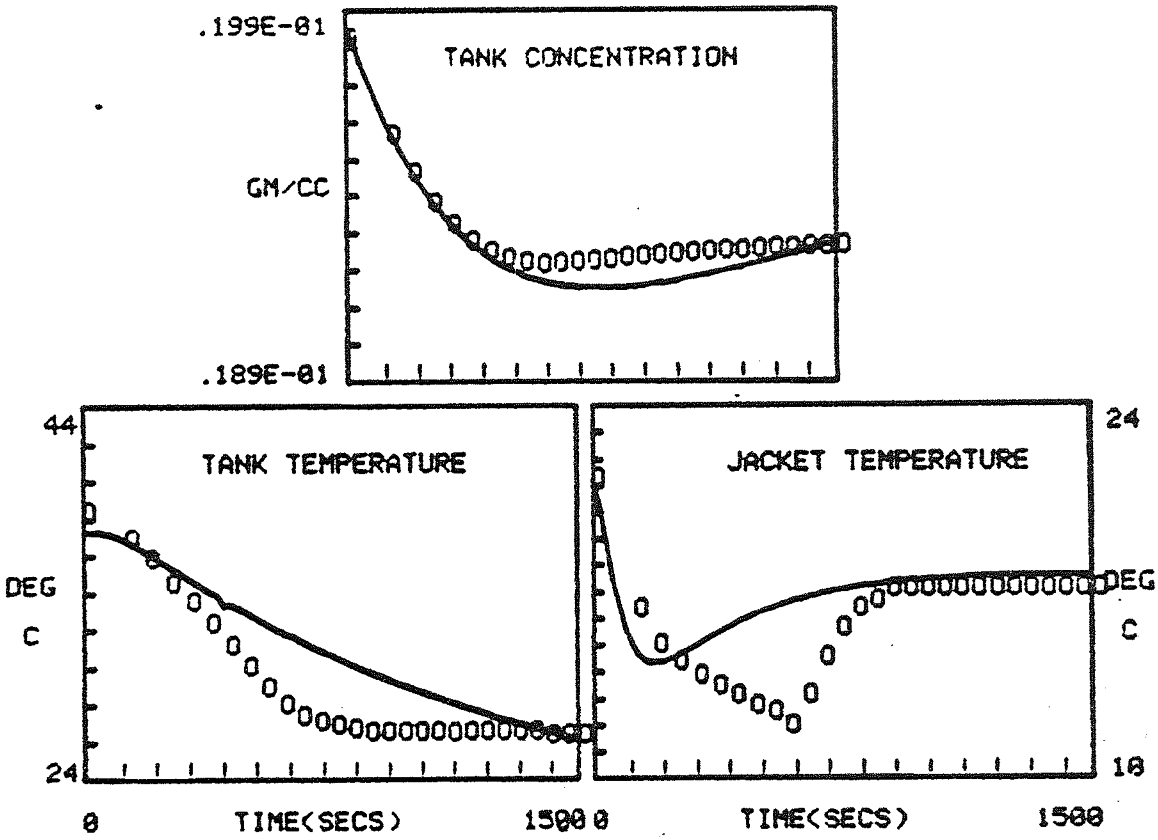


FIG.A.6.2.21 EXPERIMENT NO:36

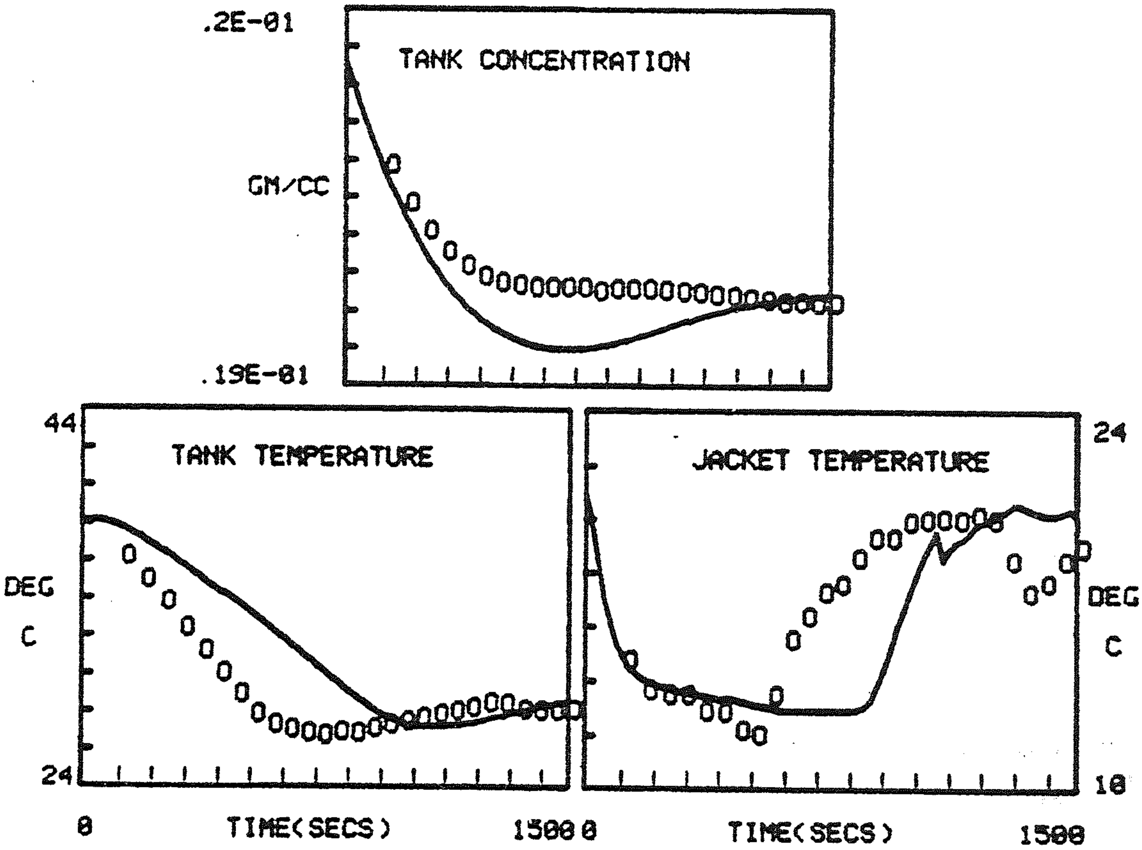


FIG.A.6.2.22 EXPERIMENT NO:37

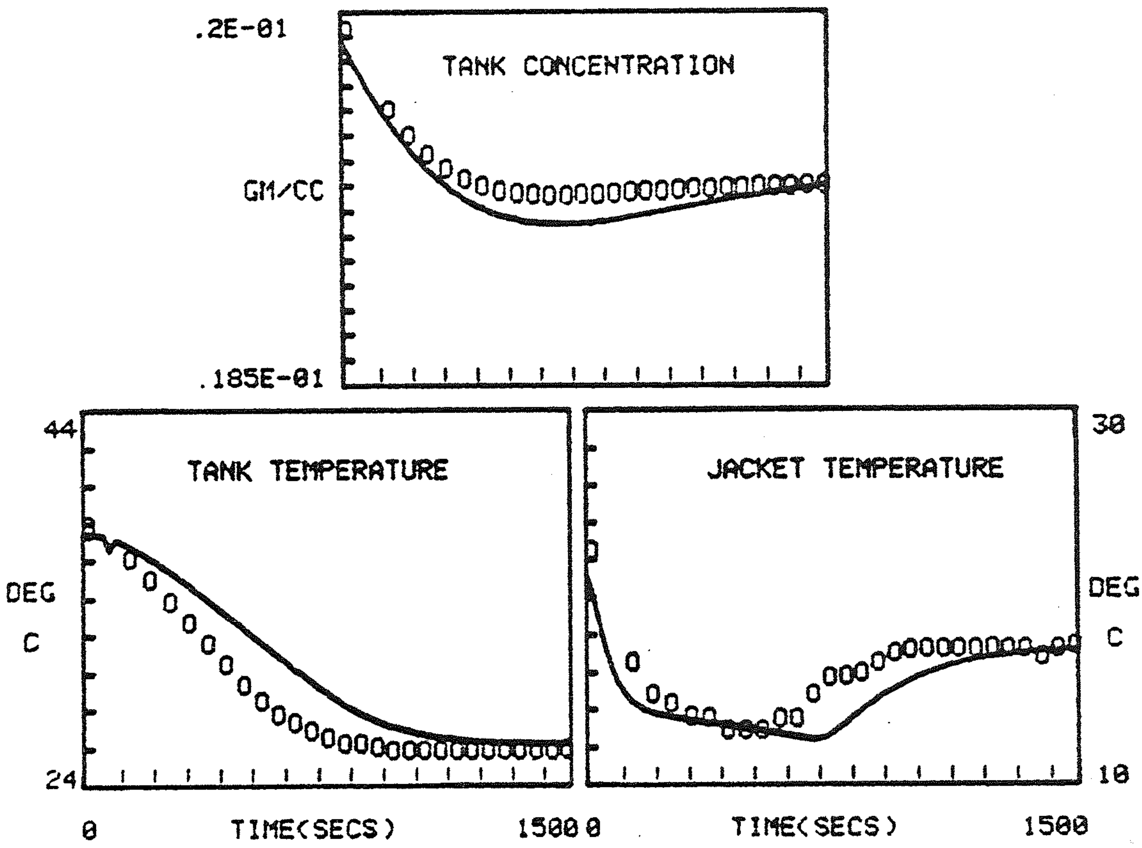


FIG.A.6.2.23 EXPERIMENT NO:38

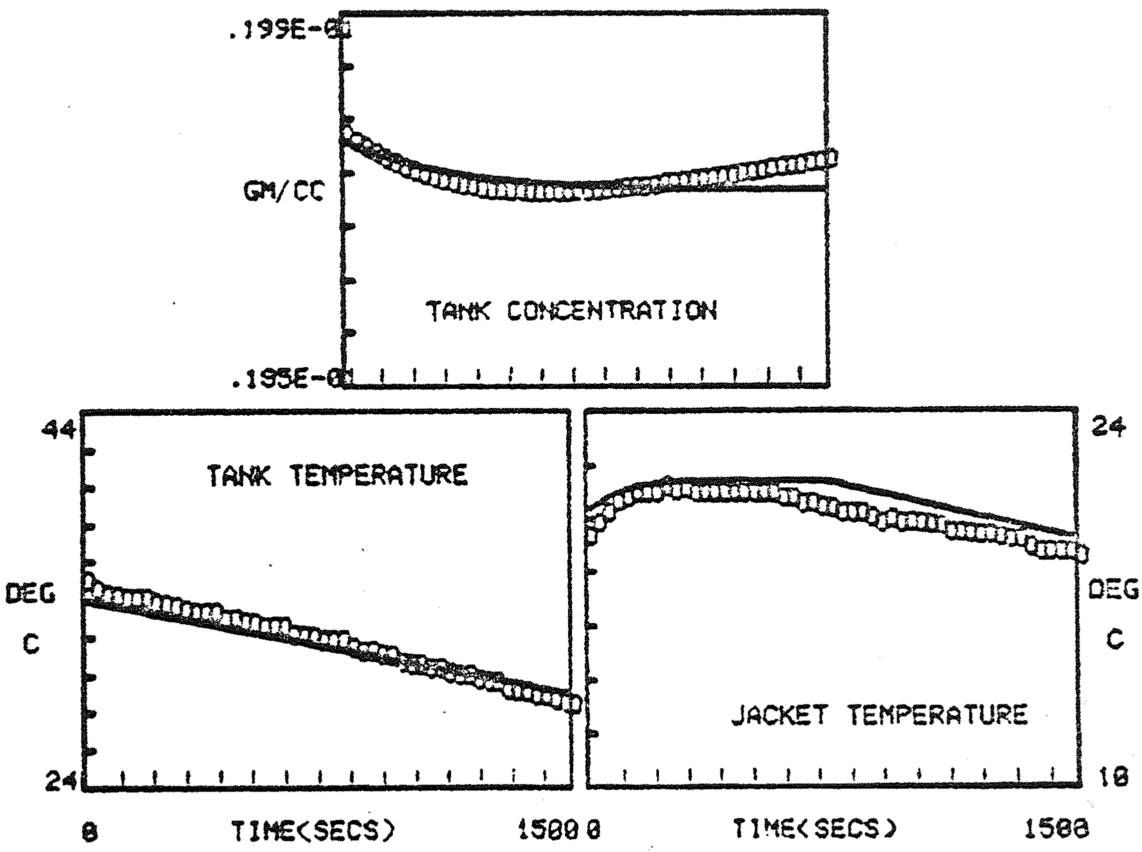


FIG.A.6.2.24 EXPERIMENT NO:48

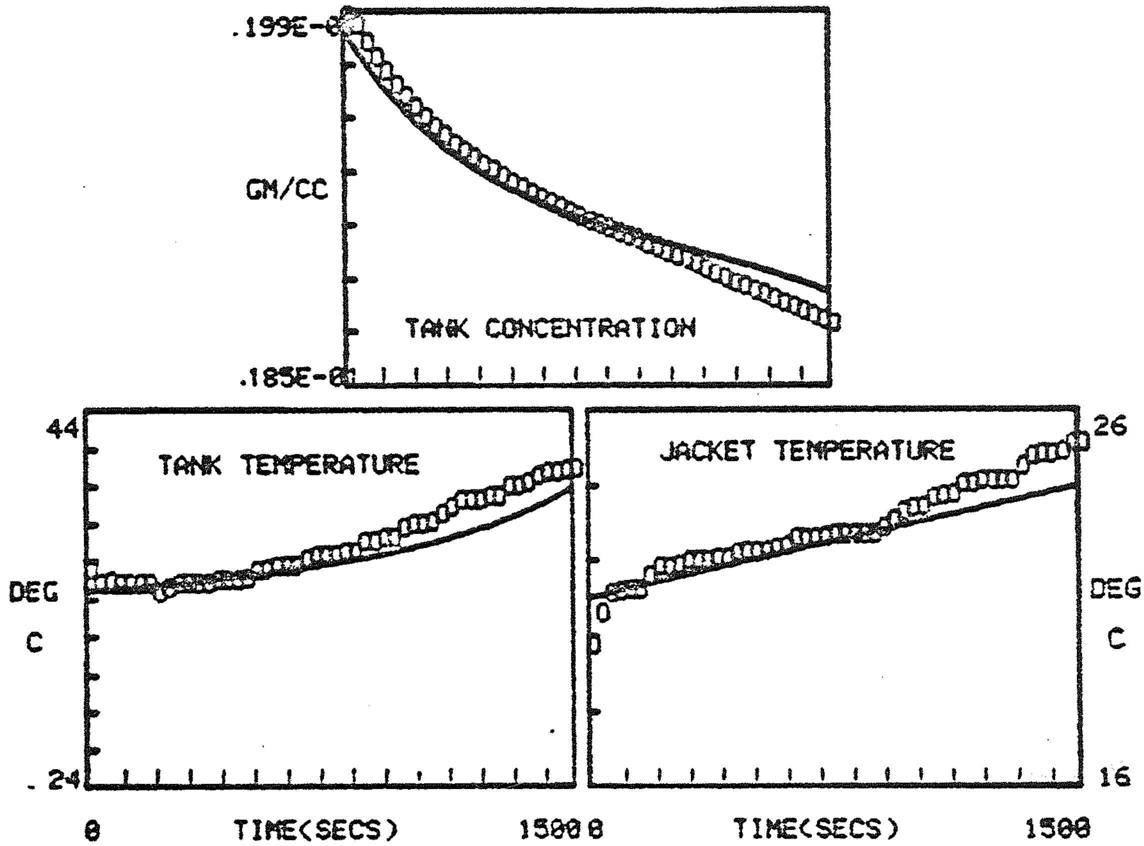


FIG.A.6.2.25 EXPERIMENT NO:49

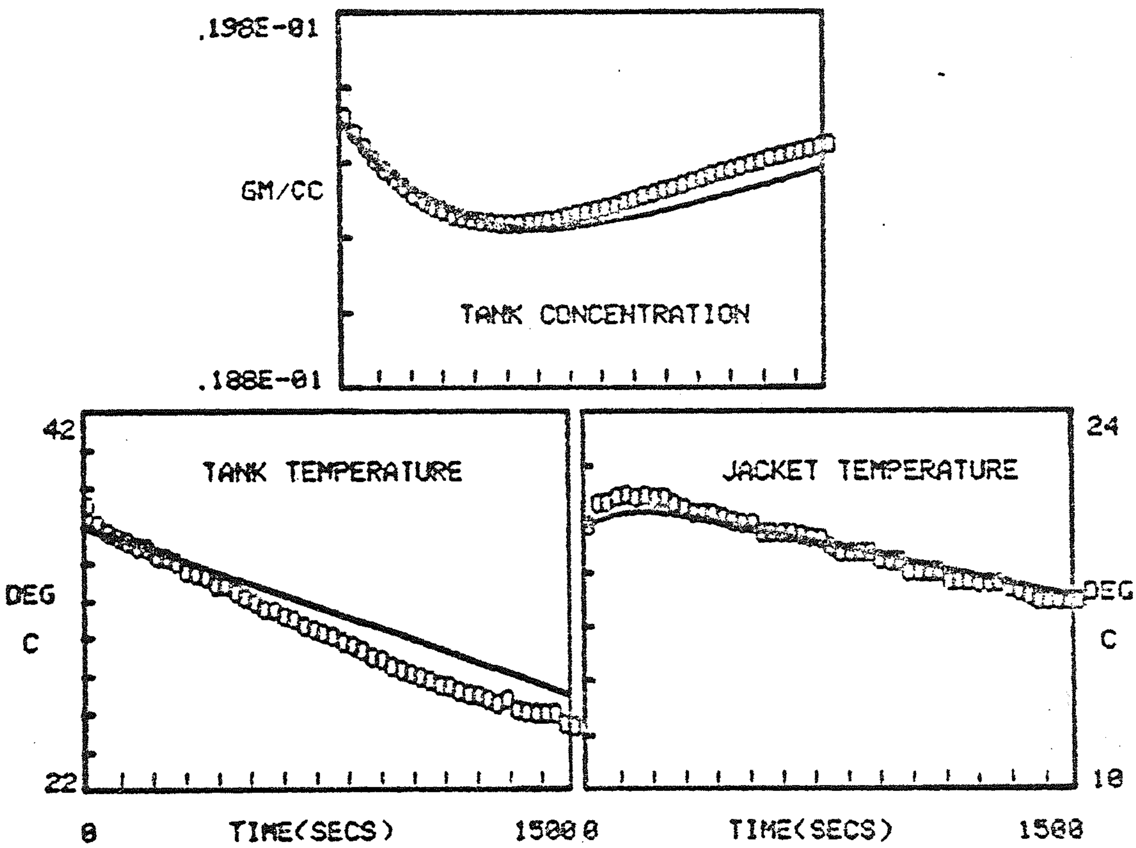


FIG.A.6.2.26 EXPERIMENT NO:50

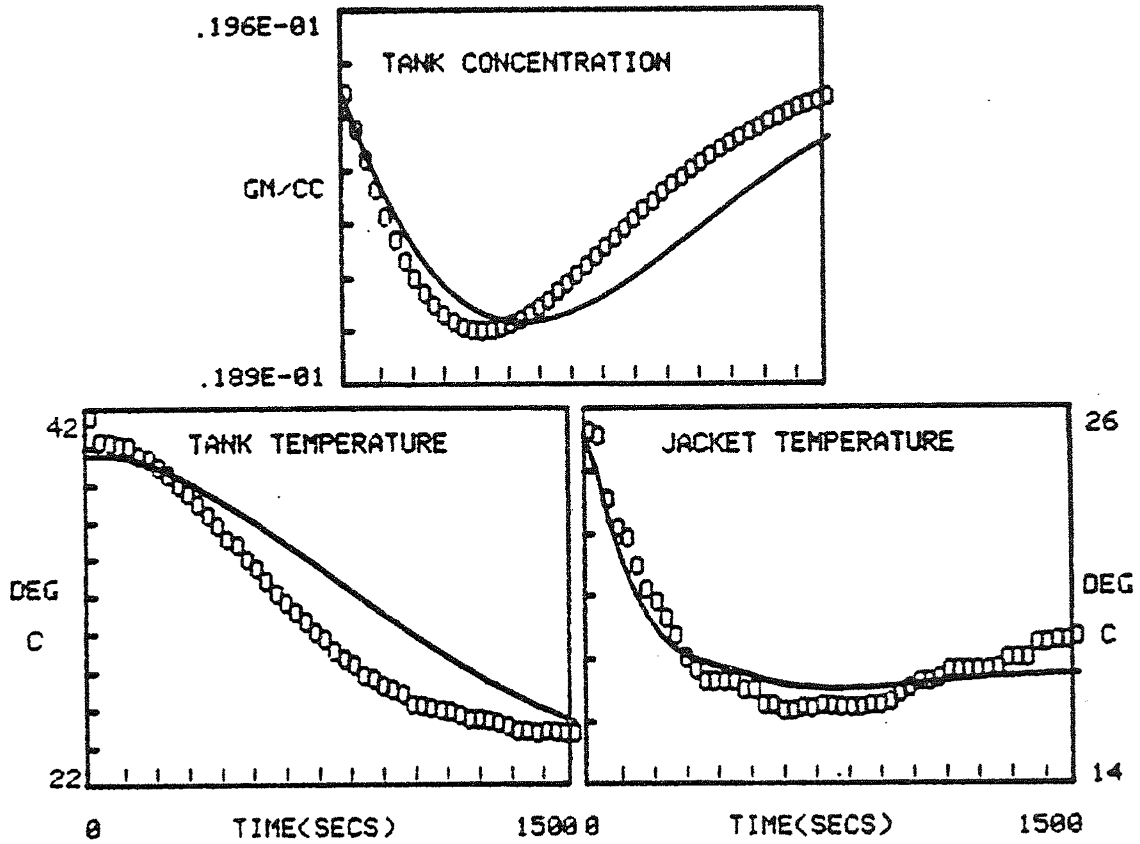


FIG.A.6.2.27 EXPERIMENT NO:54

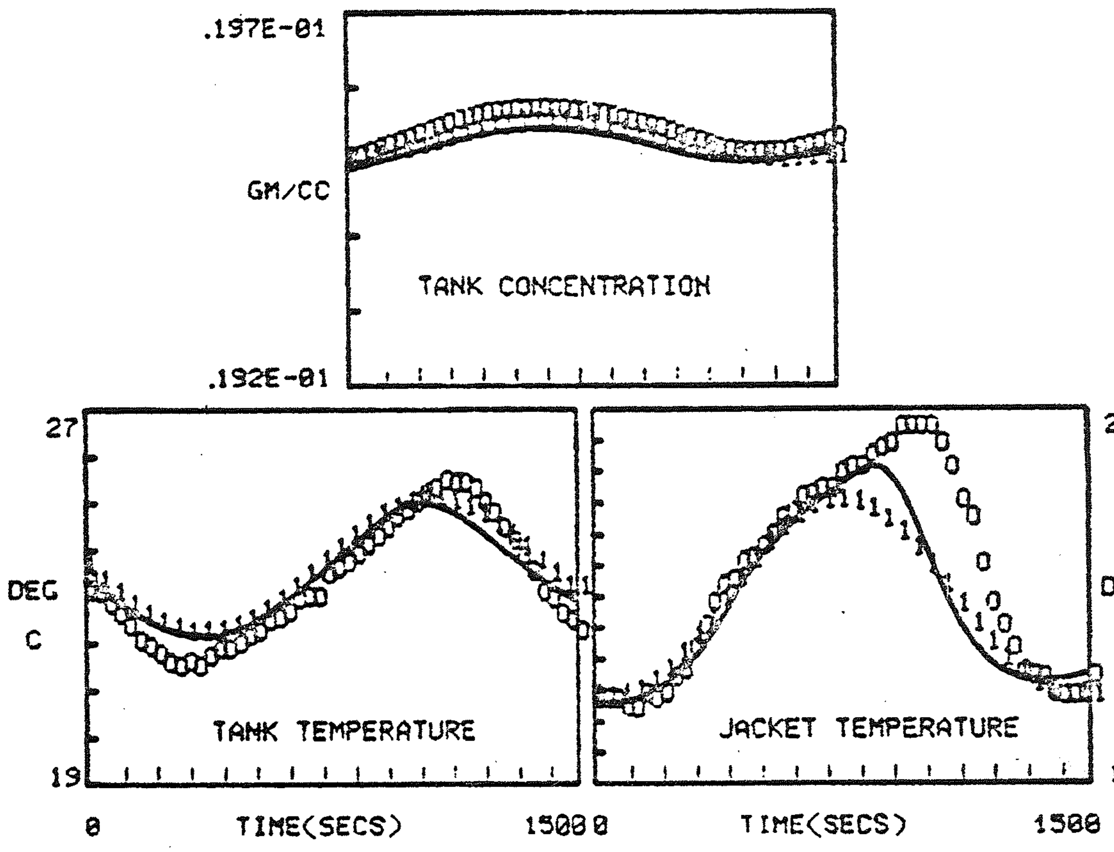


FIG.A.6.2.28 EXPERIMENT NO:55

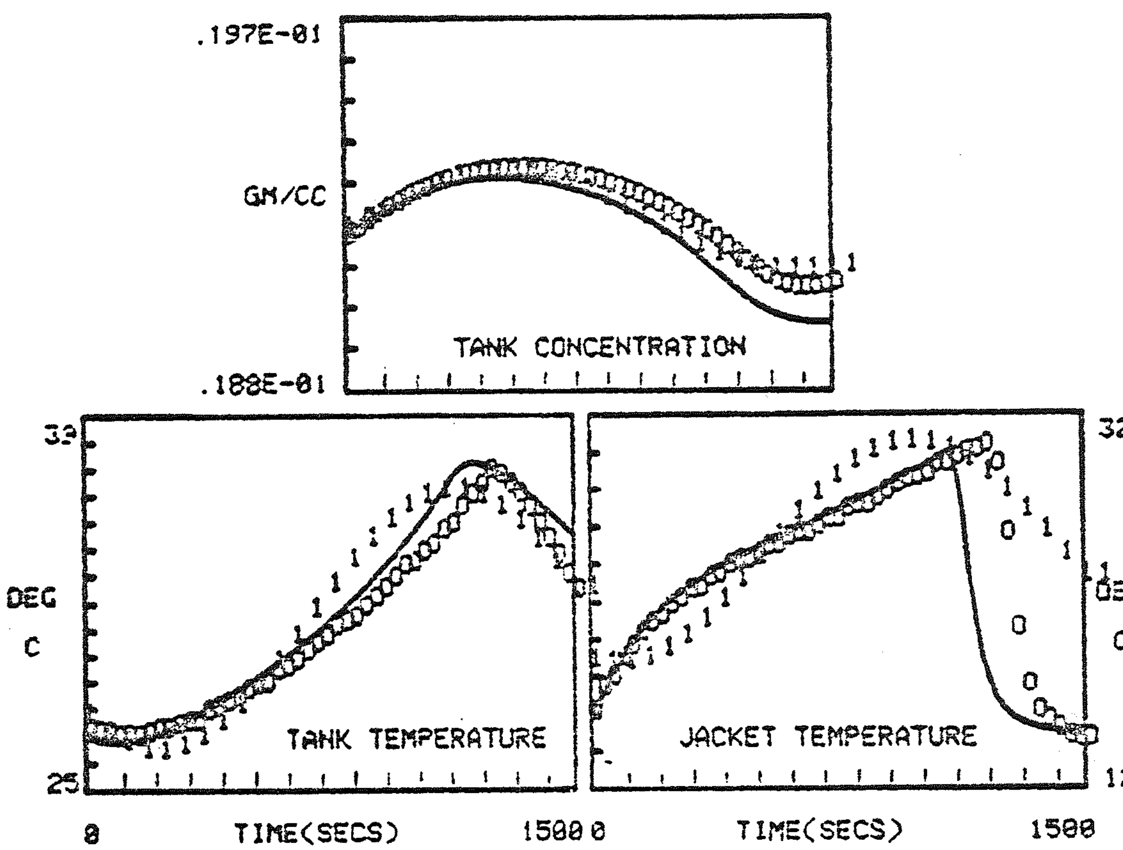


FIG.A.6.2.29 EXPERIMENT NO:56

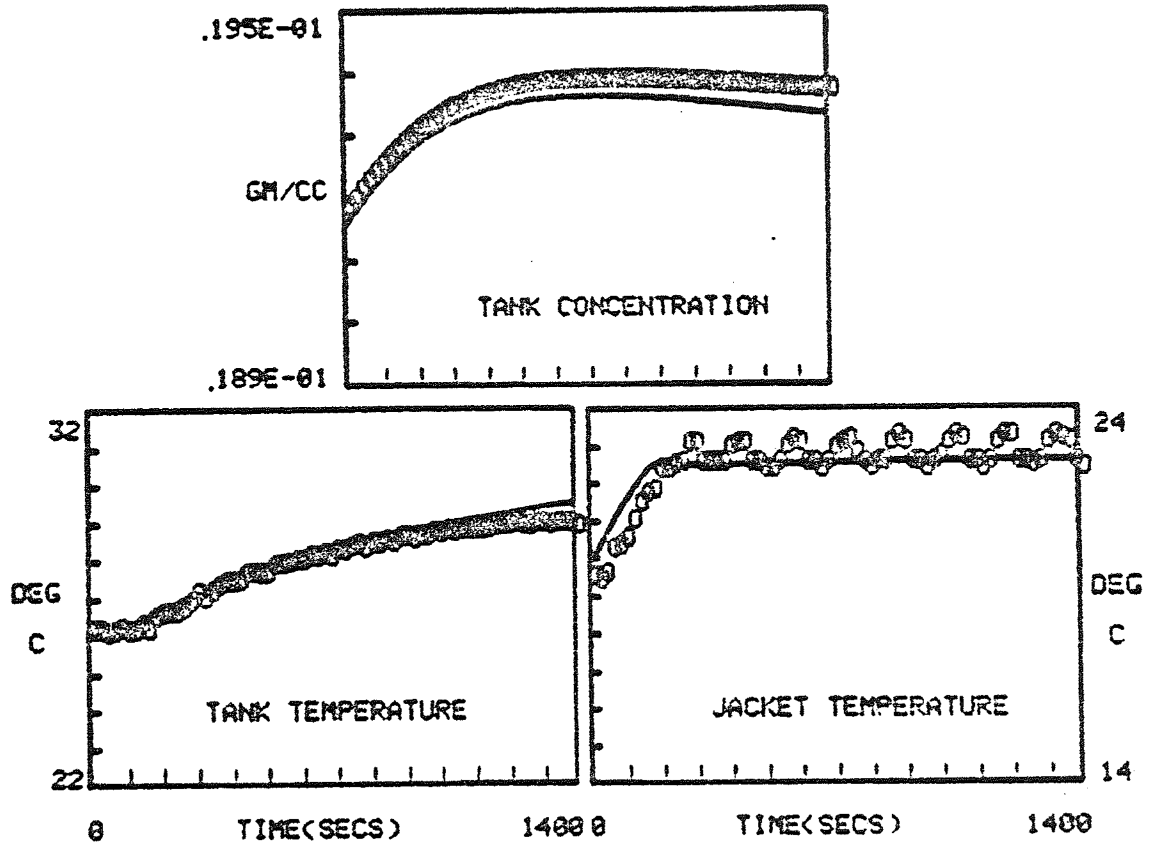


FIG.A.6.2.30 EXPERIMENT NO:60

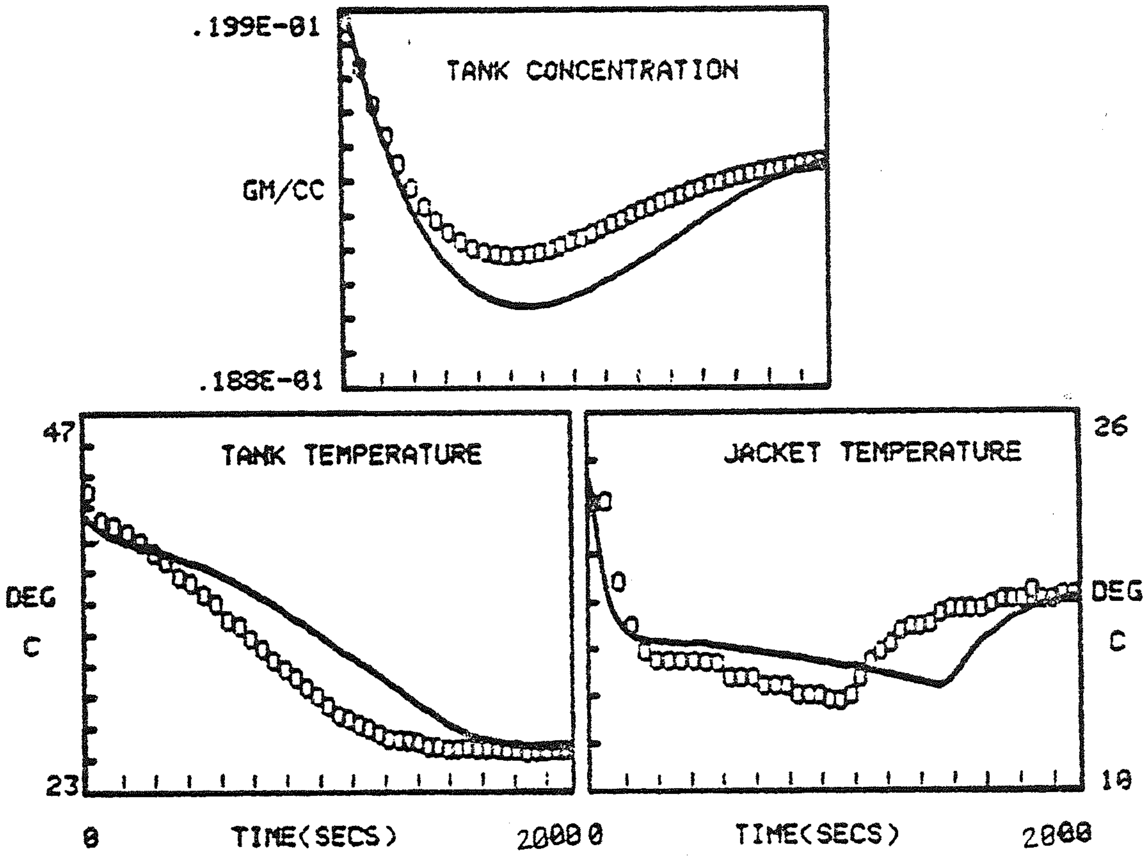


FIG.A.6.2.31 EXPERIMENT NO:62

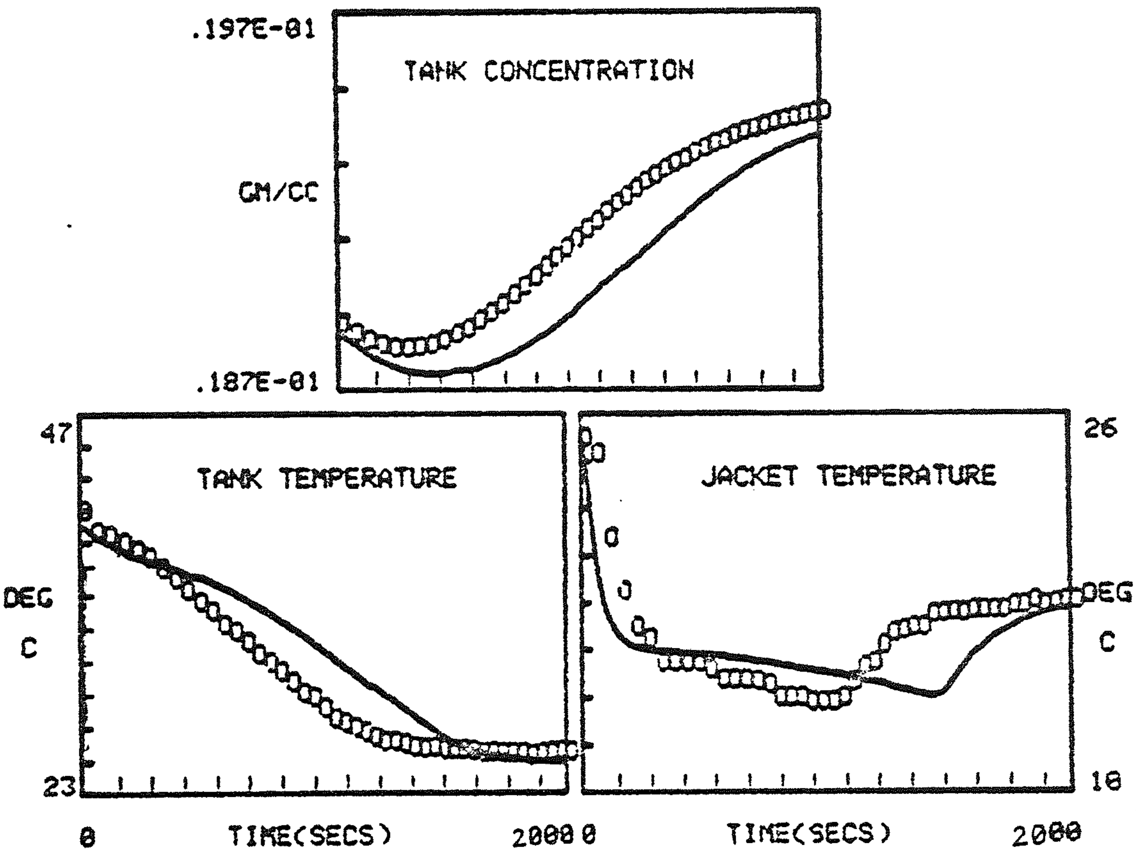


FIG.A.6.2.32 EXPERIMENT NO:63

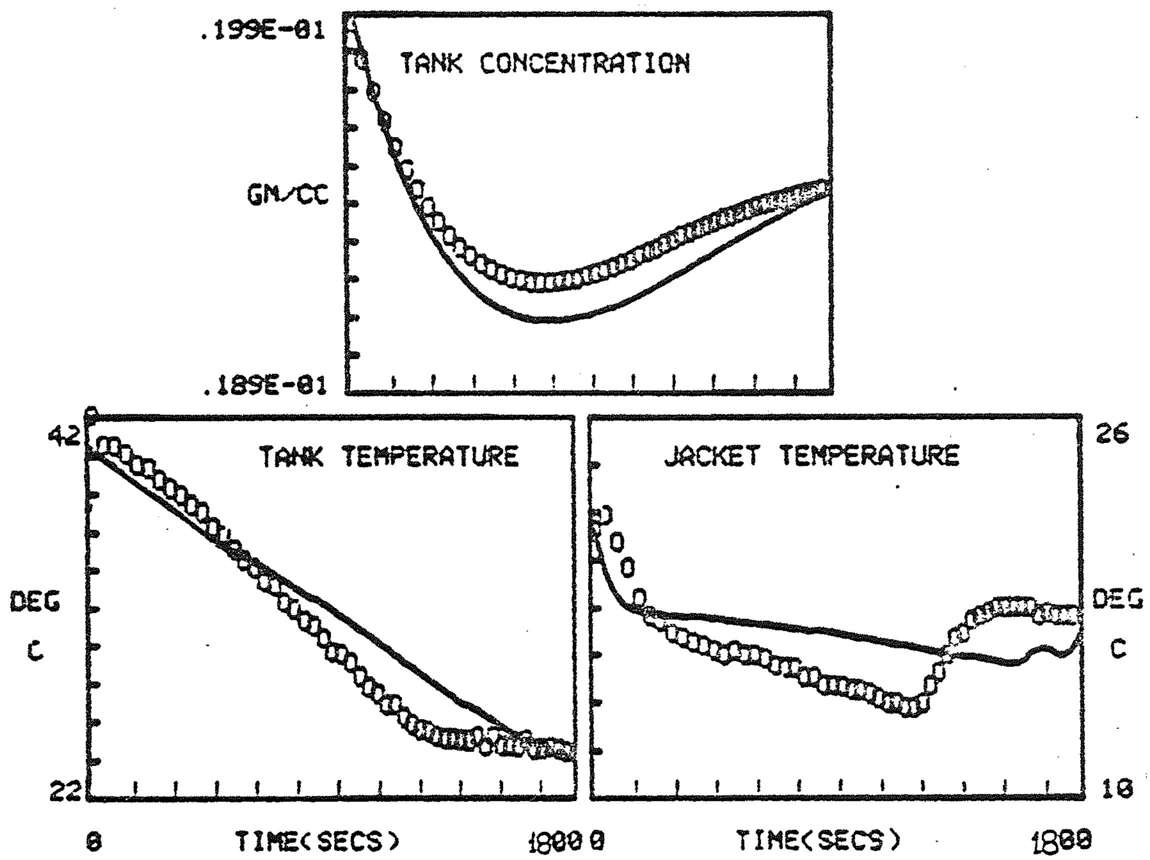


FIG.A.6.2.33 EXPERIMENT NO:65

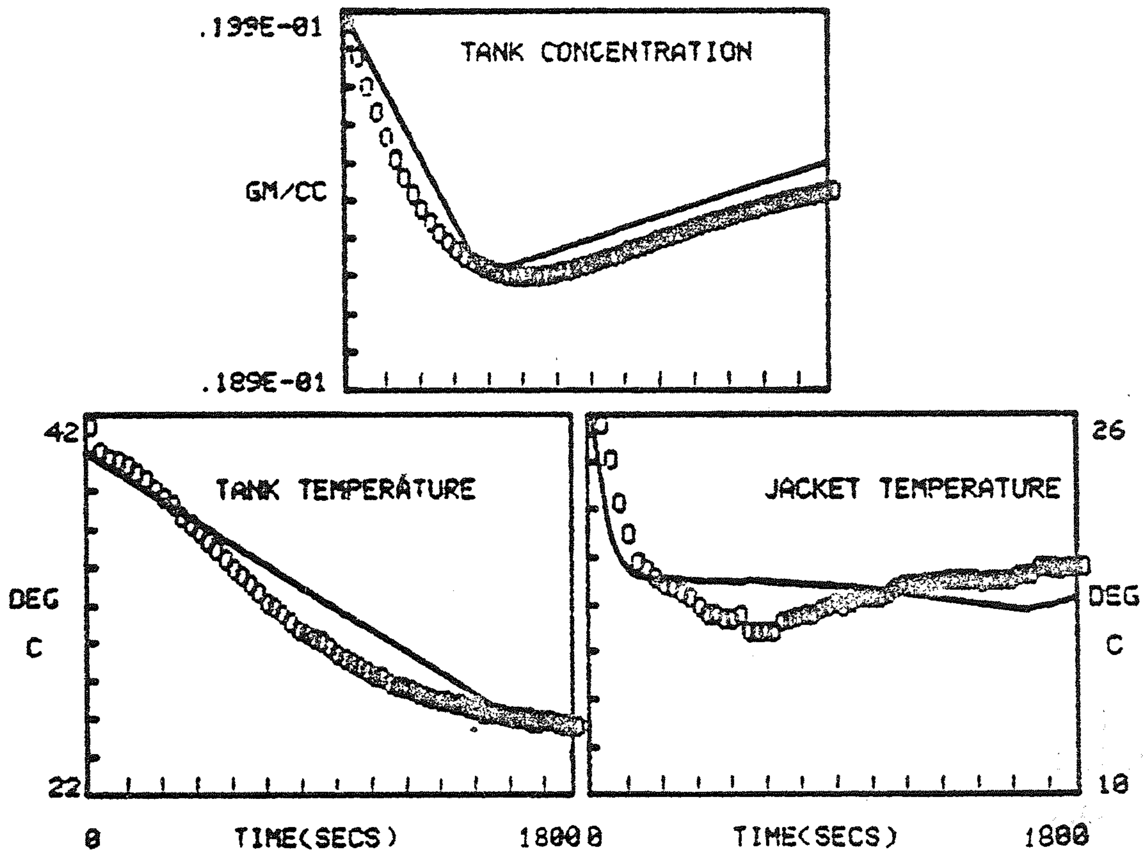


FIG.A.6.2.34 EXPERIMENT NO:66

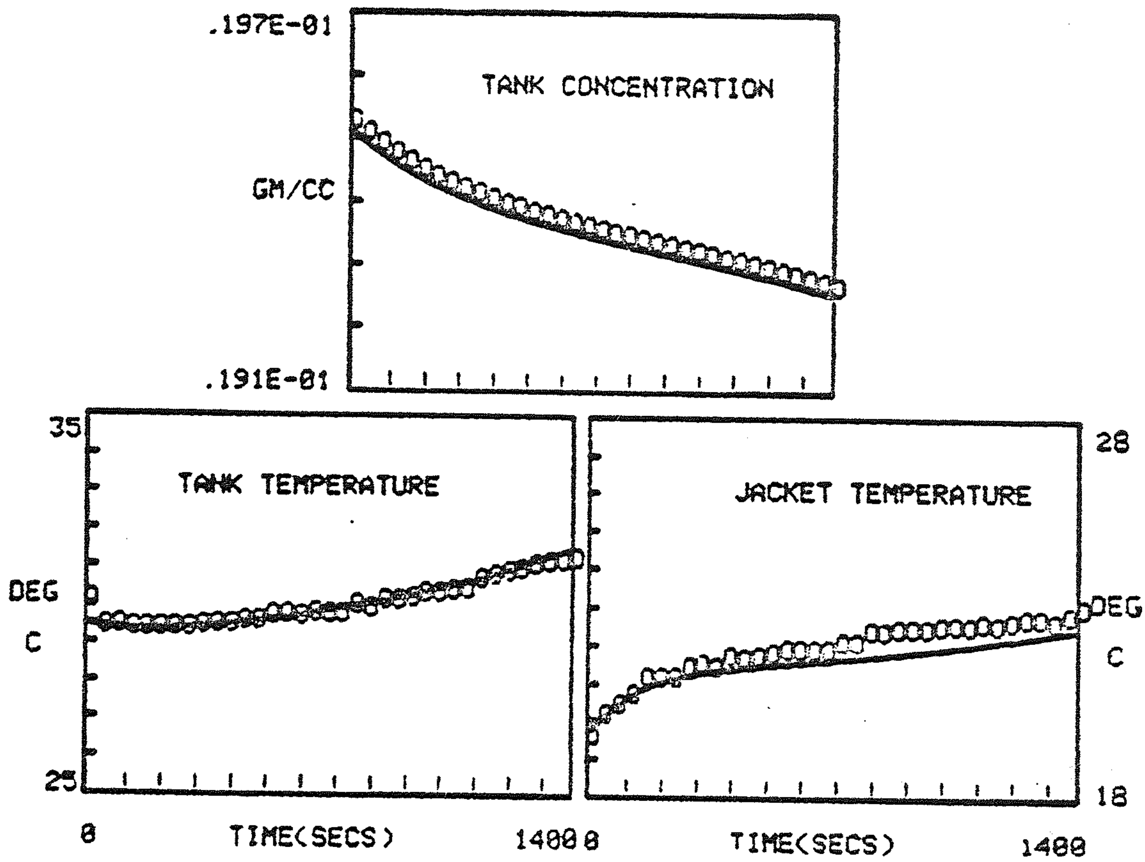


FIG.A.6.2.35 EXPERIMENT NO:69

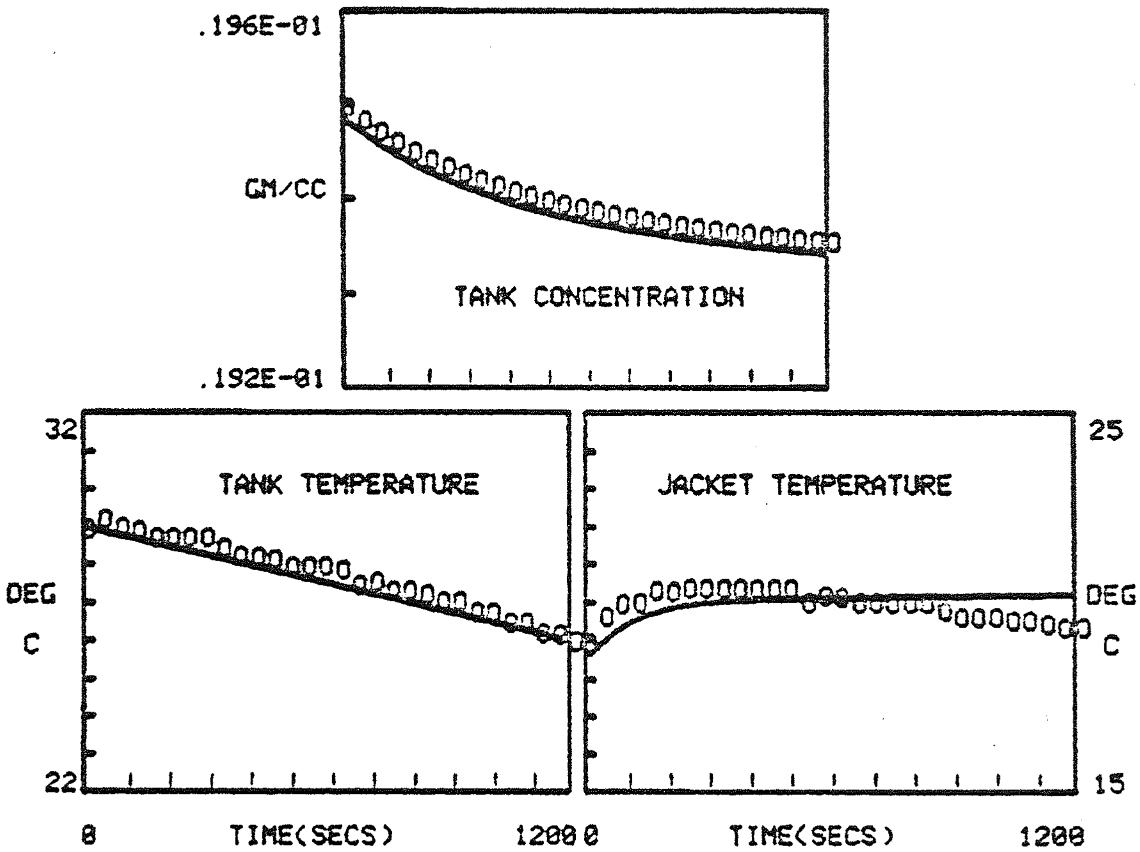


FIG.A.6.2.36 EXPERIMENT NO:71

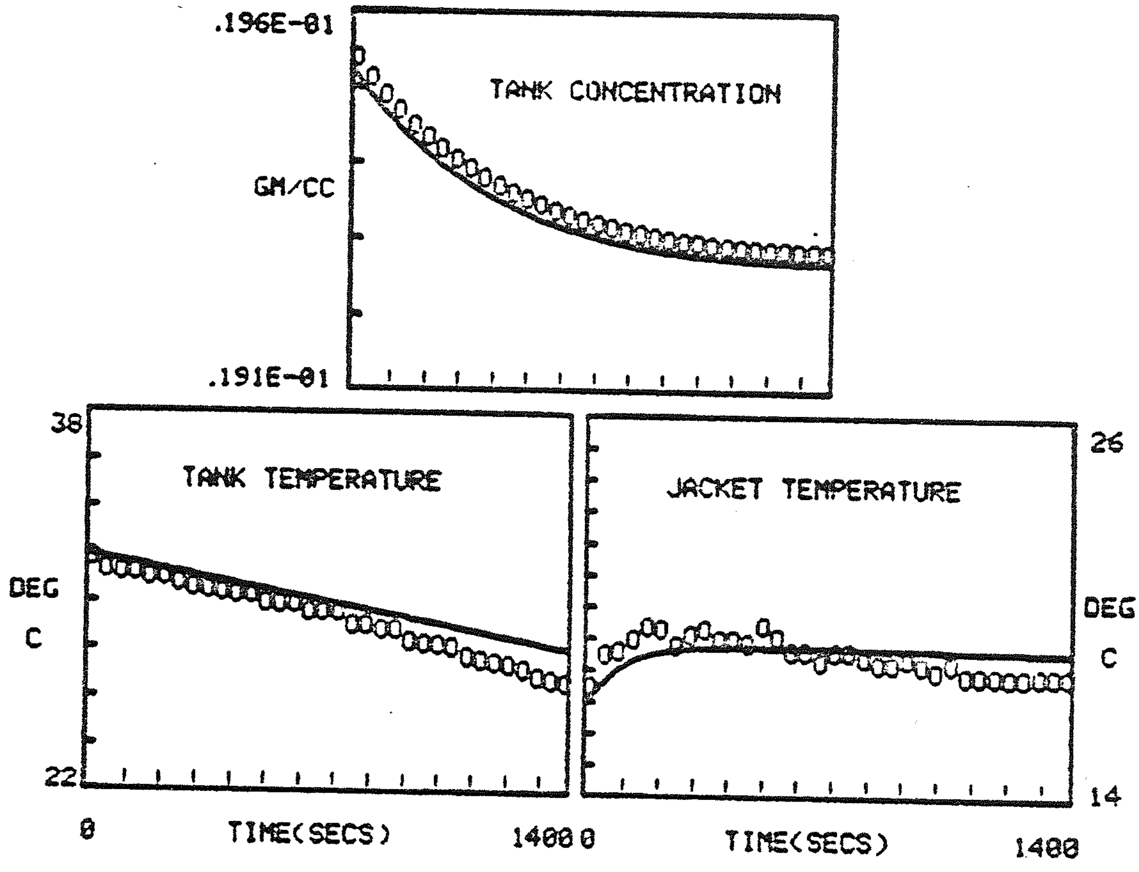


FIG.A.6.2.37 EXPERIMENT NO:73

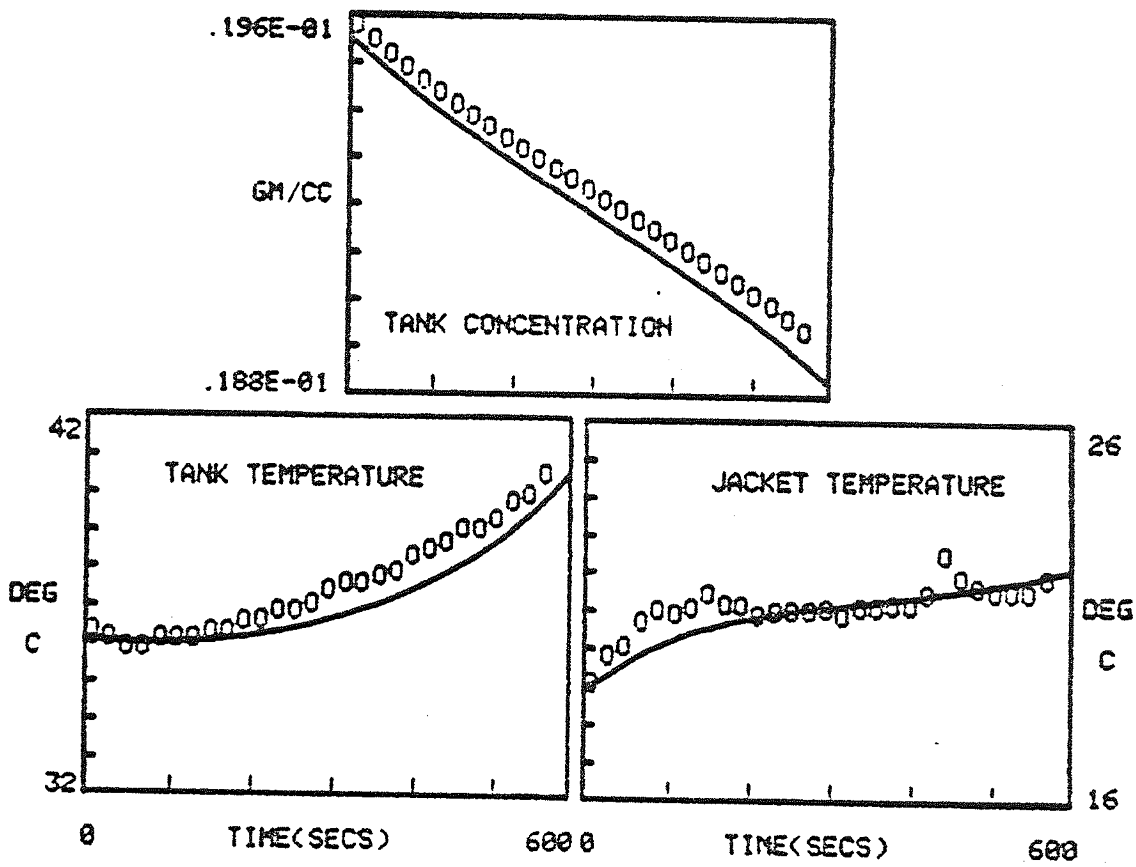


FIG.A.6.2.38 EXPERIMENT NO:74

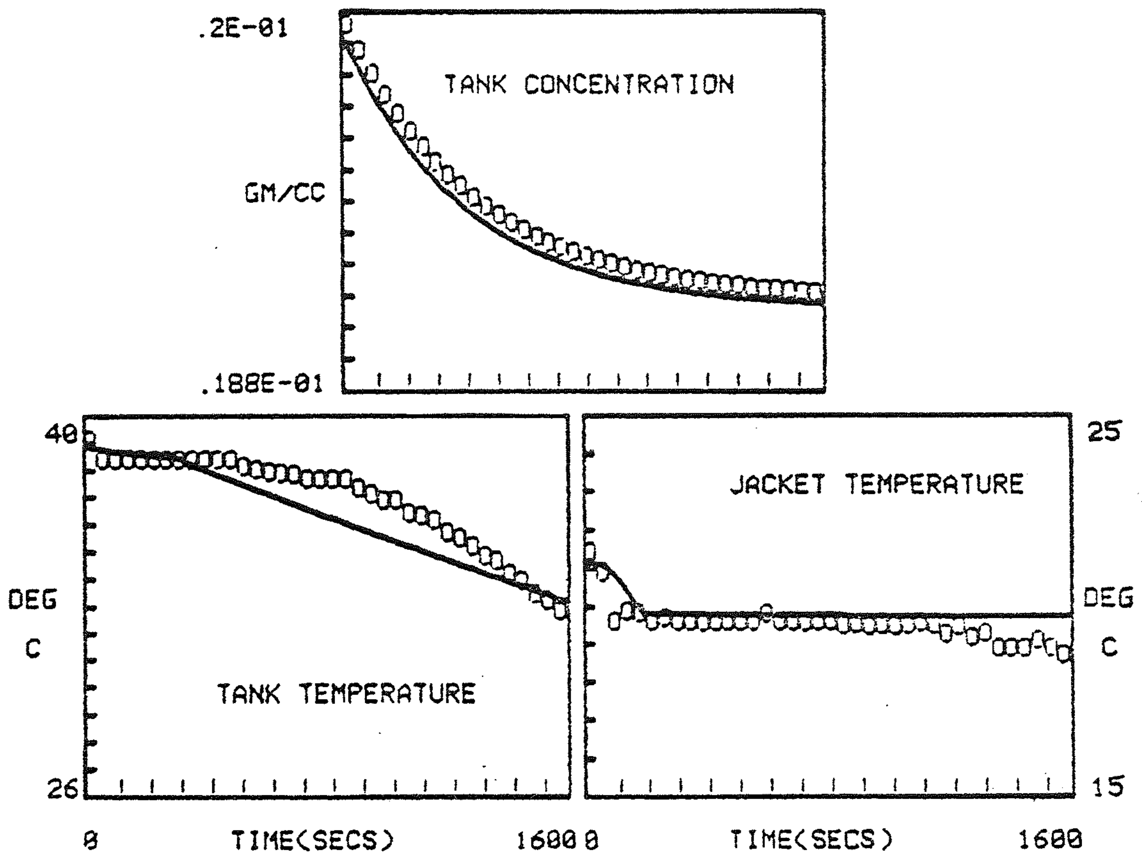


FIG.A.6.2.39 EXPERIMENT NO:76

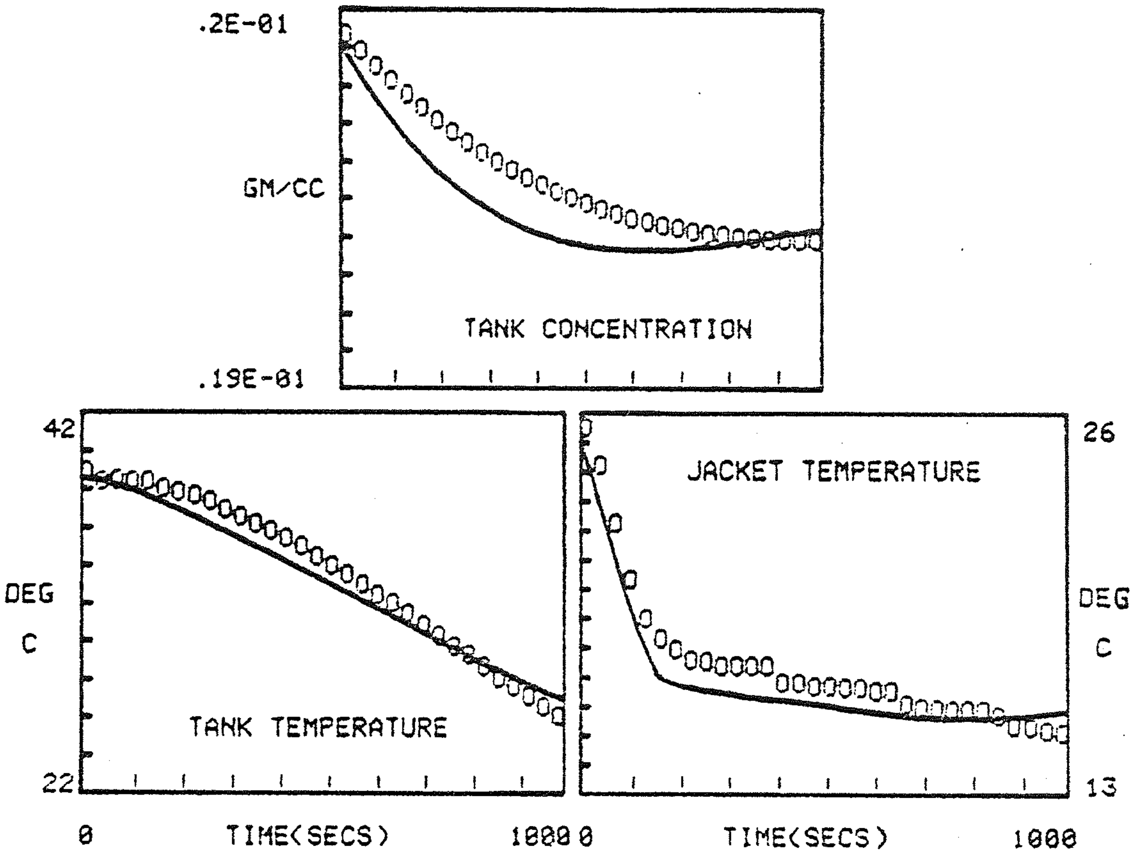


FIG.A.6.2.40 EXPERIMENT NO:77

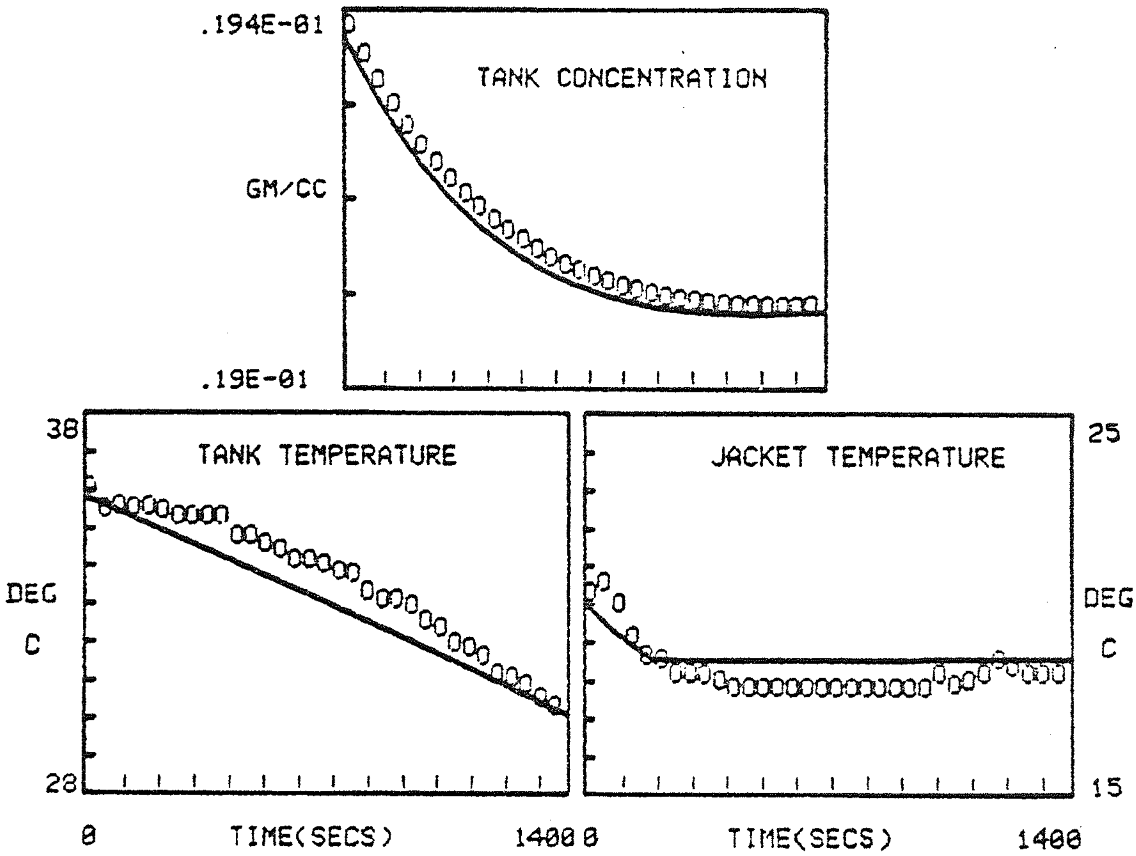


FIG.A.6.2.41 EXPERIMENT NO:80

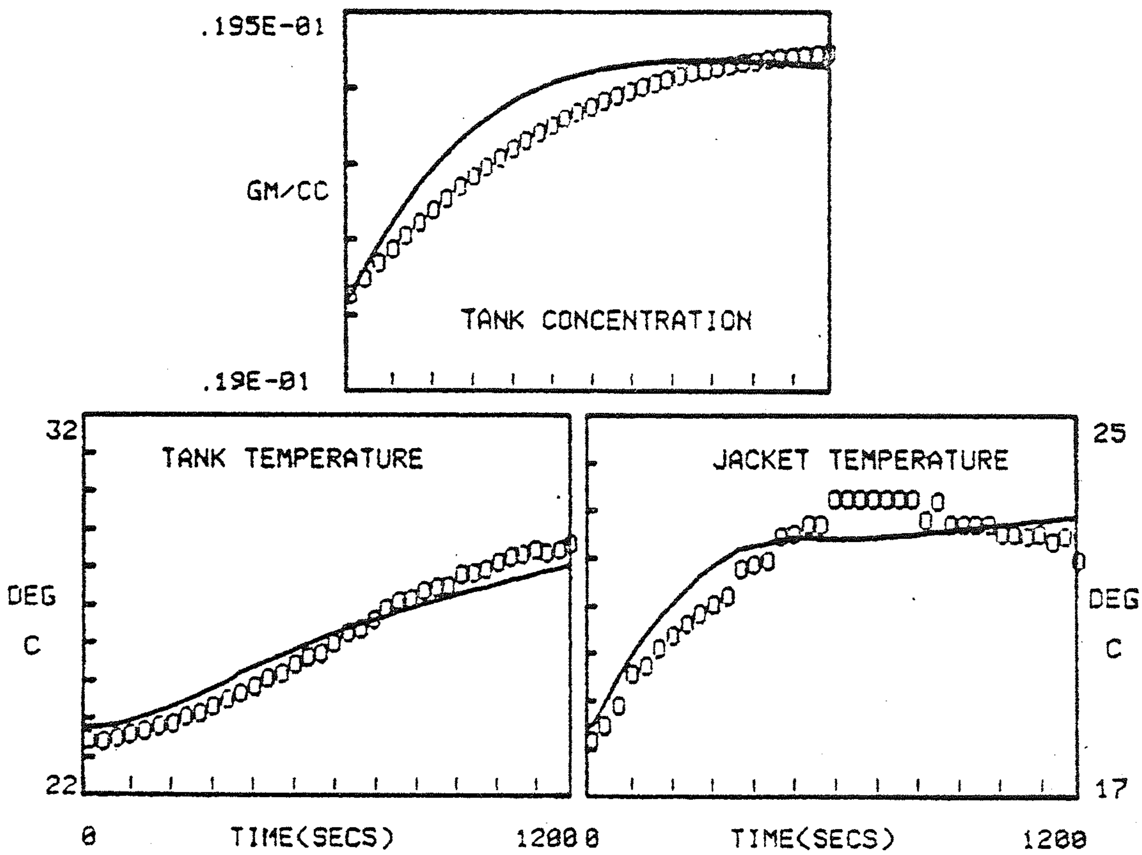


FIG.A.6.2.42 EXPERIMENT NO:83

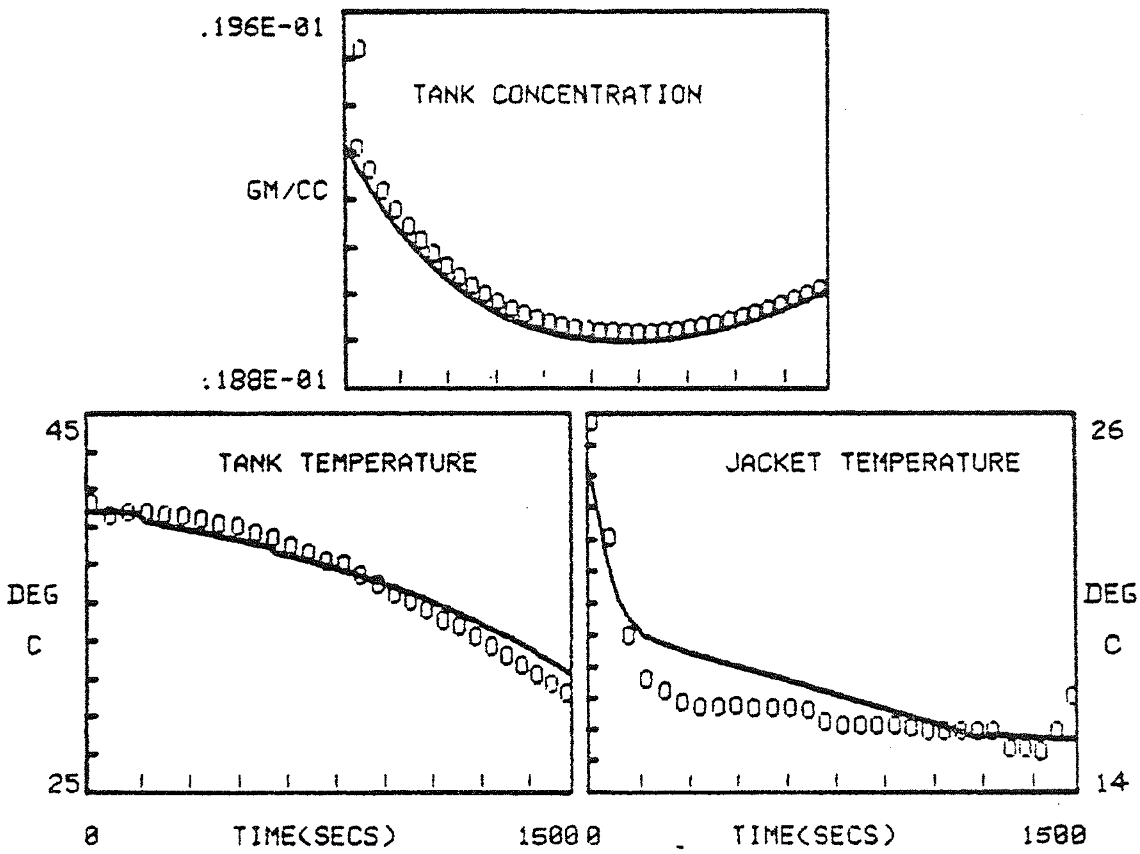


FIG.A.6.2.43 EXPERIMENT NO:84

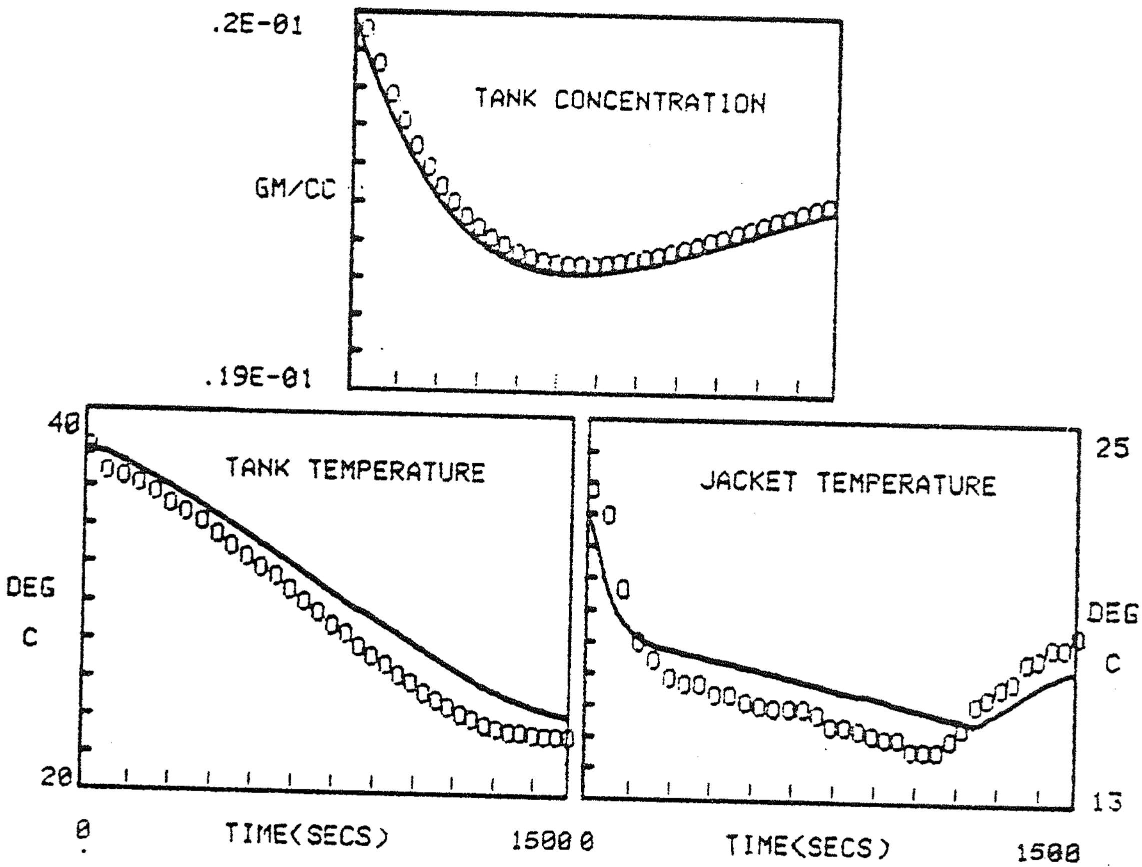


FIG.A.6.2.44 EXPERIMENT NO:85

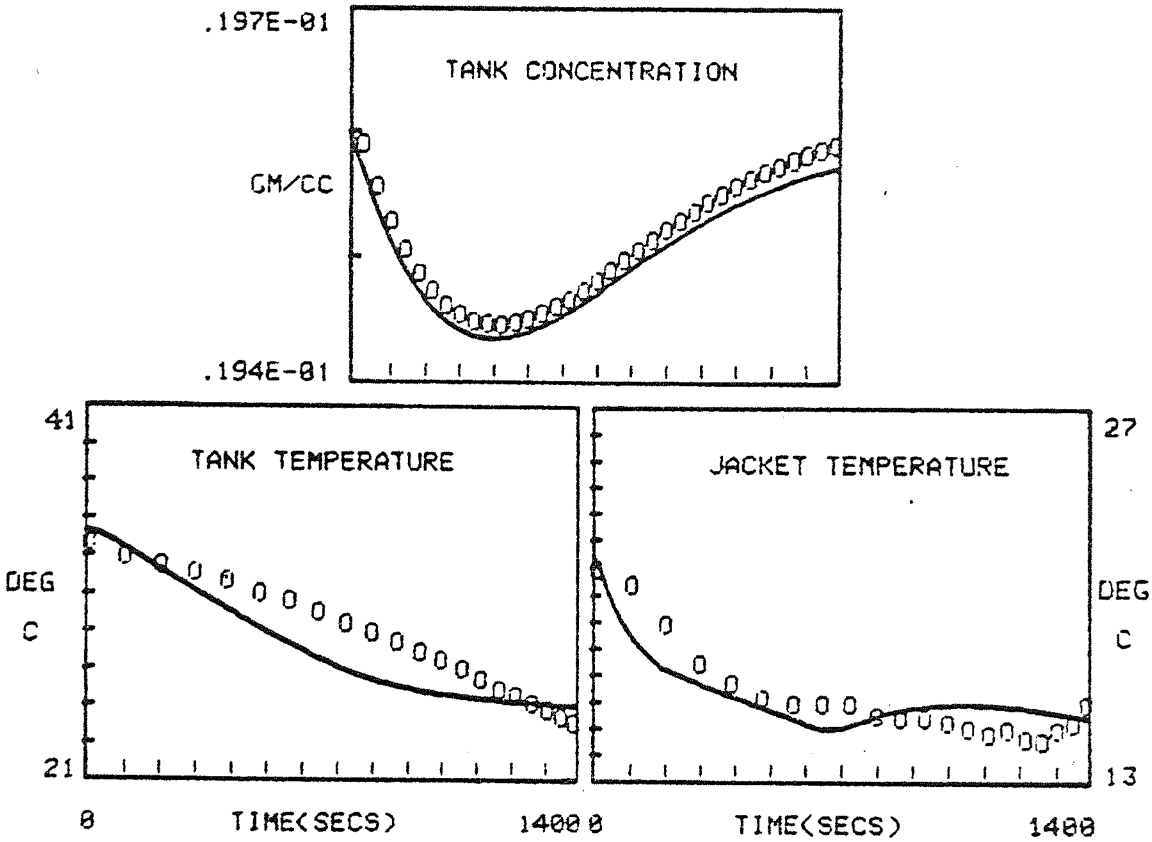


FIG.A.6.2.45 EXPERIMENT NO:88

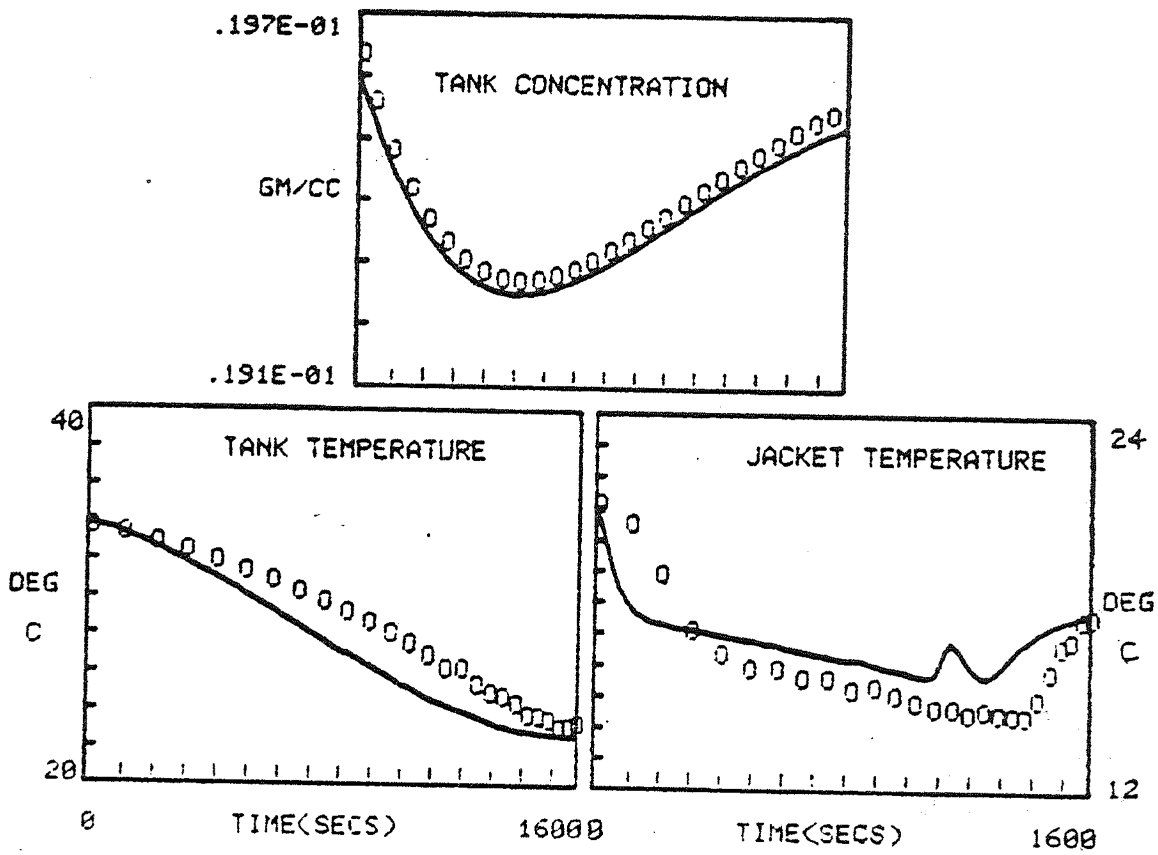


FIG.A.6.2.46 EXPERIMENT NO:91

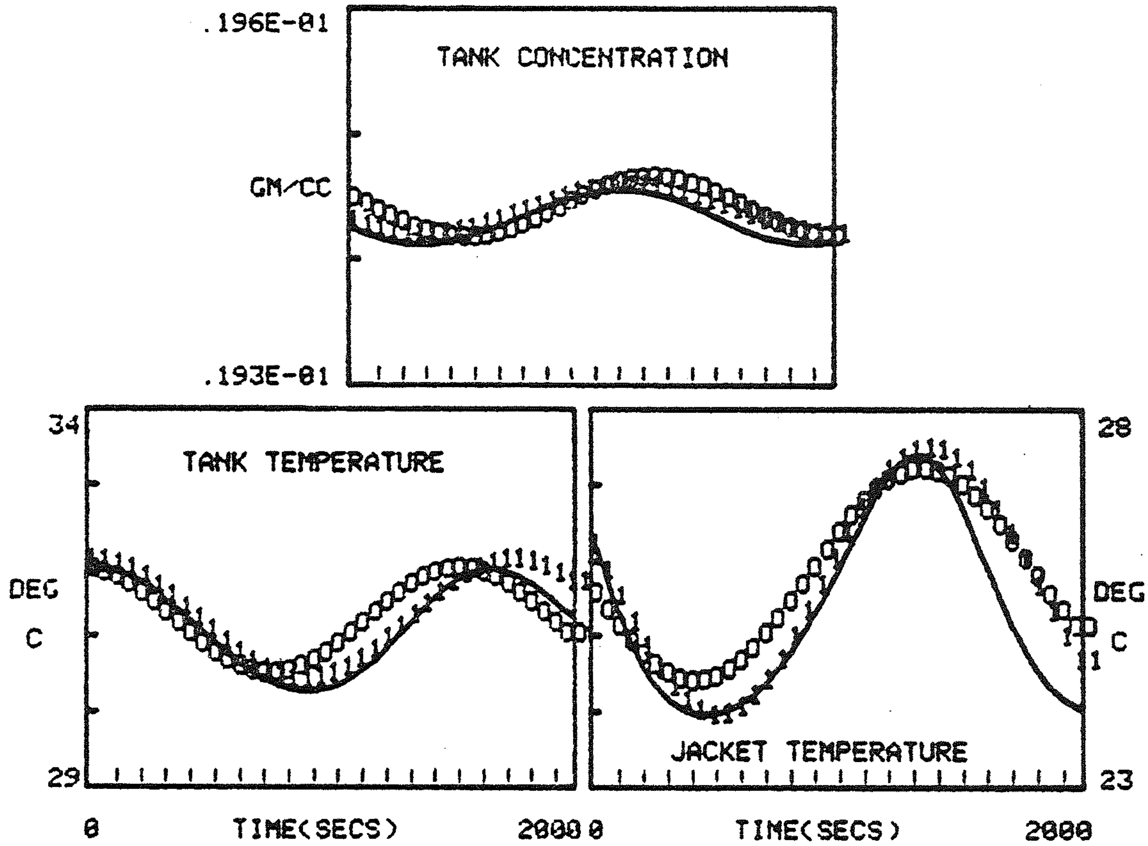


FIG.A.6.2.47 EXPERIMENT NO:92

APPENDIX 7

COMPARISON OF DECOUPLING AND INVARIANCE TYPE CONTROLS WITH CONVENTIONAL CONTROLLERS

APPENDIX 7

COMPARISON OF DECOUPLING AND INVARIANCE TYPE CONTROLS WITH CONVENTIONAL CONTROLLERS

Figure A.7.1 gives a conventional feedback and feed-forward multiloop control. The scheme has two feed-forward paths for the two load disturbances entering the system. For a P + I + D control the equation for the feedback path is given by

