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SIMULATION OF PERIODIC TANK REACTORS

BY

NOSHIR PIROJSHAW MISTRY

A DISSERTATION

PRESENTED IN PARTIAL FULFILLMENT OF

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ABSTRACT

Normally it is assumed that the steady state mode of operation is most desirable for the design of the chemical reactor system. However it appears that this assumption may not be correct in many cases.

In the present work disturbances of various types were externally created and forced on a system comprising an isothermal continuous stirred tank reactor. The effects of these purposefully created disturbances were investigated by mathematically modelling the system and simulating it on a digital computer.

The change in reactor performance, as defined by the percentage change in the production rate from the steady state value, can be either an improvement or deterioration compared to the steady state operation depending on the parameters like inlet feed concentration, flow rate, combination of both, reactor temperature etc., on which the disturbance is forced. Of the various parameters considered, feed concentration disturbance resulted in the most improved performance.

The investigation of the various form of disturbances like sinusoidal, ramp, and different types of step disturbance variations, showed that the form of the disturbance can profoudly change the reactor performance. The results indicated that of all the disturbances considered, the simple full

step type of disturbance gives the maximum change in performance. The percentage improvement brought about by full step concentration disturbance was almost twice as much as that due to sinusoidal disturbance, which is the next best in terms of performance.

The study of the effect of the order of reaction showed that improving performance results for concentration disturbance with increasing order of reaction, due to the increasing non-linearity of the system.

APPROVAL OF DISSERTATION

SIMULATION OF PERIODIC TANK REACTORS

BY

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FOR

DEPARTMENT OF CHEMICAL ENGINEERING

NEWARK COLLEGE OF ENGINEERING

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

In the development of chemical processes, operating conditions are commonly fixed prior to the design of the equipment and subsequent efforts are made to maintain the processes at the chosen steady state condition, primarily because it is normally assumed that steady state operation is always the most desirable. As disturbances occur in the input feed streams, they are taken care of either by elaborate control systems or by surge tanks so that the specified steady state conditions are regained. However recent investigations have shown that for some processes such as extraction, distillation, adsorbtion, unsteady state operation improves the performance. Horn (5,6) has shown that the over all stage efficiency of periodically operated distillation and extraction columns depends in a complicated way on the number of stages in the column as well as on equilibrium and transport parameters, and that the performance of such columns can be improved considerably by periodic operation. Wilheim, Rice and Bendelins (9) have indicated that in a column of adsorptive particles, the coupling effect of velocity and thermal fluctuations can be used to improve the separation.

Recently several investigators have extended this concept of unsteady state operation to the chemical reactor system. Douglas (2, 3, 4) in his study on the backmix reactor has shown that, under certain circumstances, it is sometimes preferable to permit the disturbances to enter the

reactor system rather than to damp them out with the control system, for they result in improved performance, however small, which tends to be profitable. Chang and Bankoff (1) have reported same results for tubular jacketed reactors. Laurence and Vasudevan (7) and Ray (8) have suggested that the periodic operation of a polymerizer could result in a product not obtainable from an isothermal steady state polymerizer and hence could be an attractive means of carrying out polymerization.

The question thereupon arises whether there might be any way in which such minimally improved performance can be improved still further. Why should the system upsets occur only at the whim of random chance? Even an inexperienced operator knows it is no difficult task to induce disturbances in a system. It may be advisable, therefore, to create the disturbances externally and make them follow a predetermined pattern through the system. In this way the best disturbances, in terms of the optimally improved performances, can be forced and the magnitude of such disturbances can then be carried to the limits of feasibility. In this work an attempt has been made to investigate these propositions.

The system discussed here is an isothermal, continuous stirred tank reactor for the general, irreversible reaction $nA \rightarrow$ Products. It is assumed that the system has been optimized based on some design for steady state operation prior to forcing the disturbances. Possible variations on which the disturbances can be imposed for such a reactor system are the concentration of the feed, the input

flow rate, combinations of both of these and the temper-
ature in the reactor. The system parameters considered
here were chosen to be the same as those employed by
Douglas (2, 3) to facilitate the comparison of results.
Douglas indicated that periodic fluctuations in input result
in small improvements in performance. One obvious way to
increase the performance would be to force periodic dis-
turbances of greater amplitudes ; however, there could be
a limit to this from the viewpoint of feasibility of
operation. Another technique is to consider the effect of
the form of the disturbance itself.

CHAPTER 2

METHOD OF SOLUTION

Introduction

For a second order irreversible reaction of the
type   2A ——→   Products
taking place in a single, isothermal, constant volume CSTR
under forced concentration disturbance, the differential
equation for the unsteady state mass balance on the
reactant A is given by

$$(\; dY/dt + Q/V + 2kA_s \;) \; Y + kY^2 = (Q/V) \; F(t) \qquad \ldots \; (1)$$

where $F(t)$ is the function representing the type of
disturbance forced.

For a flow rate type of disturbance the unsteady
state mass balance on the reactant A results in the
differential equation

$$dY/dt = F_1 \; (t) \; (A_{os} - A_s) \; / \; V -$$
$$(\; ((Q_s + F_1 \; (t) \;) \; / \; V \;) + 2kA_s \;) \; Y - kY^2 \qquad \ldots \; (2)$$

The above two equations are derived and explained
in detail in the subsequent chapters. The purpose of
introducing them here is to indicate the type of
differential equations that will be encountered in the
present work. As can