$$\bar{F}_c = K_c Y + \frac{1}{T_I} \int Y dt + T_D \quad dY/dt \qquad (A.7.1)$$

The equation for the first feed-forward path is given by

$$\bar{F}_c = K_c \beta_o + \frac{1}{T_I} \int \beta_o \, dt + T_D \frac{d\beta_o}{dt} \qquad (A.7.2)$$

and for the second feed-forward path by

$$\bar{F}_c = K_c \gamma_o + \frac{1}{T_I} \int \gamma_o \, dt + T_D \frac{d\gamma_o}{dt} \qquad (A.7.3)$$

The controllers are generally tuned for optimum settings. Figs. (A.7.2) and (A.7.3) respectively give the configuration of the decoupling and invariance type control schemes discussed in the text. The two new control schemes, have feed-forward paths but differ from conventional feed-forward control in that the controller action is, in each case, derived from the state equations of the system. In addition decoupling control is a multivariable scheme with a feedback loop.

Thus for decoupling control

$$\bar{F}_c = \{\dot{Z} + \tau_2 Z - Y/\tau_I - \gamma_o/\tau_c\} \frac{V_c}{(\gamma_{oss} + \gamma_o - \gamma_{ss} - Z)} \tag{3.49}$$

where Z is given by equation (3.50) and for invariance control

$$\bar{F}_c = \frac{\{\gamma_o/\tau_c + \beta_o(\tau_o/\tau)\tau_2\}V_c}{\{\gamma_{ss} - \gamma_{oss} - \gamma_o - \beta_o\tau_o/\tau\}} \tag{3.54}$$

Decoupling and complete invariance cannot be achieved with conventional feed-forward/feedback schemes and the present work investigates the improvements obtained with these new schemes.

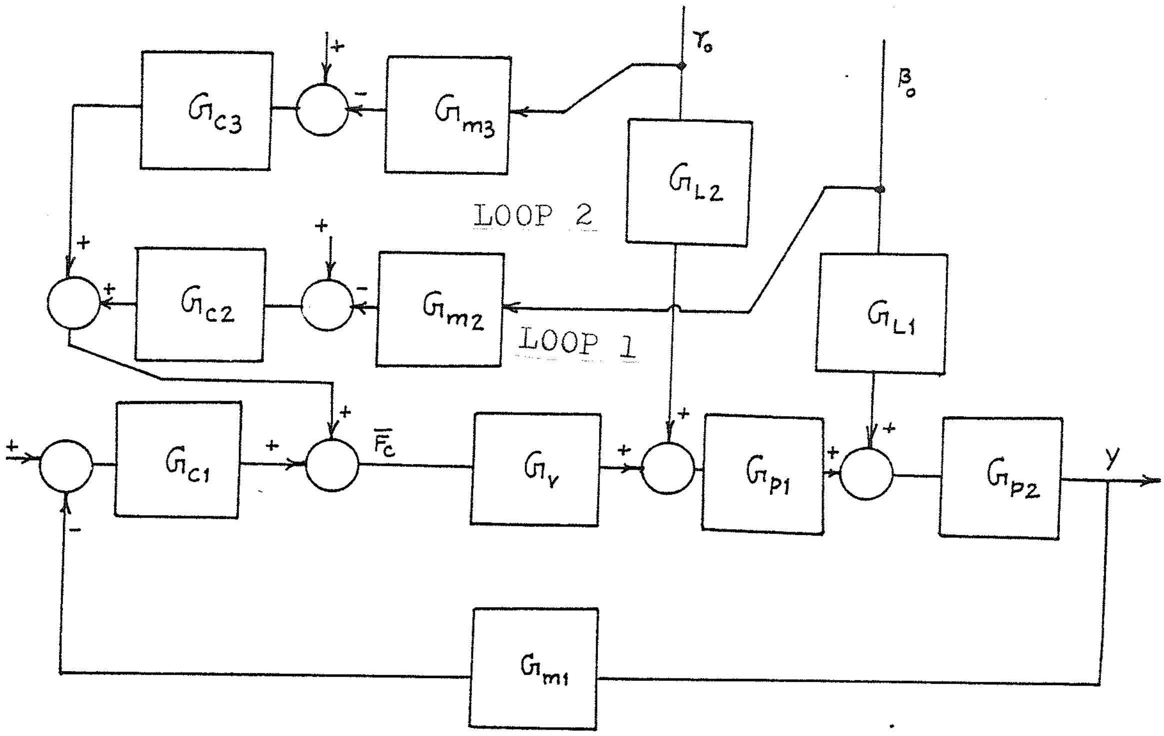


FIG. A.7.1 CONVENTIONAL FEEDBACK/FEED-FORWARD CONTROL

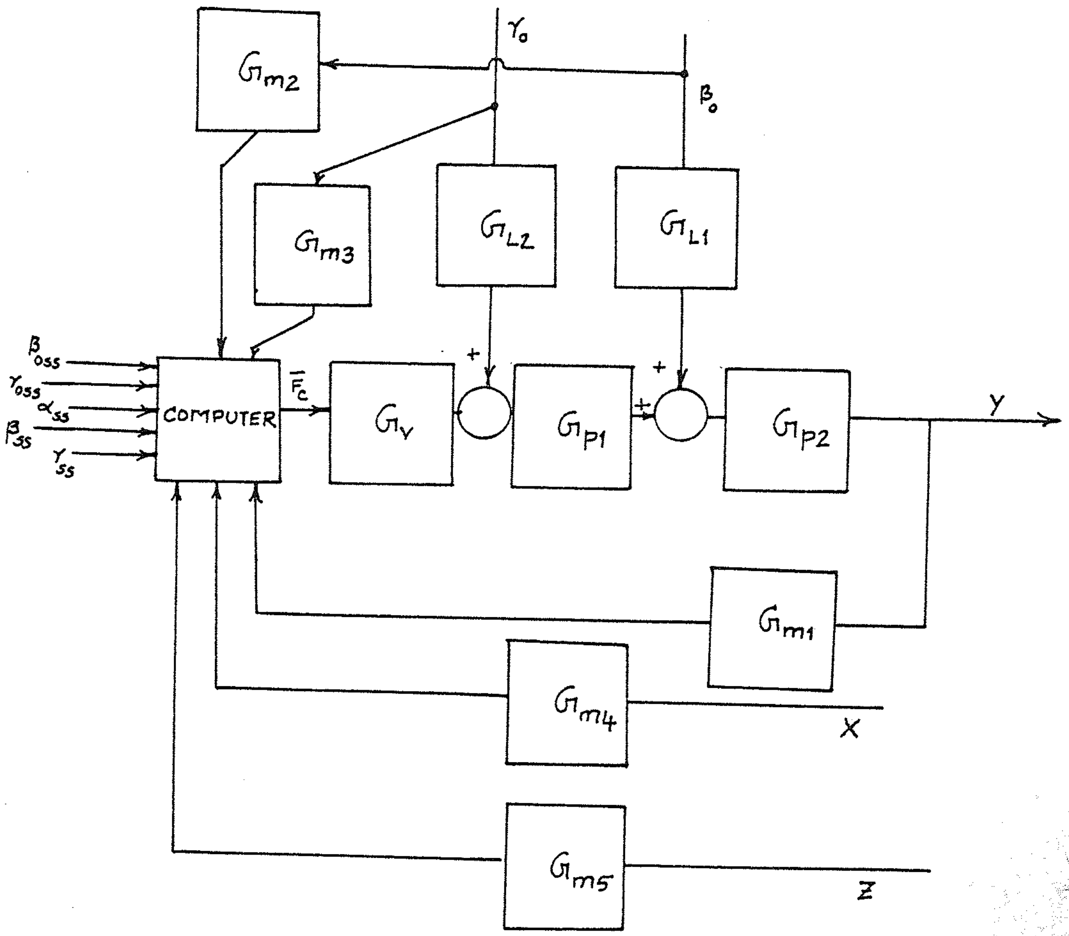


FIG. A.7.2 DECOUPLING TYPE CONTROL

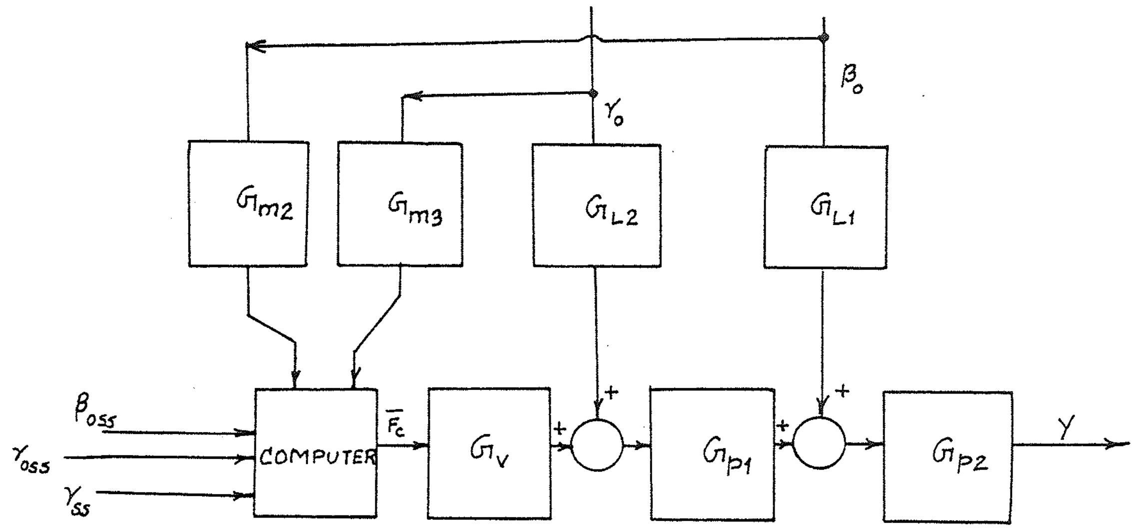
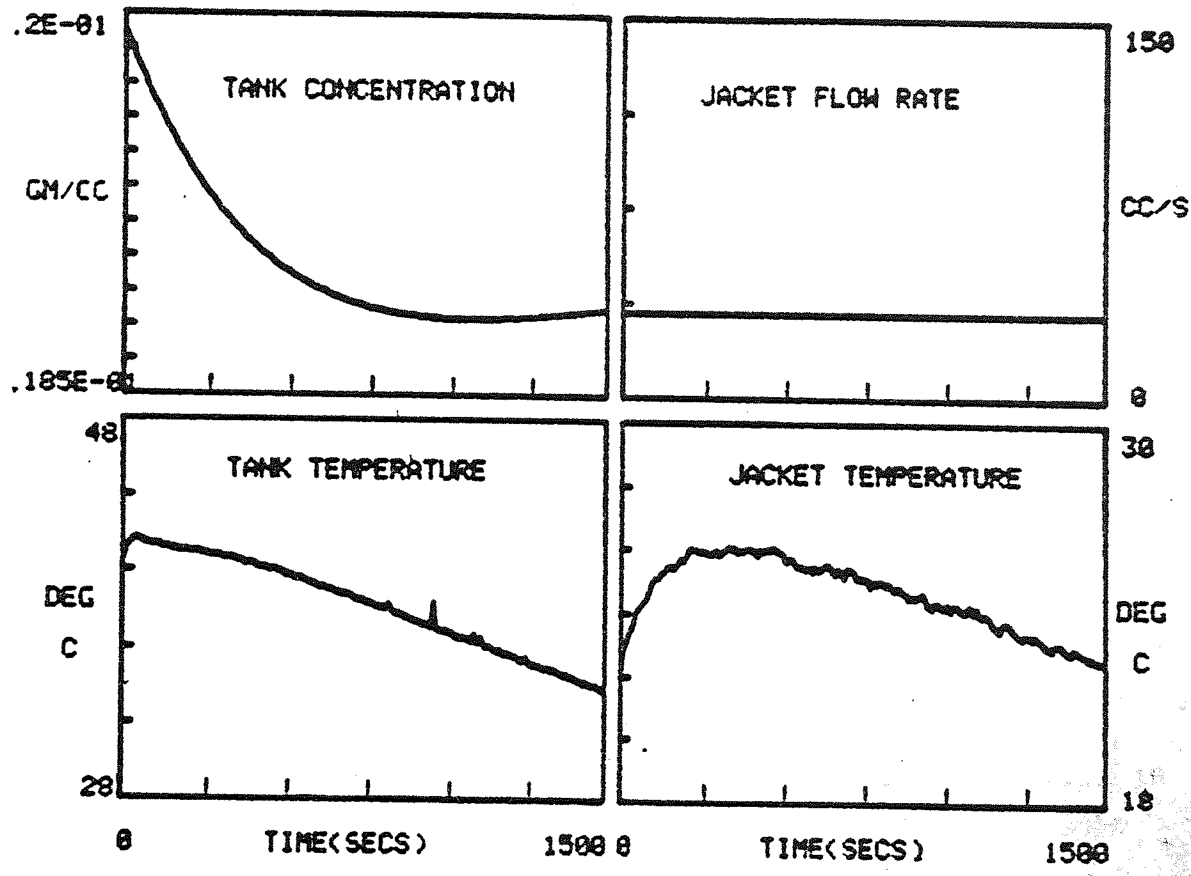


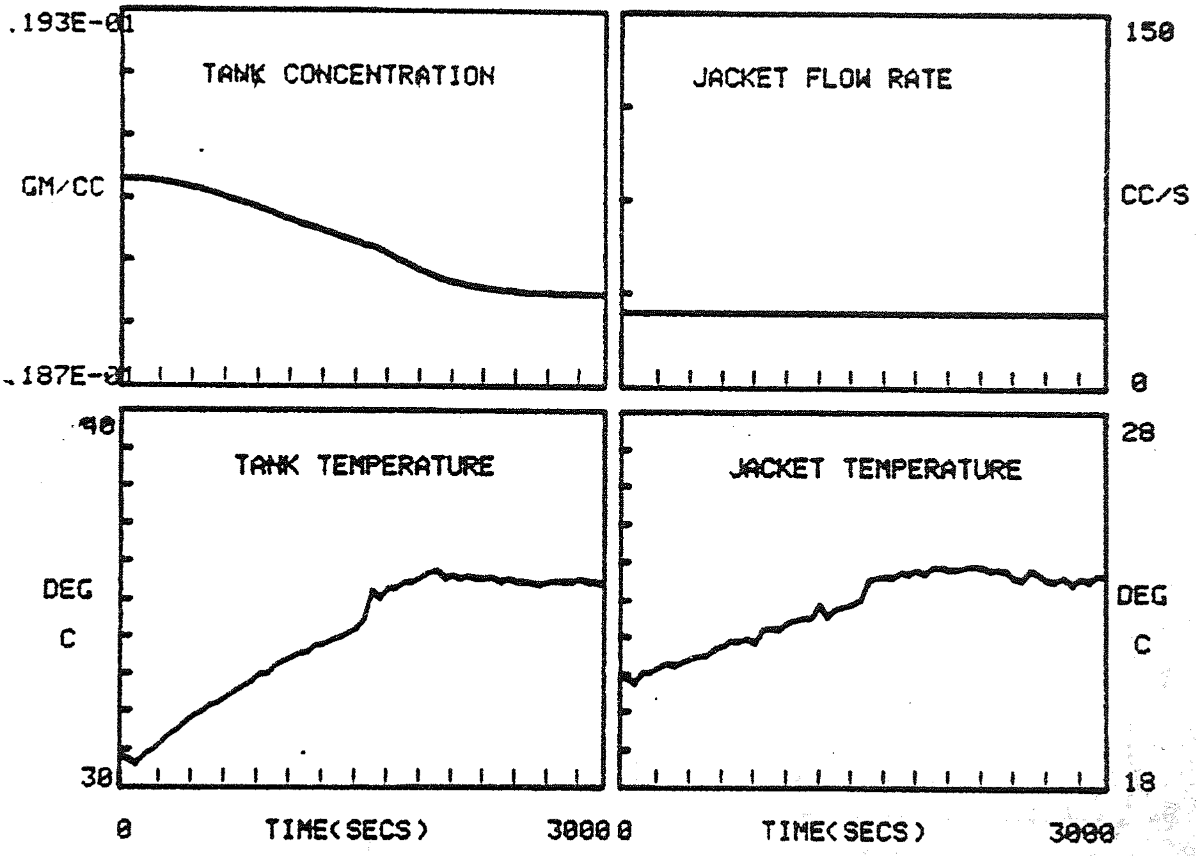
FIG. A.7.3 INVARIANCE TYPE CONTROL

G_V	=	valve transfer function
G_{p1}, G_{p2}	=	process transfer function
G_{m1} to G_{m5}	=	measuring element transfer function
G_{L1}, G_{L2}	=	load transfer function
G_{C1} to G_{C3}	=	controller transfer function



Reaction order = 2
Open loop studies
Initial perturbations in state variables

FIG.A.6.1.2 EXPERIMENT NO:2

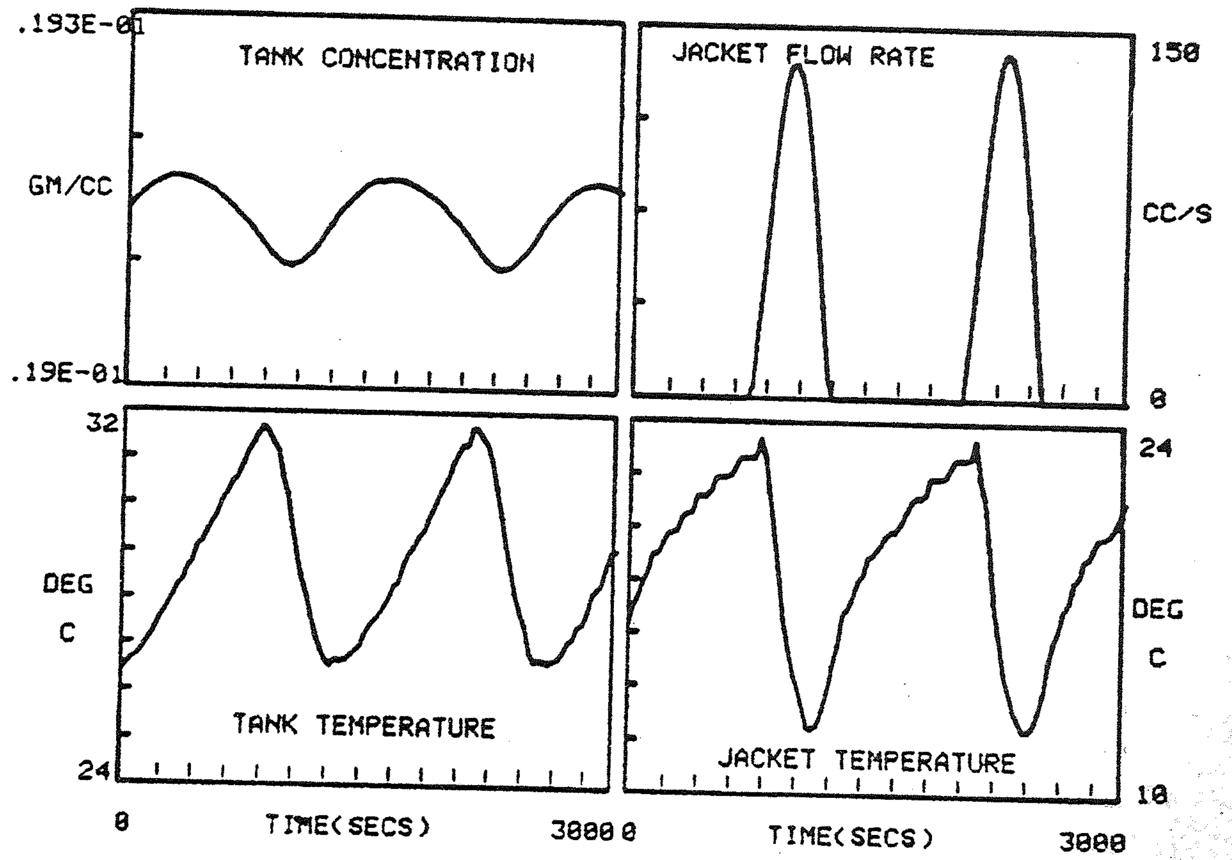


Reaction order = 2

Open loop studies

Step in tank inlet temperature = 2.5 K

FIG.A.6.1.3 EXPERIMENT NO:3

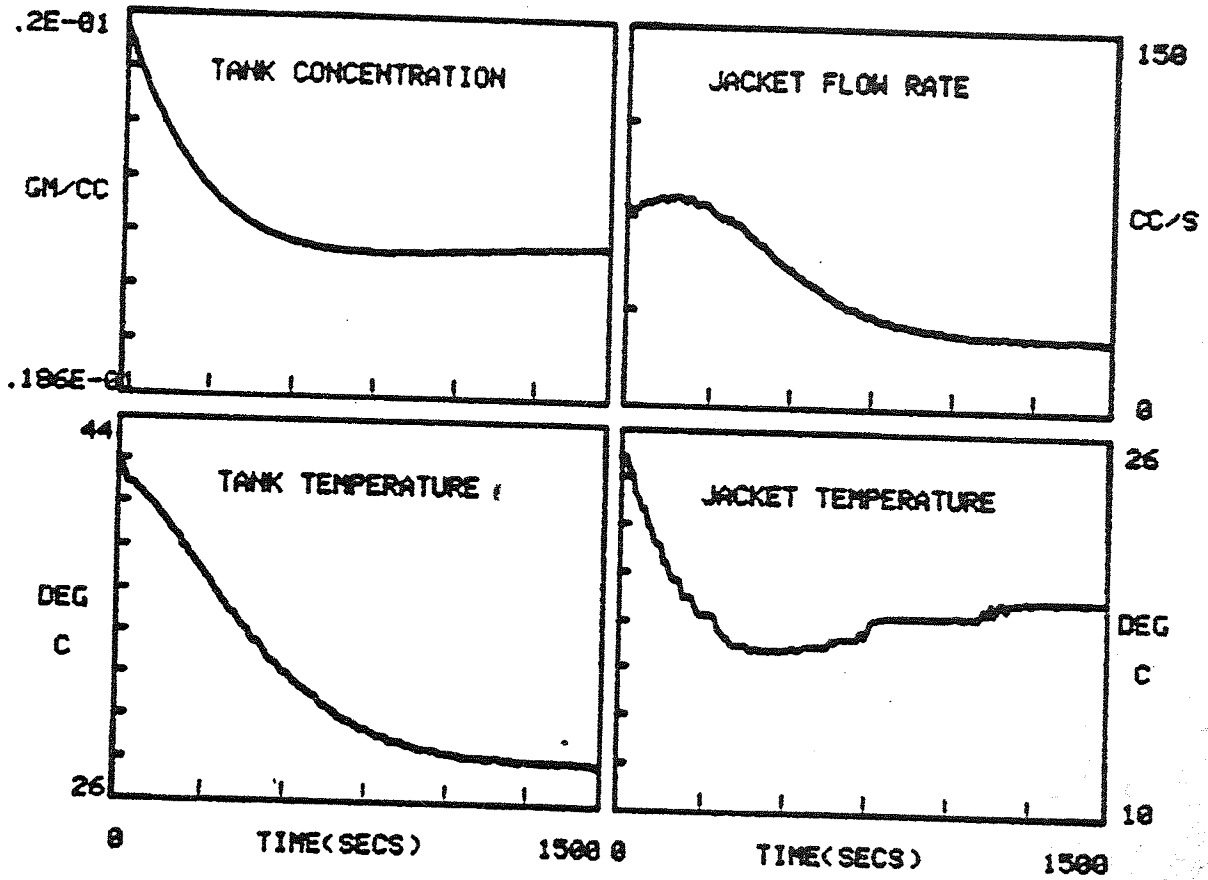


Reaction order = 2

Limit-cycle around open loop stable operating point

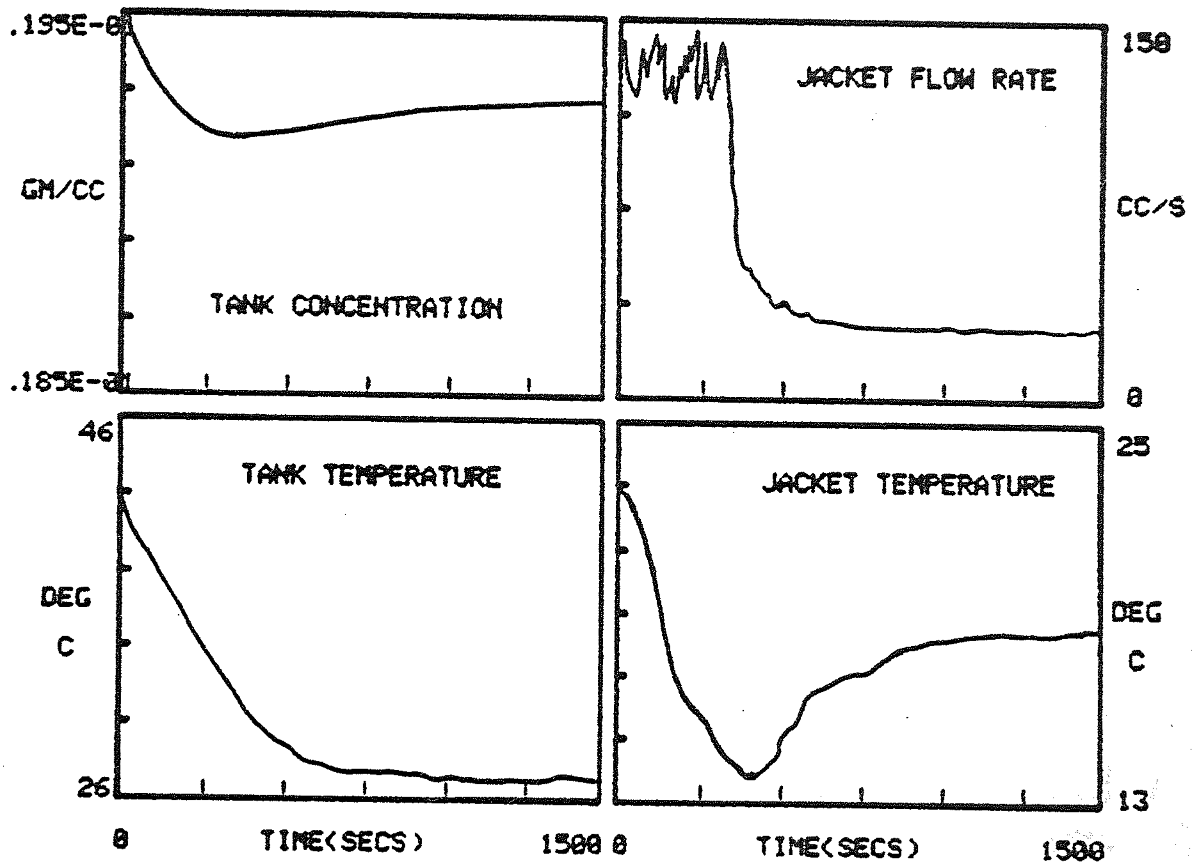
Gain (K_c=0.09)

FIG.A.6.1.4 EXPERIMENT NO:4



Reaction order = 2
Controller equation derived from stablity conditions(eqn.(3.38))
Initial perturbations in state variables

FIG.A.6.1.5 EXPERIMENT NO:5

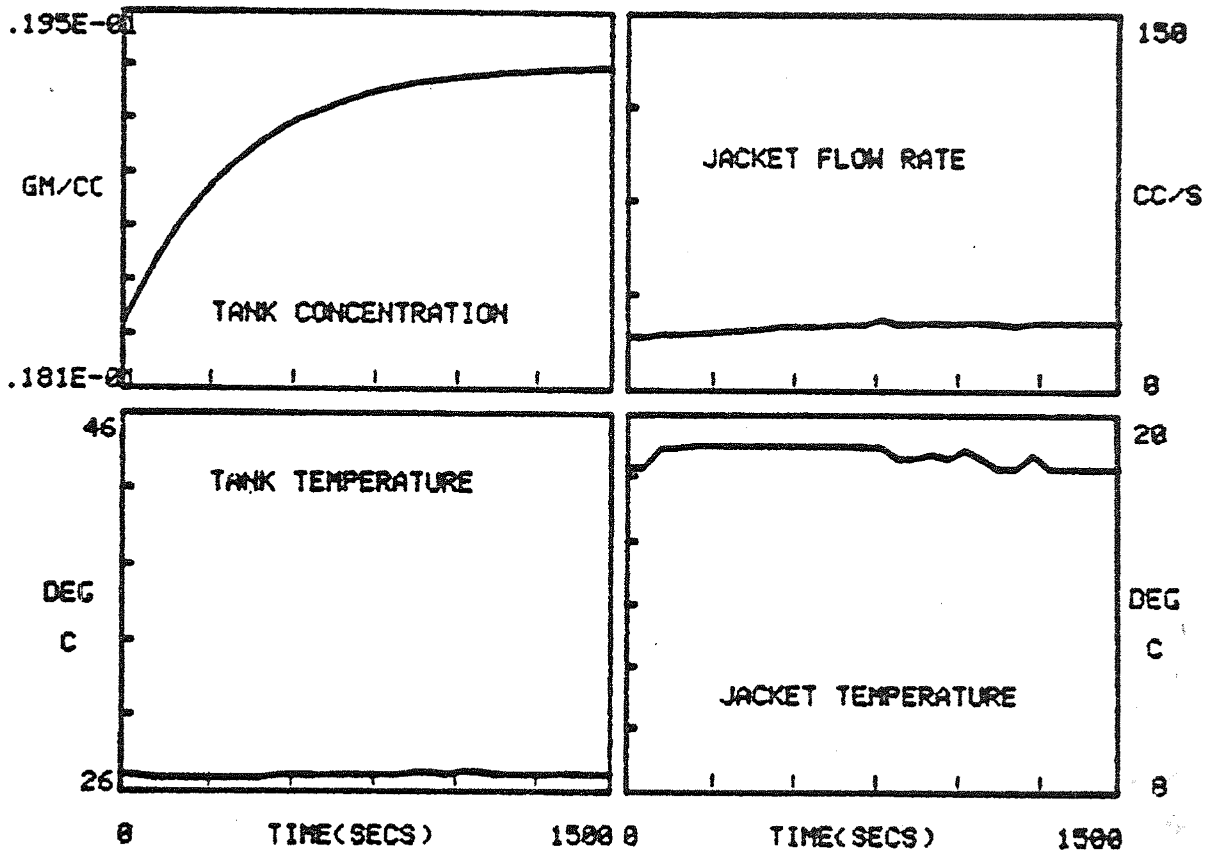


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.6 EXPERIMENT NO:6

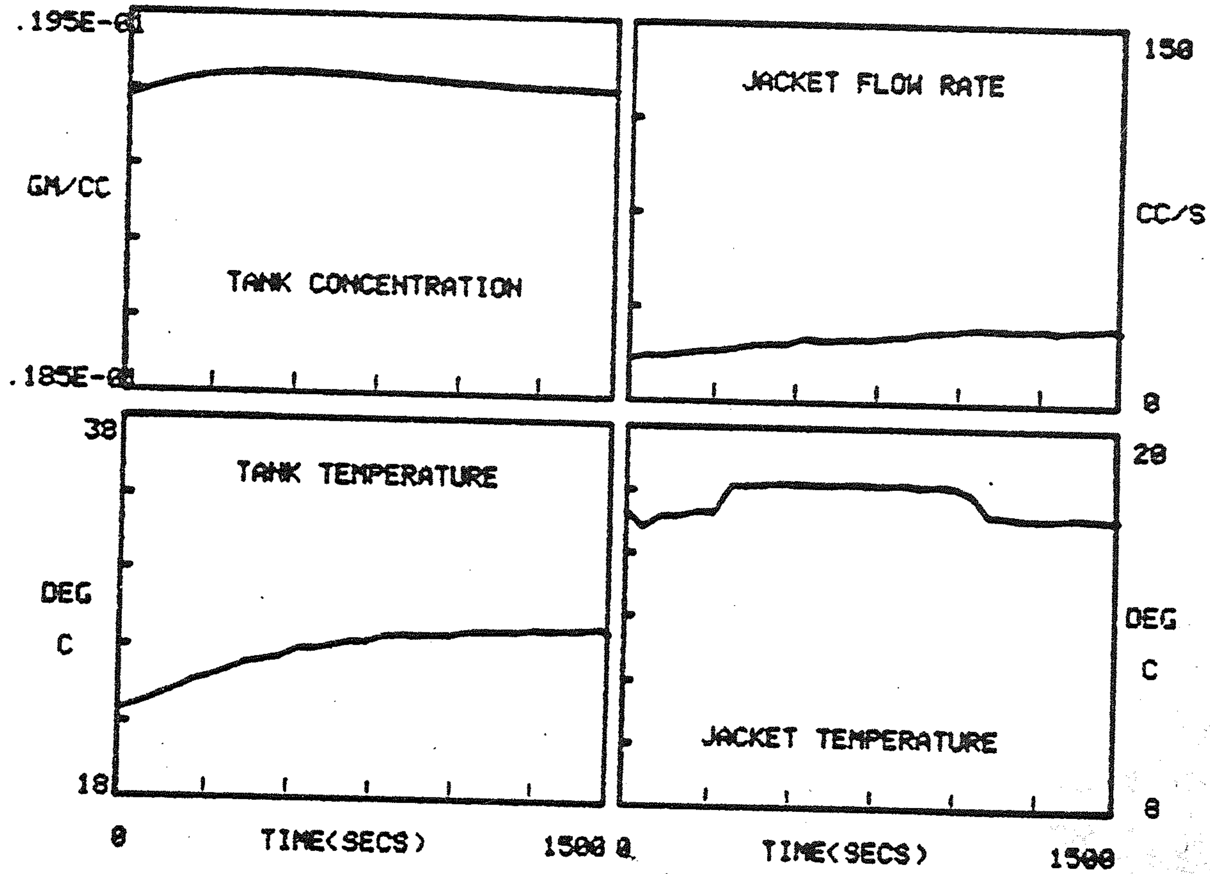


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.7 EXPERIMENT NO:7

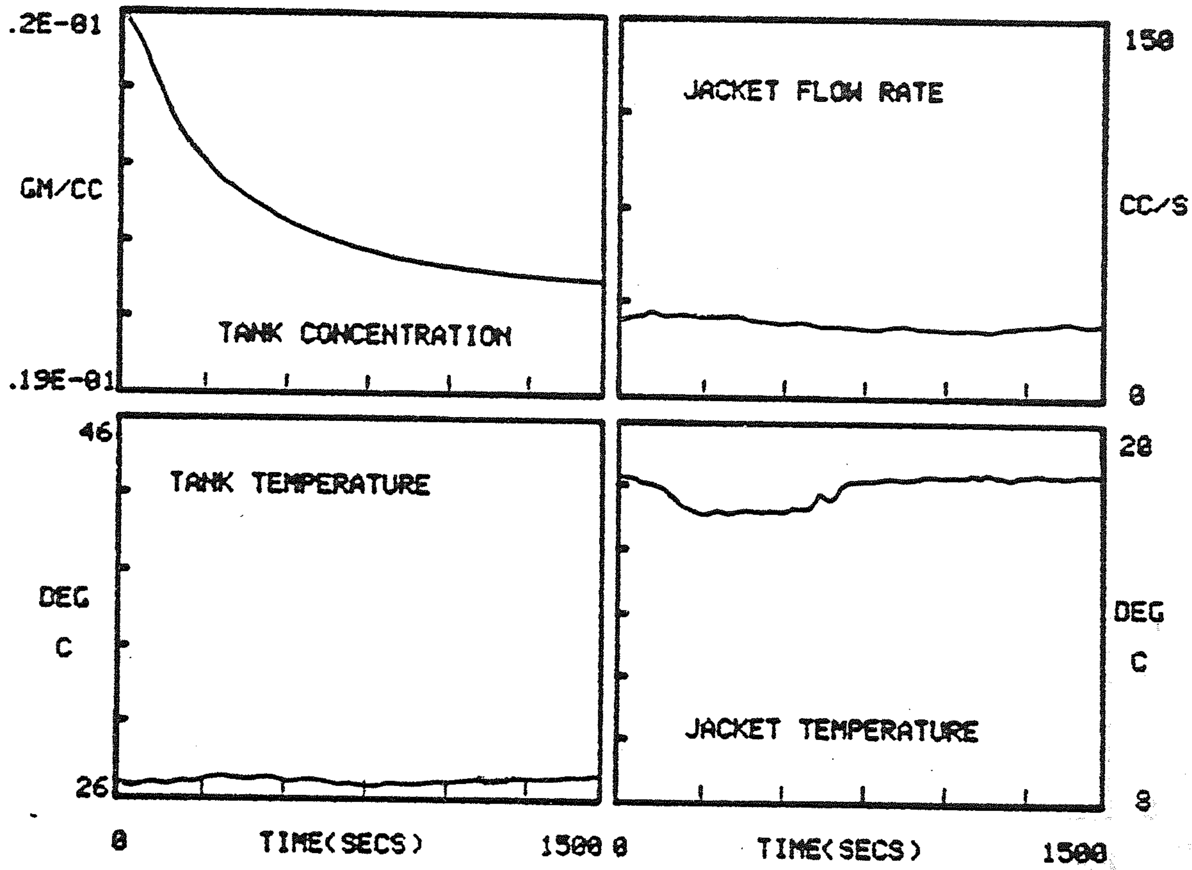


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.8 EXPERIMENT NO:8

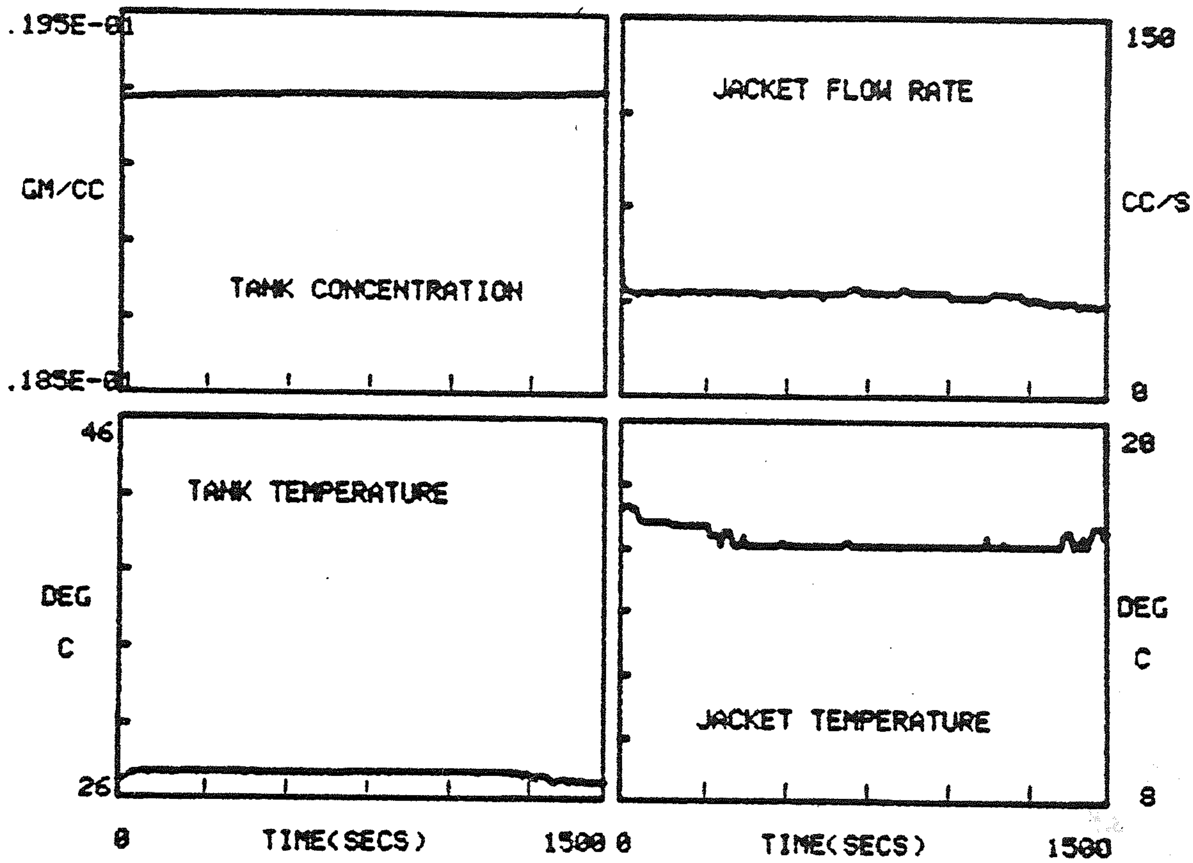


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.9 EXPERIMENT NO:9

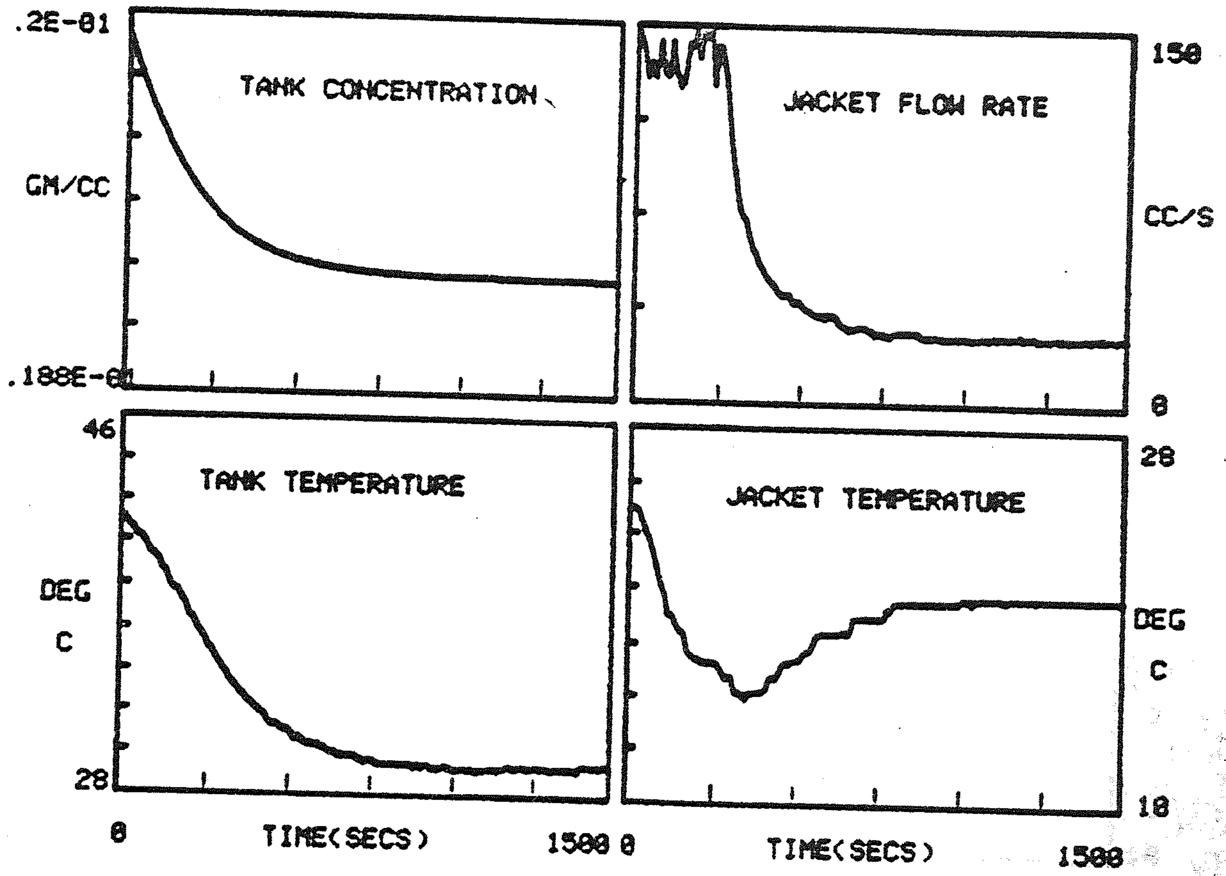


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.007)

Step in tank inlet temperature = 3 K

FIG.A.6.1.10 EXPERIMENT NO:10

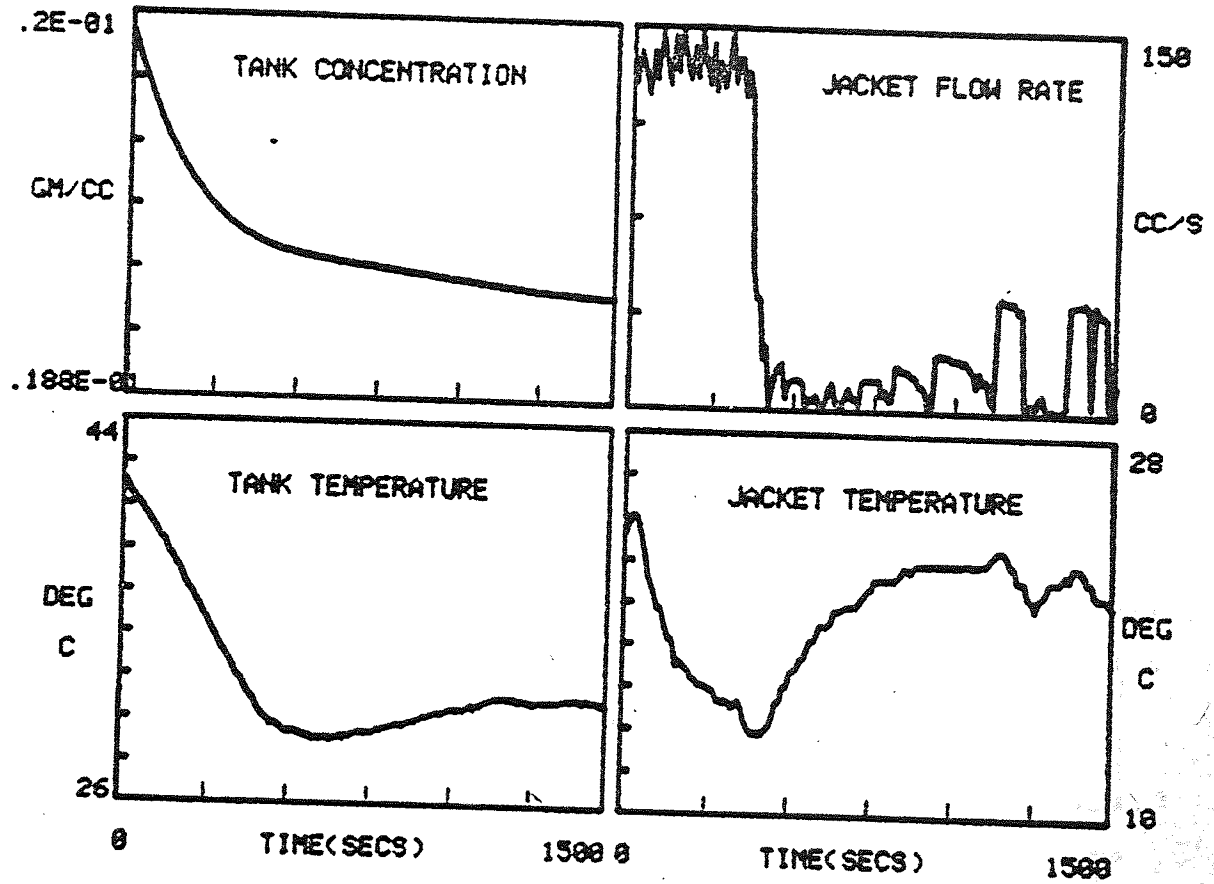


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.005)

Initial perturbations in state variables

FIG.A.6.1.11 EXPERIMENT NO:11

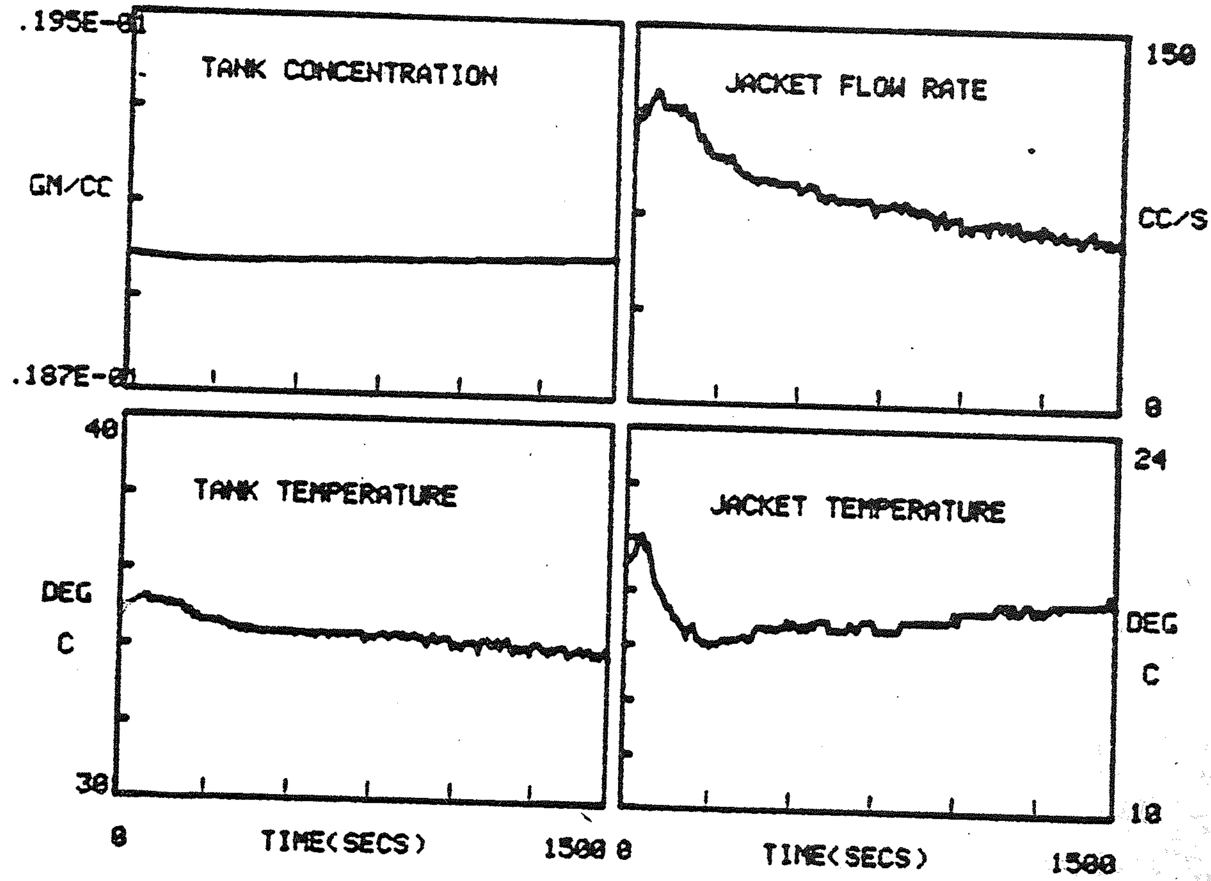


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.015)

Initial perturbations in state variables

FIG.A.6.1.12 EXPERIMENT NO:12

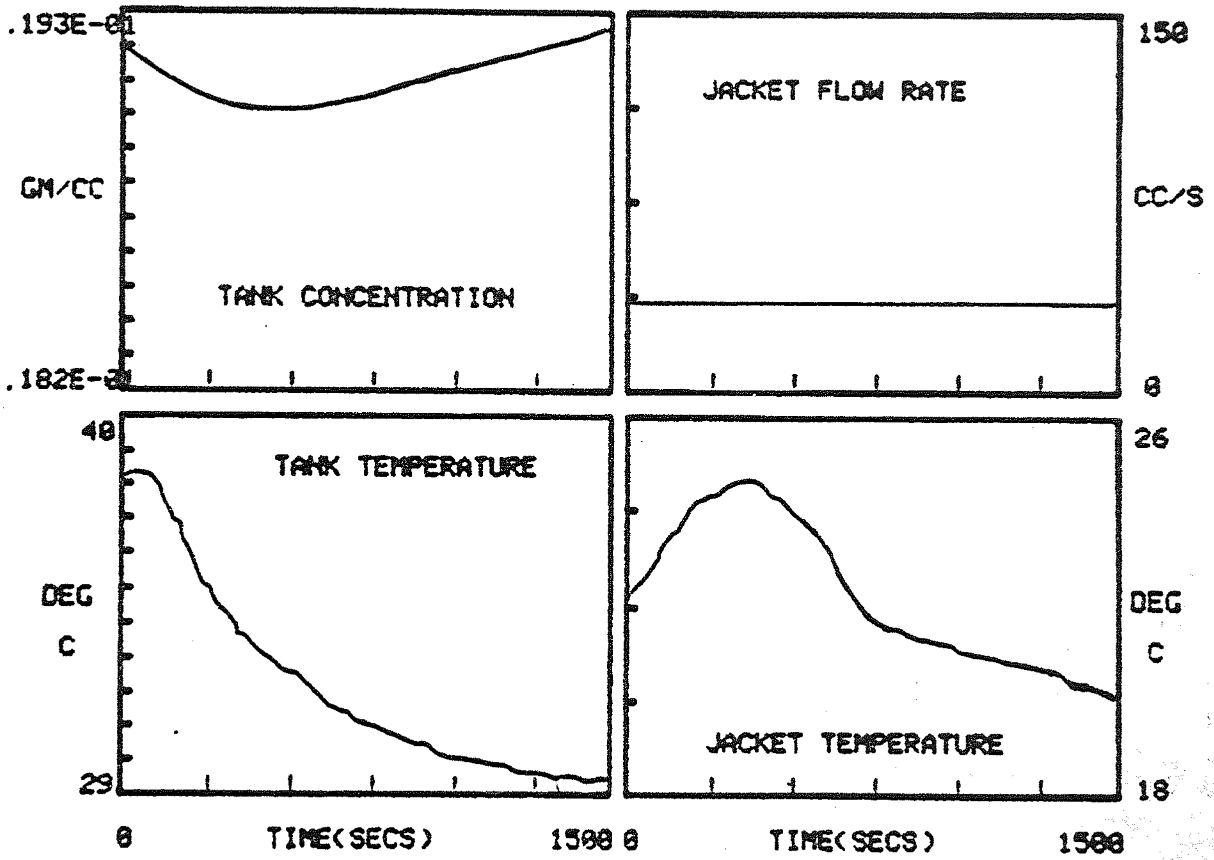


Reaction order = 2

Decoupling type control of tank temperature(D_{max}=.007)

Step in tank inlet temperature =4.75 K

FIG.A.6.1.13 EXPERIMENT NO:13

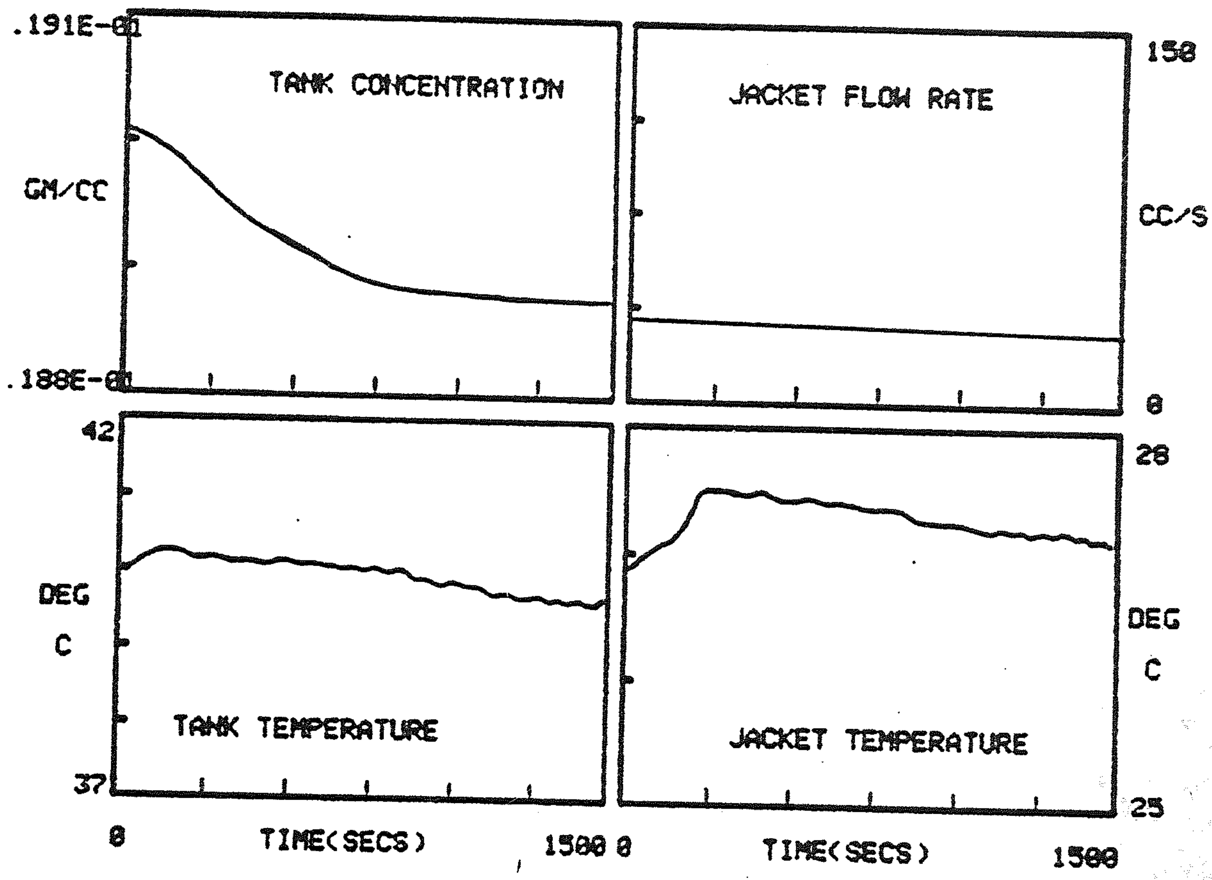


Reaction order = 1

Open loop studies

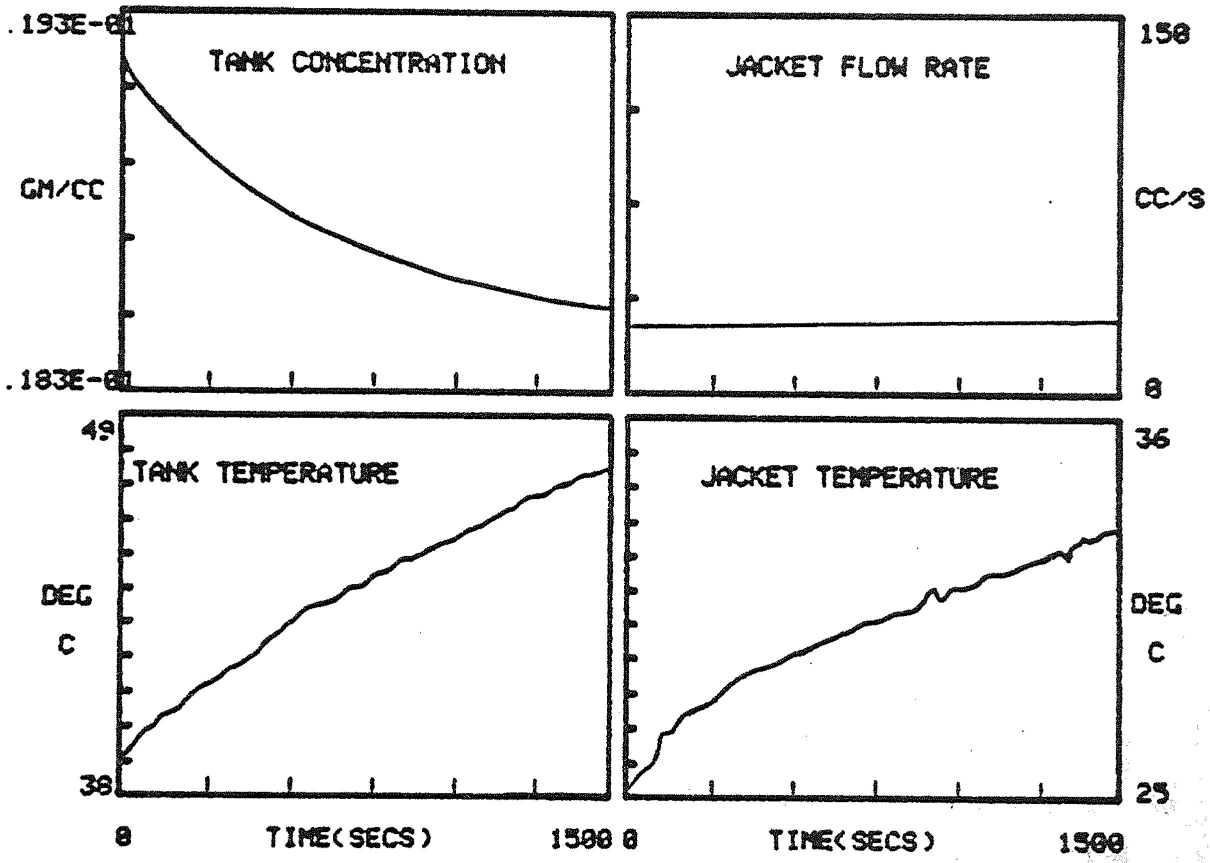
Initial perturbations in state variables

FIG.A.6.1.14 EXPERIMENT NO:14



Reaction order = 1
Open loop studies
Initial perturbations in state variables

FIG.A.6.1.15 EXPERIMENT NO:15

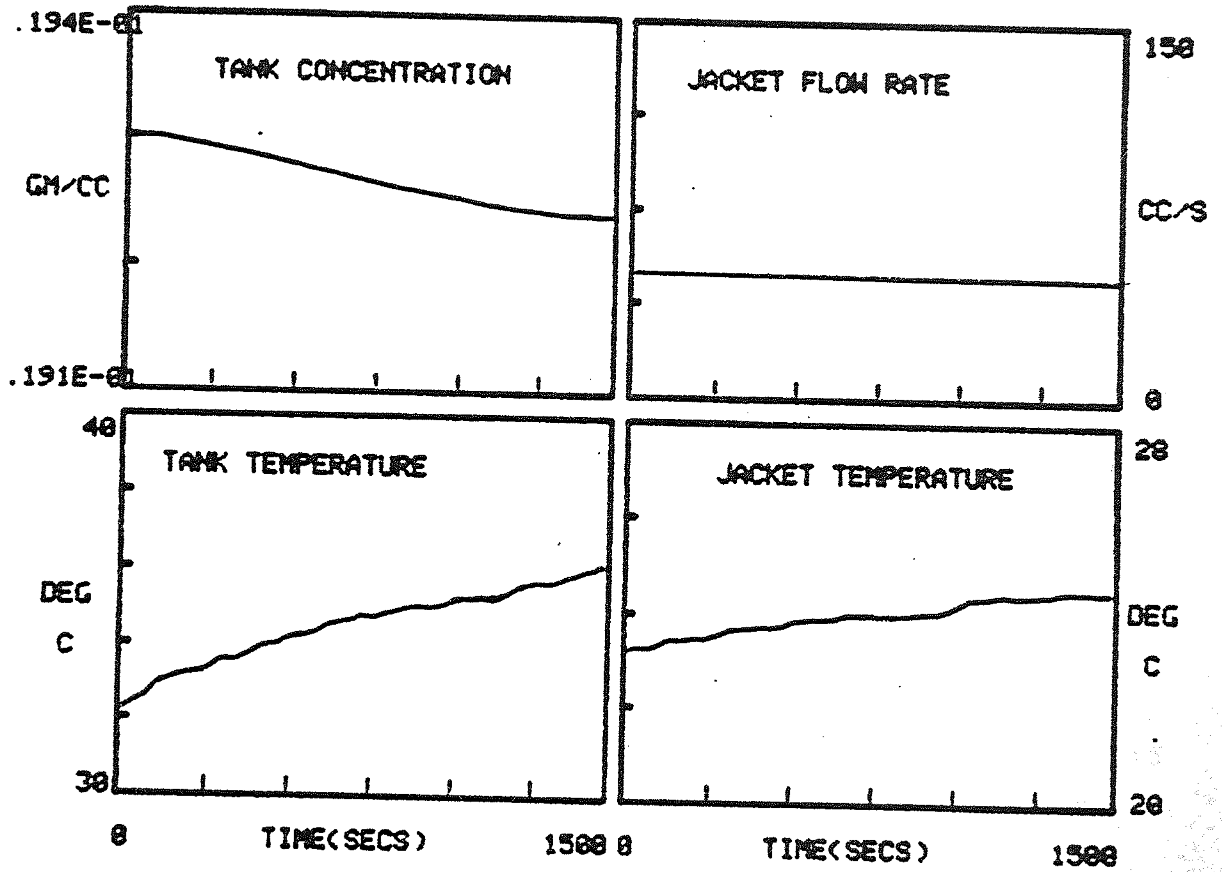


Reaction order = 1

Open loop studies

Initial perturbations in state variables

FIG.A.6.1.16 EXPERIMENT NO:16

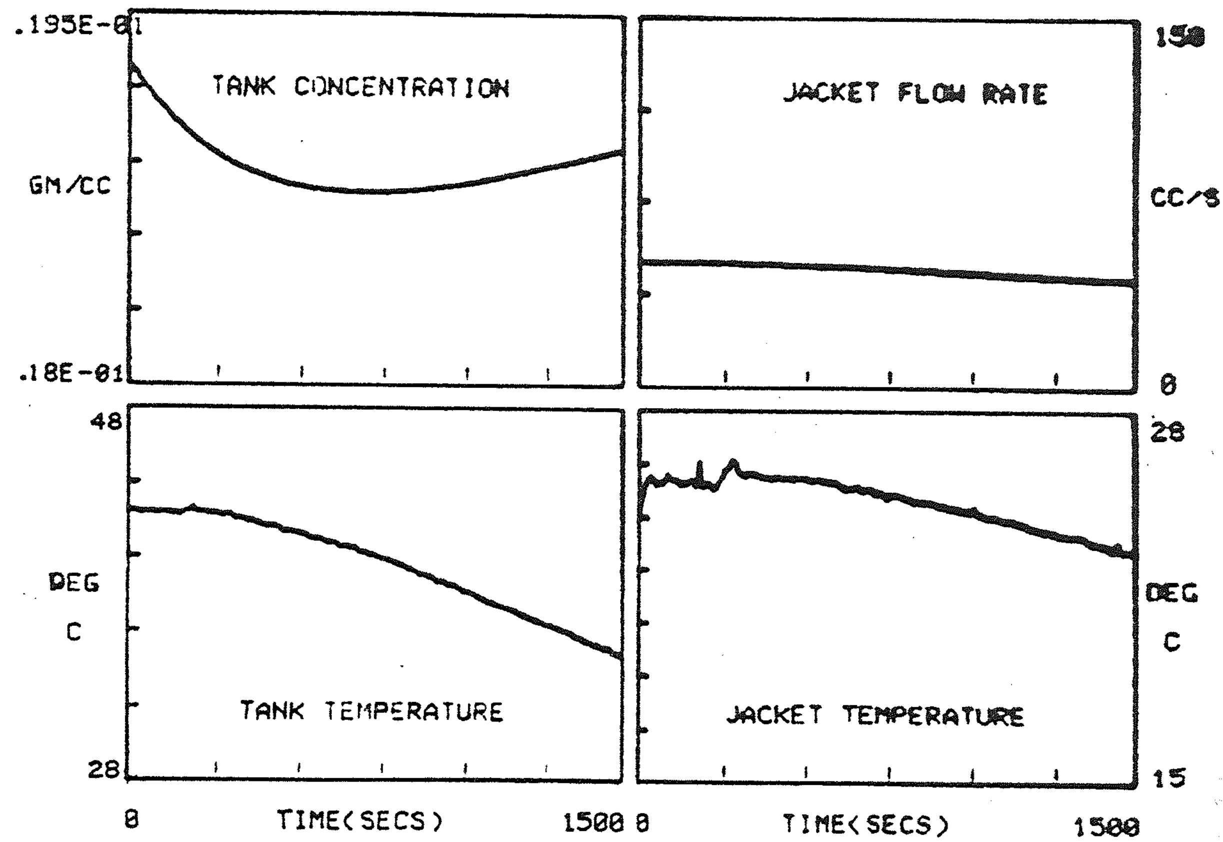


Reaction order = 1

Open loop studies

Step in tank inlet temperature = 2.75 K

FIG.A.6.1.17 EXPERIMENT NO:17

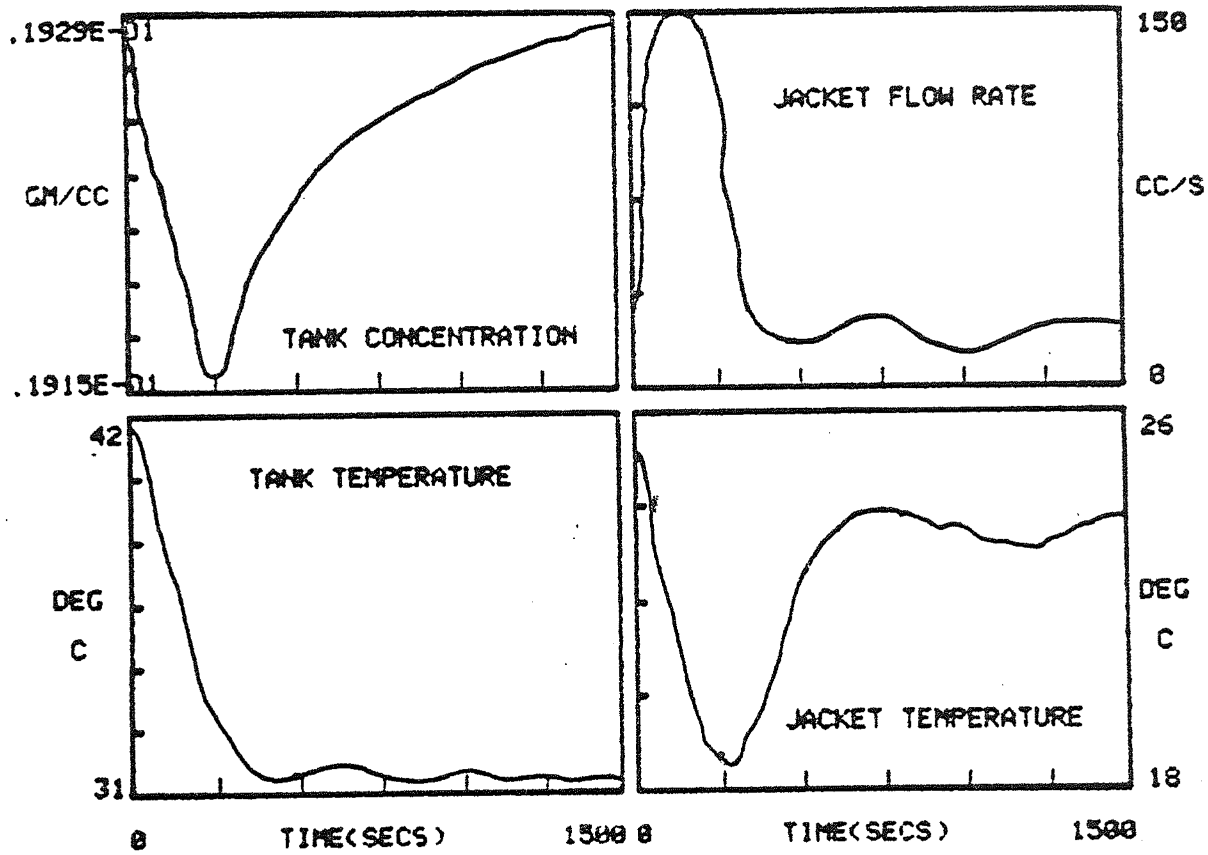


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.0005)

Initial perturbations in state variables

FIG.A.6.1.18 EXPERIMENT NO:18

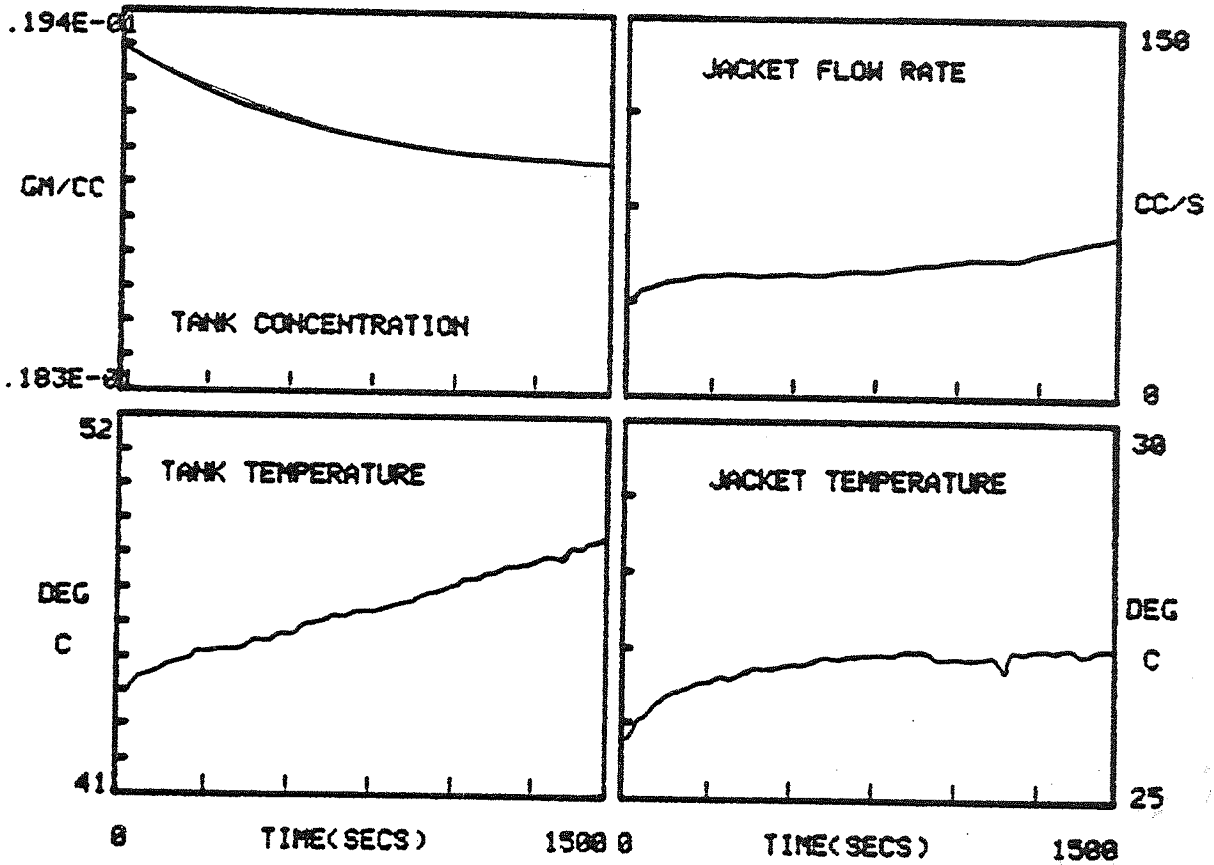


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.03)

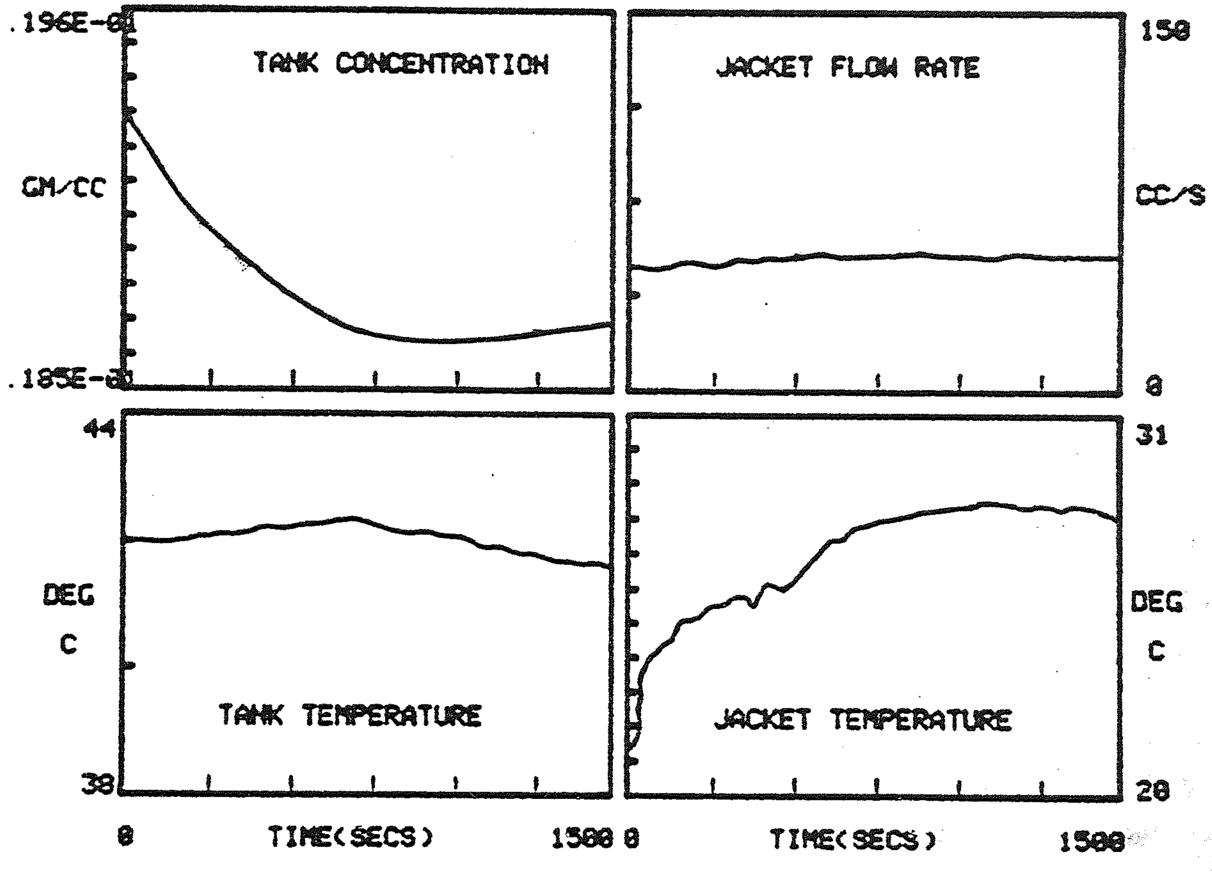
Initial perturbations in state variables

FIG.A.6.1.19 EXPERIMENT NO:19



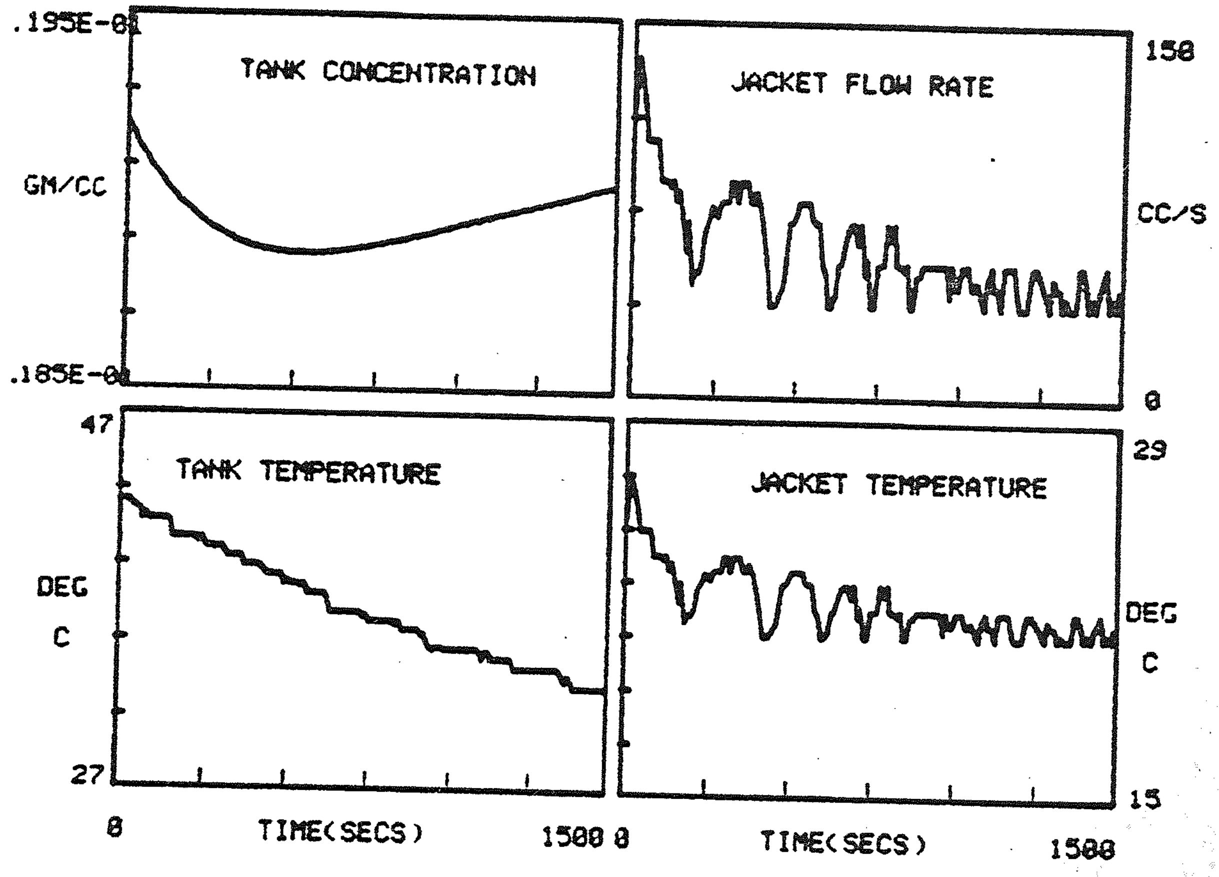
Reaction order = 1
Proportional feedback control of tank temperature(K_c=.0005)
Initial perturbations in state variables

FIG.A.6.1.20 EXPERIMENT NO:20



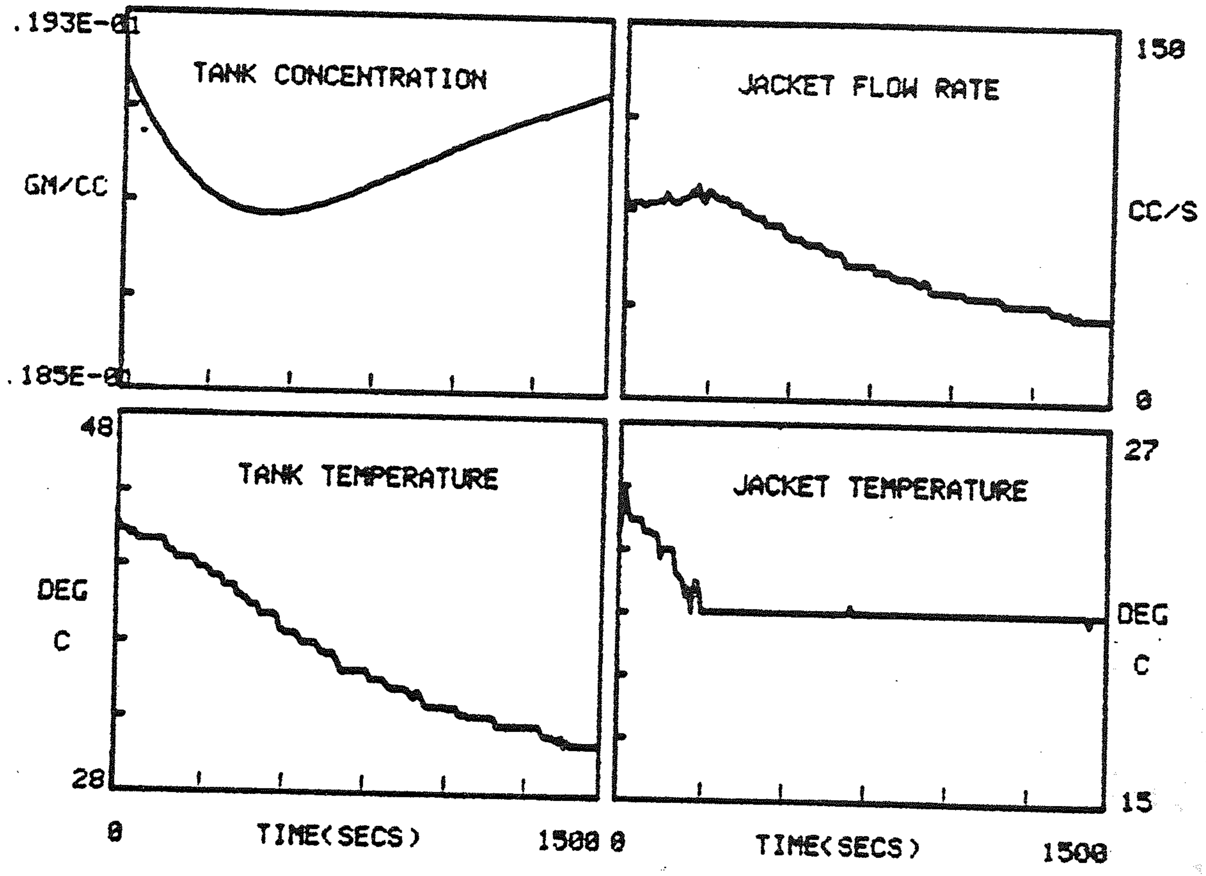
Reaction order = 1
Proportional feedback control of jacket temperature(K_c=.001)
Initial perturbations in state variables

FIG.A.6.1.21 EXPERIMENT NO:21



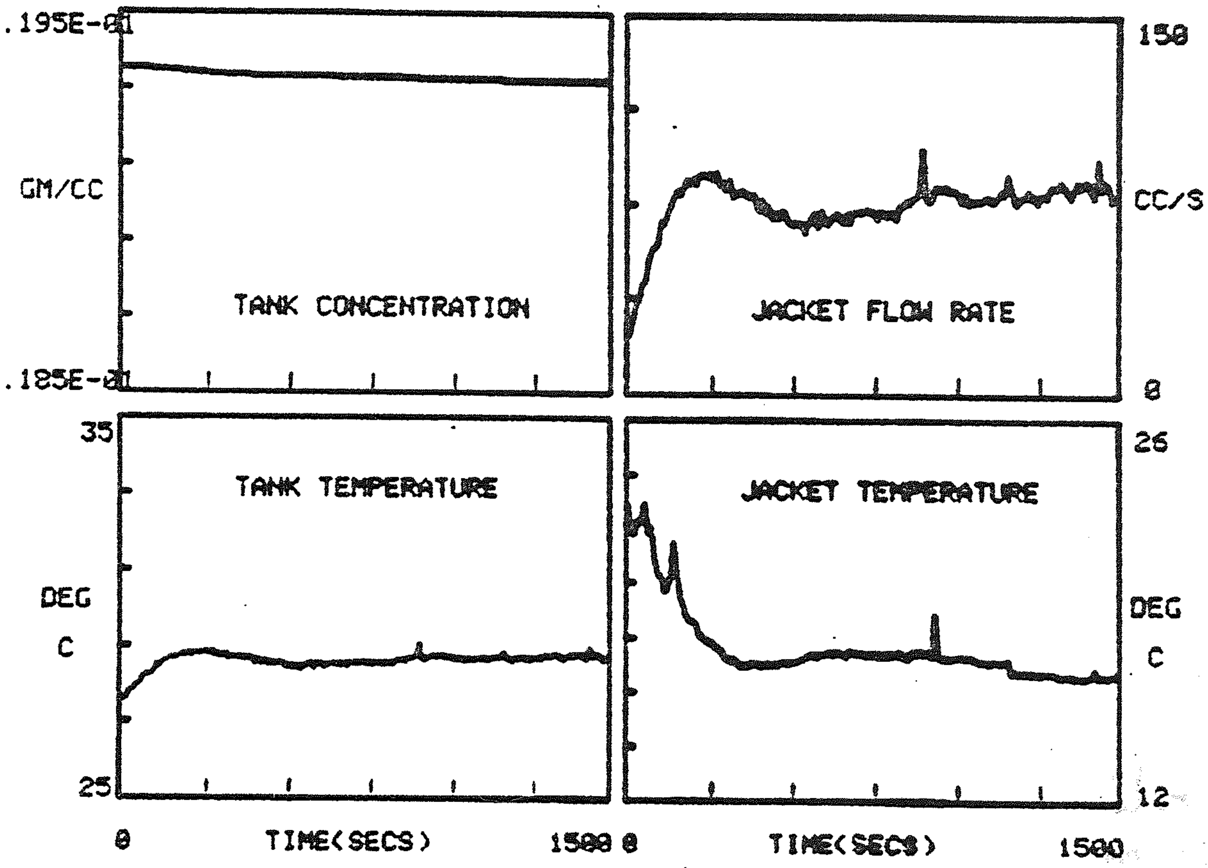
Reaction order = 1
Proportional feedback control of jacket temperature(K_c=.01)
Initial perturbations in state variables

FIG.A.6.1.22 EXPERIMENT NO:22



Reaction order = 1
Controller equation derived from stability conditions(eqn.(3.38))
Initial perturbations in state variables

FIG.A.6.1.23 EXPERIMENT NO:23

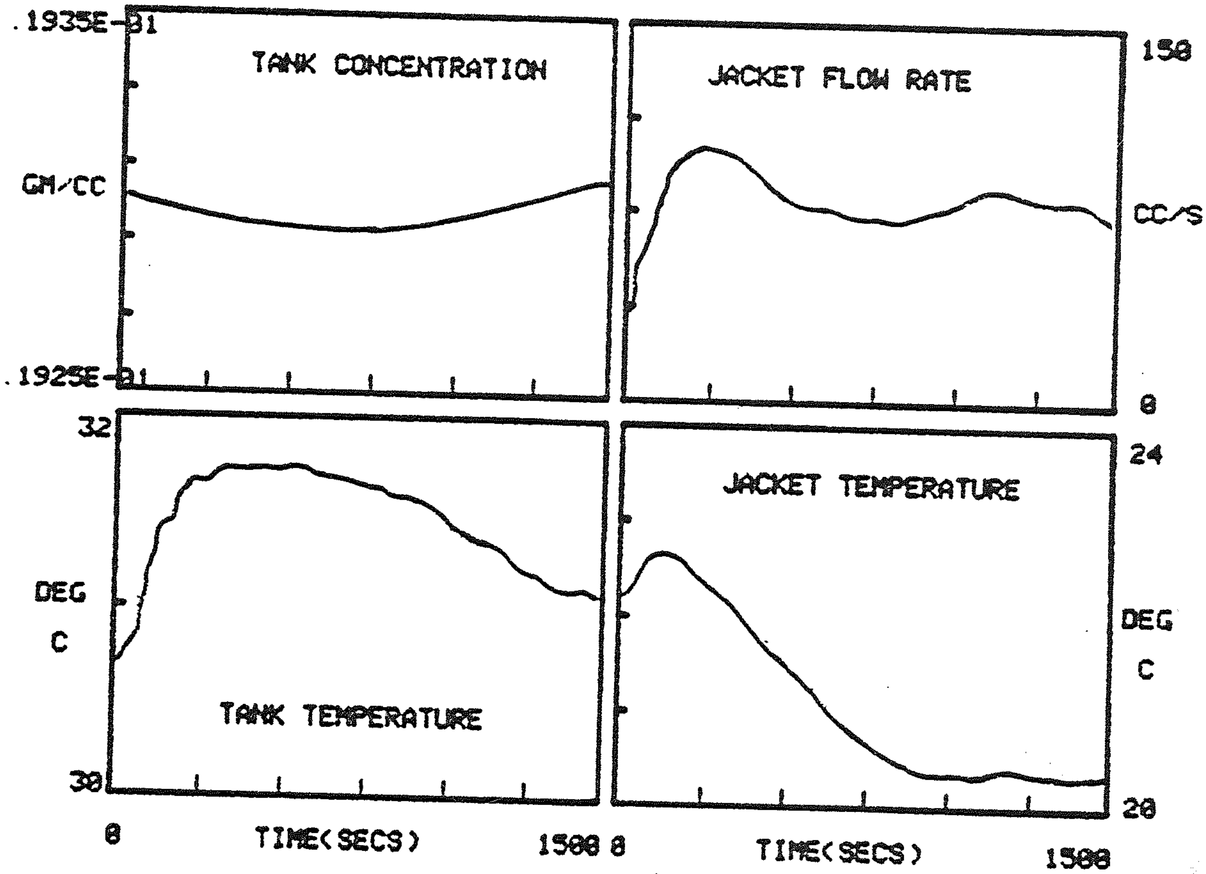


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.03)

Step in tank inlet temperature = 4.6 K

FIG.A.6.1.24 EXPERIMENT NO:24

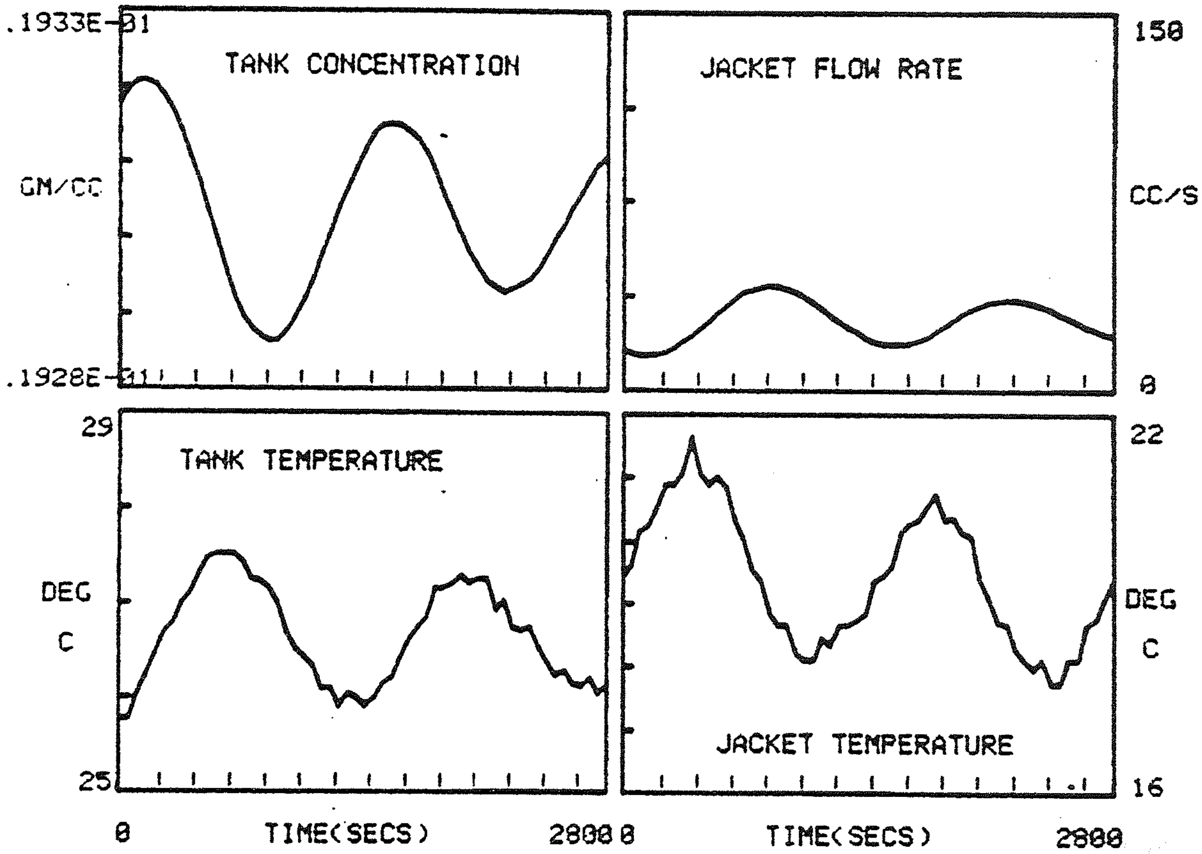


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.05)

Step in tank inlet temperature = 3.5 K

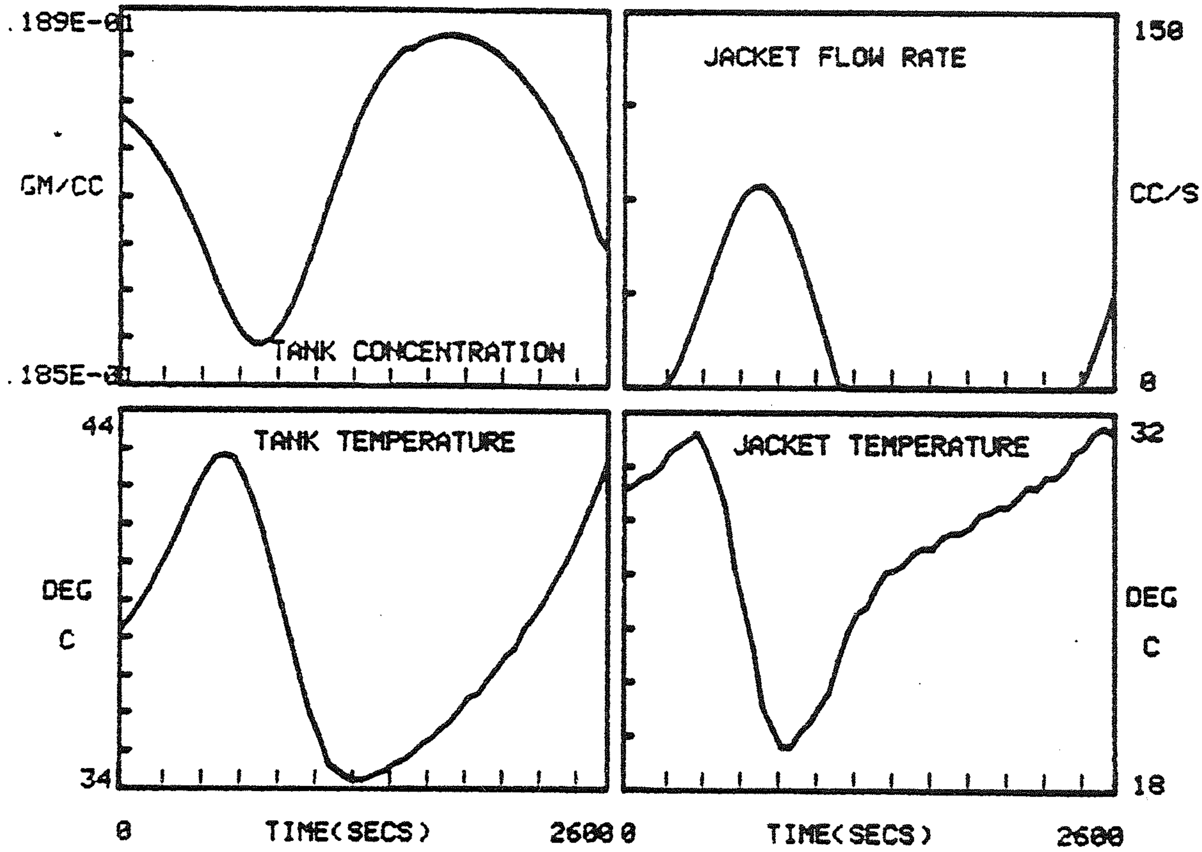
FIG.A.6.1.25 EXPERIMENT NO:25



Reaction order = 1

Limit-cycle behaviour around open loop stable operating point(K_c=.016)

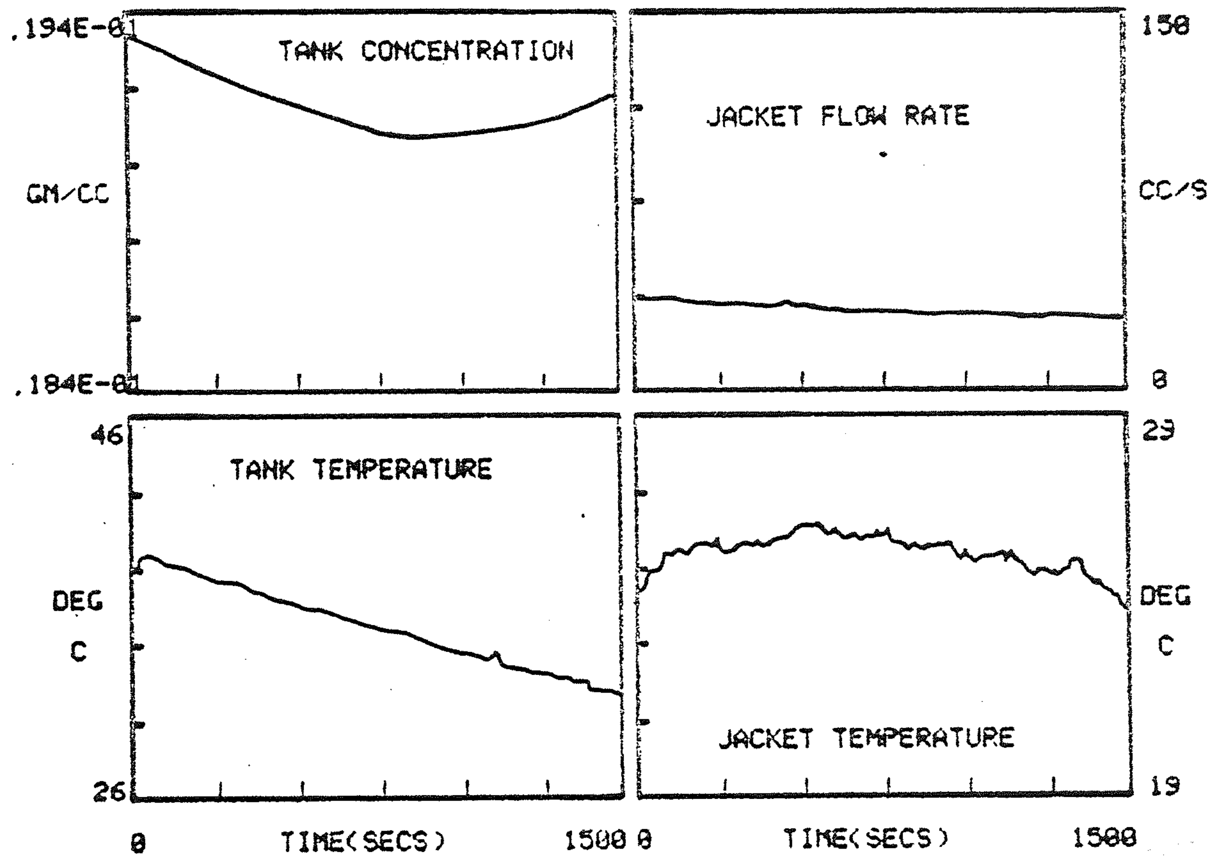
FIG.A.6.1.26 EXPERIMENT NO:26



Reaction order = 1

Limit-cycle behaviour around open loop unstable operating point(K_c=.0086)

FIG.A.6.1.27 EXPERIMENT NO:27

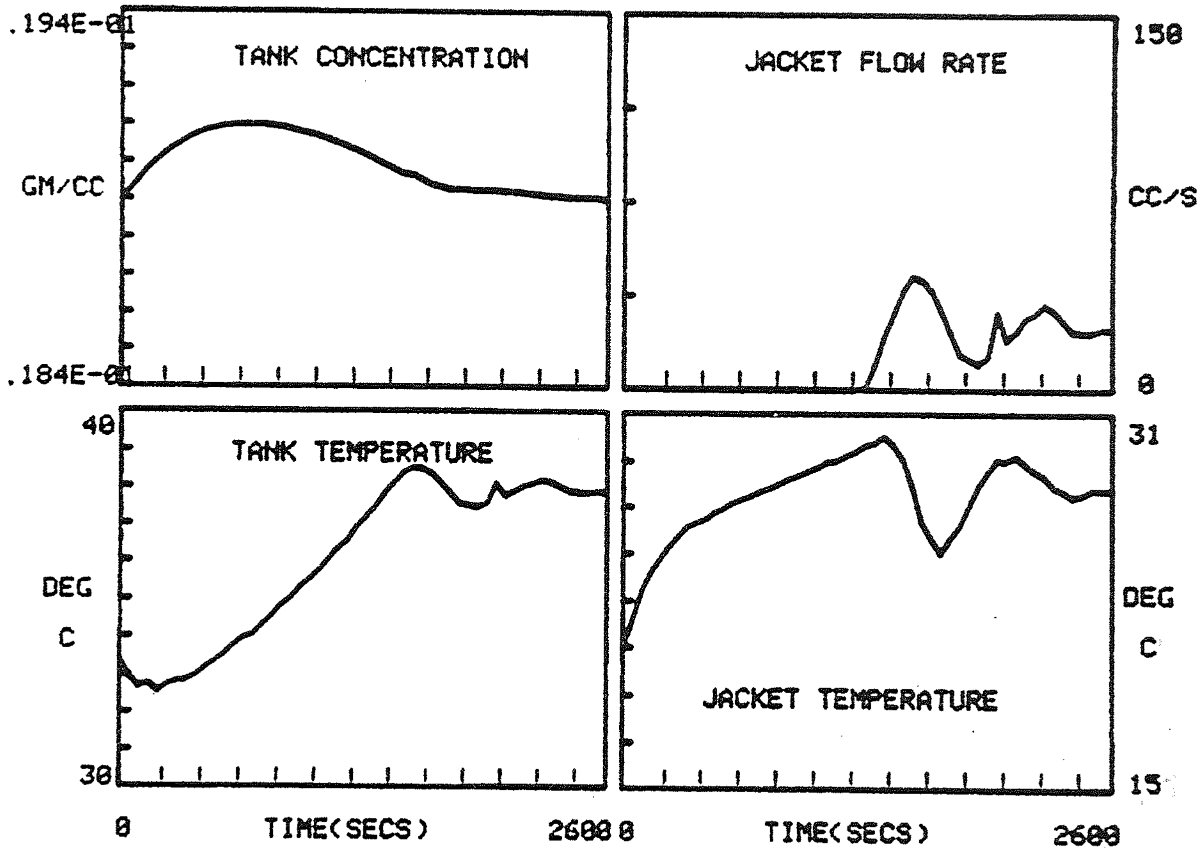


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.0005)

Stabilising open loop unstable operating point

FIG.A.6.1.28 EXPERIMENT NO:28

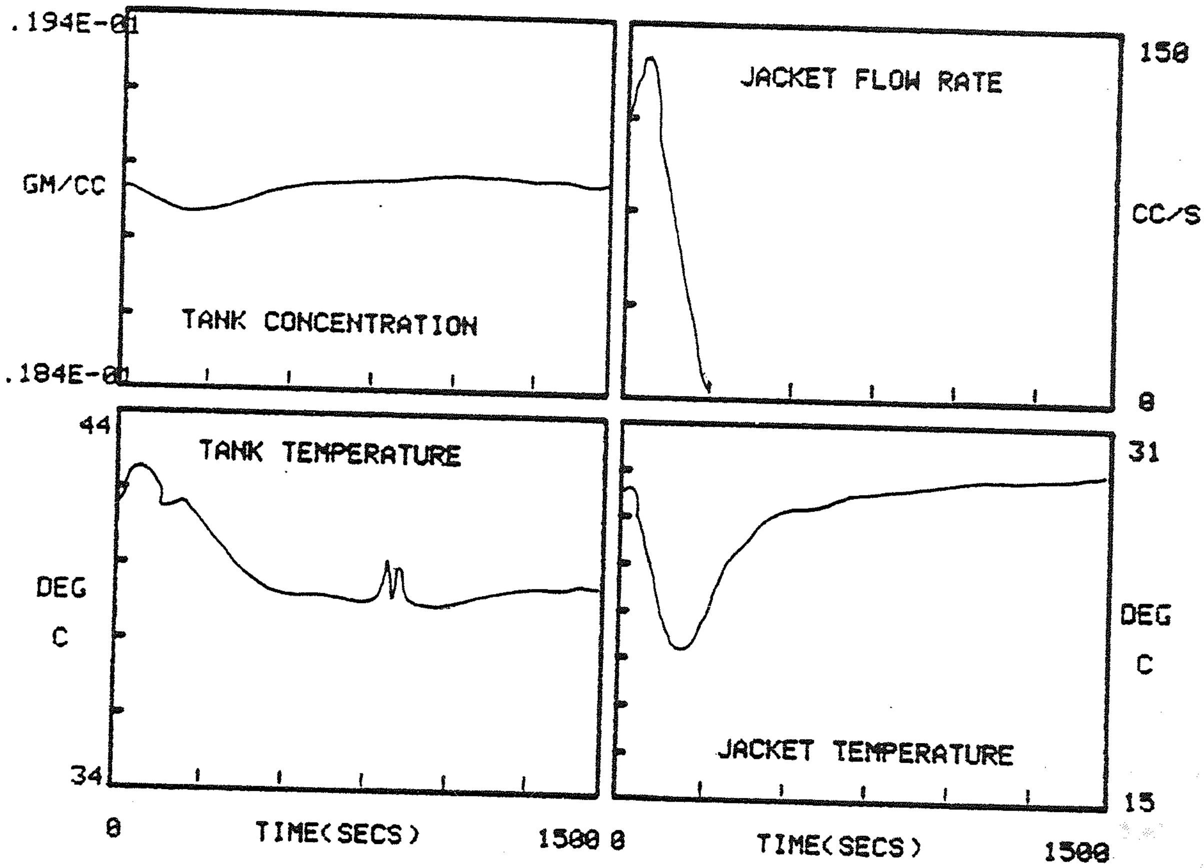


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.02)

Stabilising open loop unstable operating point

FIG.A.6.1.29 EXPERIMENT NO:29

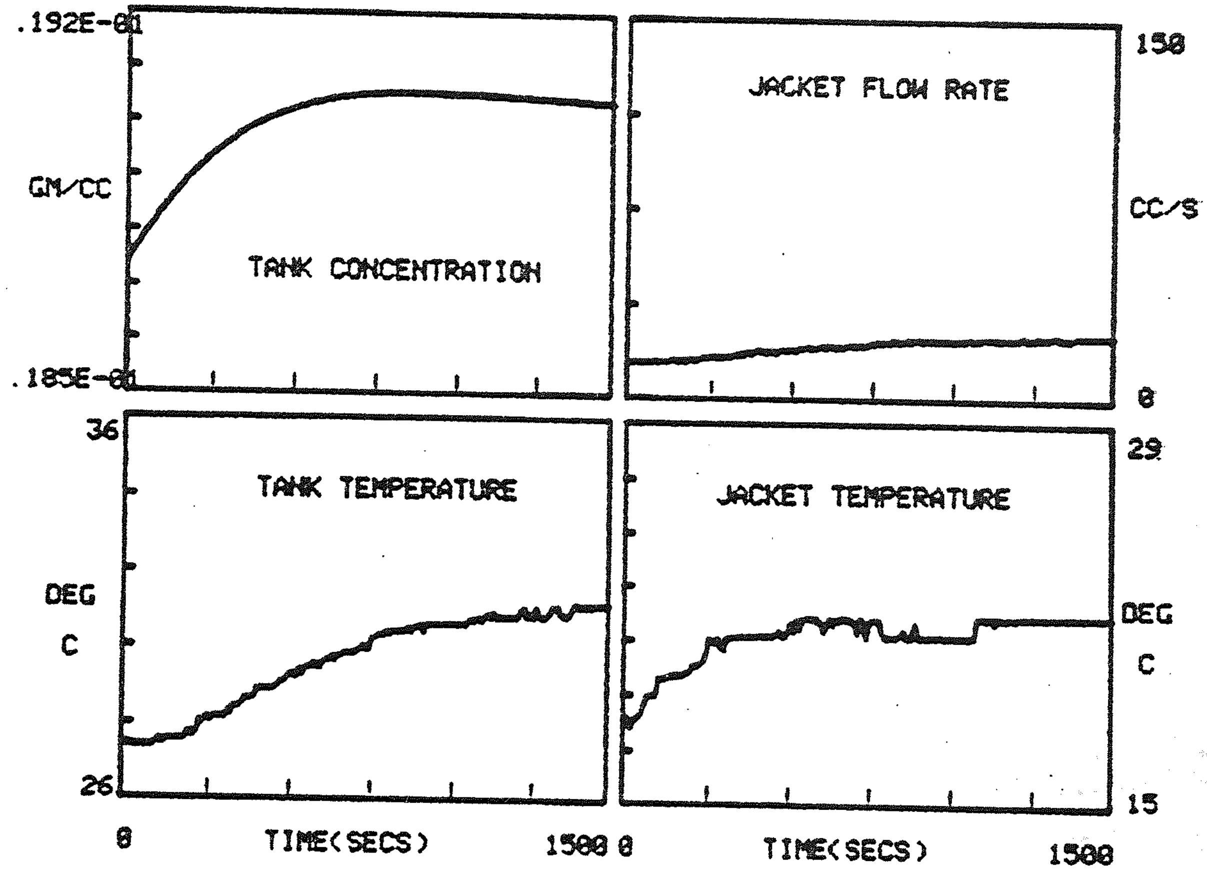


Reaction order = 1

Proportional feedback control of tank temperature(K_c=.02)

Stabilising open loop unstable operating point

FIG.A.6.1.30 EXPERIMENT NO:30



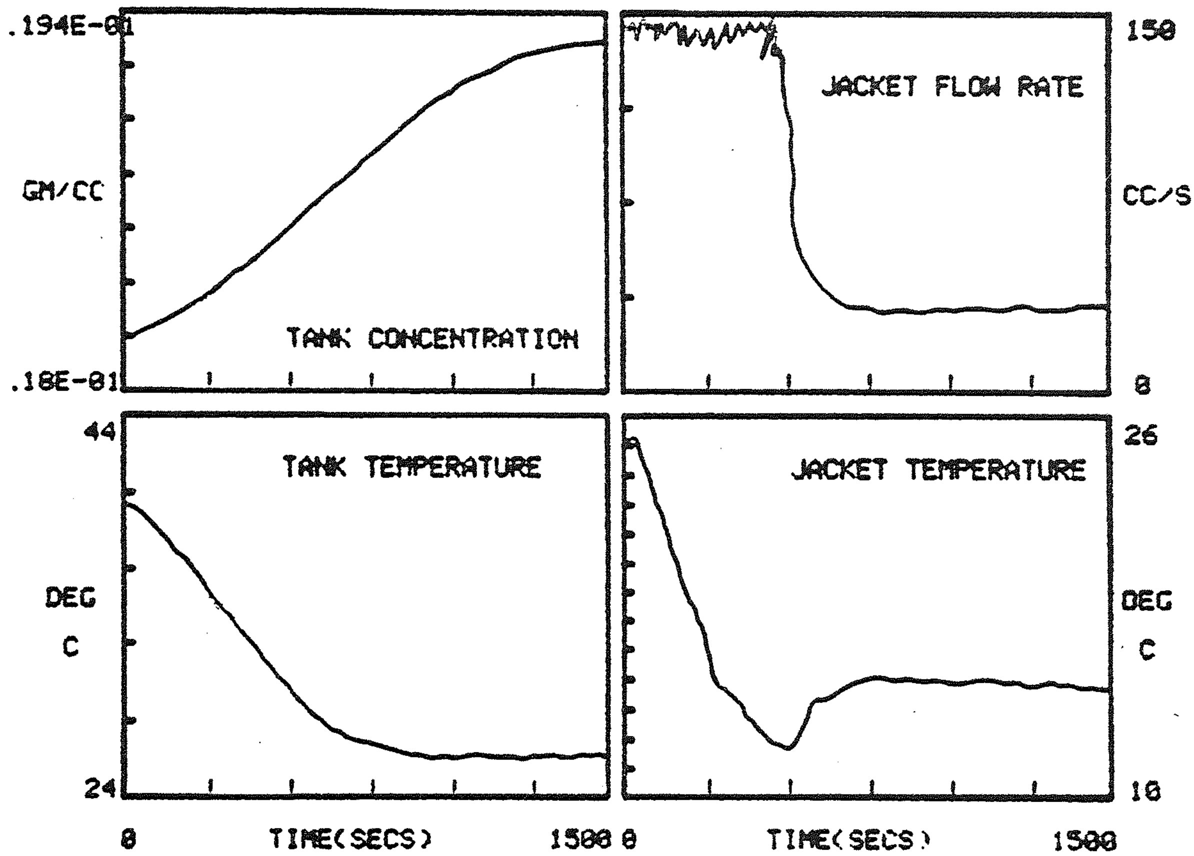
Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

Stabilising open loop unstable operating point

FIG.A.6.1.31 EXPERIMENT NO:31

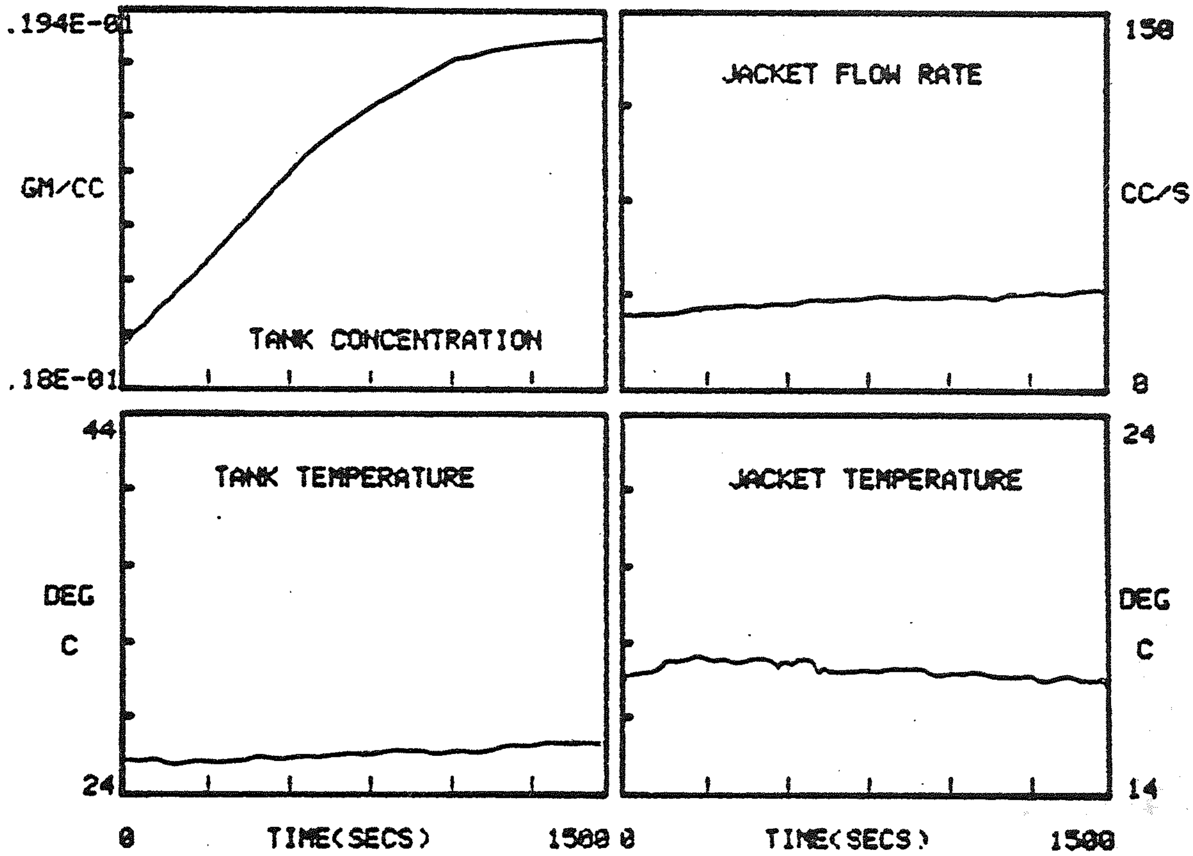


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.32 EXPERIMENT NO:32

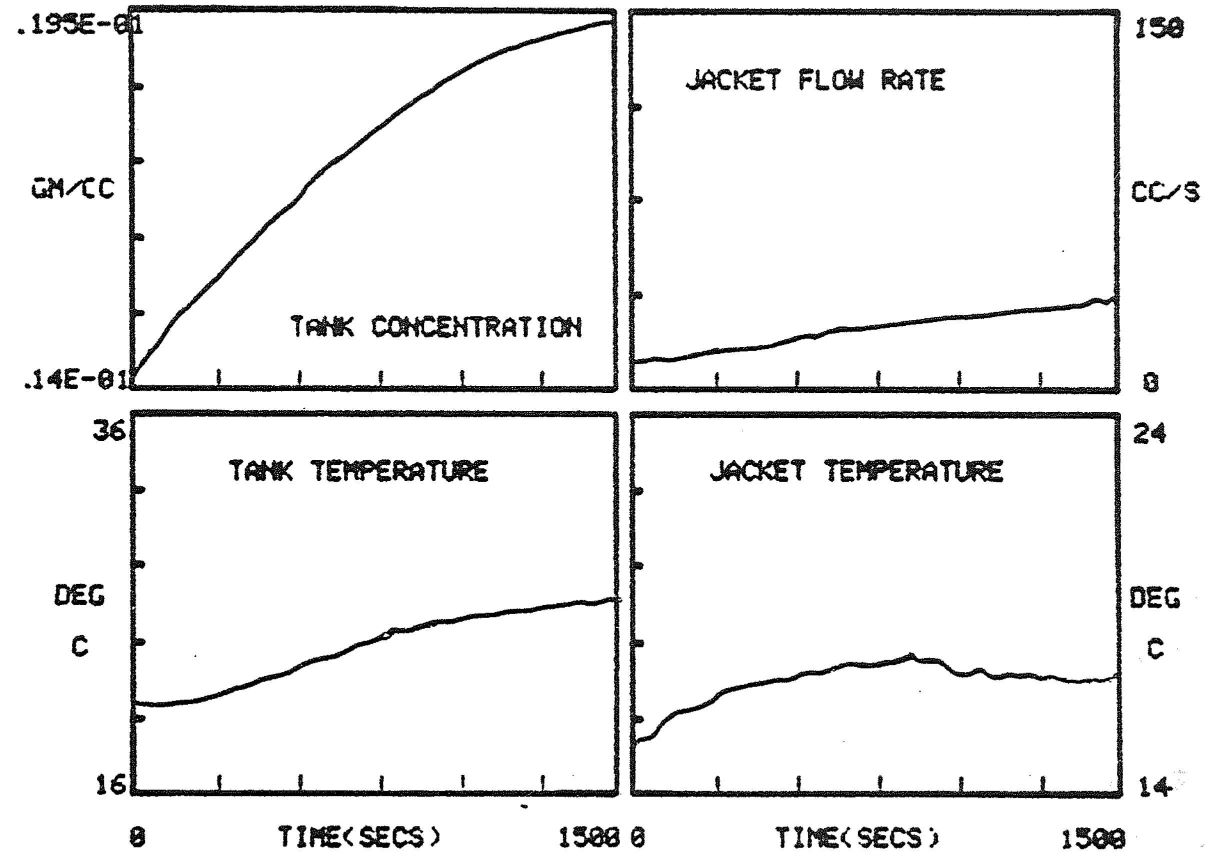


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.007)

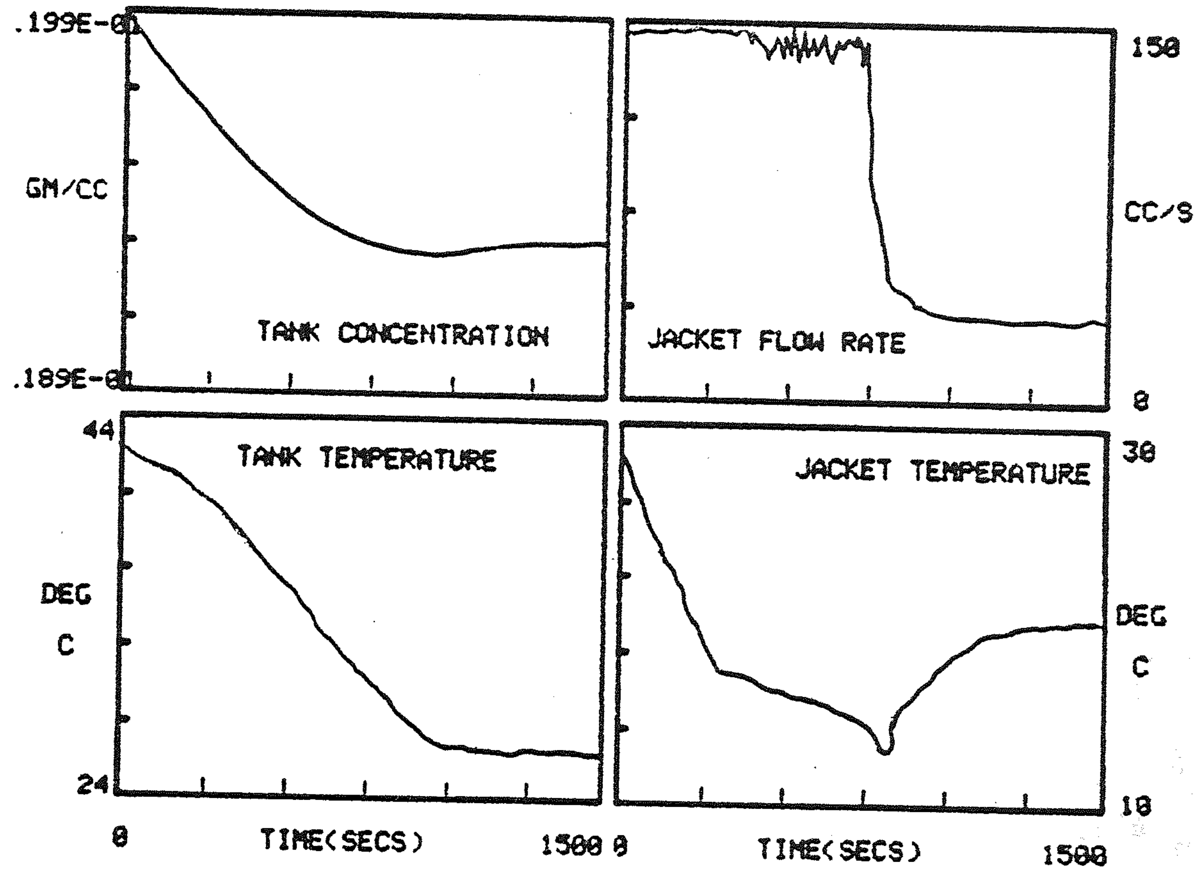
Initial perturbation in a state variable

FIG.A.6.1.33 EXPERIMENT NO:33



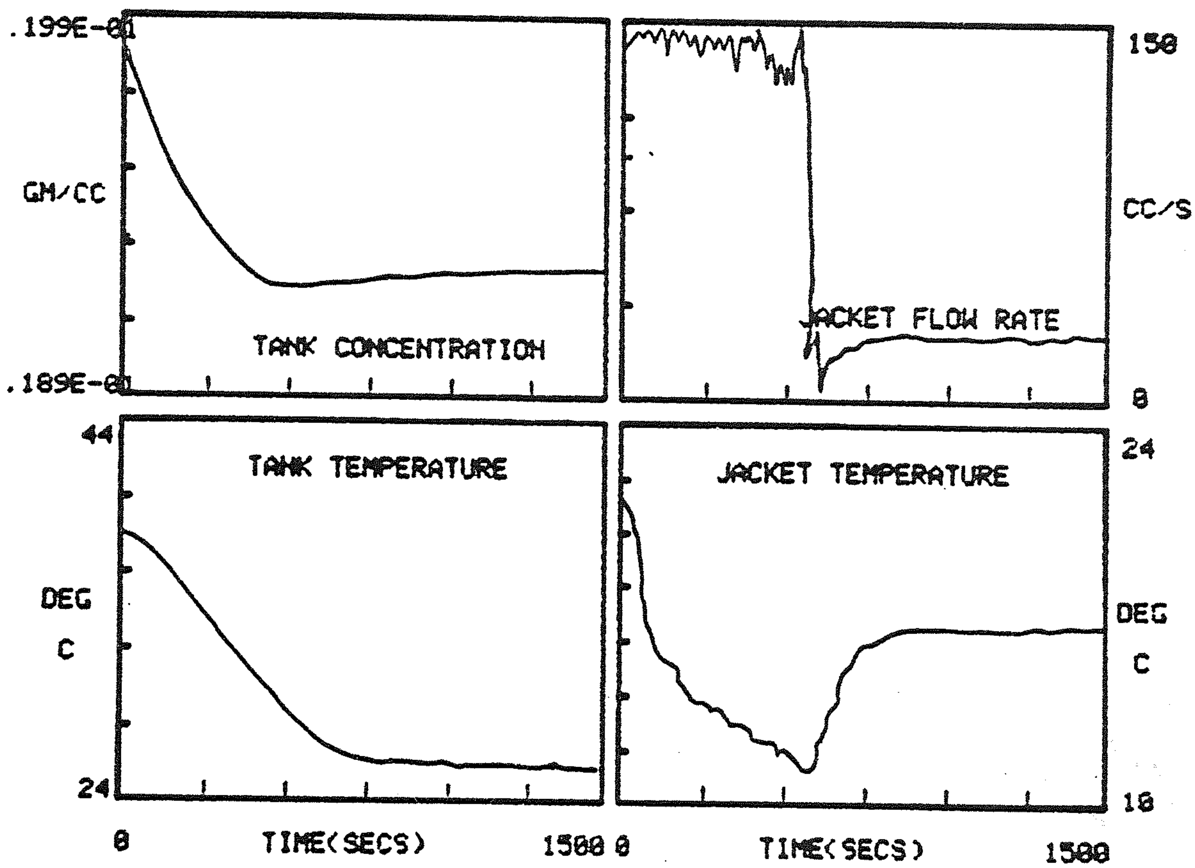
Reaction order = 1
Decoupling type control of tank temperature(D_{max}=.007)
Initial perturbations in state variables

FIG.A.6.1.34 EXPERIMENT NO:34



Reaction order = 1
Decoupling type control of tank temperature(D_{max}=.007)
Initial perturbations in state variables

FIG.A.6.1.35 EXPERIMENT NO:35

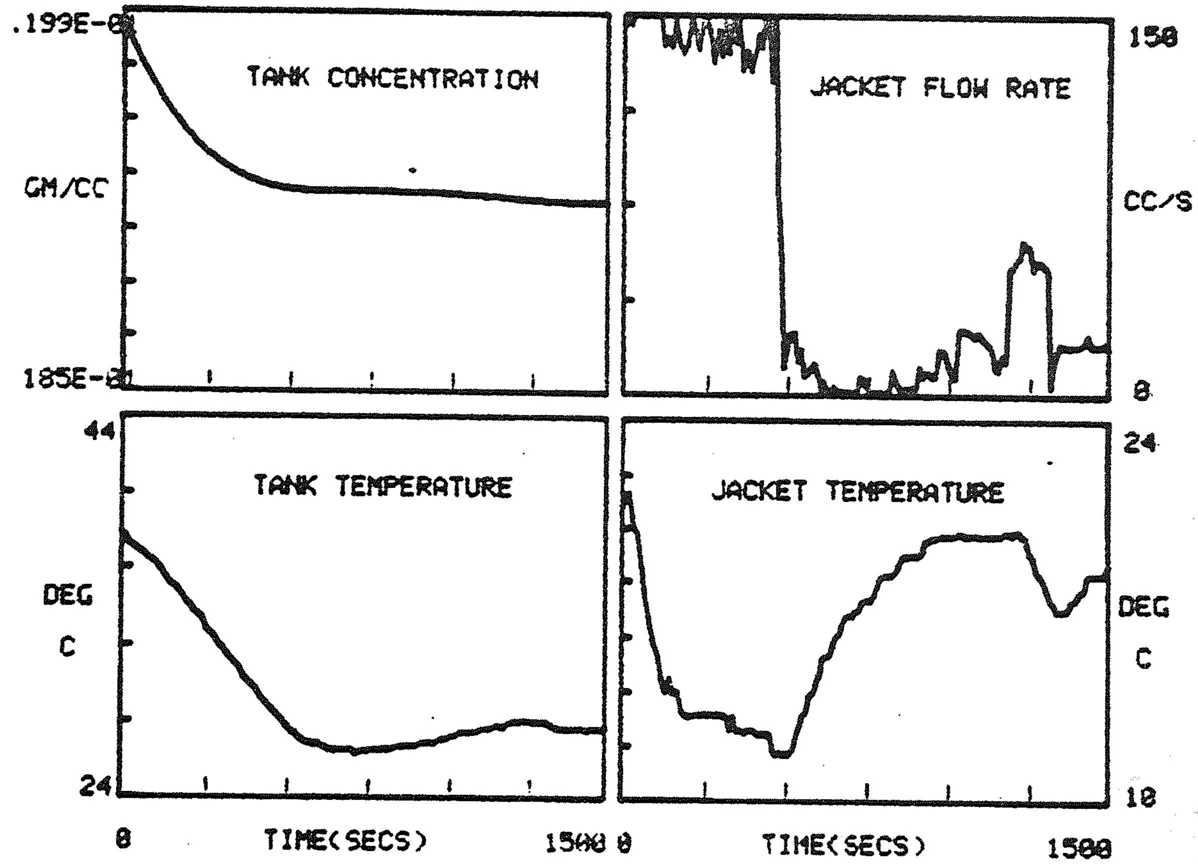


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.01)

Initial perturbations in state variables

FIG.A.6.1.36 EXPERIMENT NO:36

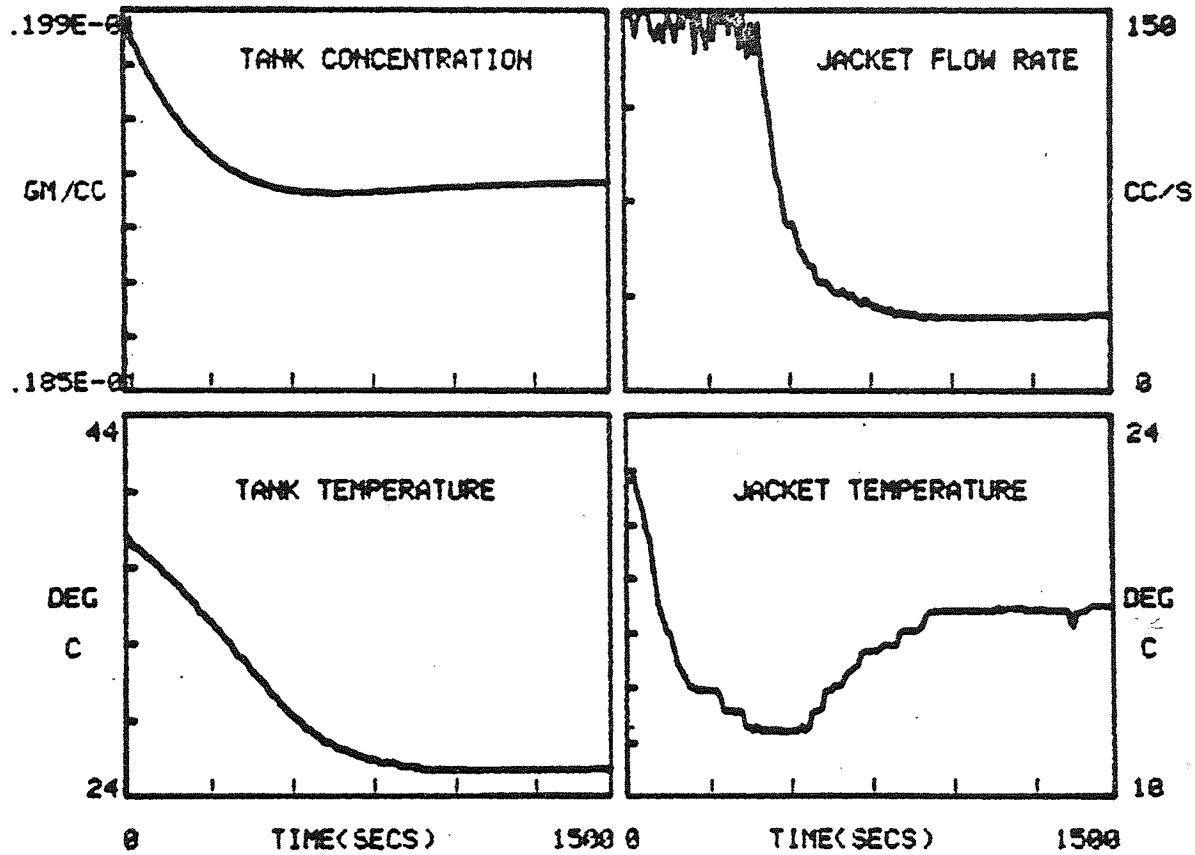


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.015)

Initial perturbations in state variables

FIG.A.6.1.37 EXPERIMENT NO:37

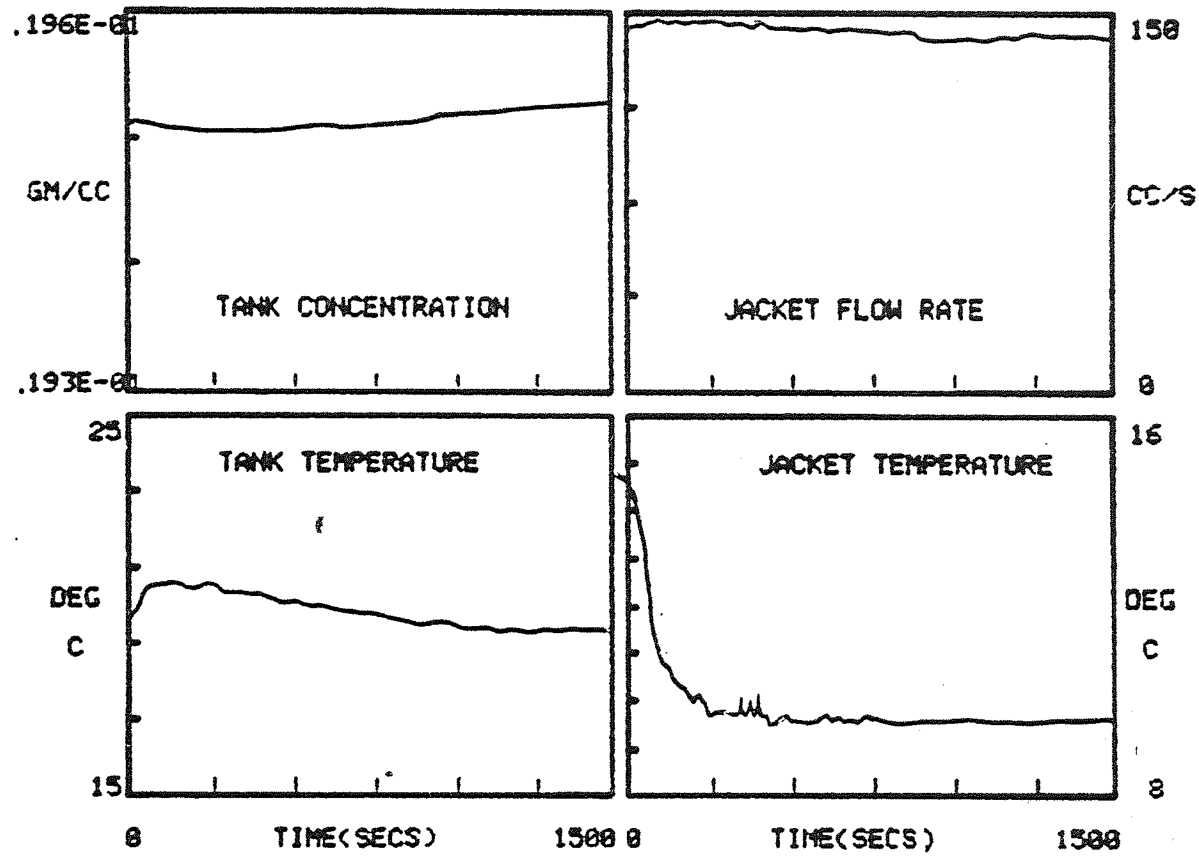


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.005)

Initial perturbations in state variables

FIG.A.6.1.38 EXPERIMENT NO:38

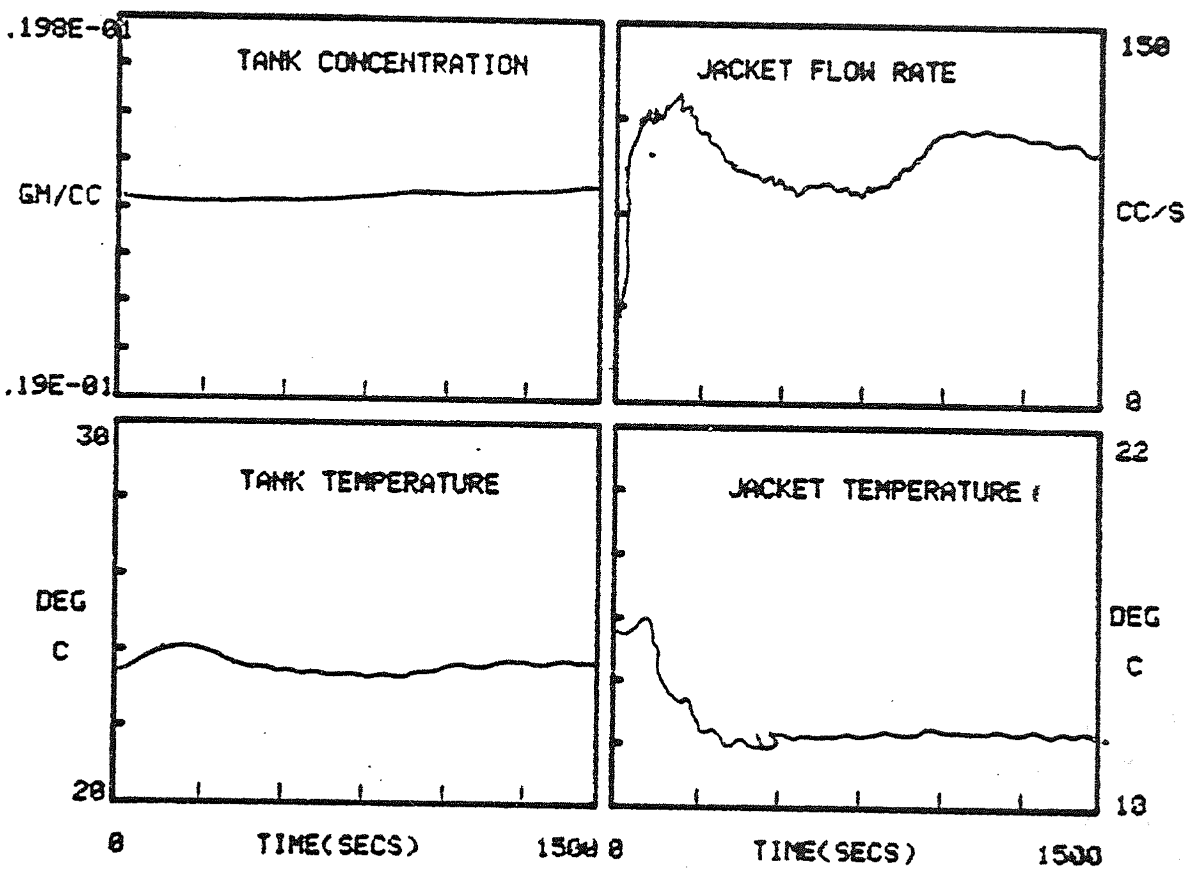


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.007)

Step in tank inlet temperature= 4.5 K

FIG.A.6.1.39 EXPERIMENT NO:39

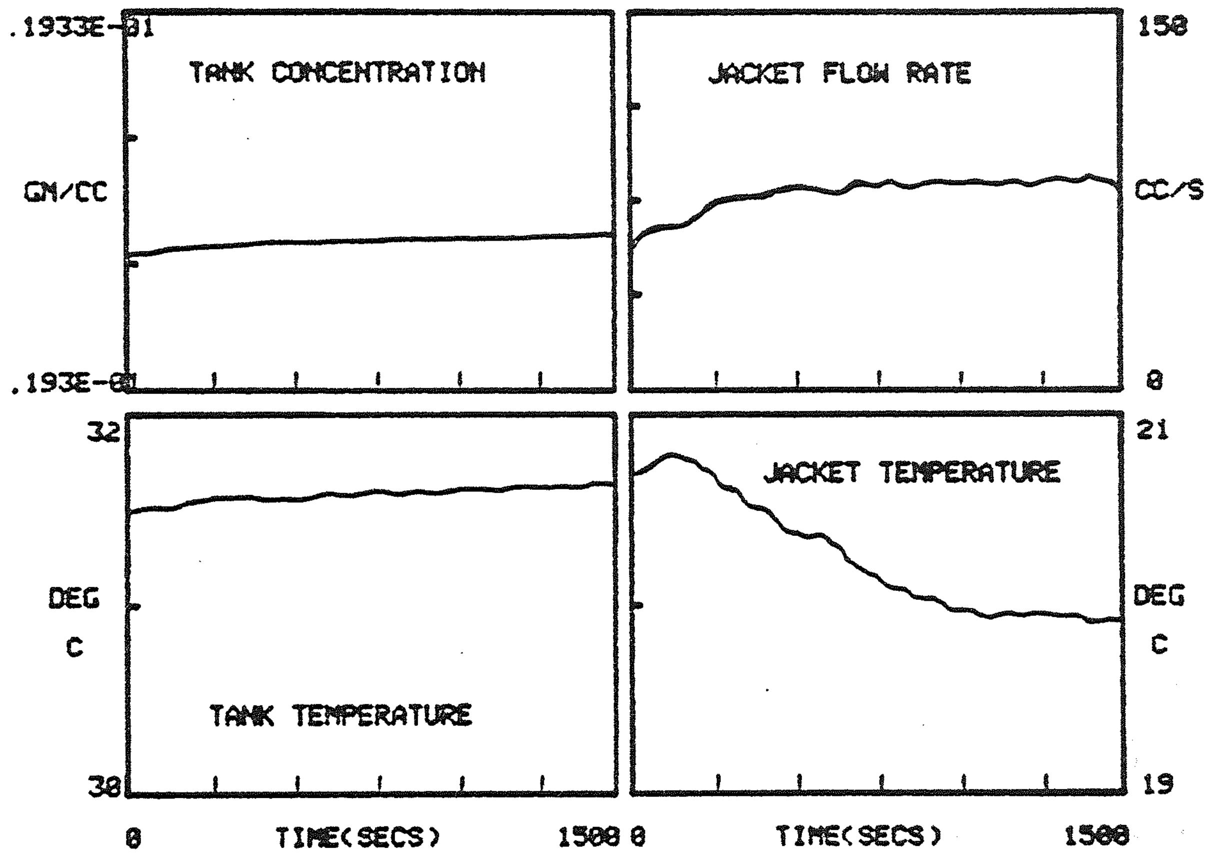


Reaction order = 1

Decoupling type control of tank temperature(D_{max}=.007)

Step in tank inlet temperature = 3.5 K

FIG.A.6.1.40 EXPERIMENT NO:40

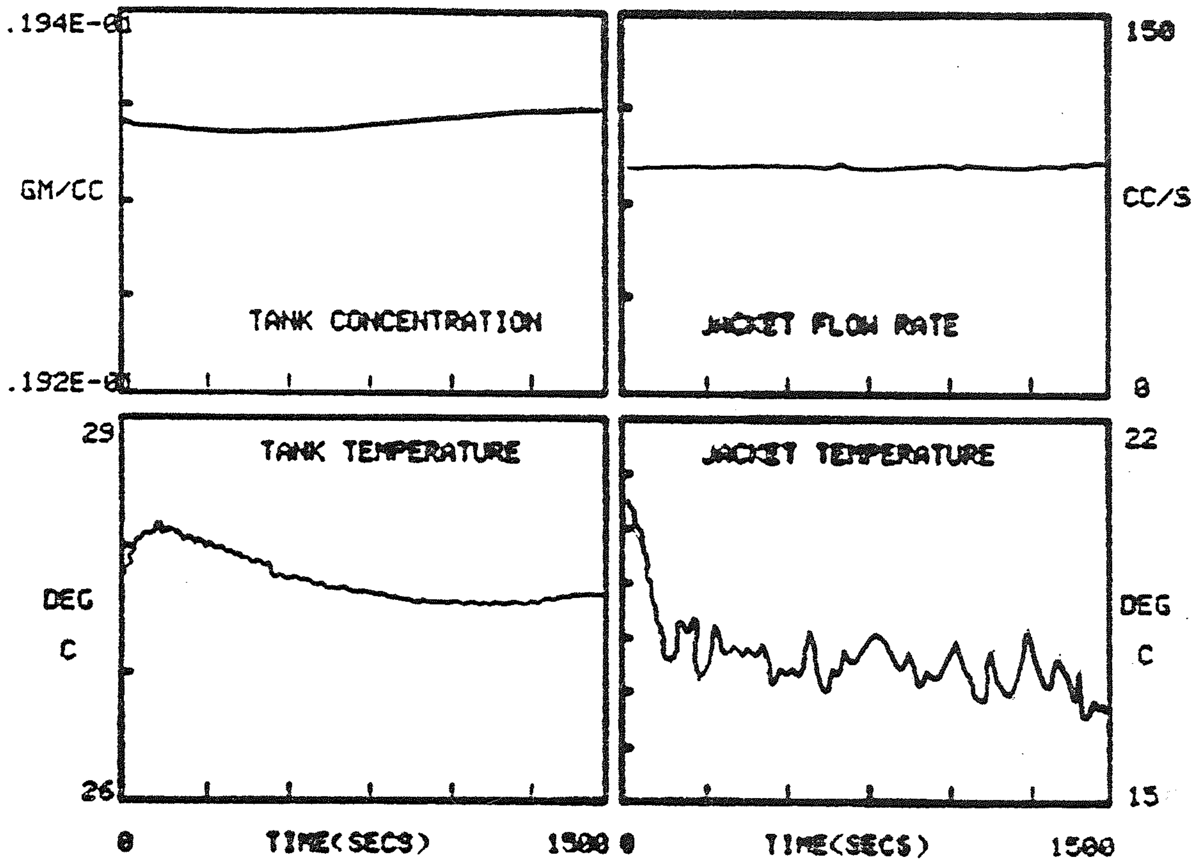


Reaction order = 1

Invariance control

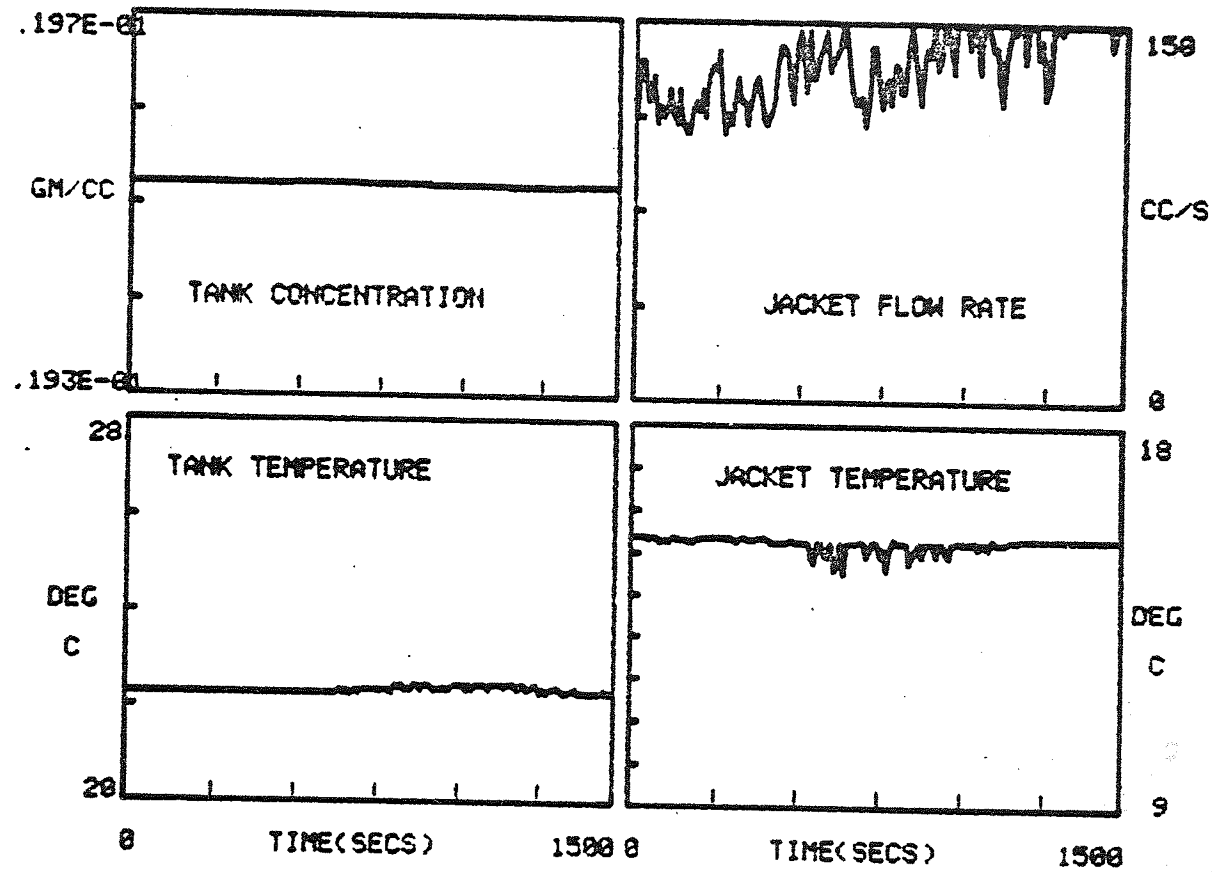
Step in tank inlet temperature = 3.4 K

FIG.A.6.1.41 EXPERIMENT NO:41



Reaction order = 1
Invariance control
Step in tank inlet temperature = 4.8 K

FIG.A.6.1.42 EXPERIMENT NO:42

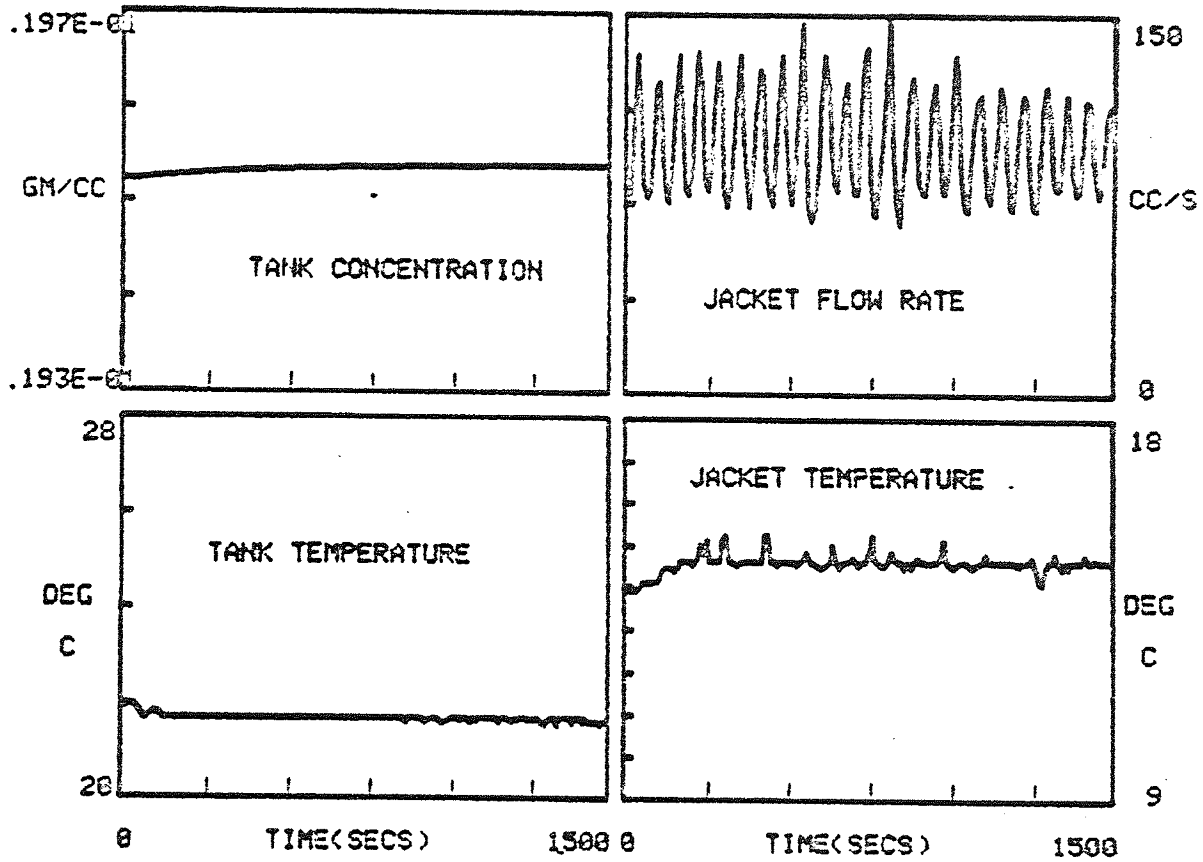


Reaction order = 1

Invariance control

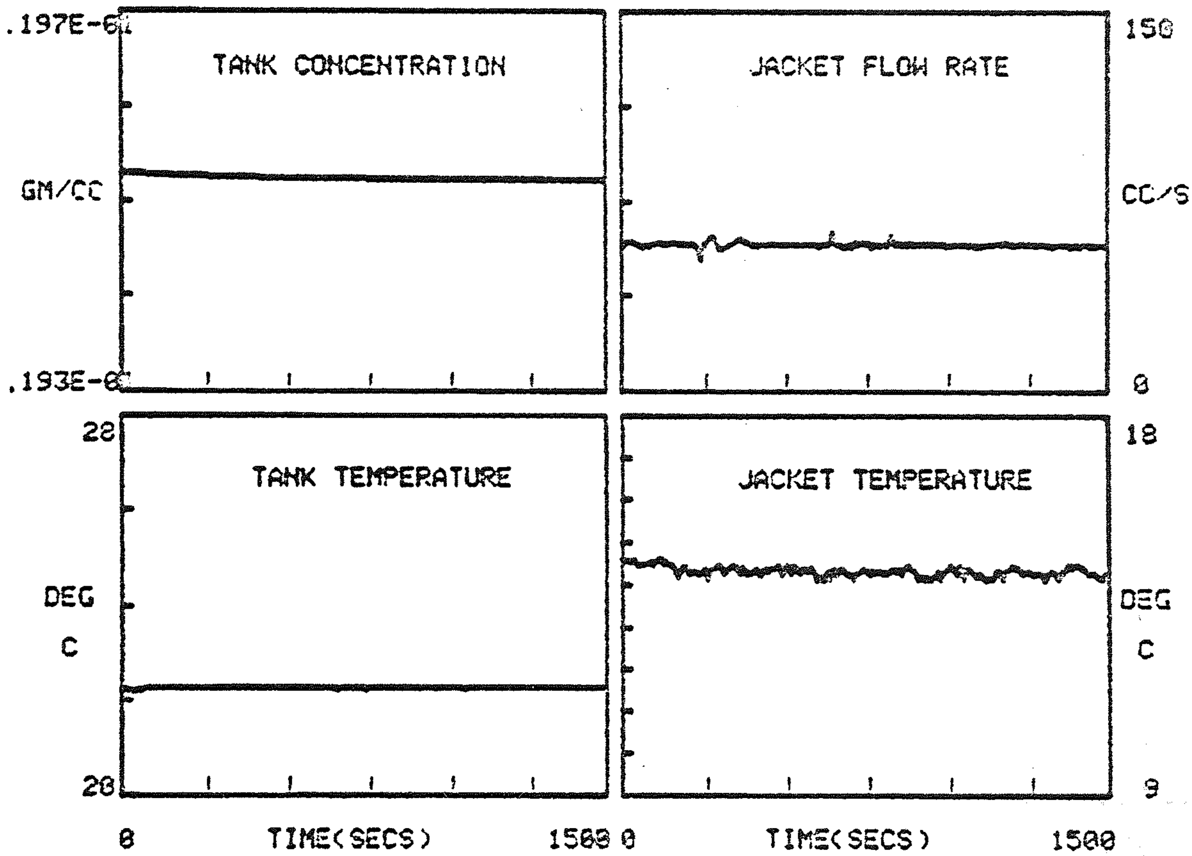
Step in jacket inlet temperature = 7 K

FIG.A.6.1.43 EXPERIMENT NO:43



Reaction order = 1
Invariance control
Step in jacket inlet temperature = 5 K

FIG.A.6.1.44 EXPERIMENT NO:44

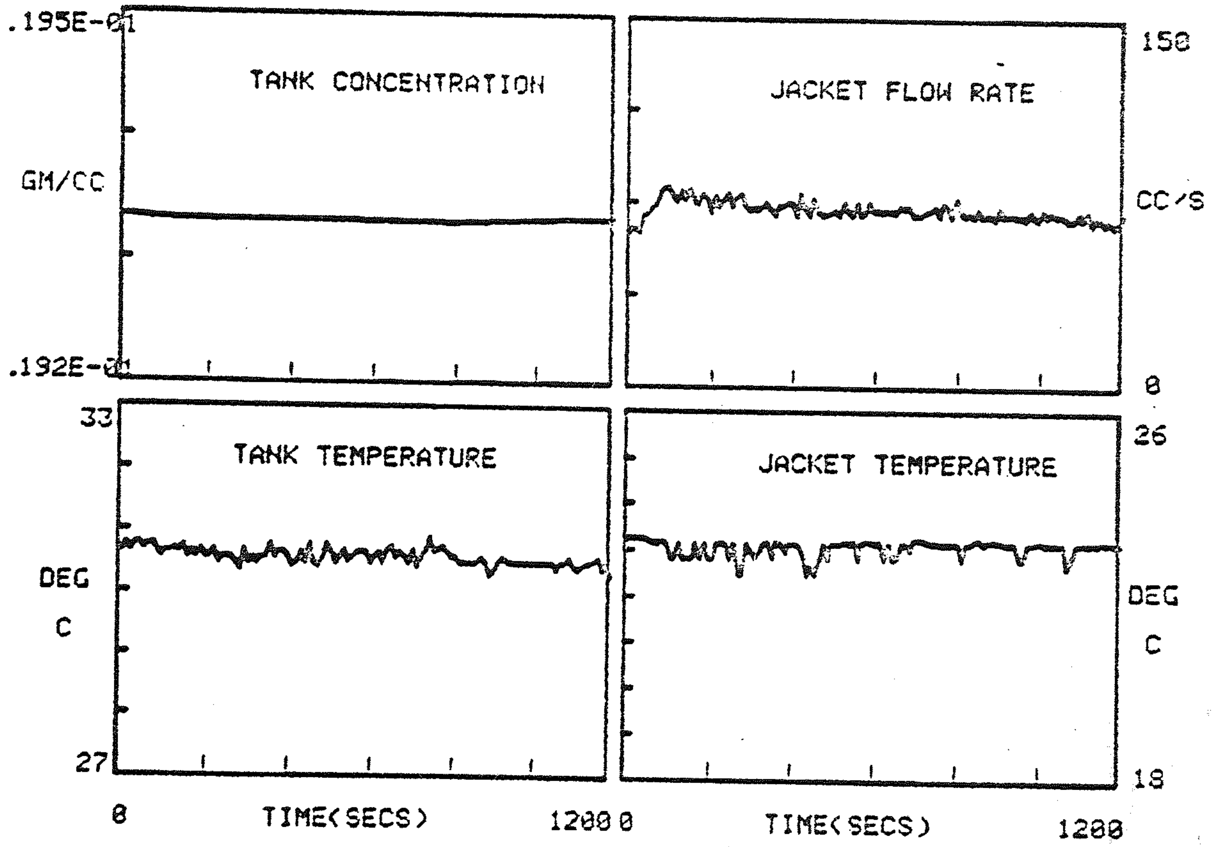


Reaction order = 1

Invariance control

Step in jacket inlet temperature = 2.5 K

FIG.A.6.1.45 EXPERIMENT NO:45



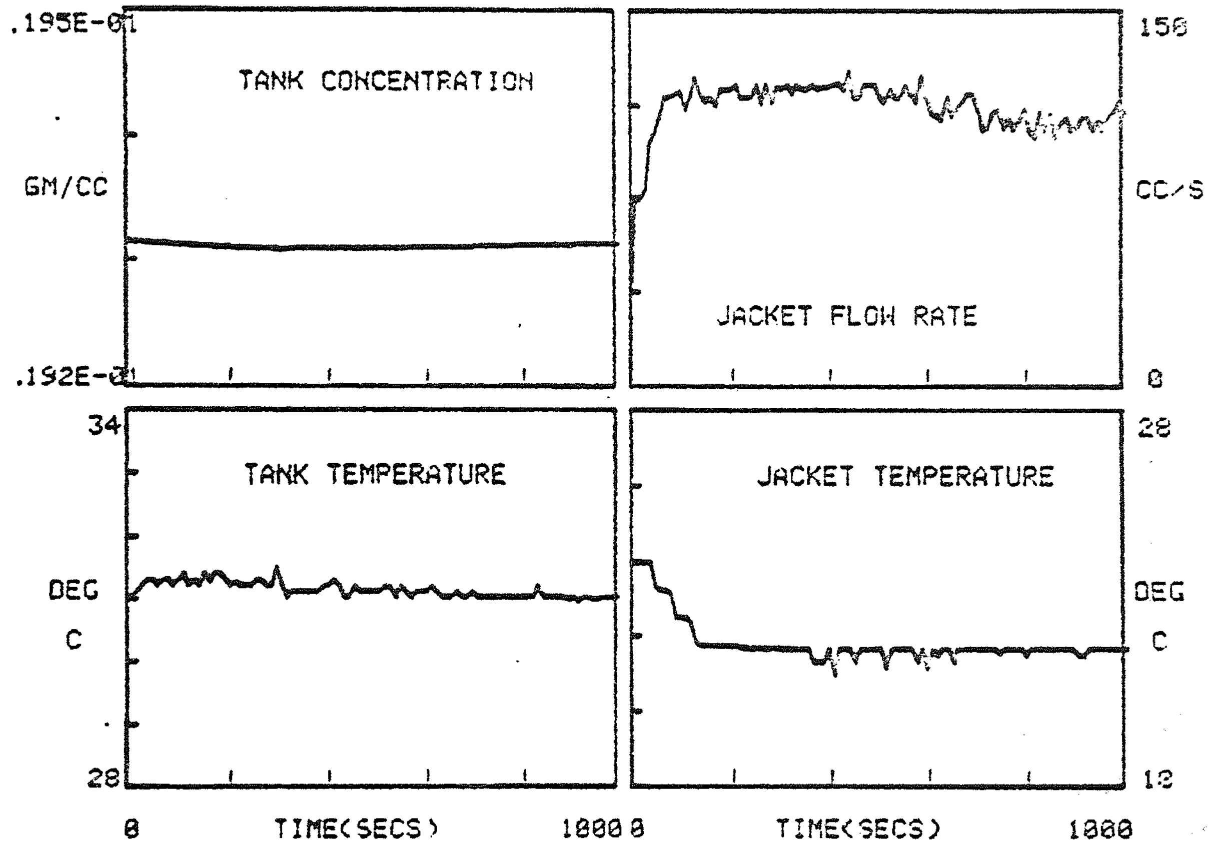
Reaction order = 1

Invariance control

Step in tank inlet temperature = .75 K

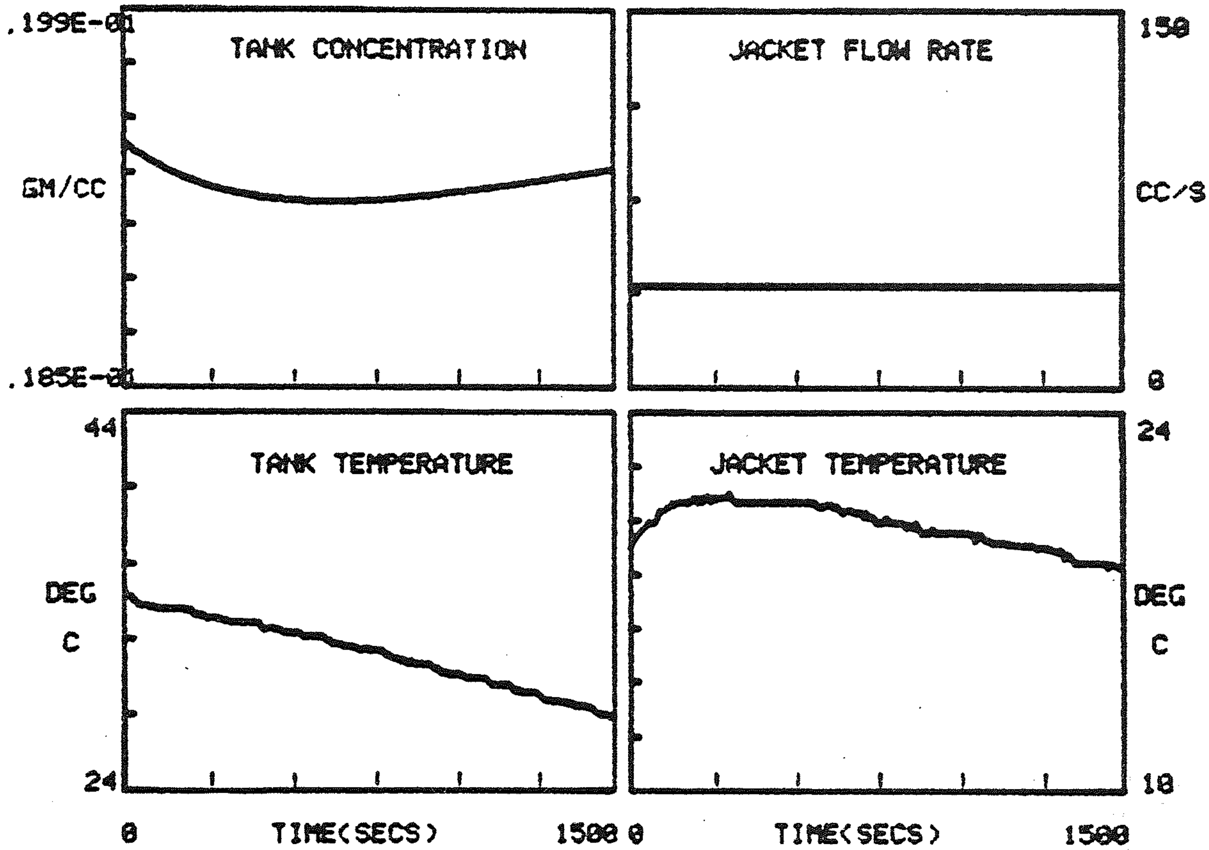
Step in jacket inlet temperature = 2.7 K

FIG.A.6.1.46 EXPERIMENT NO:46



Reaction order = 1
Invariance control
Step in tank inlet temperature = 2. K
Step in jacket inlet temperature = 2.1 K

FIG.A.6.1.47 EXPERIMENT NO:47

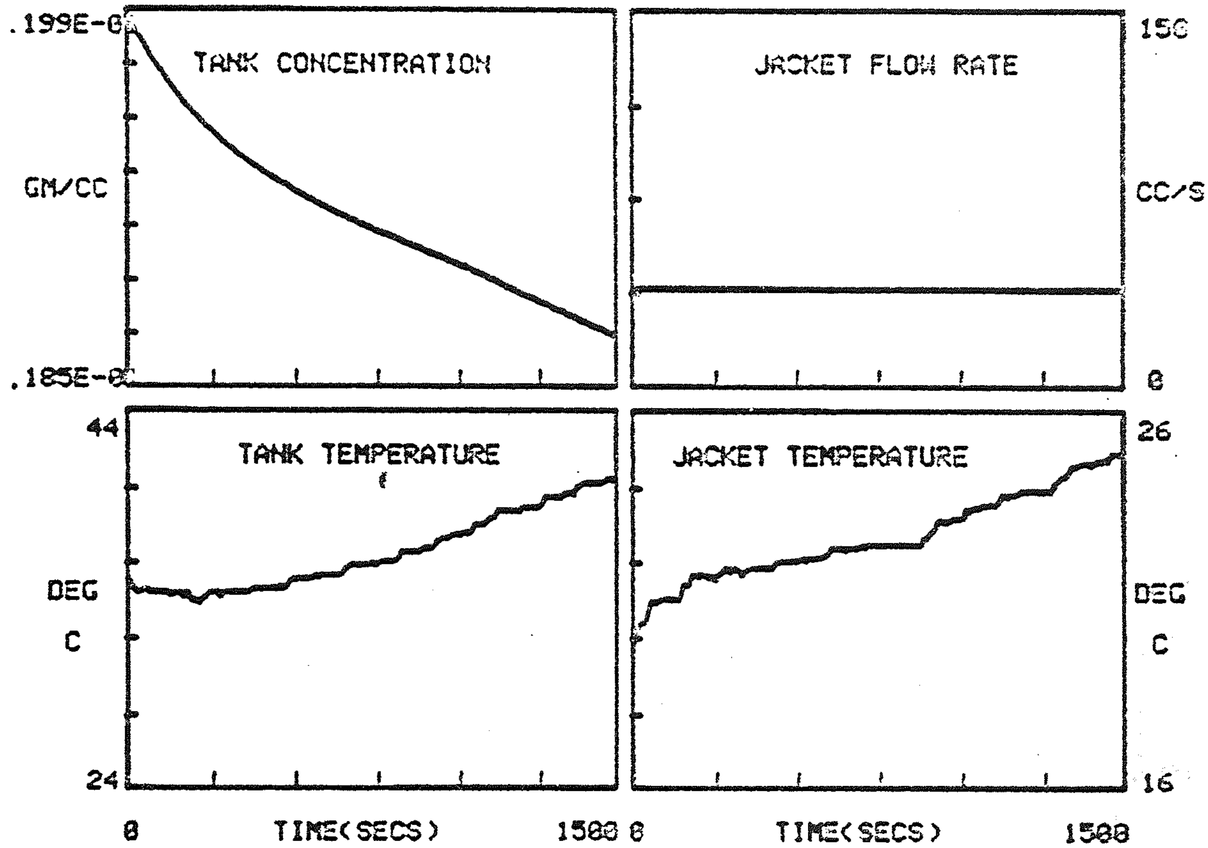


Reaction order = 0

Open loop studies

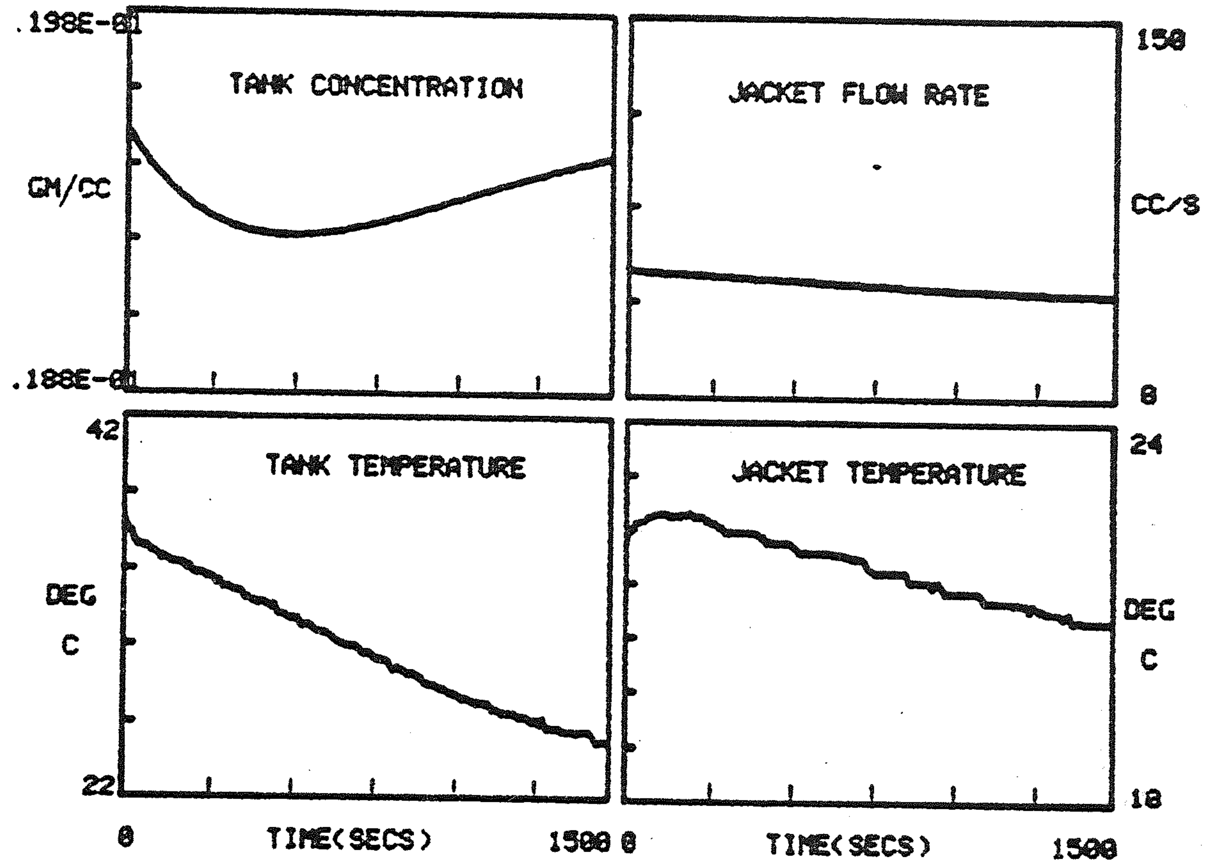
Initial perturbations in state variables

FIG.A.6.1.48 EXPERIMENT NO:48



Reaction order = 0
Open loop studies
Initial perturbations in state variables

FIG.A.6.1.49 EXPERIMENT NO:49

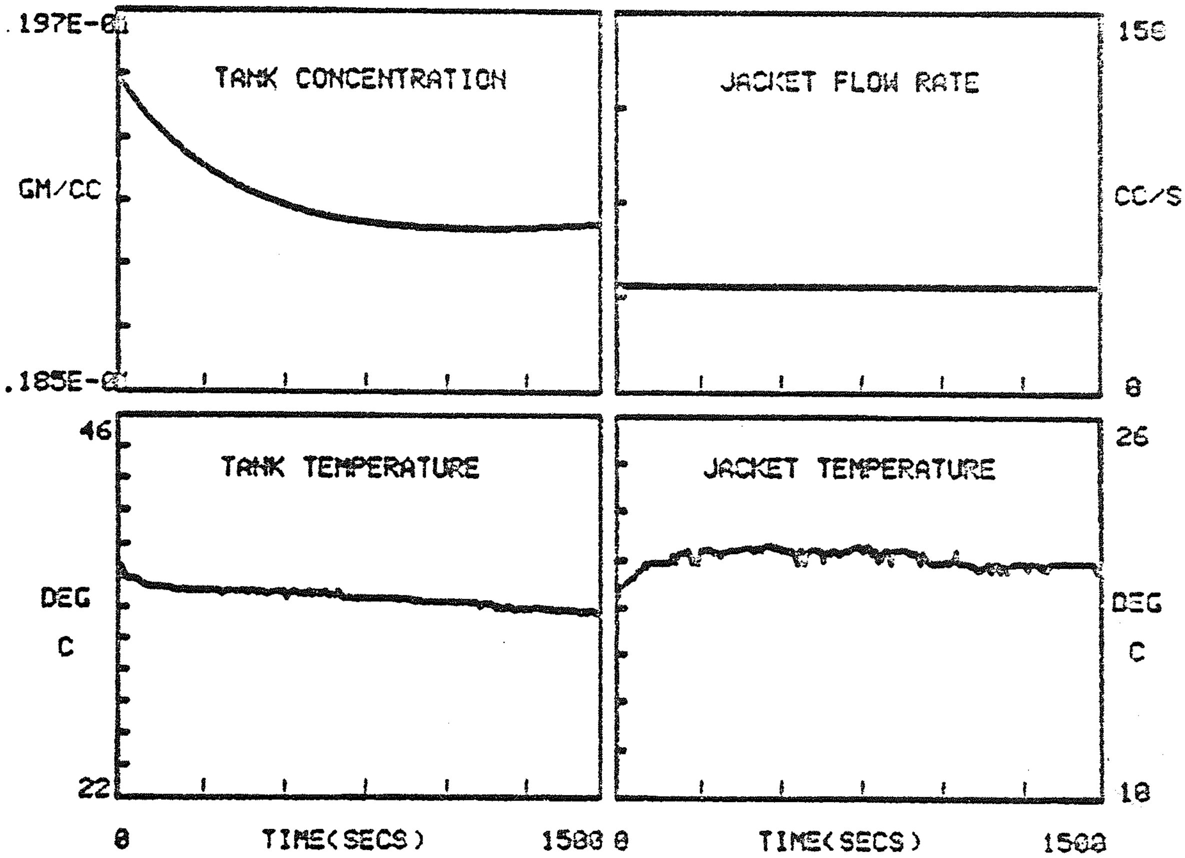


Reaction order = 0

Proportional feedback control of tank temperature(K_c=.0005)

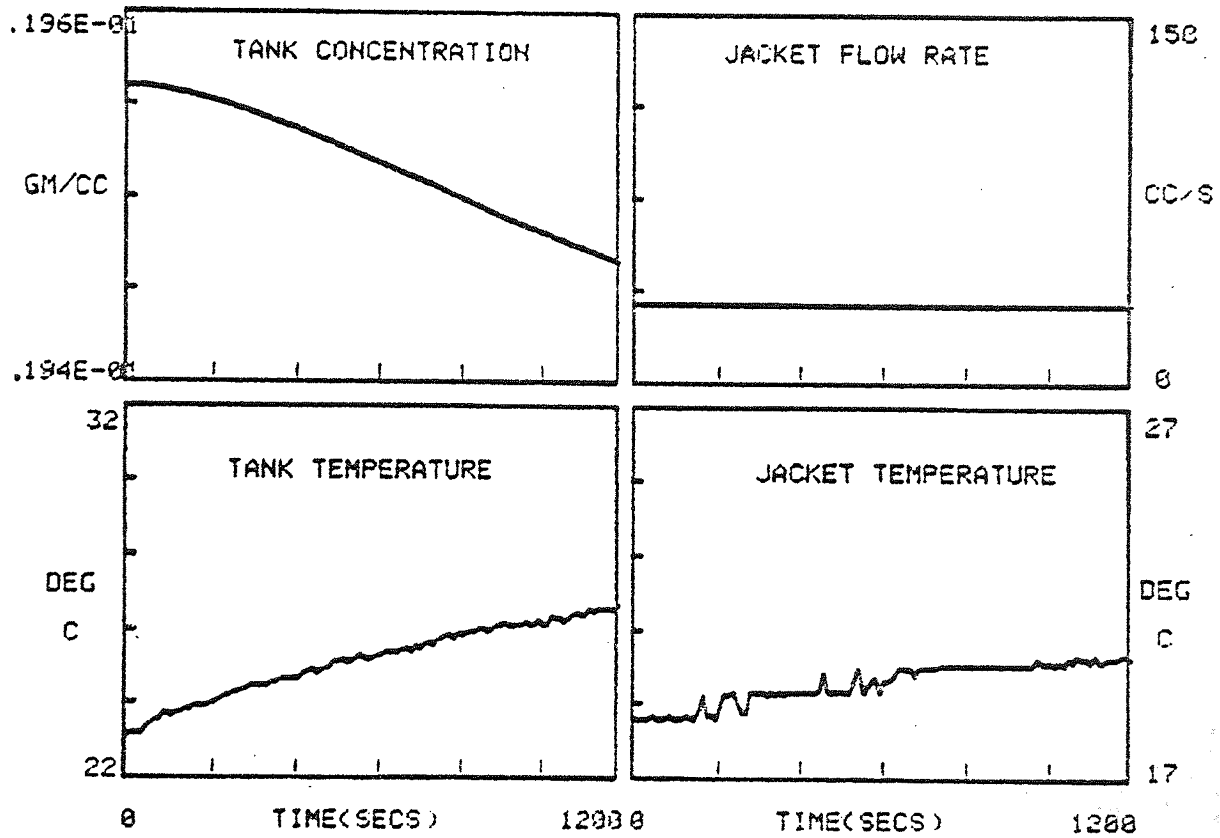
Initial perturbations in state variables

FIG.A.6.1.50 EXPERIMENT NO:50



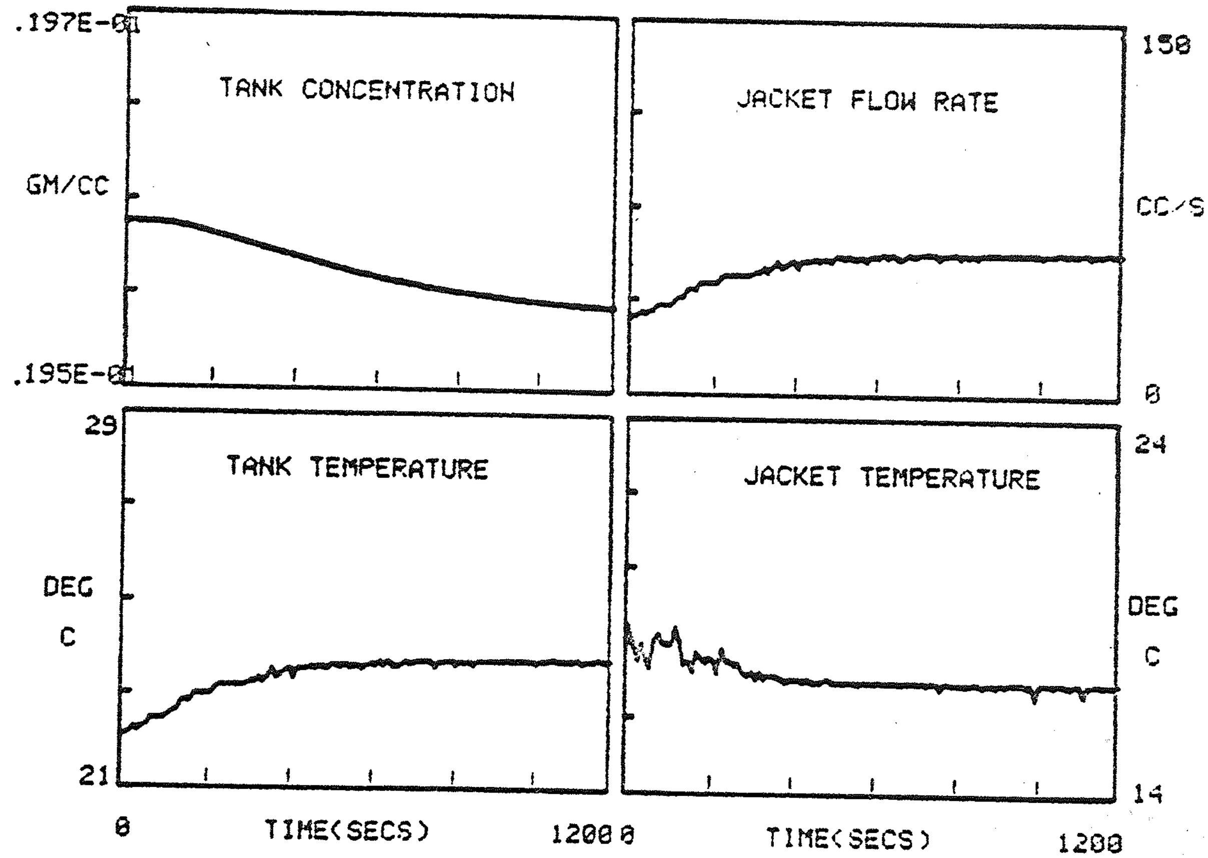
Reaction order = 0
Proportional feedback control of tank temperature(K_c=.0001)
Initial perturbations in state variables

FIG.A.6.1.51 EXPERIMENT NO:51



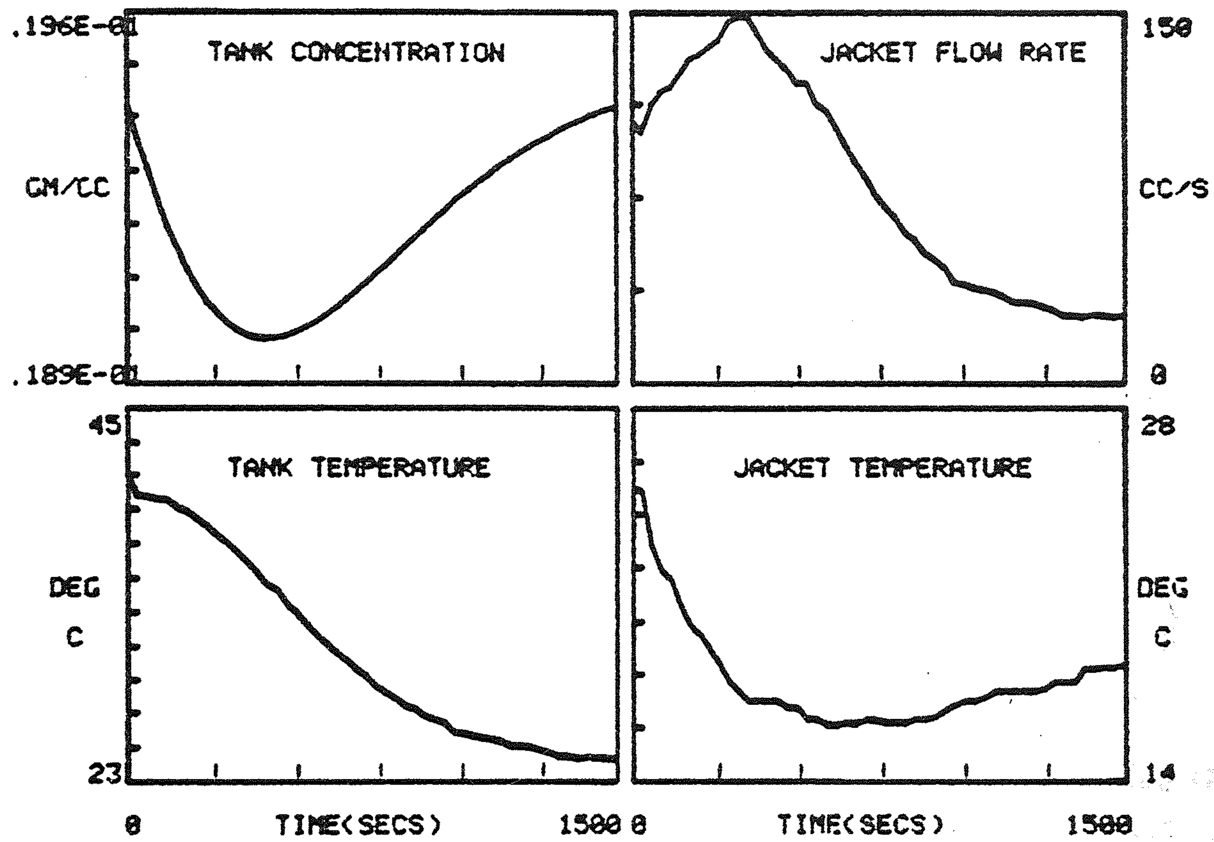
Reaction order = 0
Open loop studies
Step in tank inlet temperature = 2.6 K

FIG.A.6.1.52 EXPERIMENT NO:52



Reaction order = 0
Proportional feedback control of tank temperature(K_c=.01)
Step in tank inlet temperature = 3 K

FIG.A.6.1.53 EXPERIMENT NO:53

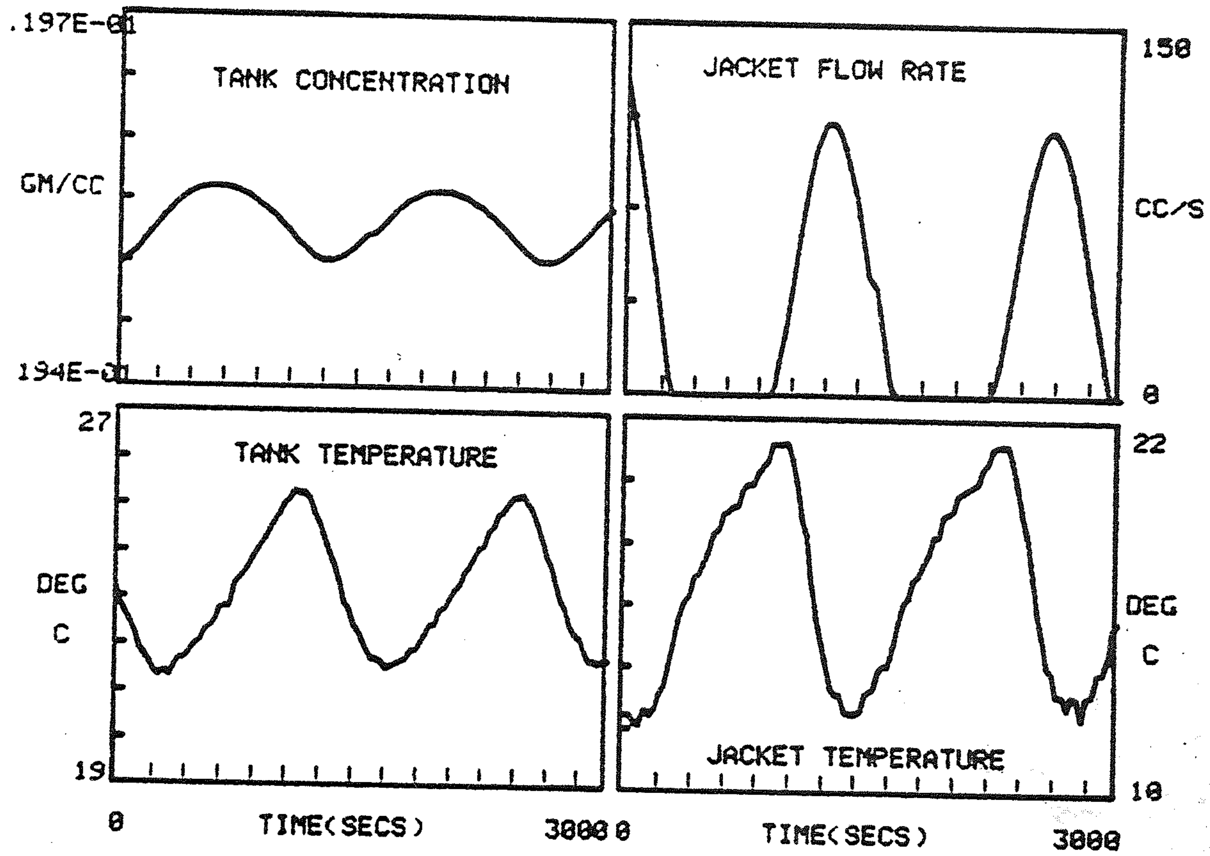


Reaction order = 0

Controller equation derived from stability conditions(eqn.(3.38))

Initial perturbations in state variables

FIG.A.6.1.54 EXPERIMENT NO:54

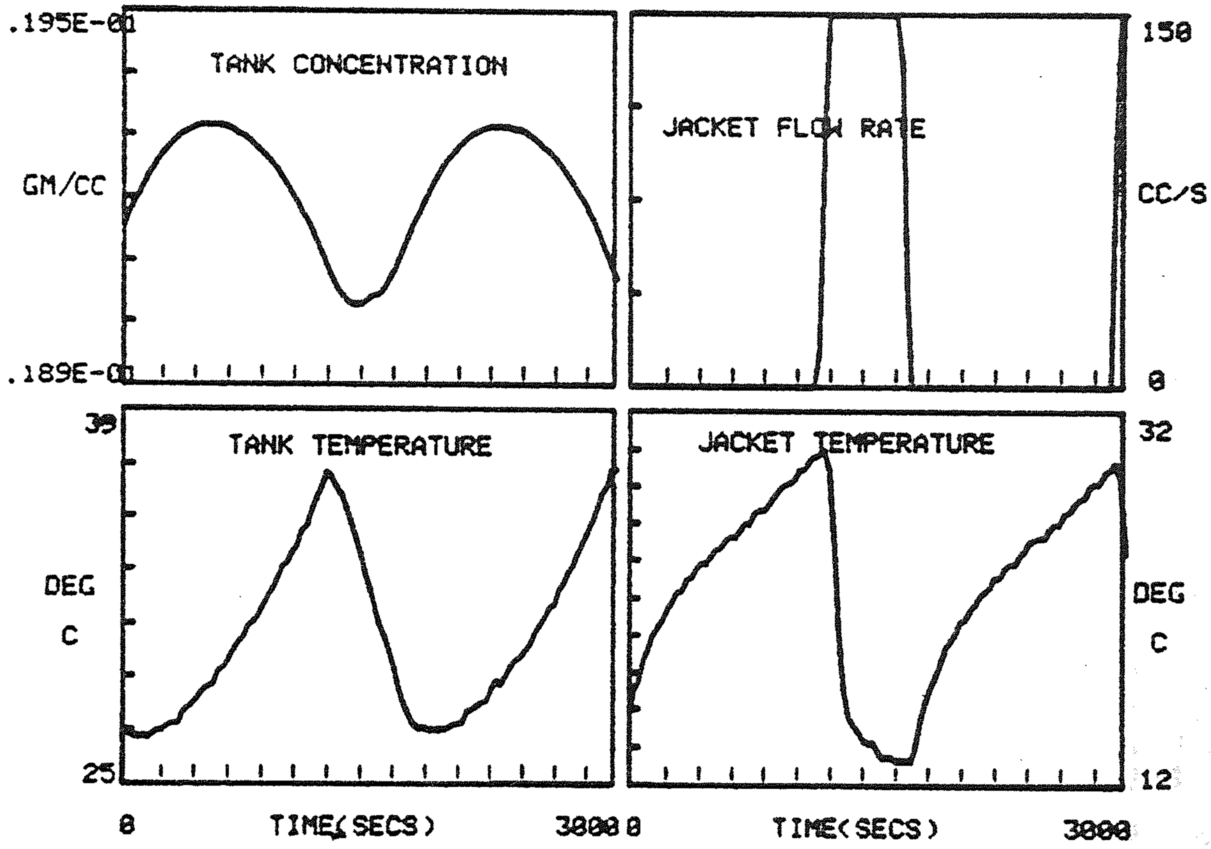


Reaction order = 0

Limit-cycle behaviour around open loop stable operating point

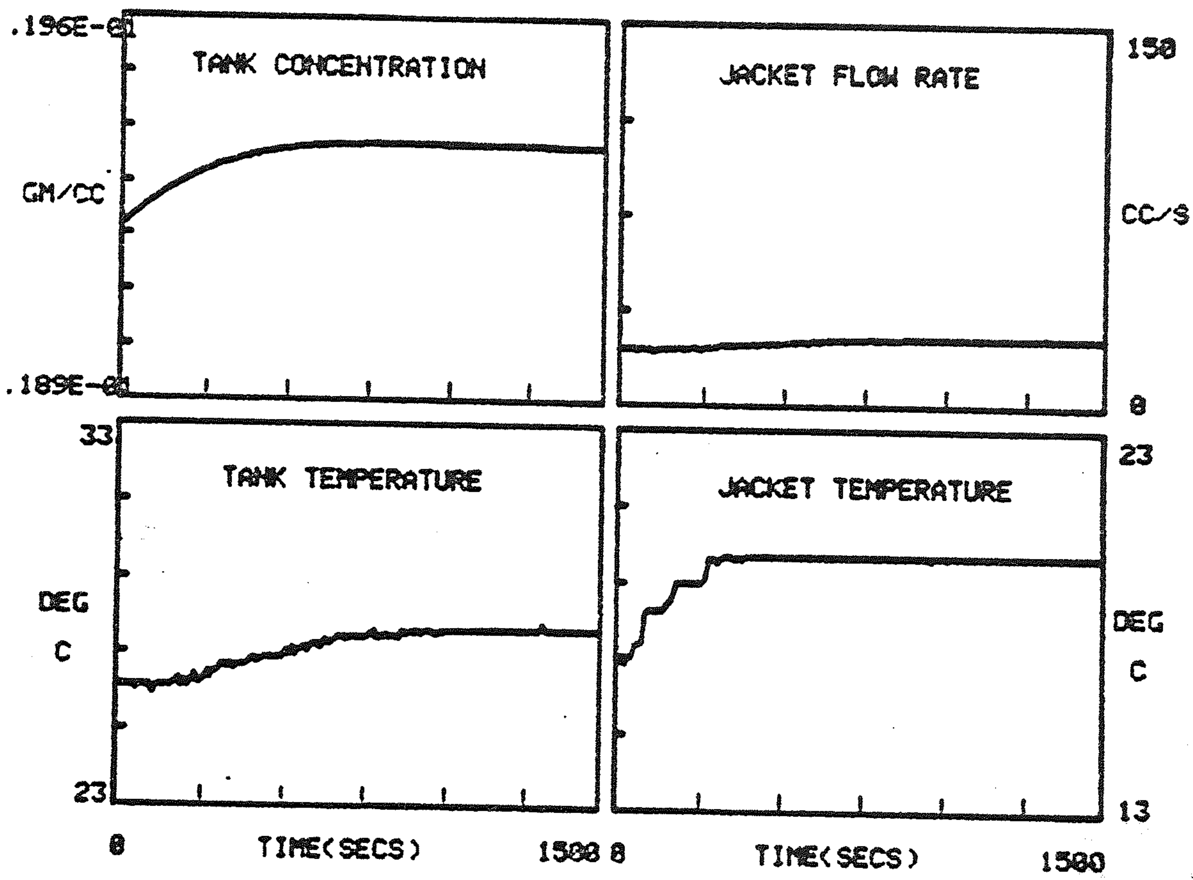
(K_c=.06)

FIG.A.6.1.55 EXPERIMENT NO:55



Reaction order = 0
Limit-cycle behaviour around open loop unstable operating point(K_c=.1)

FIG.A.6.1.56 EXPERIMENT NO:56

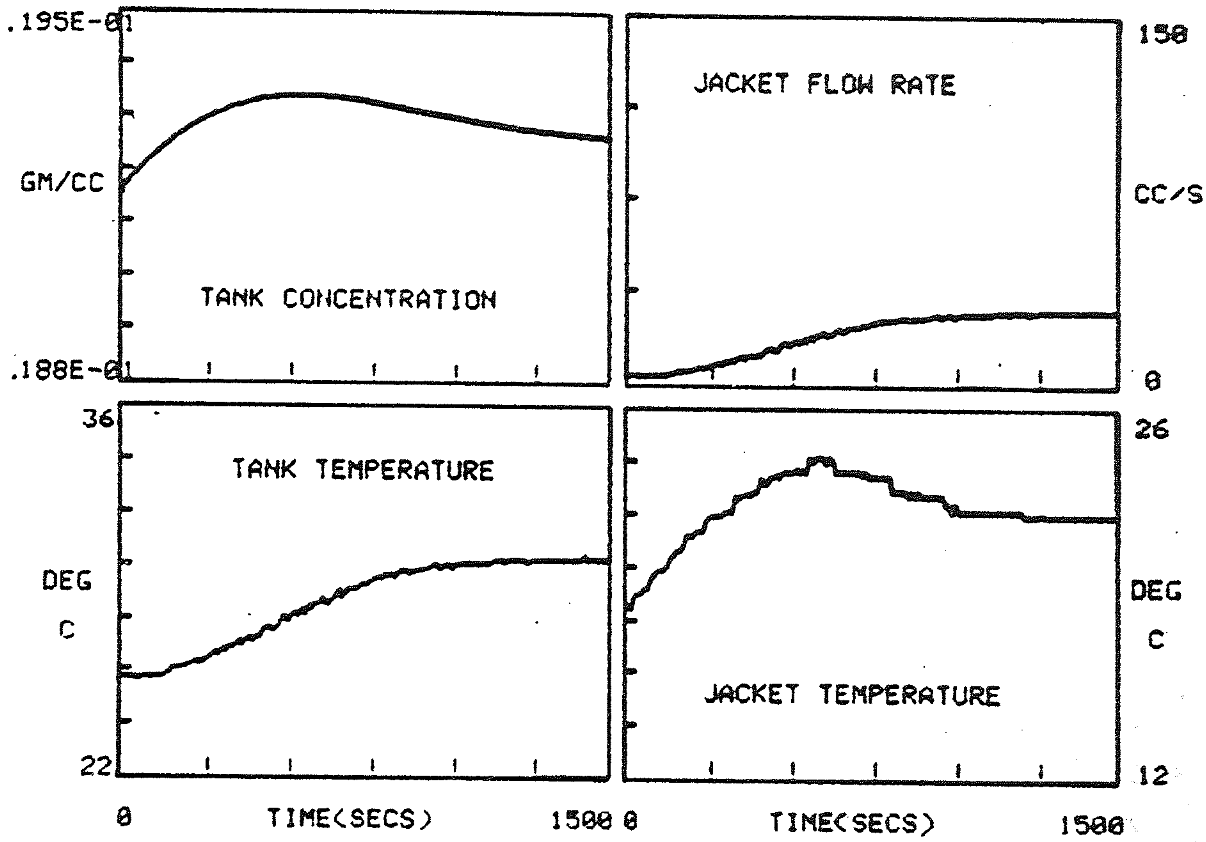


Reaction order = 0

Proportional feedback control of tank temperature(K_c=.002)

Stabilising open loop unstable operating point

FIG.A.6.1.57 EXPERIMENT NO:57

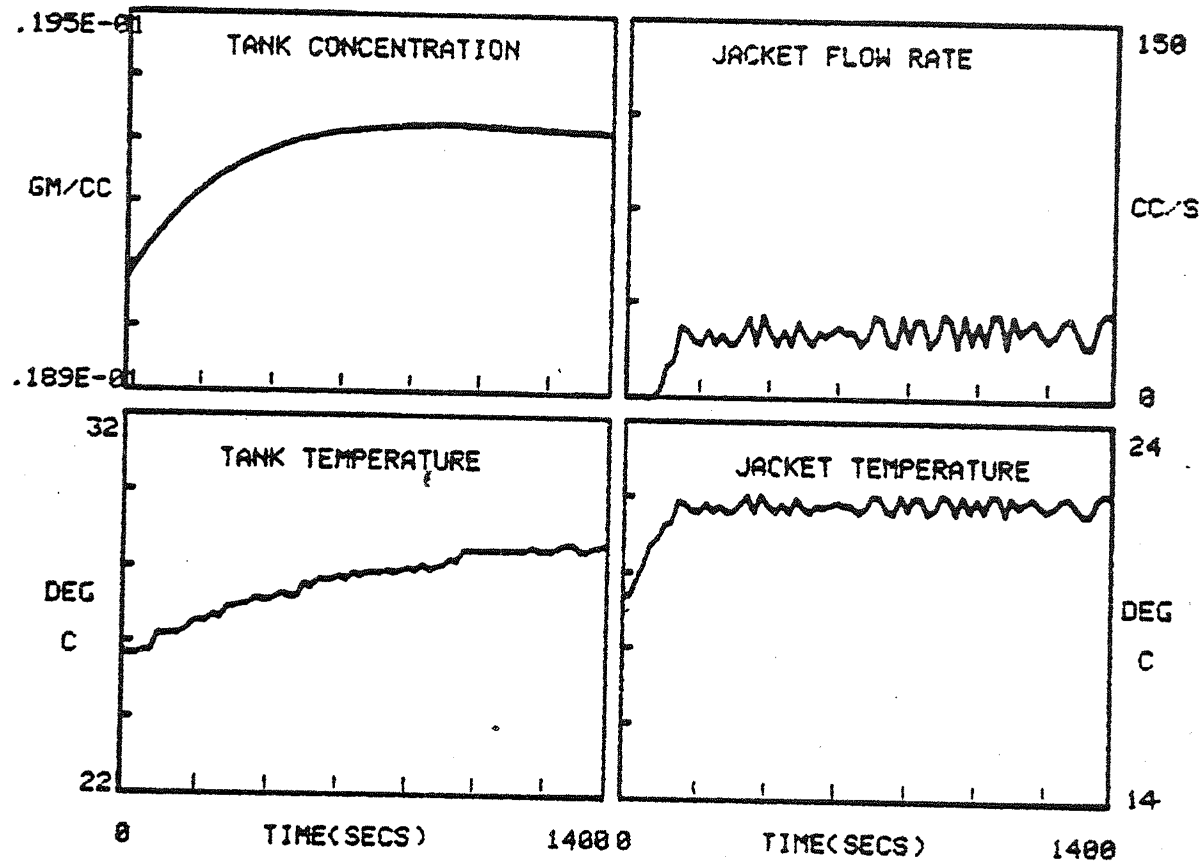


Reaction order = 0

Proportional feedback control of tank temperature(K_c=.0035)

Stabilising open loop unstable operating point

FIG.A.6.1.58 EXPERIMENT NO:58

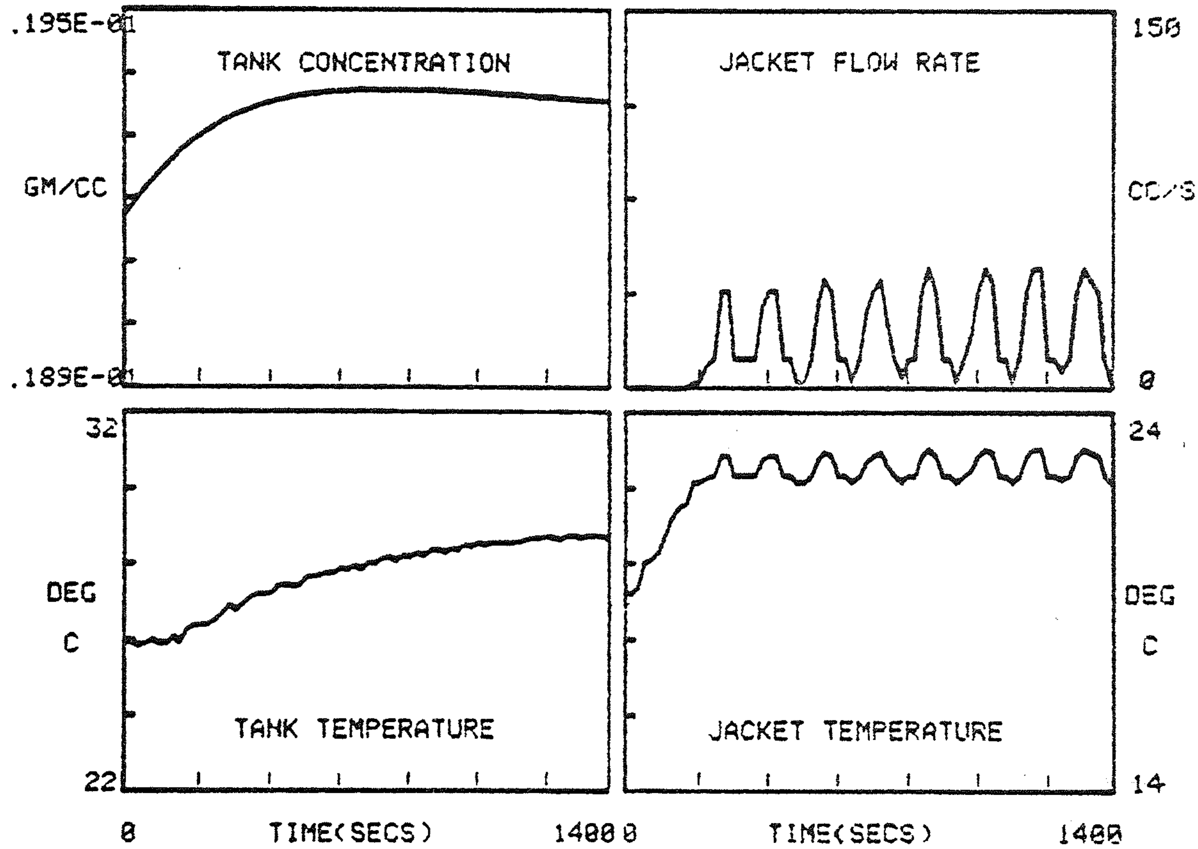


Reaction order = 0

Proportional feedback control of jacket temperature(K_c=.015)

Stabilising open loop unstable operating point

FIG.A.6.1.59 EXPERIMENT NO:59

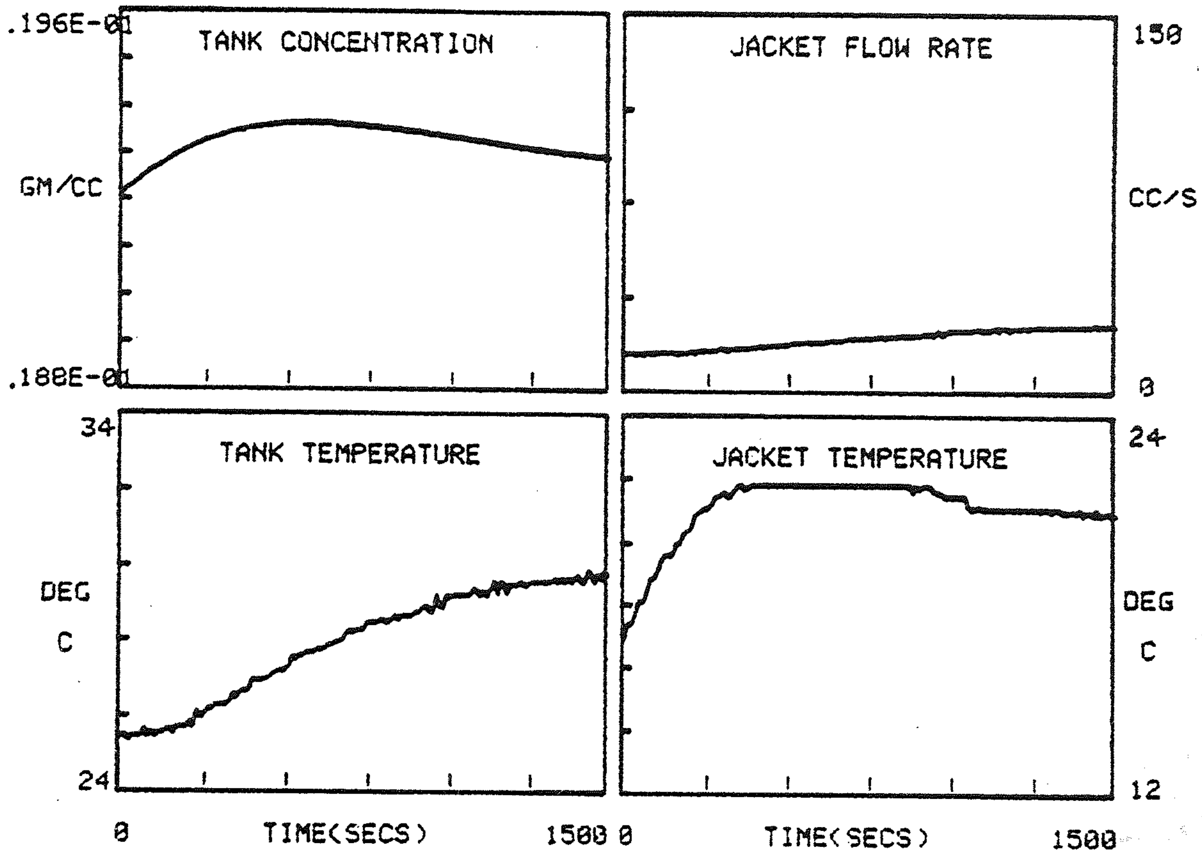


Reaction order = 0

Proportional feedback control of jacket temperature(K_c=.03)

Stabilising open loop unstable operating point

FIG.A.6.1.60 EXPERIMENT NO:60

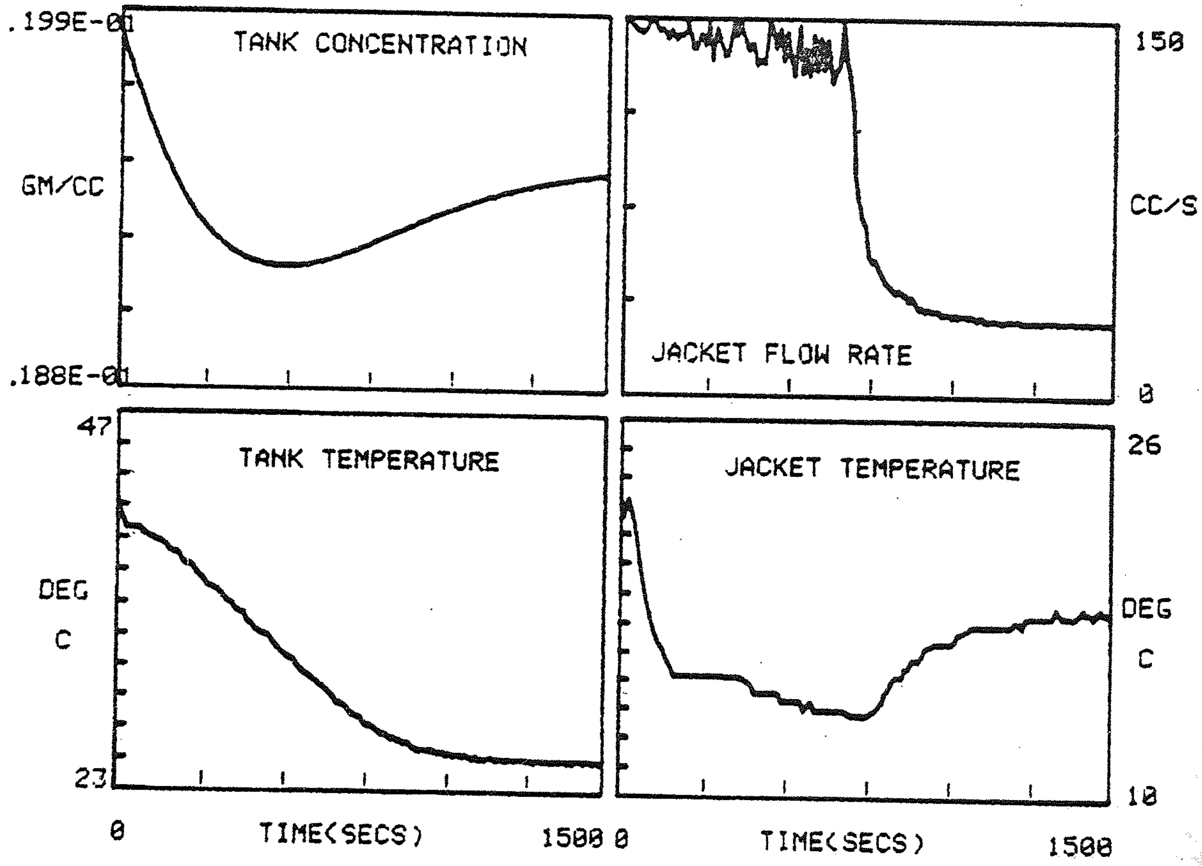


Reaction order = 0

Decoupling type control of tank temperature(D_{max}=.007)

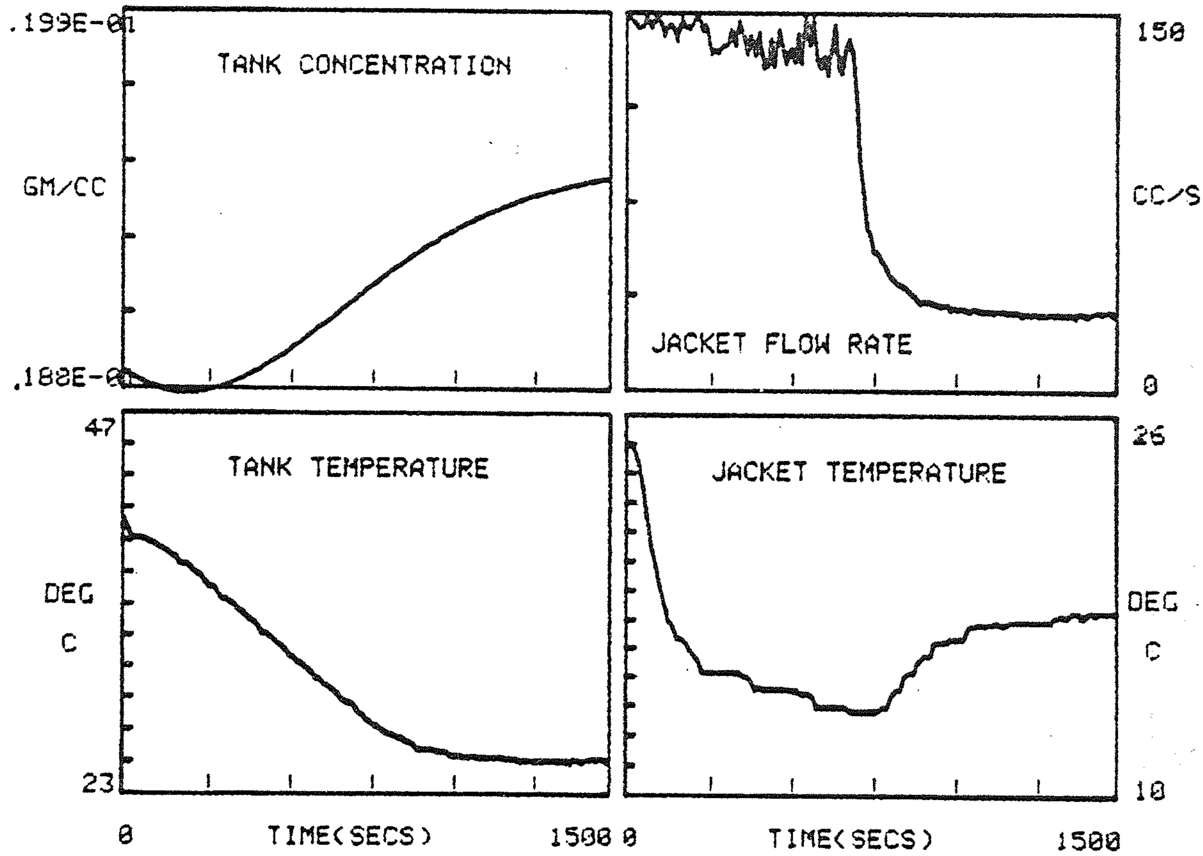
Stabilising open loop unstable operating point

FIG.A.6.1.61 EXPERIMENT NO:61



Reaction order = 0
Decoupling type control of tank temperature(D_{max}=.007)
Initial perturbations in state variables

FIG.A.6.1.62 EXPERIMENT NO:62

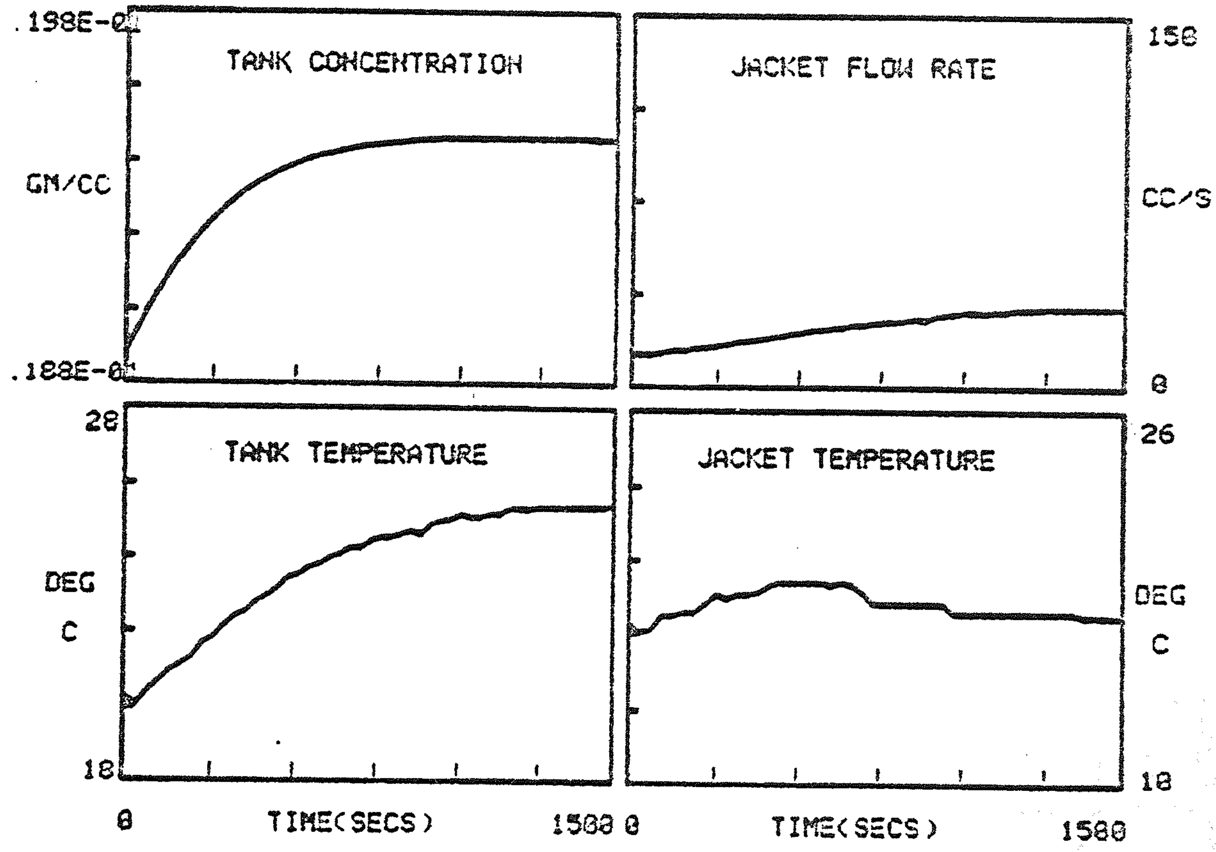


Reaction order = 0

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.63 EXPERIMENT NO:63

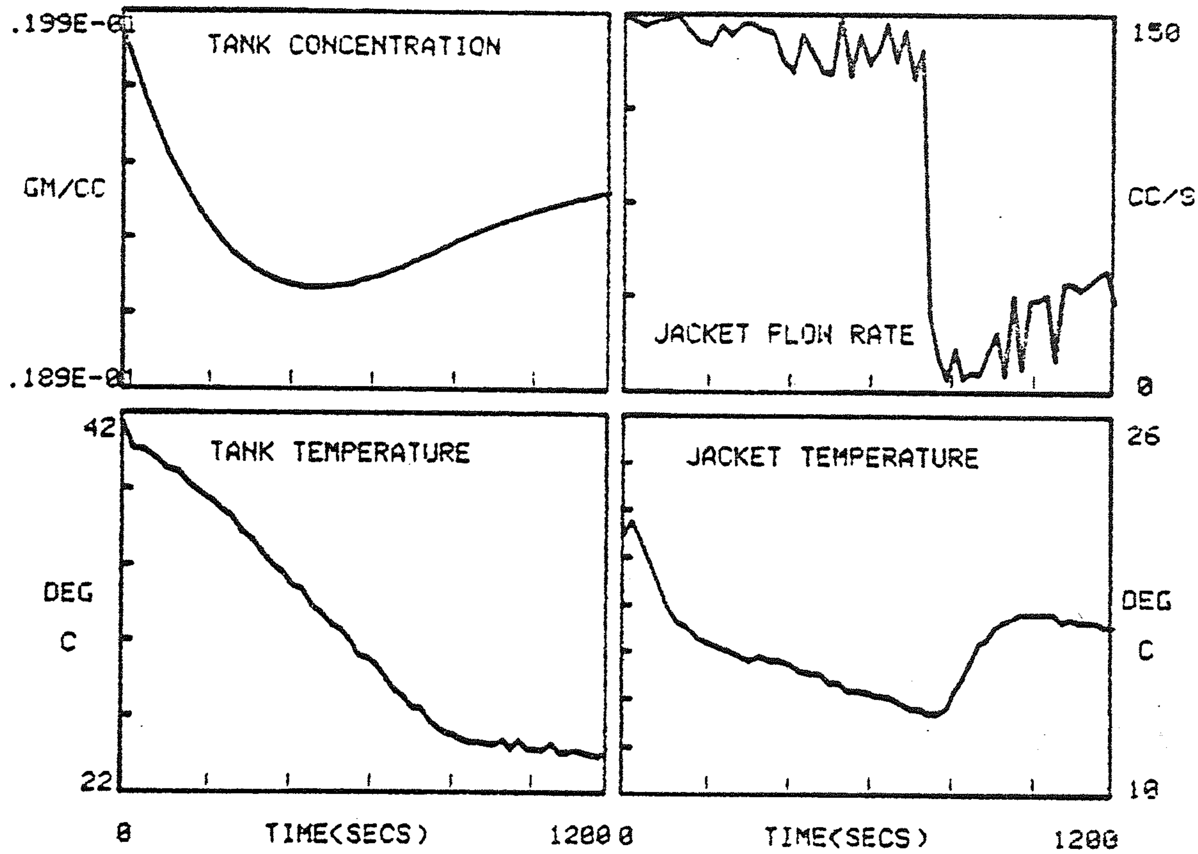


Reaction order = 0

Decoupling type control of tank temperature(D_{max}=.007)

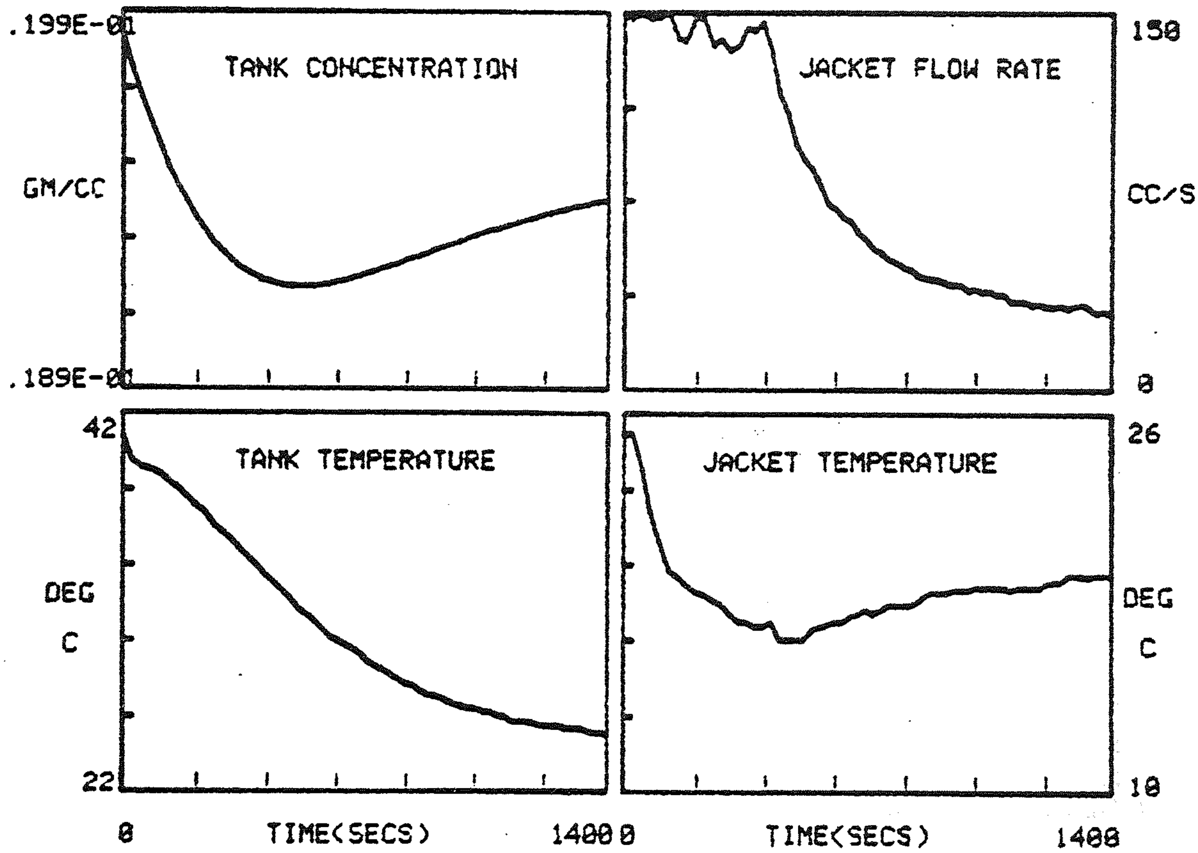
Initial perturbations in state variables

FIG.A.6.1.64 EXPERIMENT NO:64



Reaction order = 0
Decoupling type control of tank temperature(D_{max}=.016)
Initial perturbations in state variables

FIG.A.6.1.65 EXPERIMENT NO:65

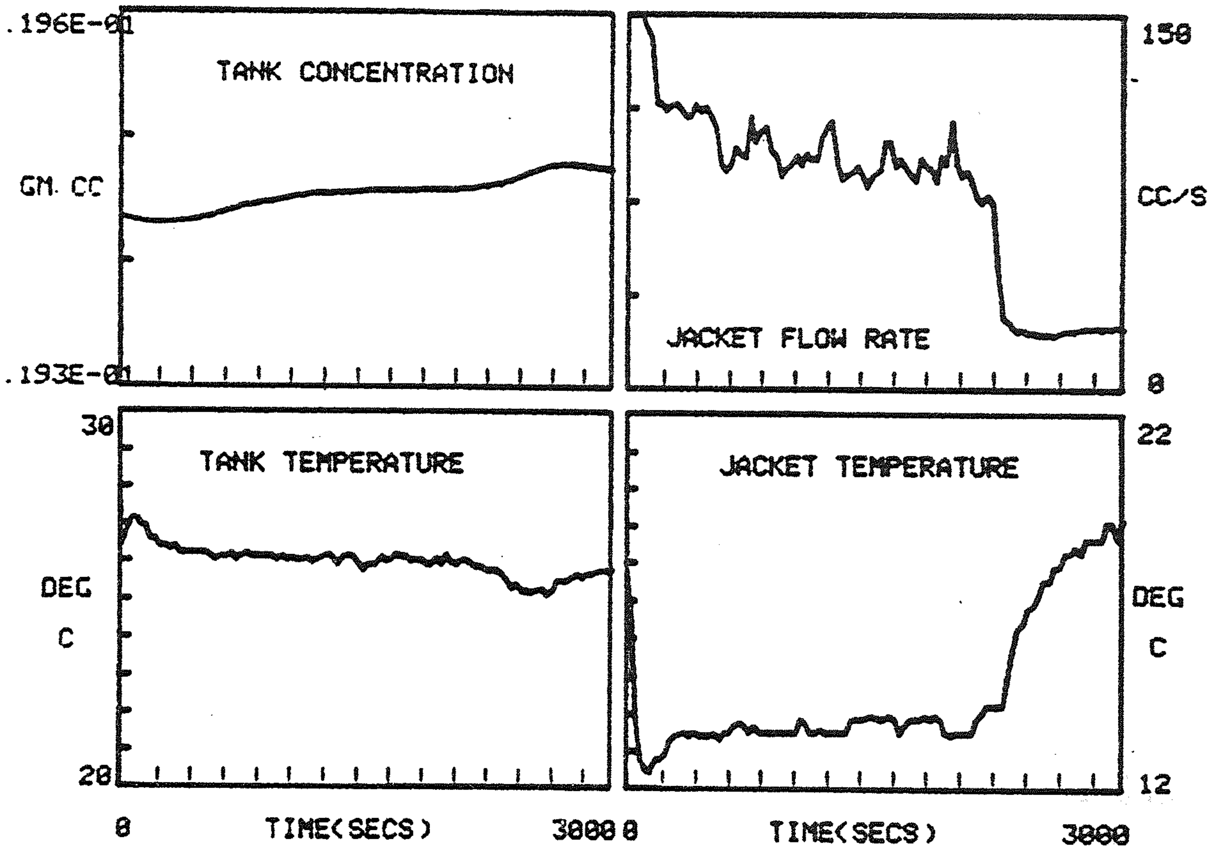


Reaction order = 0

Decoupling type control of tank temperature(D_{max}=.002)

Initial perturbations in state variables

FIG.A.6.1.66 EXPERIMENT NO:66

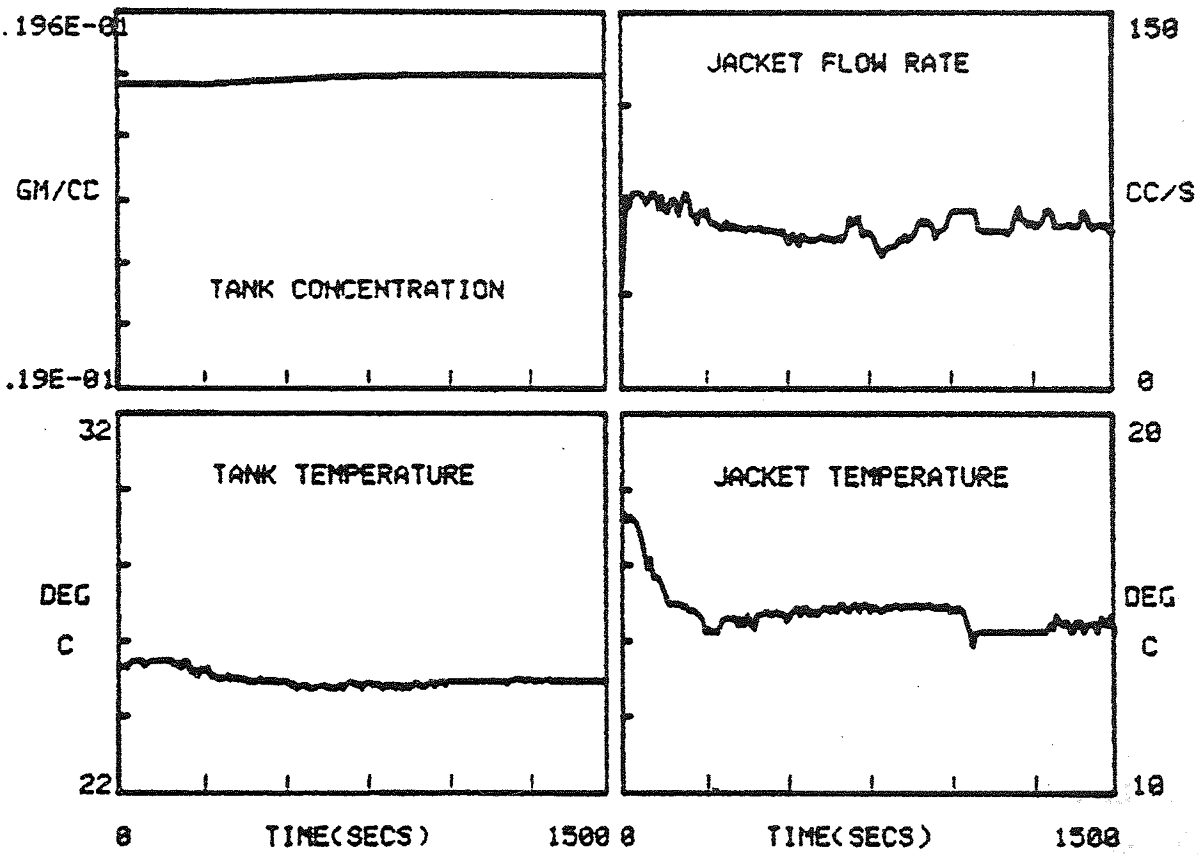


Reaction order = 0

Decoupling type control of tank temperature(D_{max}=.007)

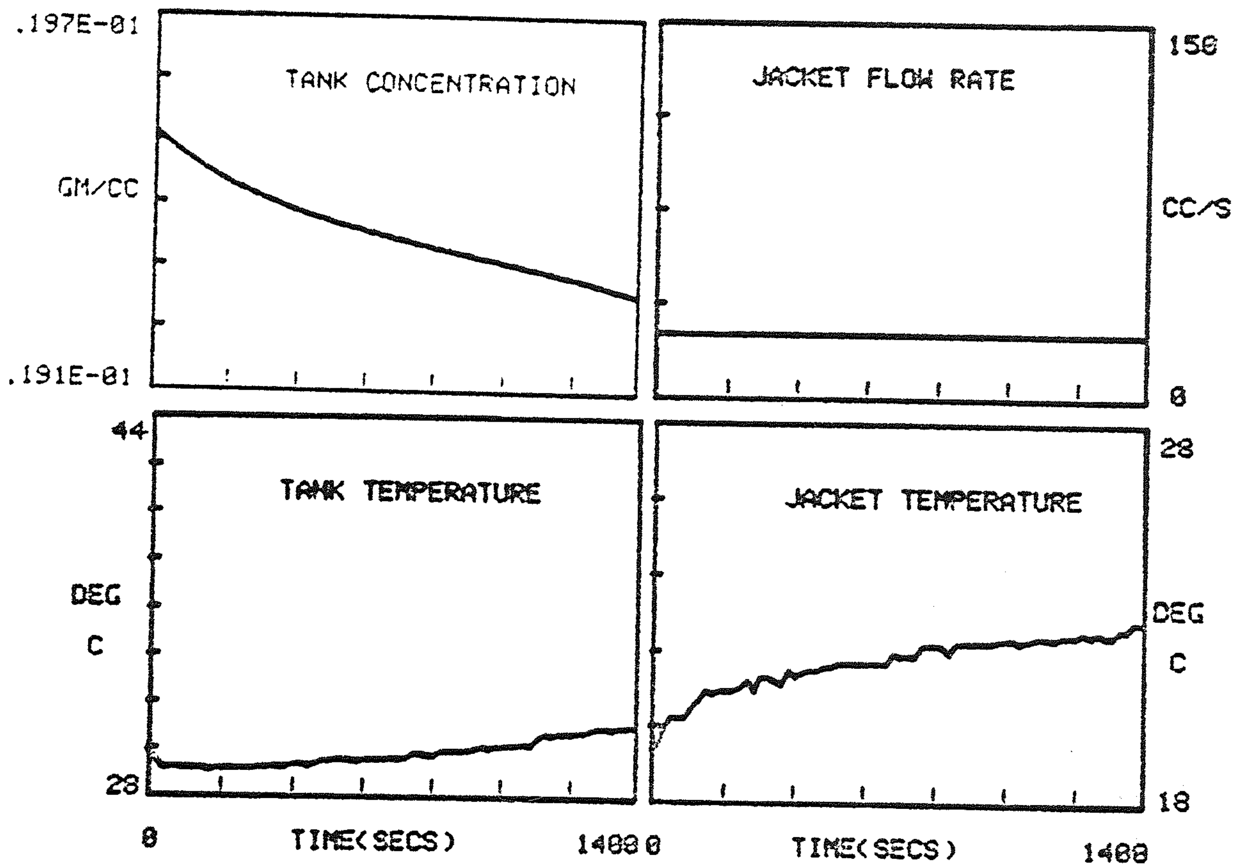
Step in tank inlet temperature = 4.2 K

FIG.A.6.1.67 EXPERIMENT NO:67



Reaction order = 0
Decoupling type control of tank temperature(D_{max}=.007)
Step in tank inlet temperature = 2.5 K

FIG.A.6.68 EXPERIMENT NO:68

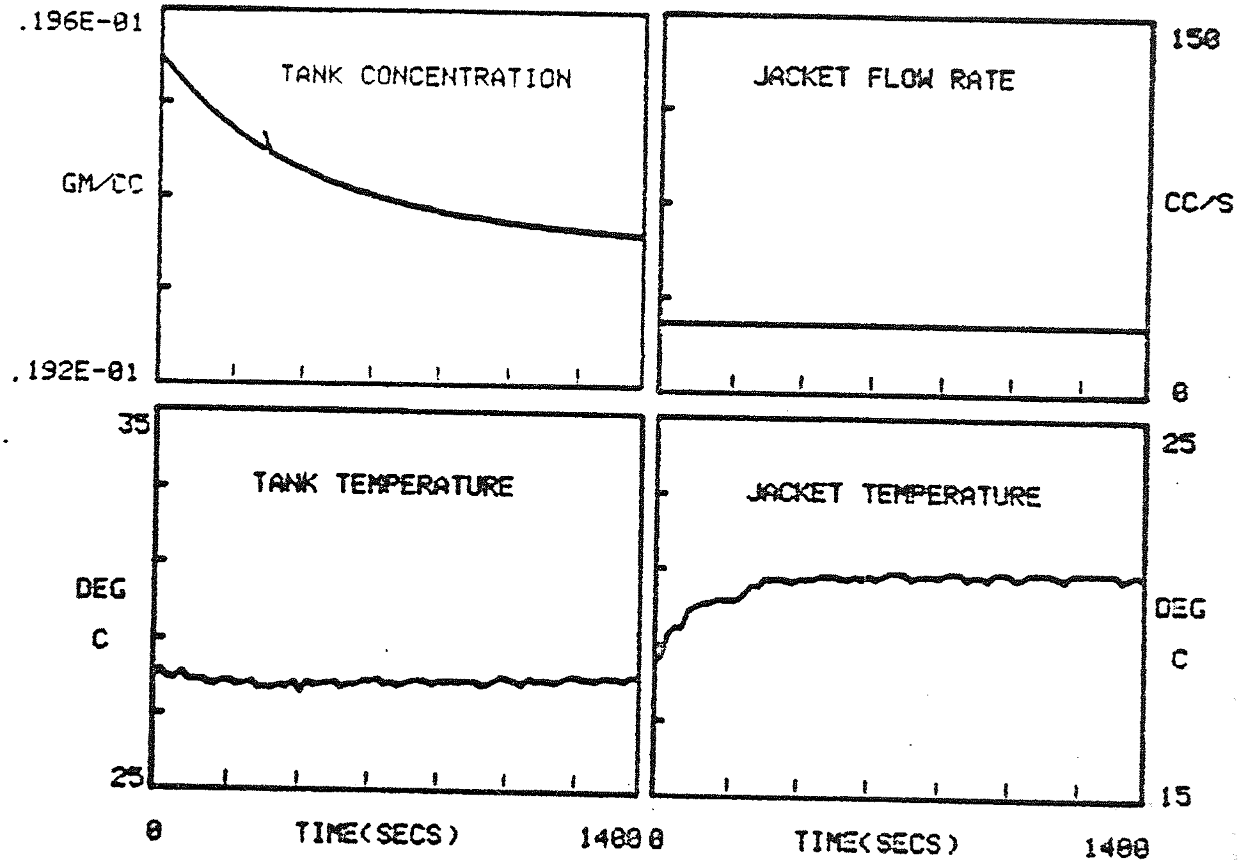


Reaction order =-1

Open loop studies

Initial perturbations in state variables

FIG.A.6.1.69 EXPERIMENT NO:69

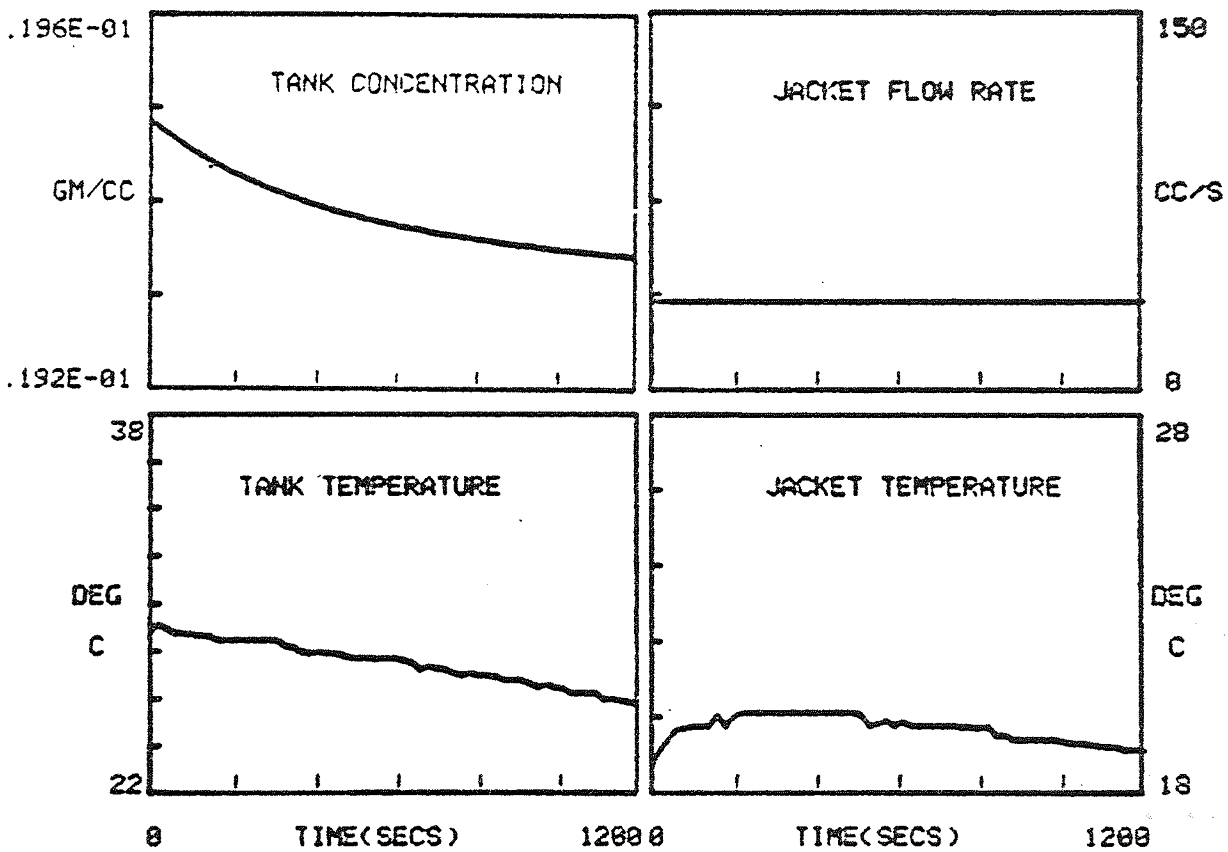


Reaction order = -1

Open loop studies

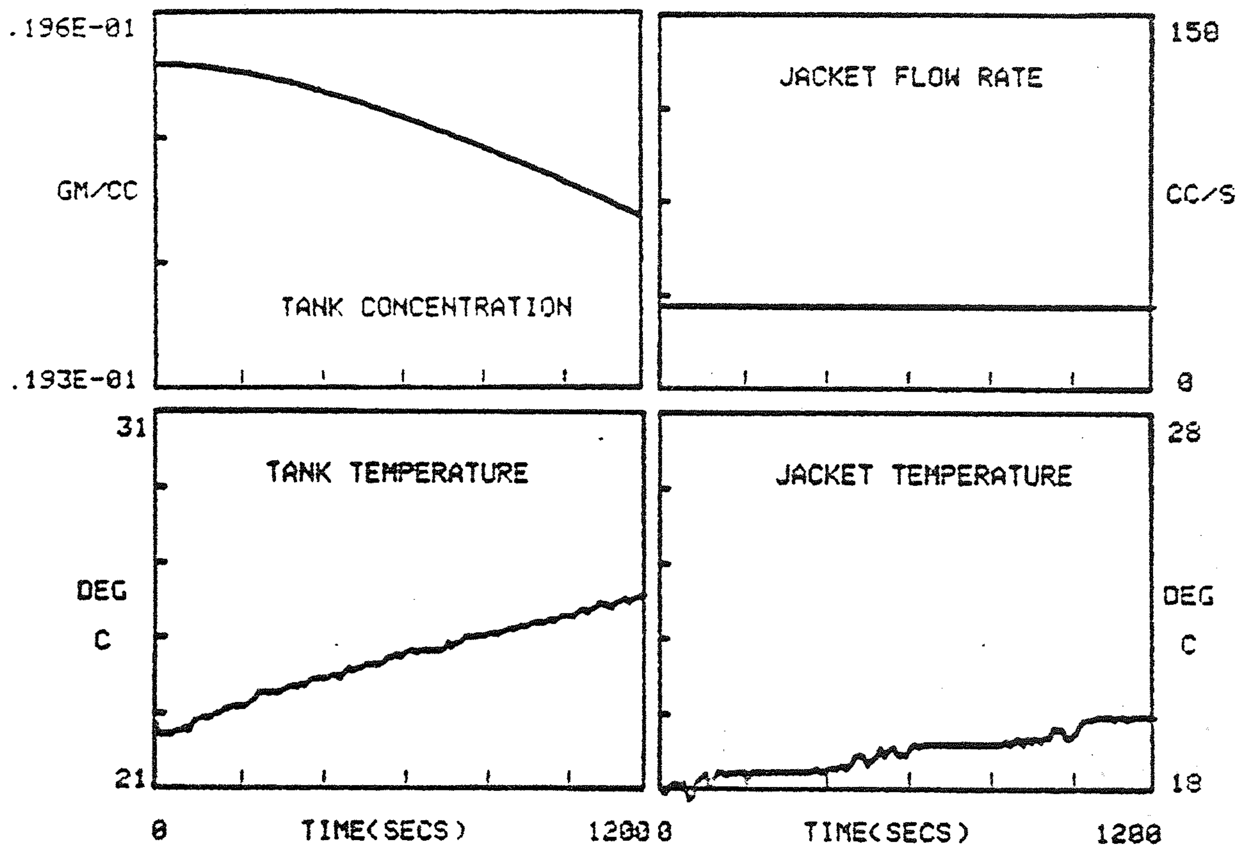
Initial perturbations in state variables

FIG.A.6.1.70 EXPERIMENT NO:70



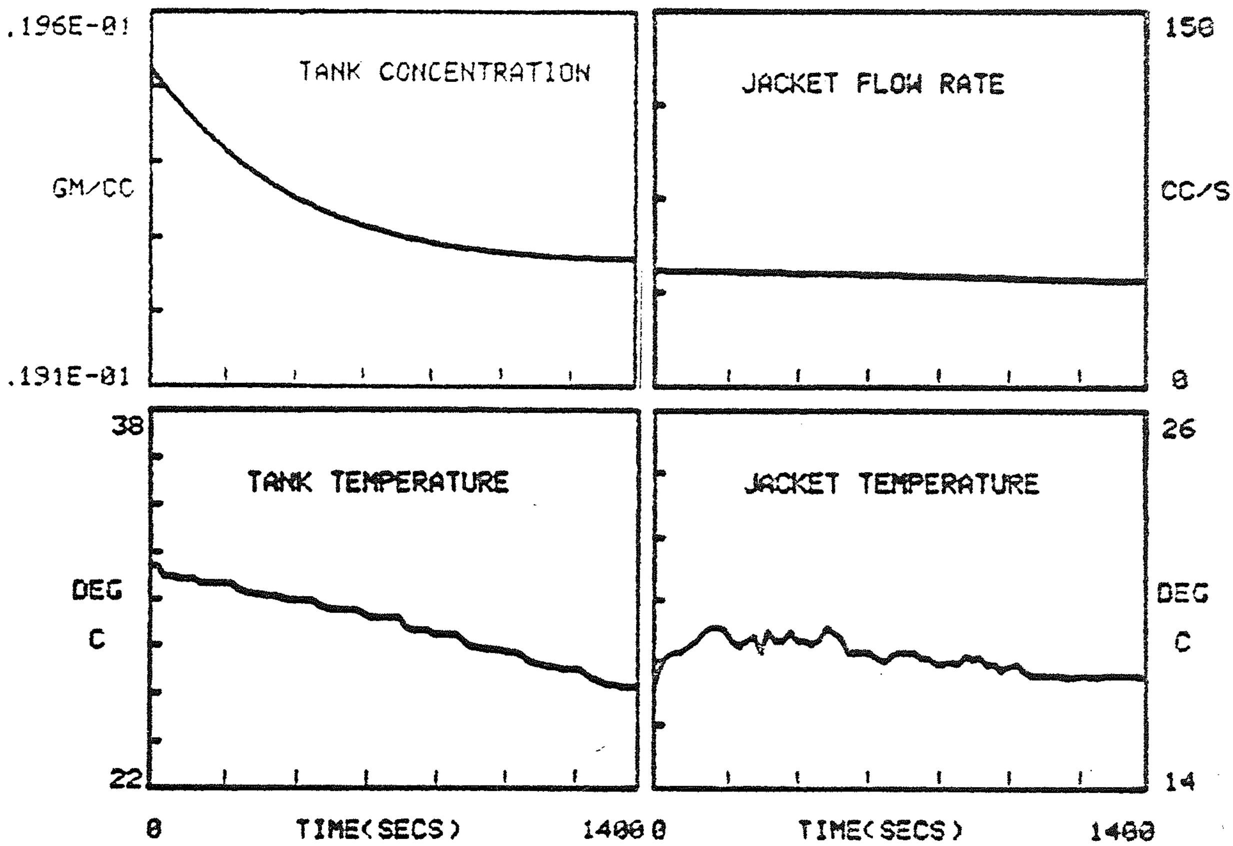
Reaction order = -1
Open loop studies
Initial perturbations in state variables

FIG.A.6.1.71 EXPERIMENT NO:71



Reaction order = -1
Open loop studies
Step in tank inlet temperature = 2.5 K

FIG.A.6.1.72 EXPERIMENT NO:72

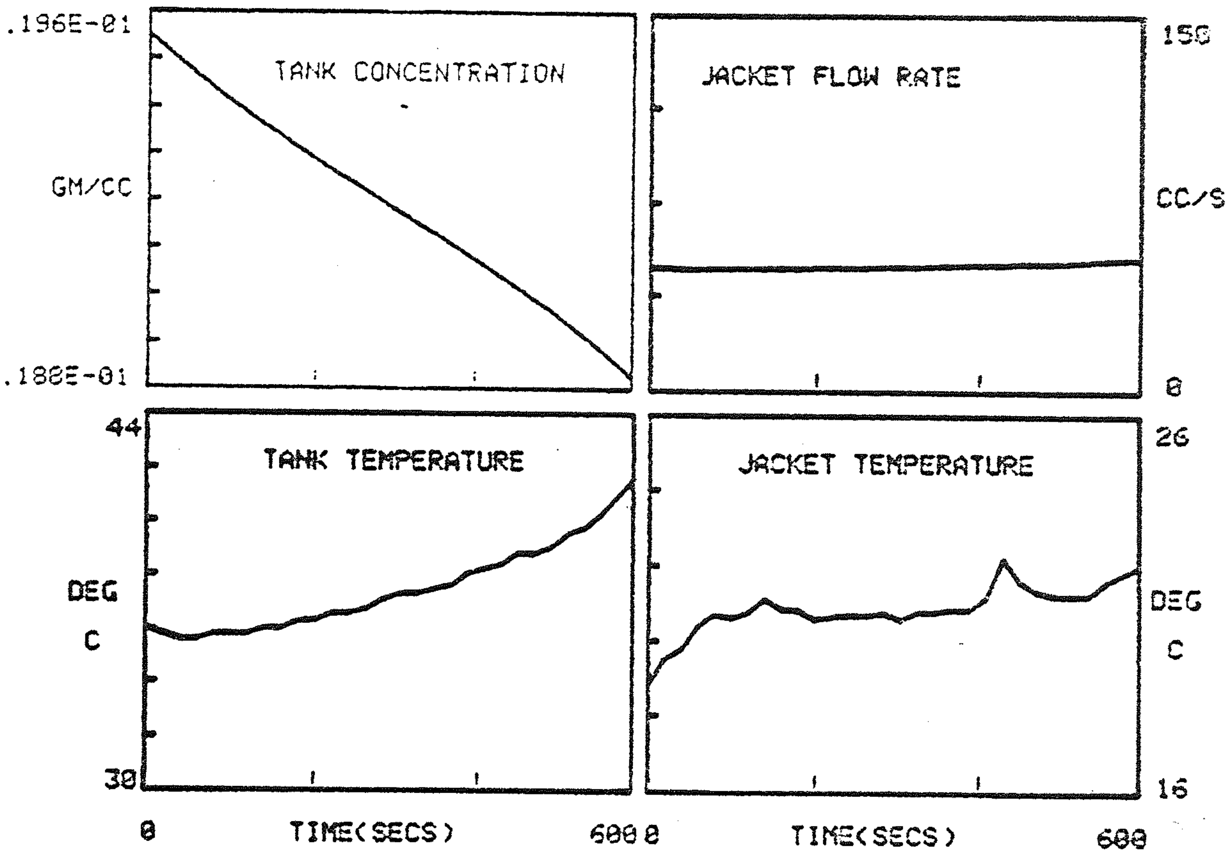


Reaction order = -1

Proportional feedback control of tank temperature(K_c=.0005)

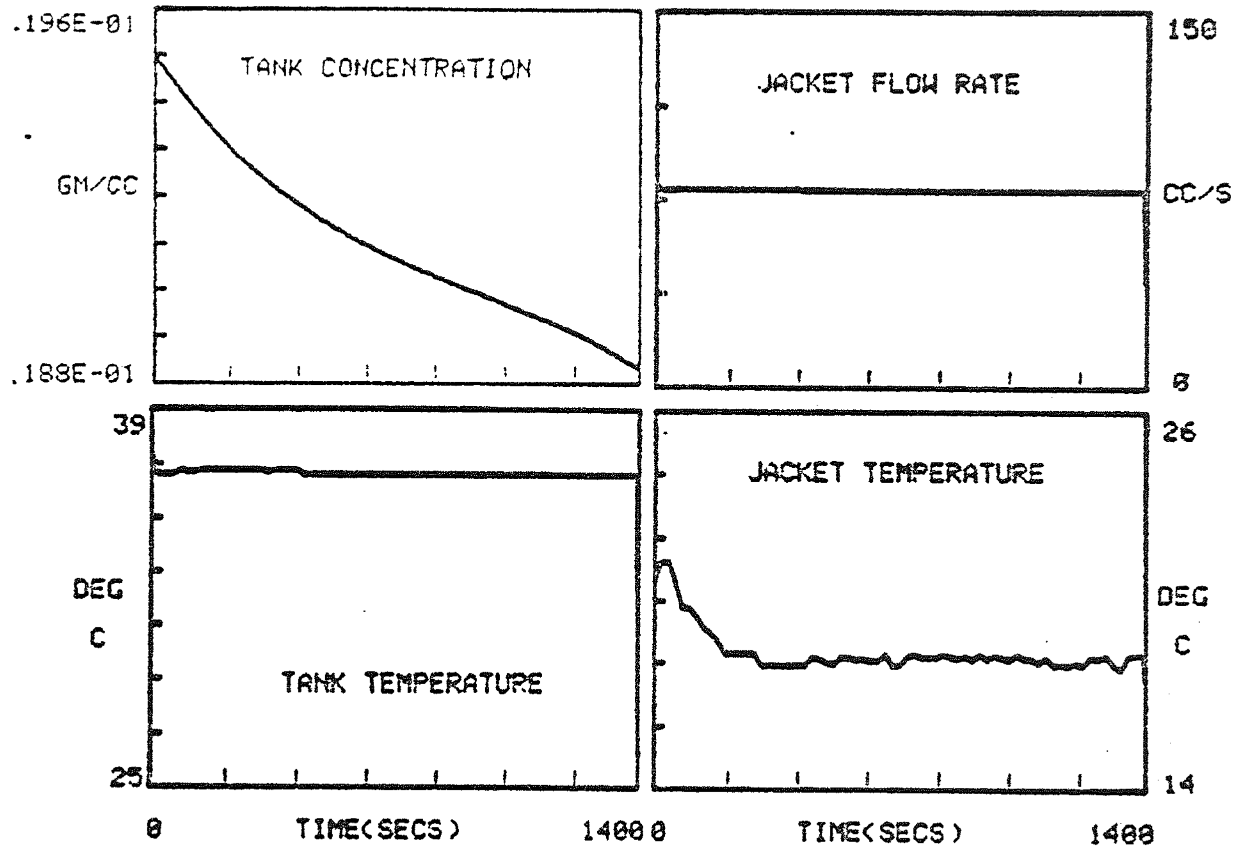
Initial perturbations in state variables

FIG.A.6.1.73 EXPERIMENT NO:73



Reaction order = -1
Proportional feedback control of tank temperature(K_c=.0005)
Initial perturbations in state variables

FIG.A.6.1.74 EXPERIMENT NO:74

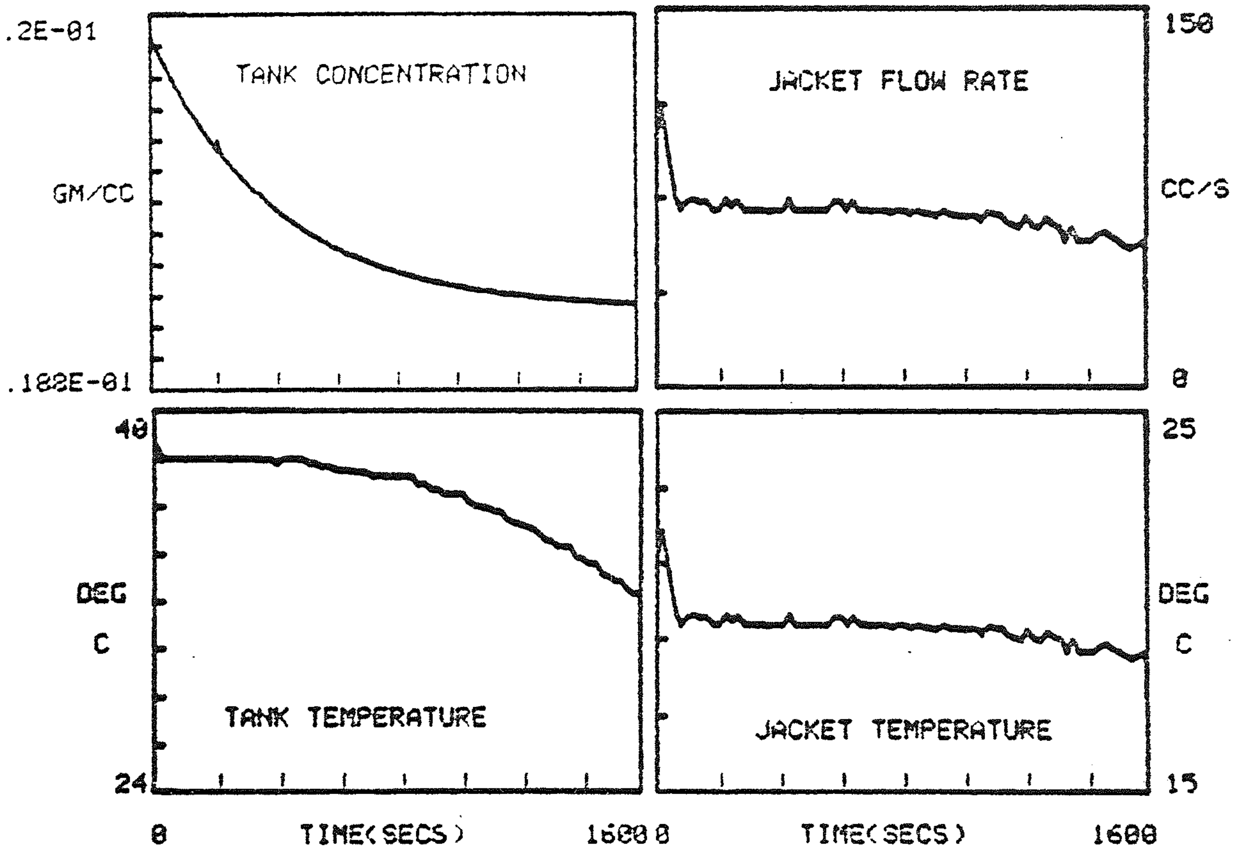


Reaction order = -1

Proportional feedback control of tank temperature(K_c=.002)

Initial perturbations in state variables

FIG.A.6.1.75 EXPERIMENT NO:75

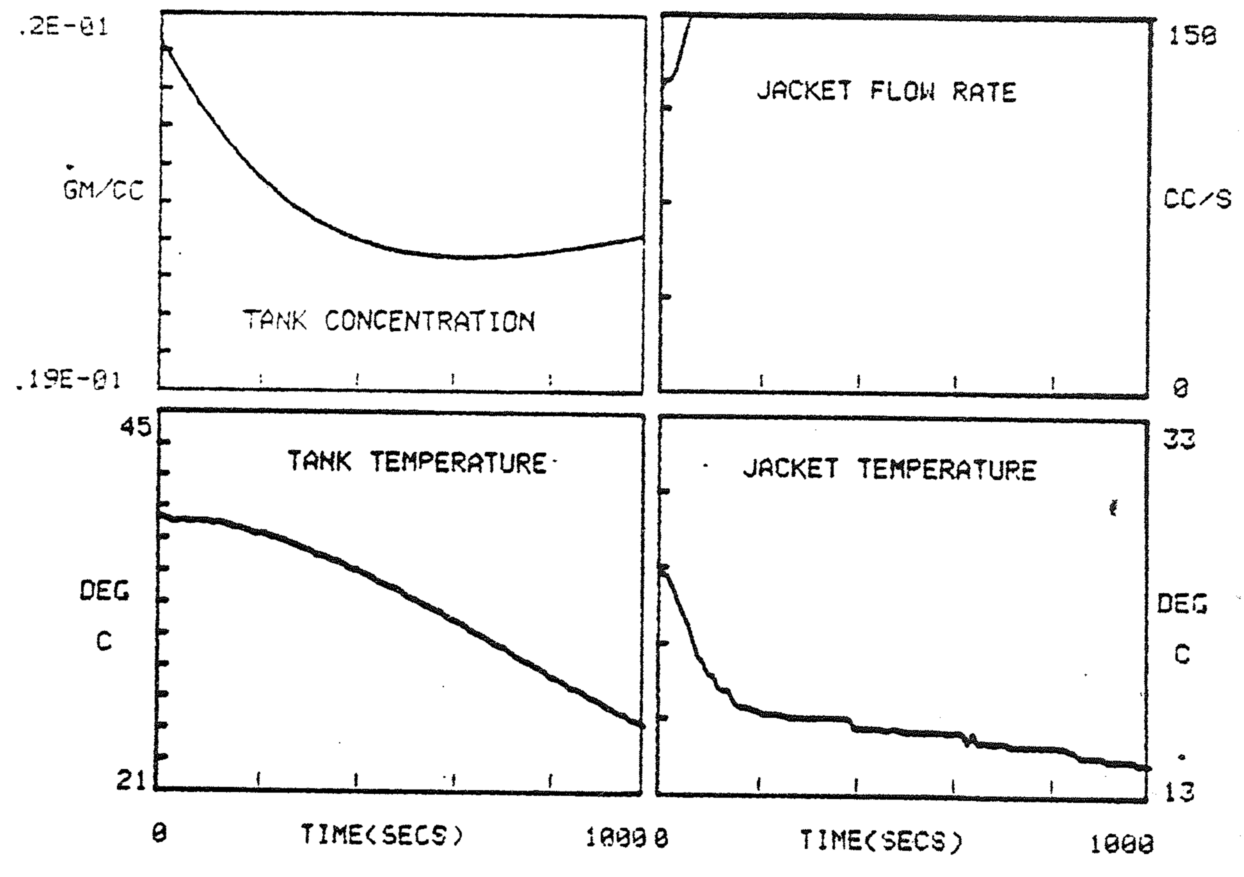


Reaction order = -1

Proportional feedback control of jacket temperature(K_c=.01)

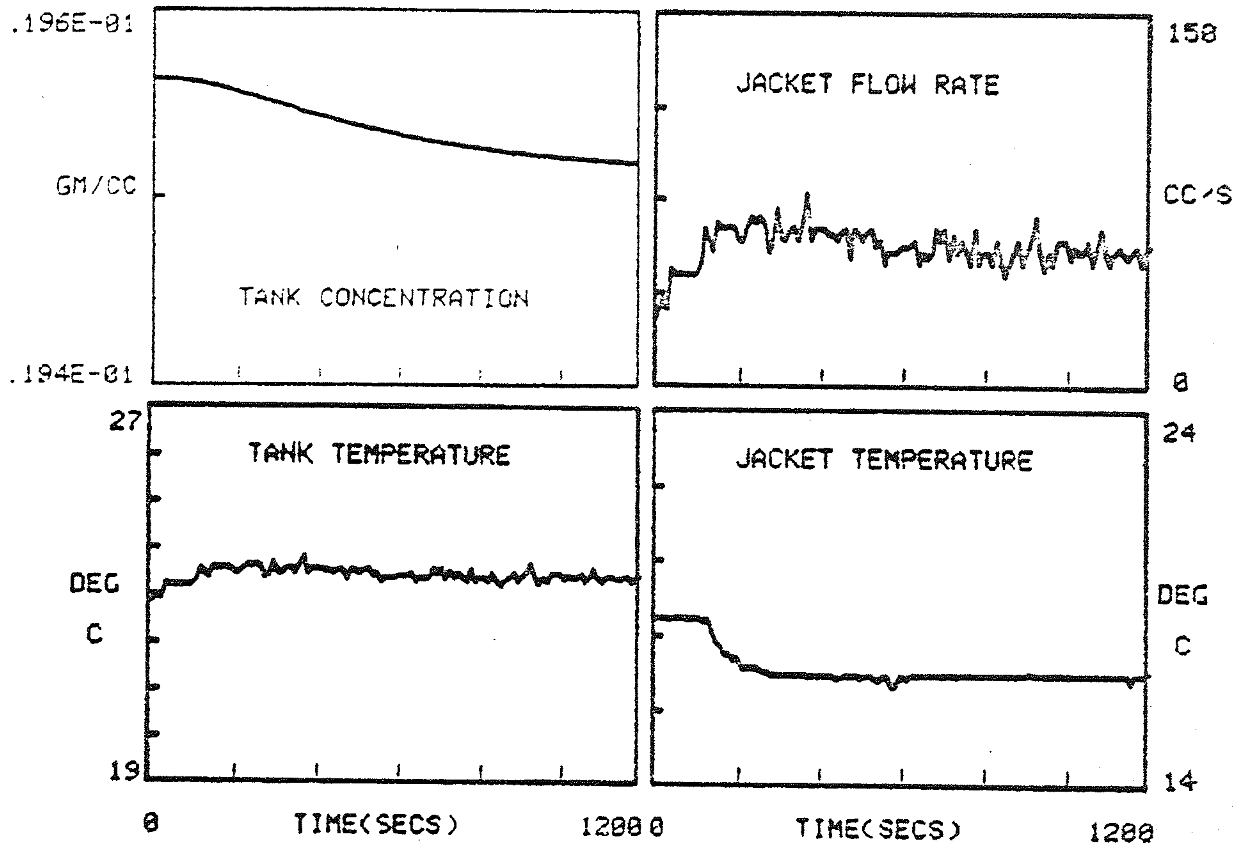
Initial perturbations in state variables

FIG.A.6.1.76 EXPERIMENT NO:76



Reaction order = -1
Controller equation derived from stability conditions(eqn.(3.38))
Initial perturbations in state variables

FIG.A.6.1.77 EXPERIMENT NO:77

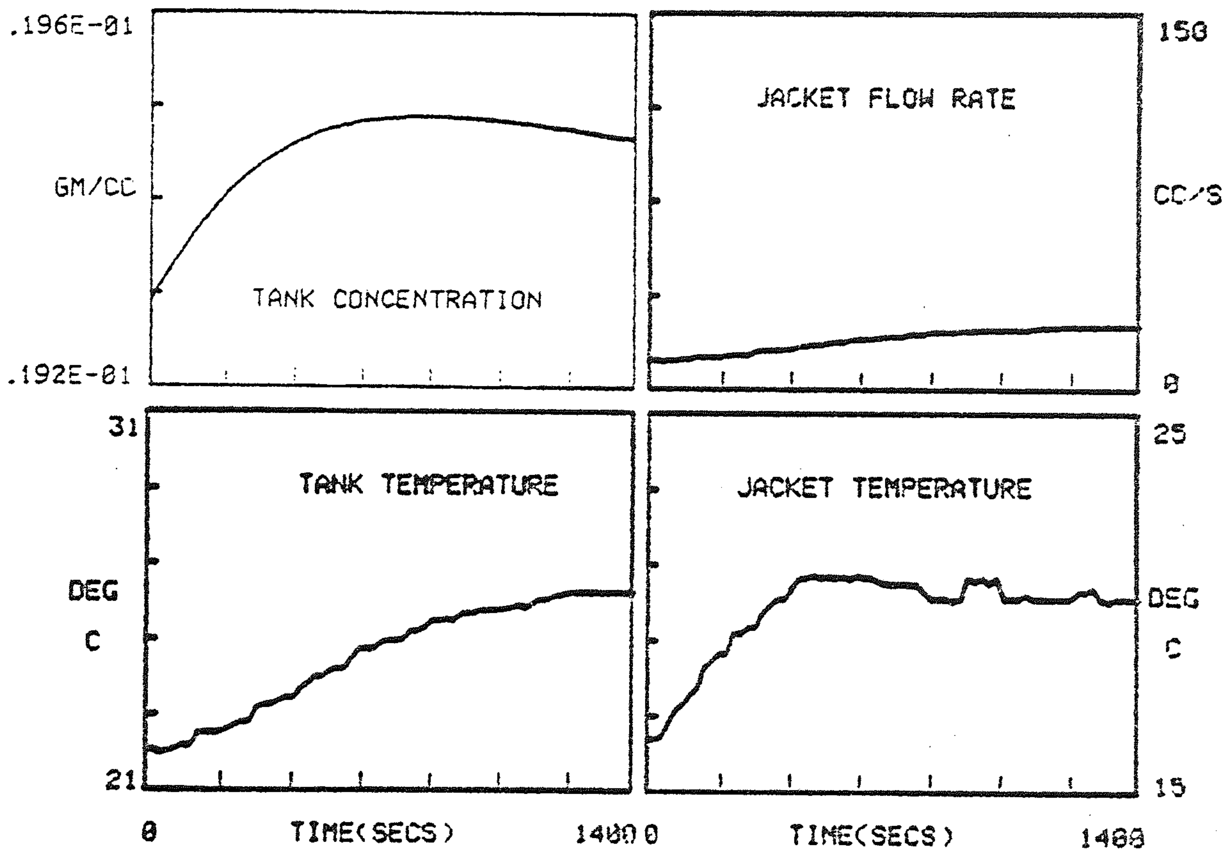


Reaction order = -1

Proportional feedback control of tank temperature(K_c=.03)

Step in tank inlet temperature = 2.6 K

FIG.A.6.1.78 EXPERIMENT NO:78

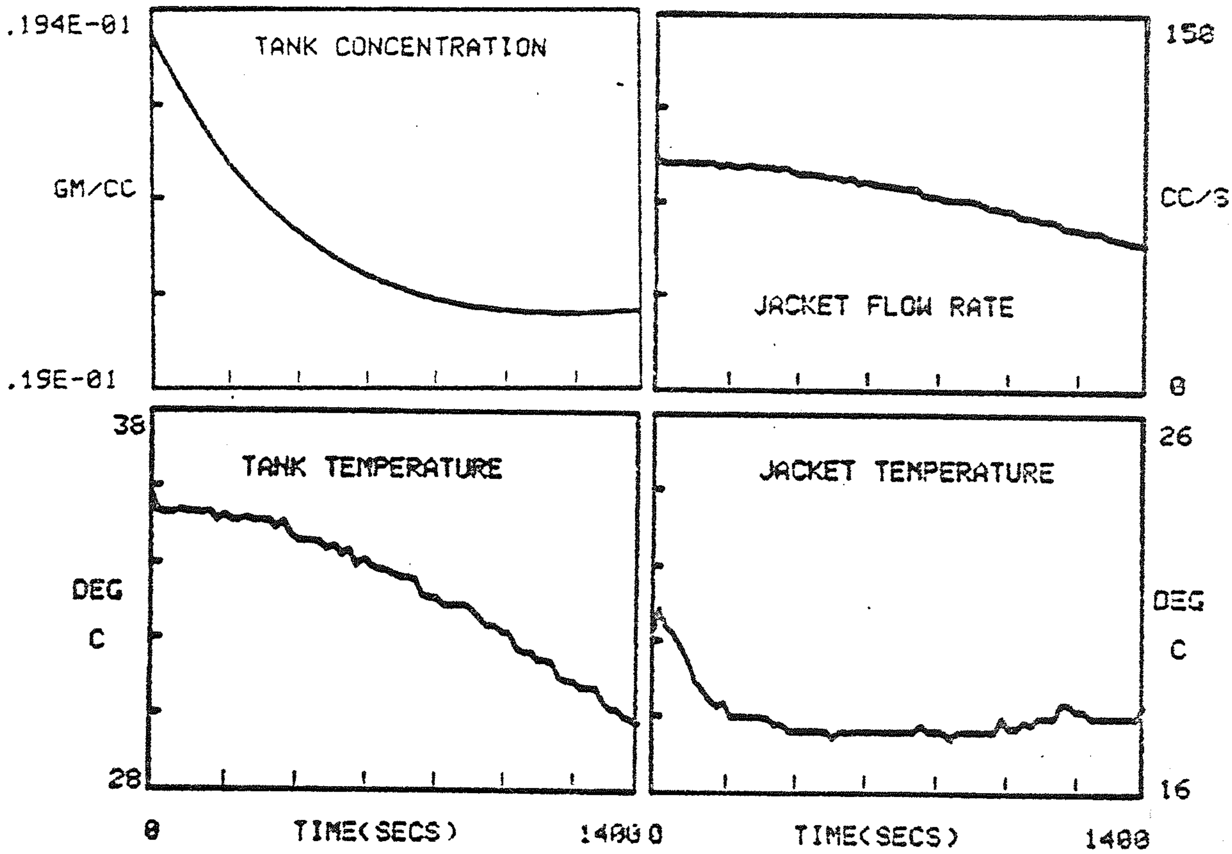


Reaction order = -1

Proportional feedback control of tank temperature(K_c=.002)

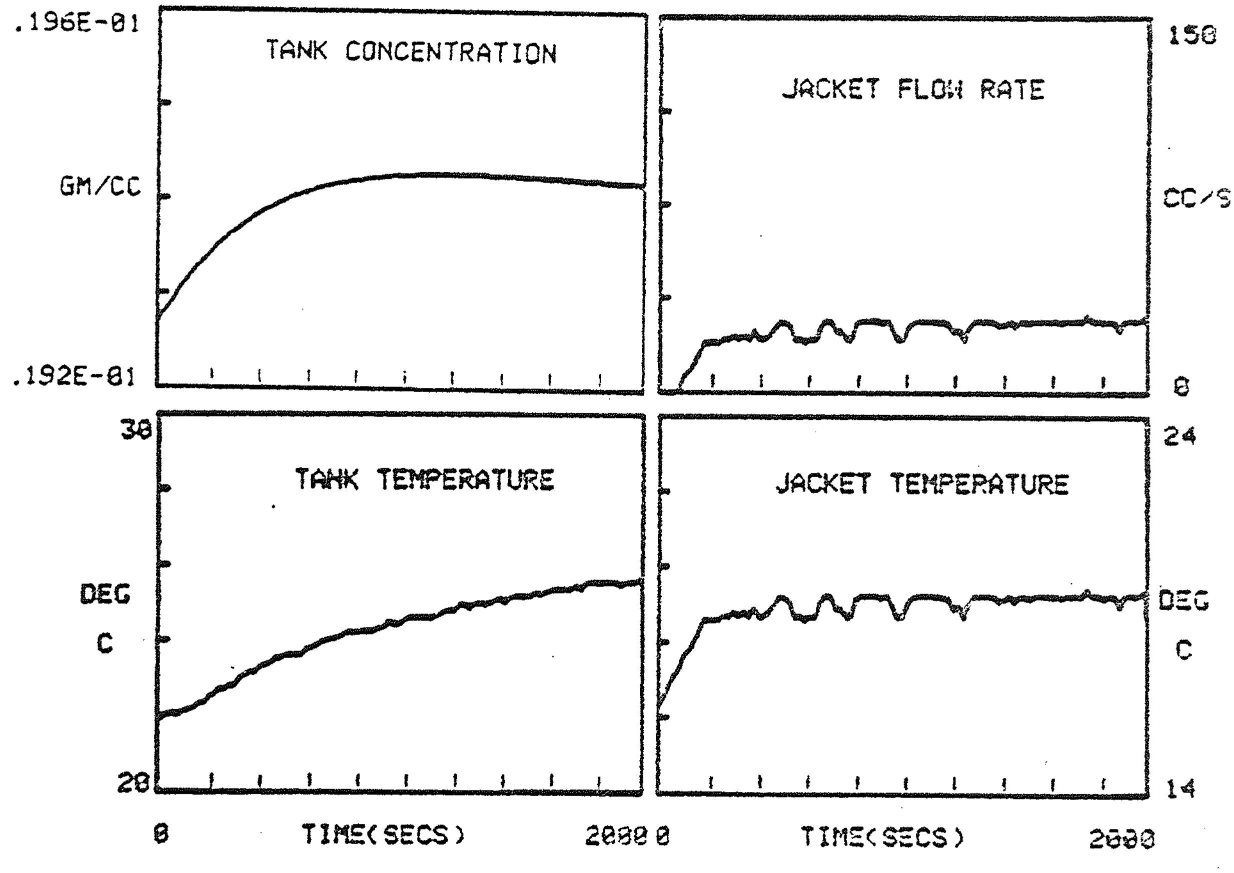
Stabilising open loop unstable operating point

FIG.A.6.1.79 EXPERIMENT 79



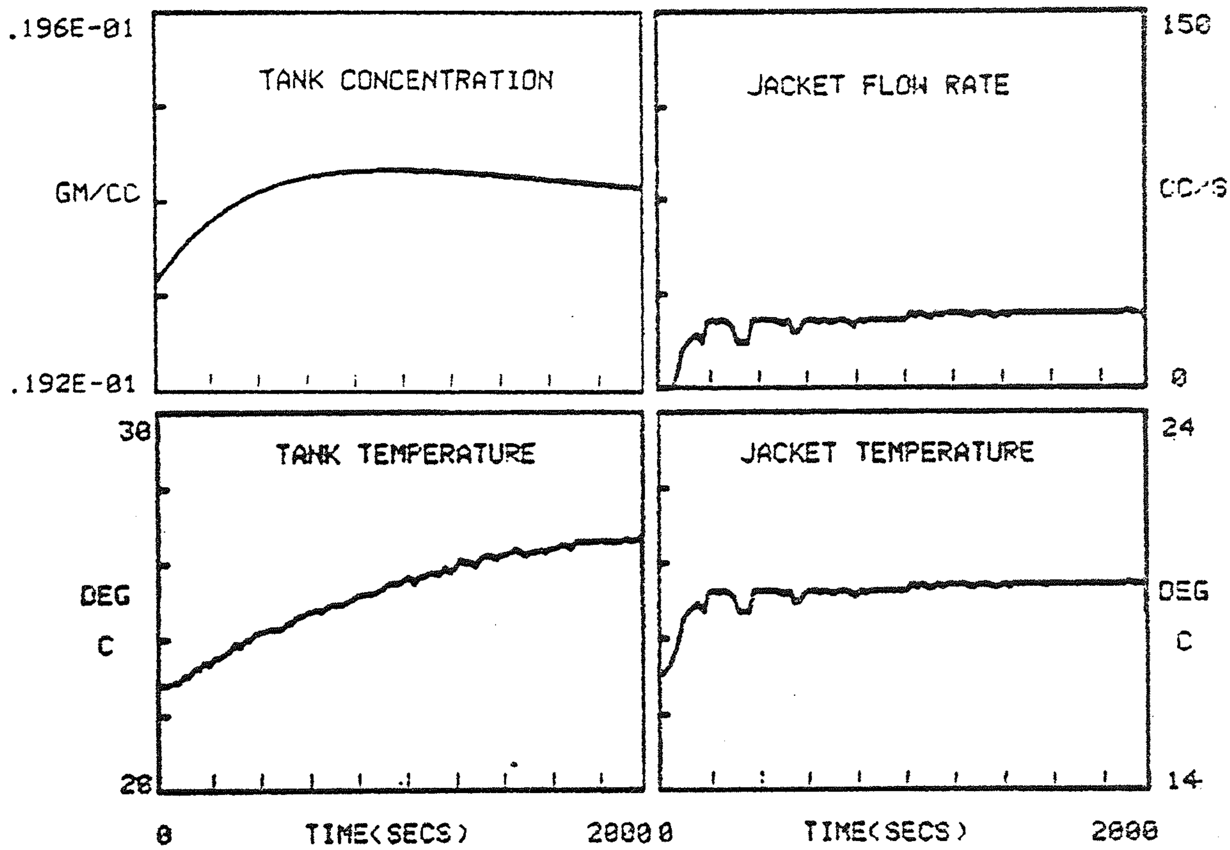
Reaction order = -1
Proportional feedback control of tank temperature(K_c=.0035)
Stabilising open loop unstable operating point

FIG.A.6.1.80 EXPERIMENT NO:80



Reaction order = -1
Proportional feedback control of jacket temperature(K_c=.008)
Stabilising open loop unstable operating point

FIG.A.6.1.81 EXPERIMENT NO:81

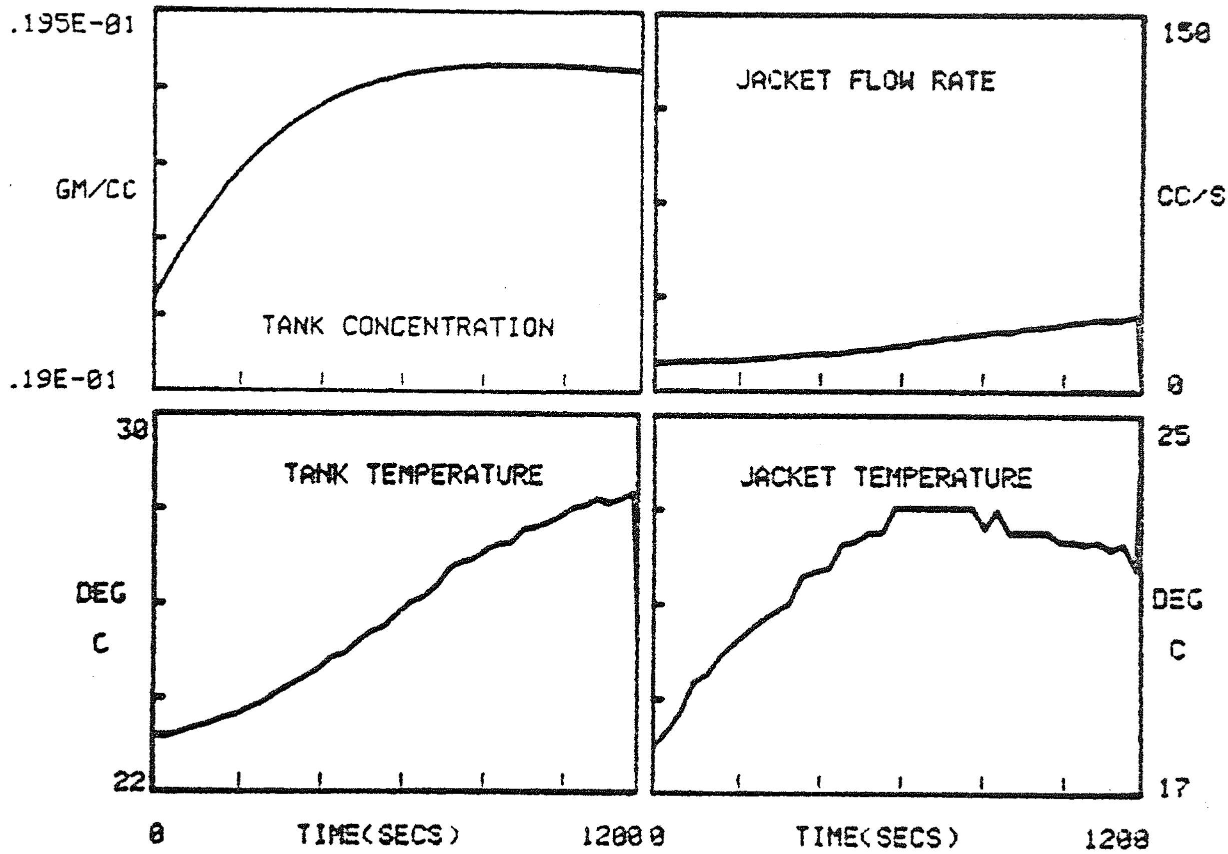


Reaction order = -1

Proportional feedback control of jacket temperature(K_c=.01)

Stabilising open loop unstable operating point

FIG.A.6.1.82 EXPERIMENT NO:82

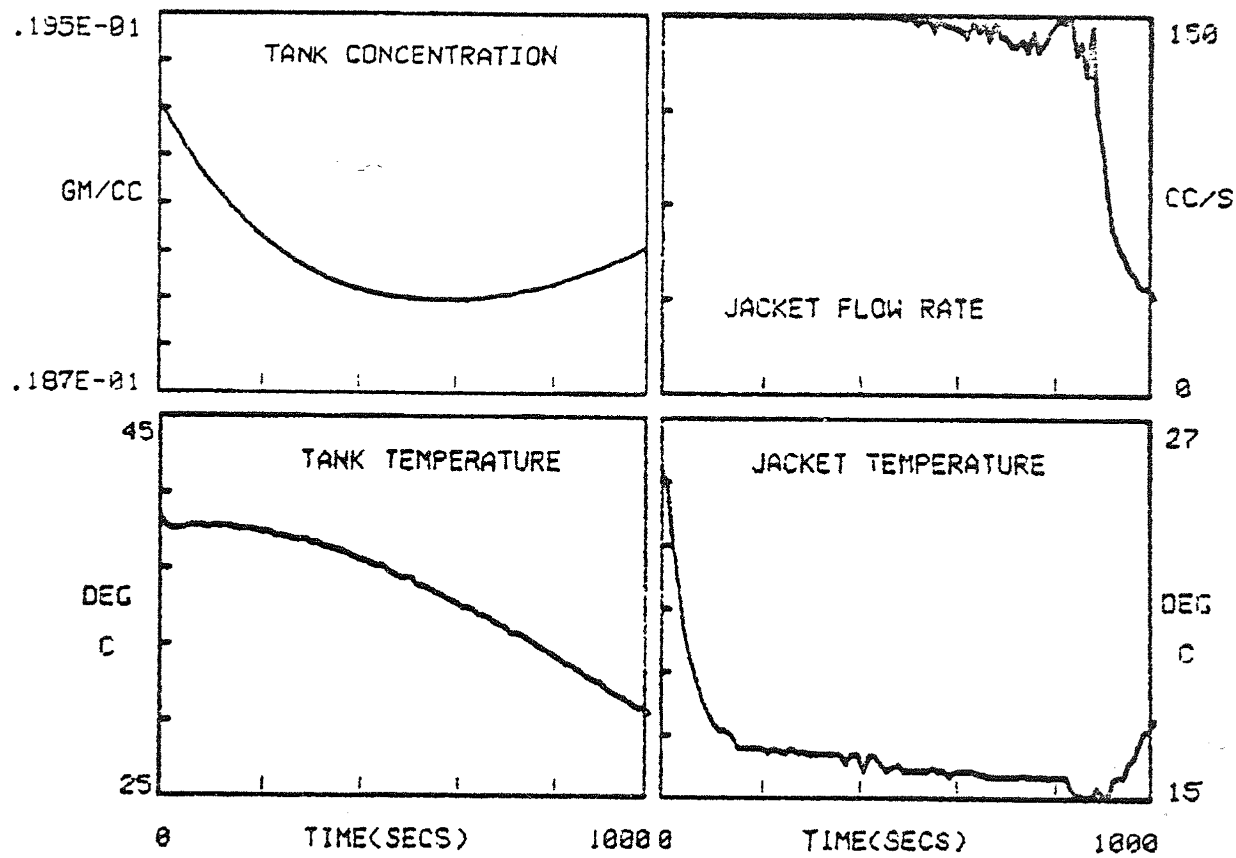


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.007)

Stabilising open loop unstable operating point

FIG.A.6.1.83 EXPERIMENT NO:83

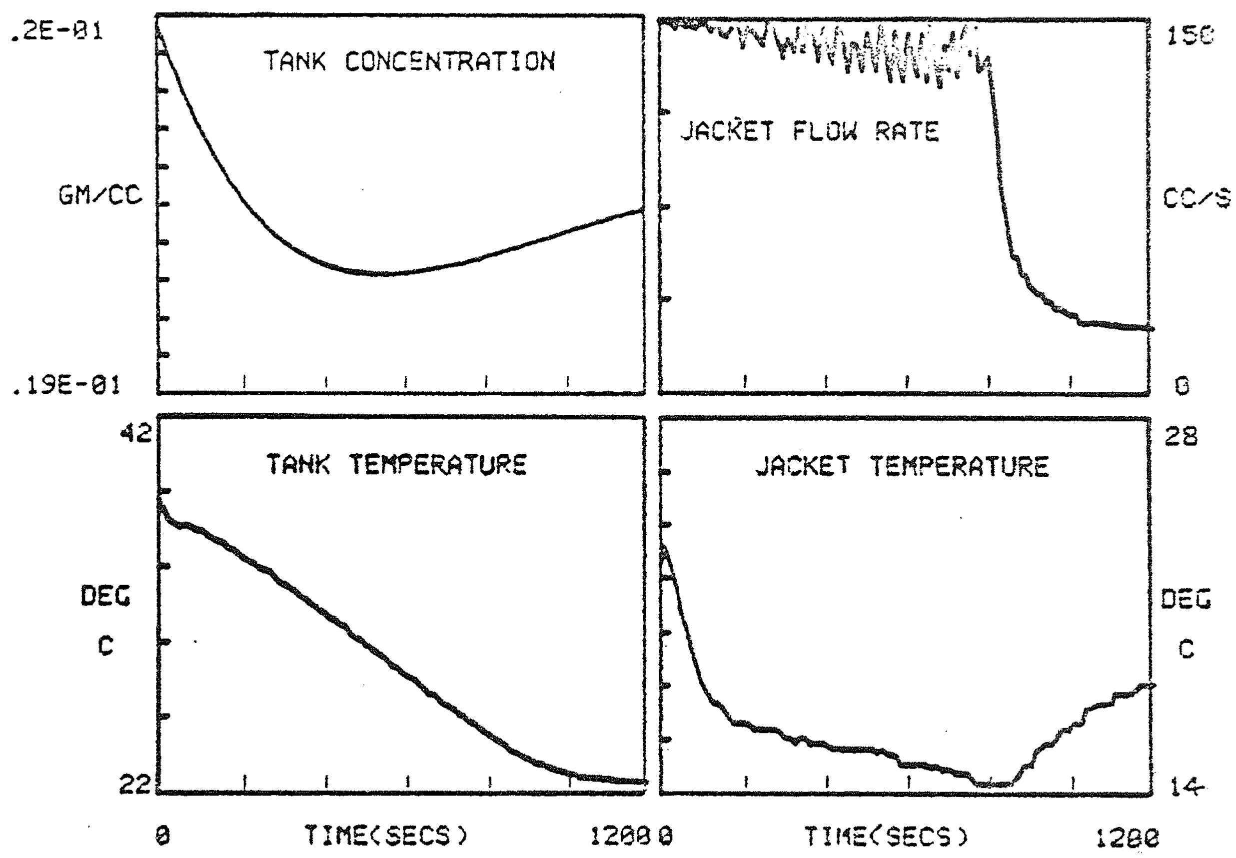


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.007)

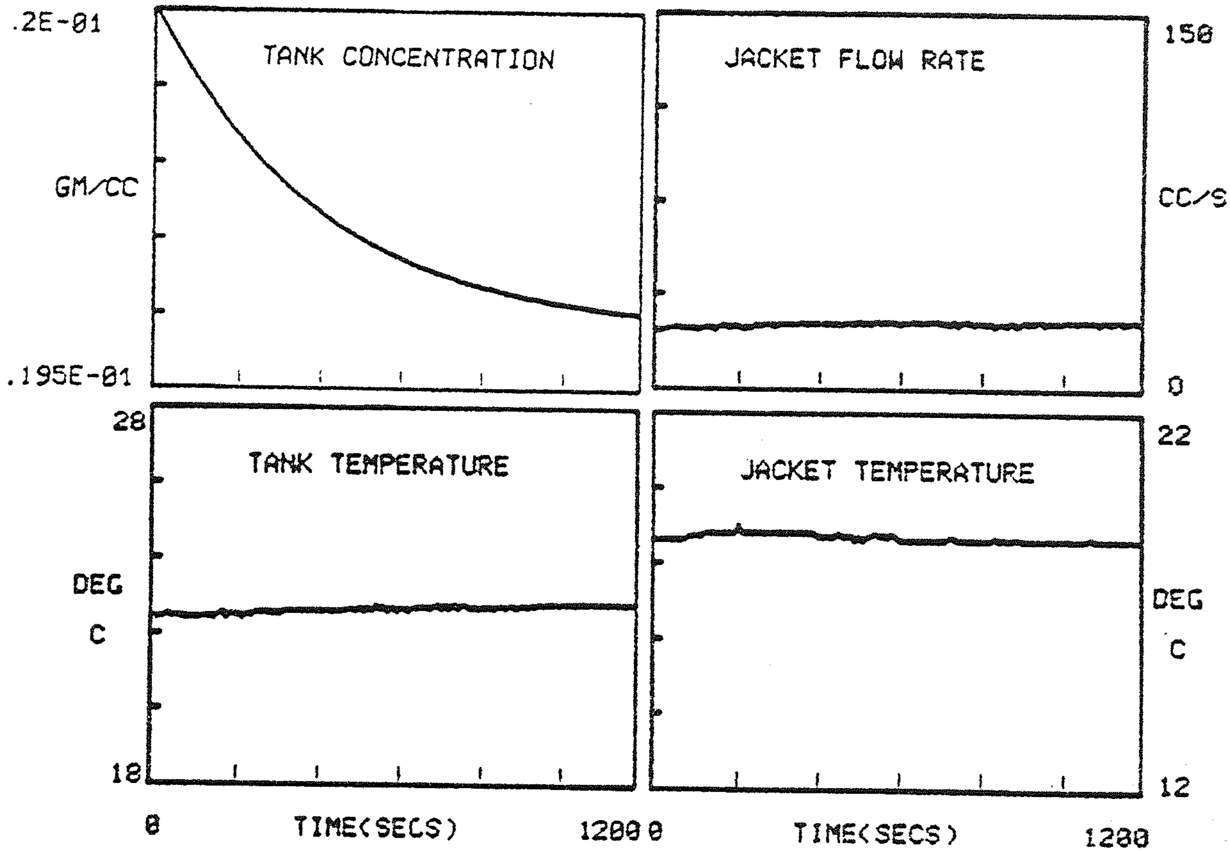
Stabilising open loop unstable operating point

FIG.A.6.1.84 EXPERIMENT NO:84



Reaction order = -1
Decoupling type control of tank temperature(D_{max}=.007)
Initial perturbations in state variables

FIG.A.6.1.85 EXPERIMENT NO:85

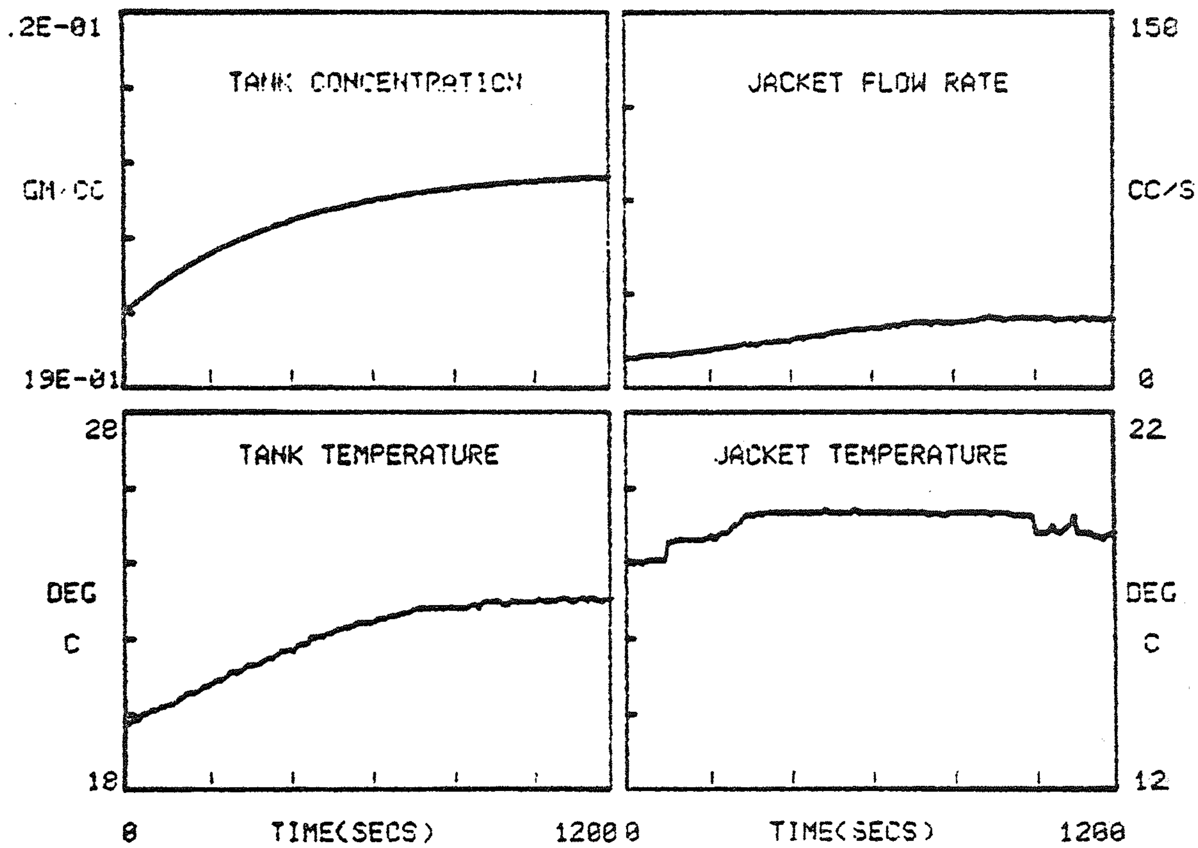


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbation in a state variable

FIG.A.6.1.86 EXPERIMENT NO:86

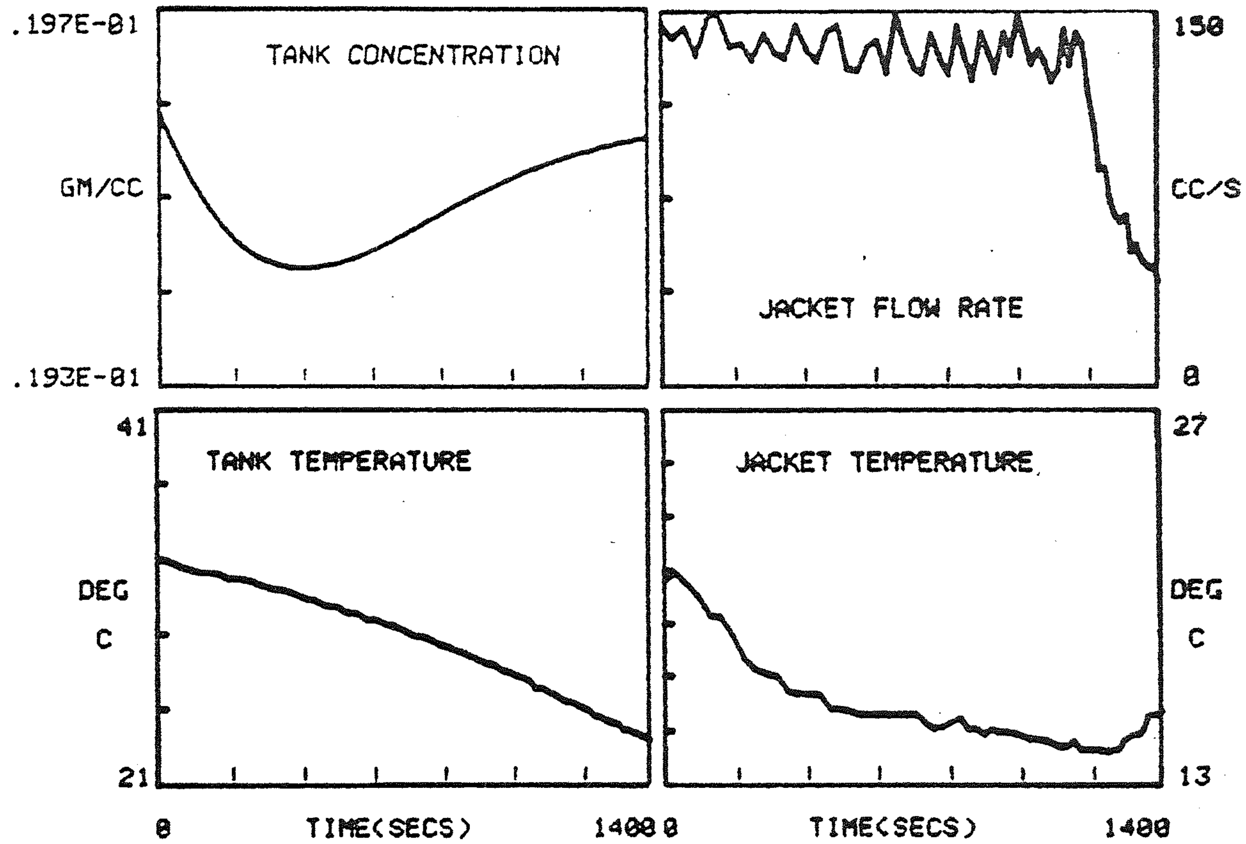


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.007)

Initial perturbations in state variables

FIG.A.6.1.87 EXPERIMENT NO:87

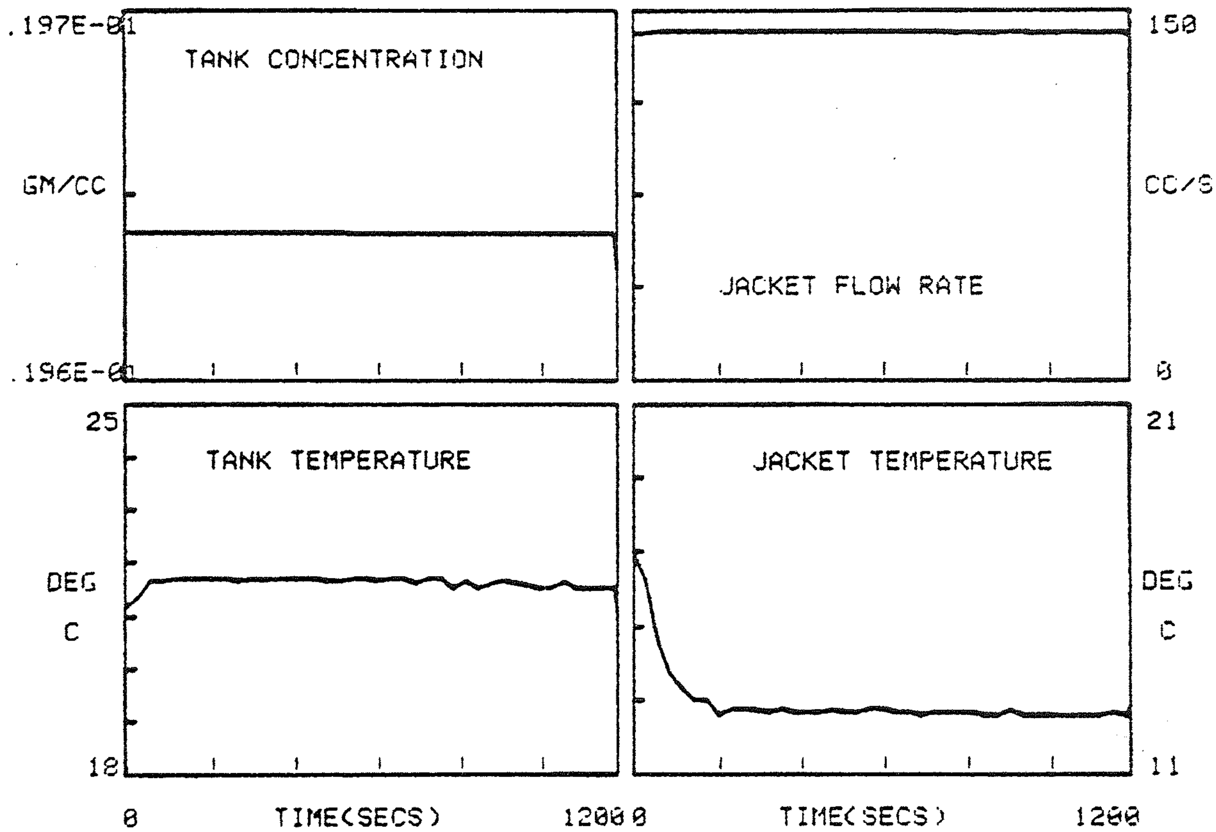


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.005)

Initial perturbations in state variables

FIG.A.6.1.88 EXPERIMENT NO:88

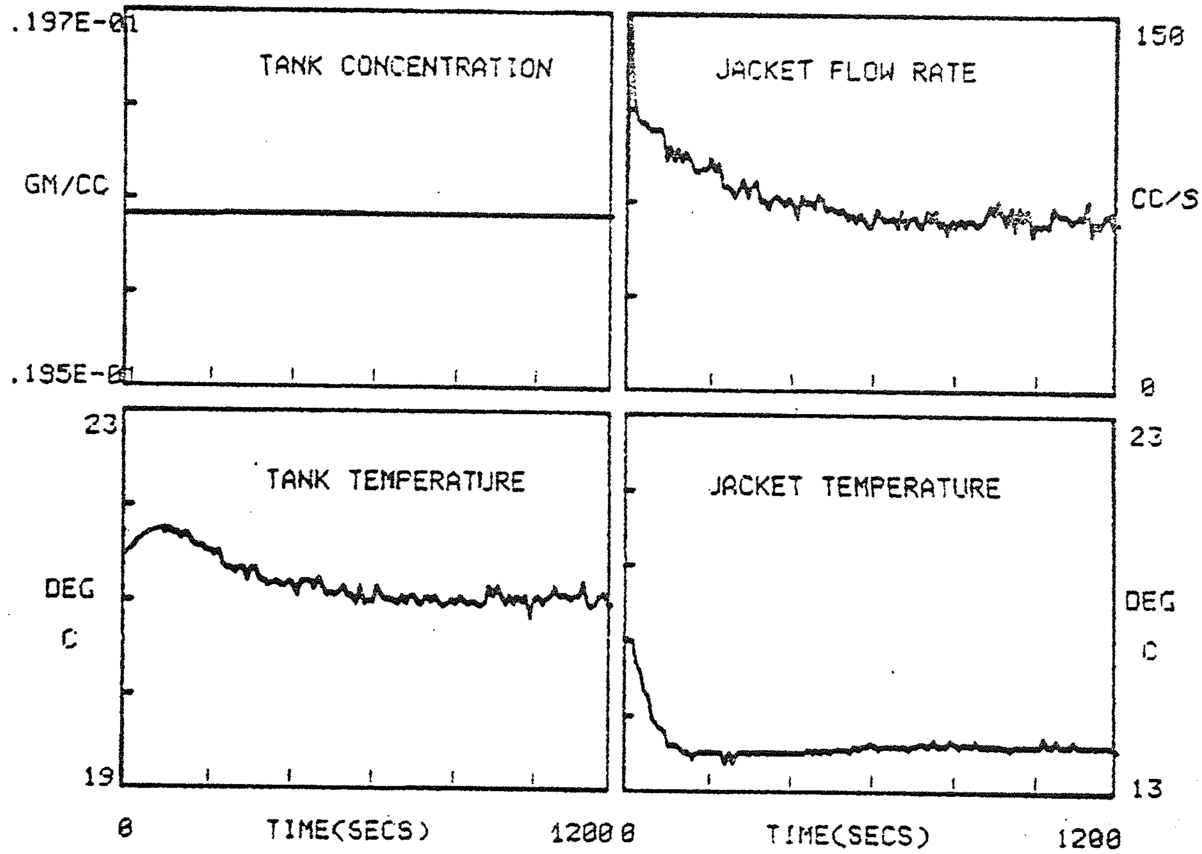


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.007)

Step in tank inlet temperature = 3.6 K

FIG.A.6.1.89 EXPERIMENT NO:89

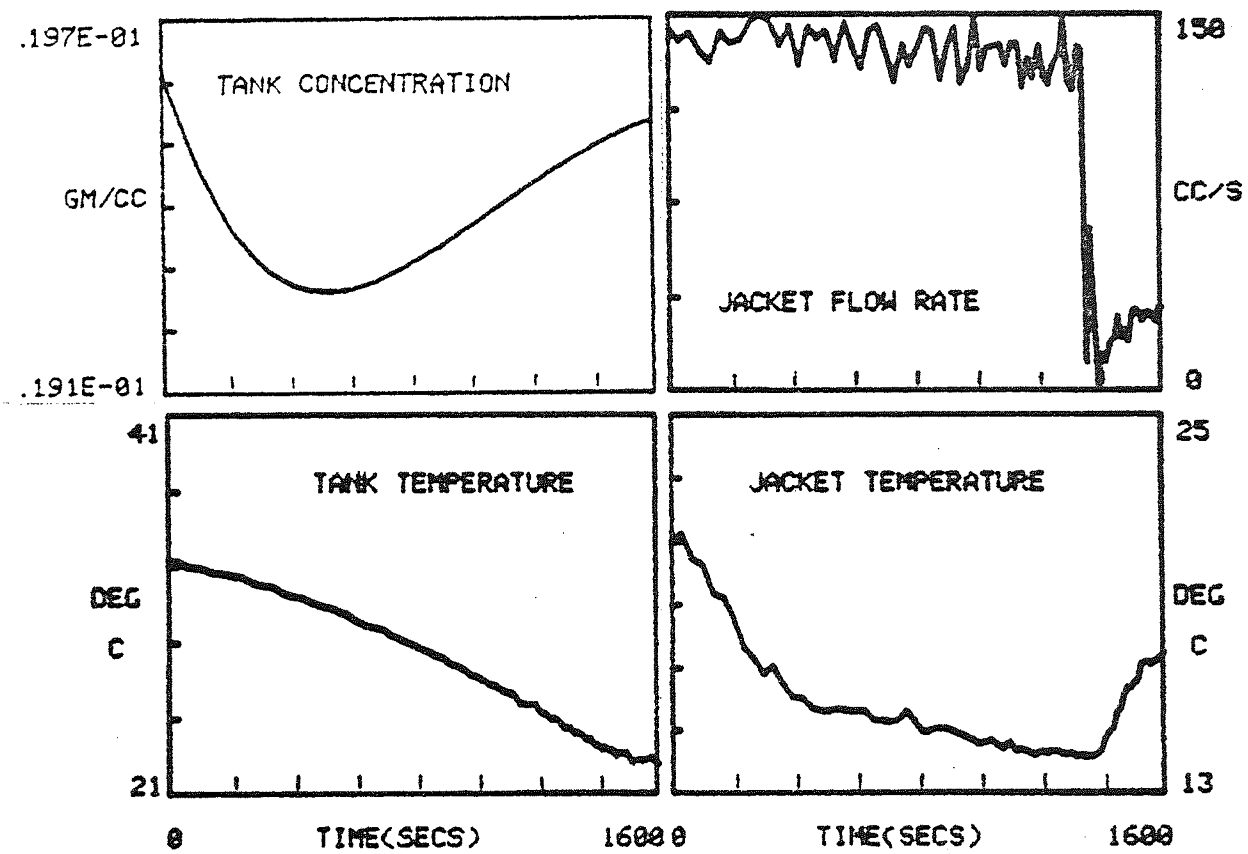


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.007)

Step in tank inlet temperature = 2.3 K

FIG.A.6.1.90 EXPERIMENT NO:90

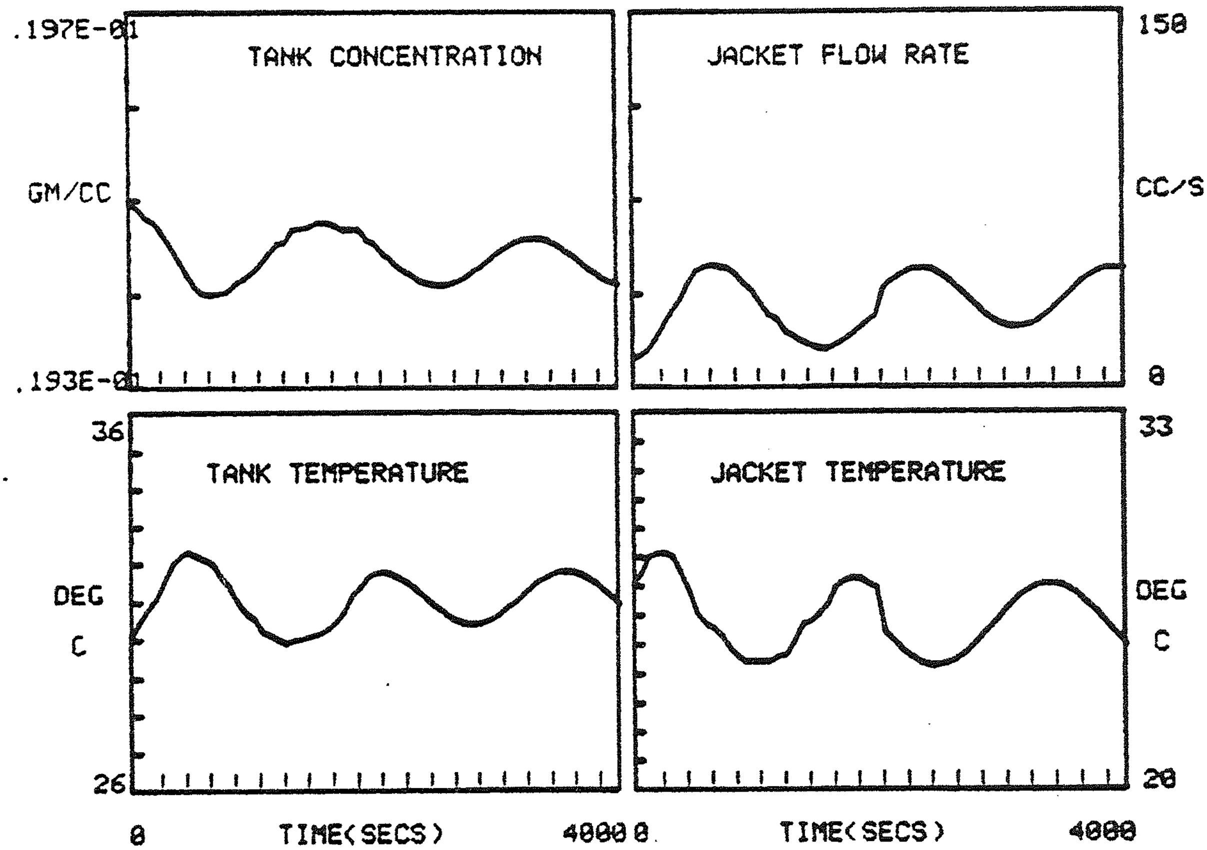


Reaction order = -1

Decoupling type control of tank temperature(D_{max}=.011)

Initial perturbations in state variables

FIG.A.6.1.91 EXPERIMENT NO:91



Reaction order = -1
Limit-cycle around open loop unstable operating point
(K_c=.028)

FIG.A.6.1.92 EXPERIMENT NO:92

A.6.2 COMPARISON OF EXPERIMENTS WITH TOTAL SIMULATION

(continuous lines indicate total simulation,

O experimental points and

1 first harmonic response

(eqn. (3.63)-(3.65)))

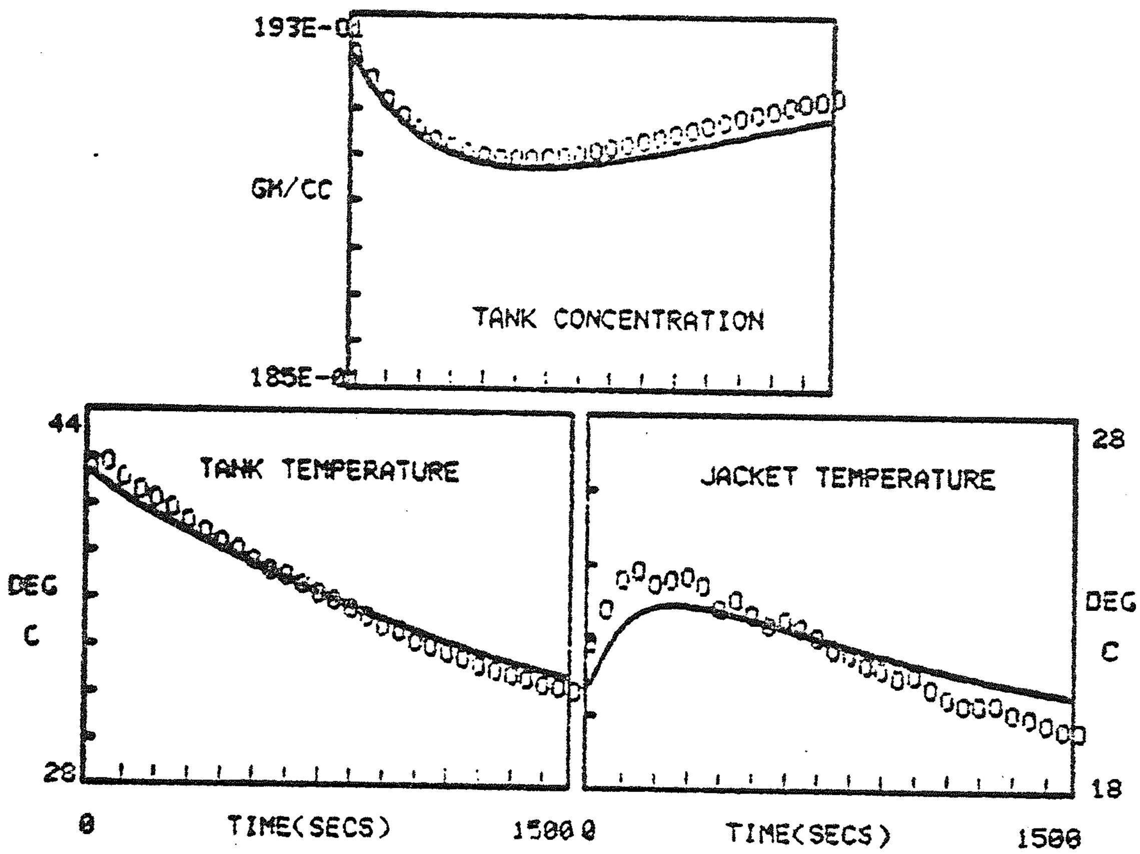


FIG.A.6.2.1 EXPERIMENT NO:1

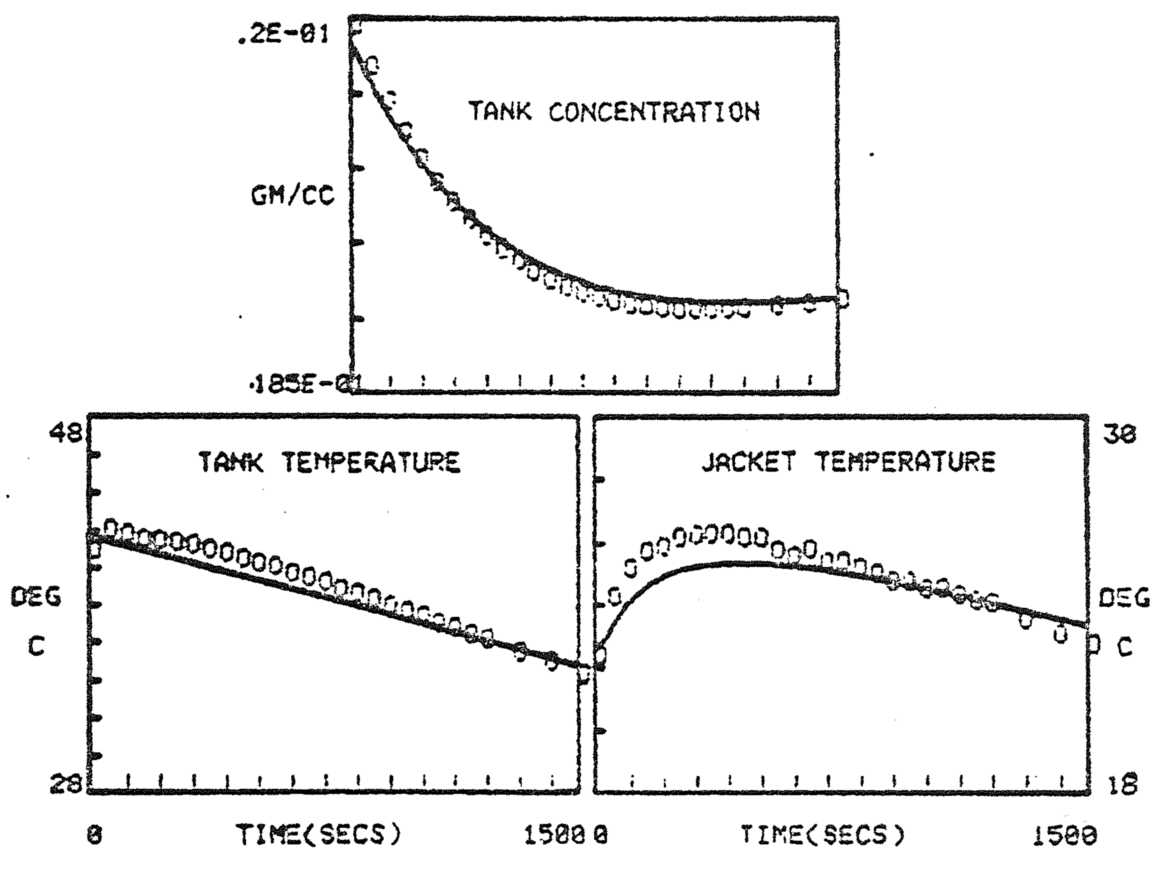


FIG.A.6.2.2 EXPERIMENT NO:2

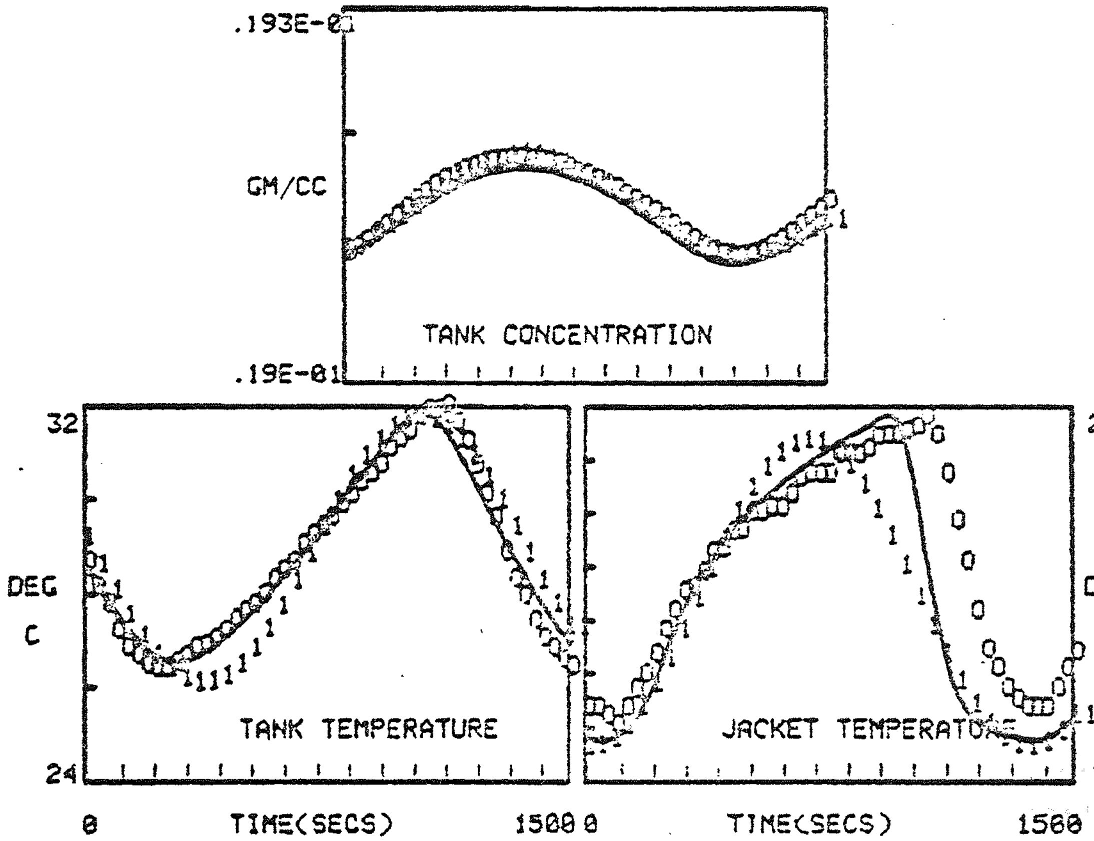


FIG.A.6.2.3 EXPERIMENT NO:4

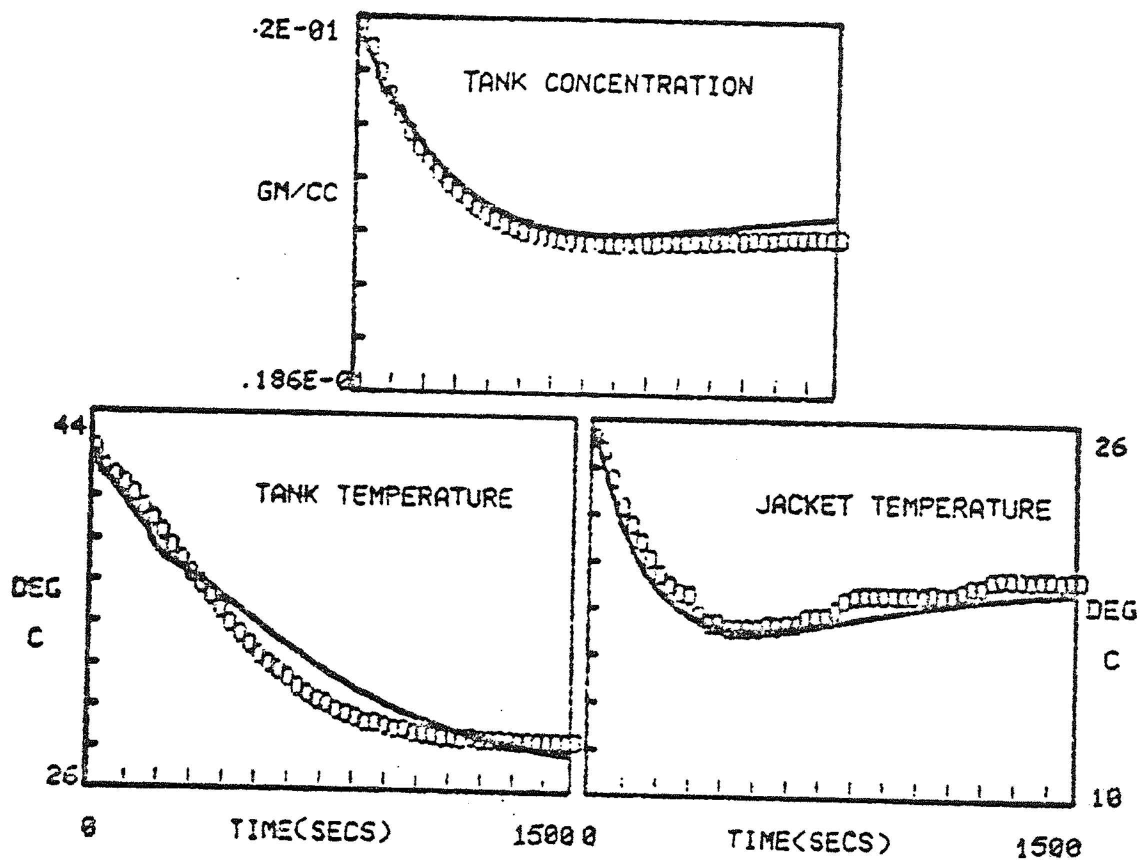


FIG.A.6.2.4 EXPERIMENT NO:5

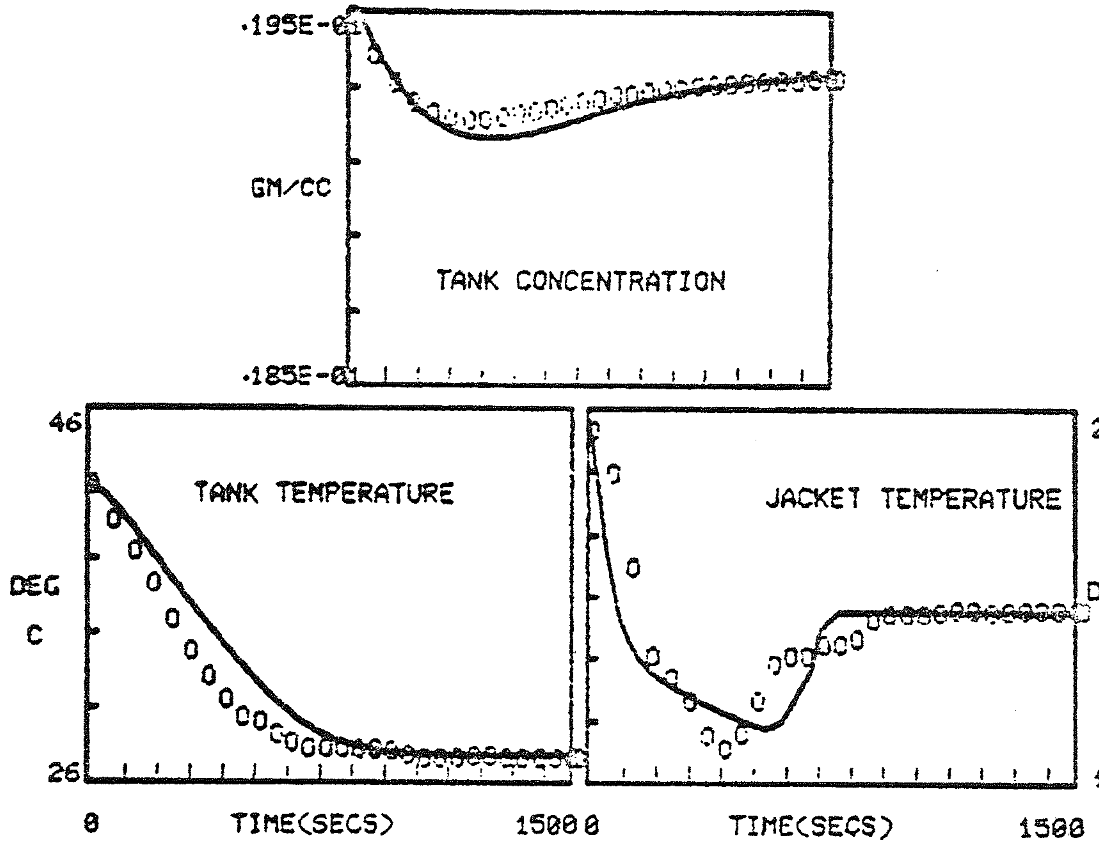


FIG.A.6.2.5 EXPERIMENT NO:6

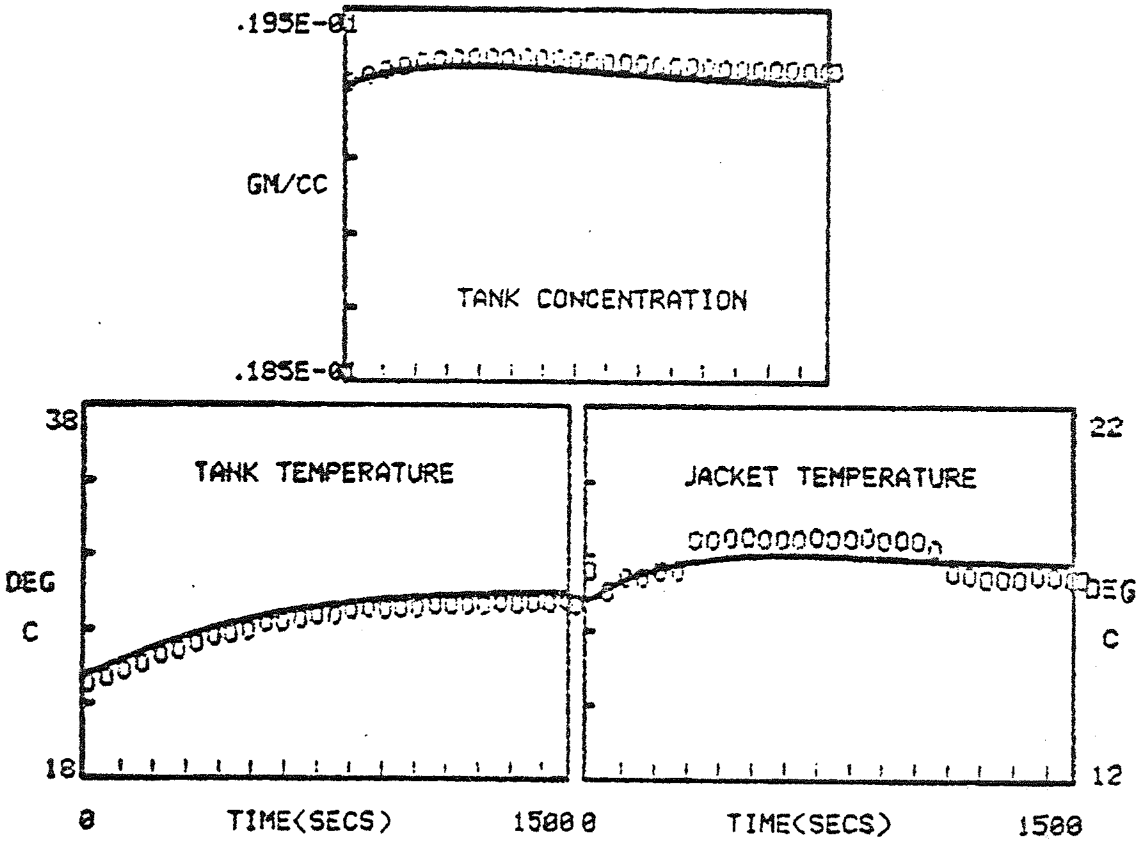


FIG.A.6.2.6 EXPERIMENT NO:8

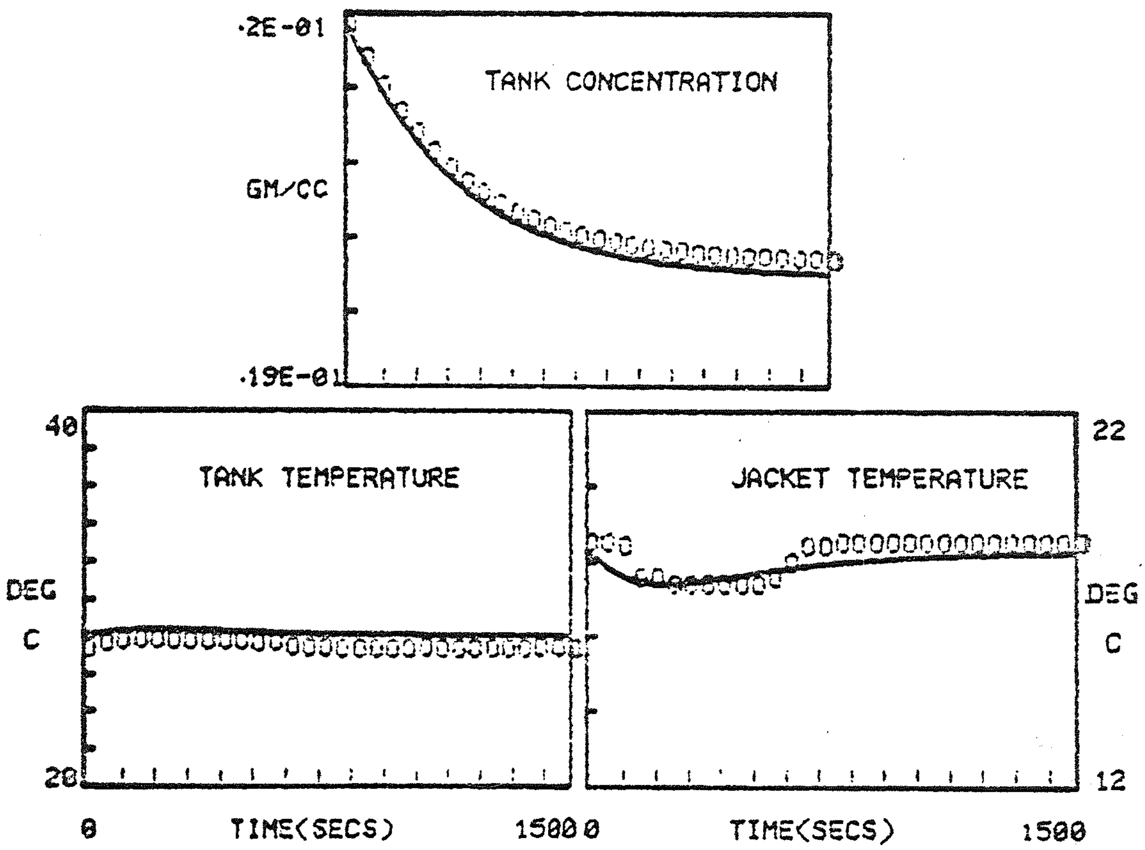


FIG.A.6.2.7 EXPERIMENT NO:9

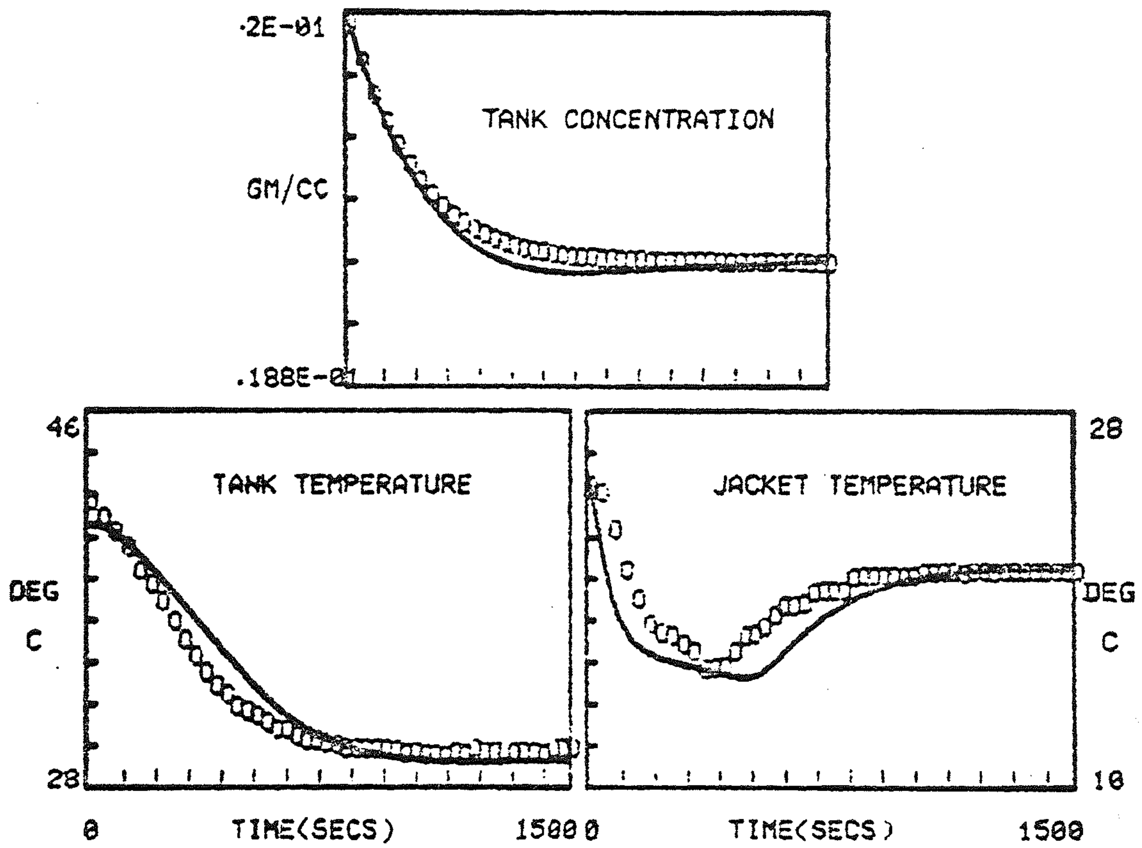


FIG.A.6.2.8 EXPERIMANT NO:11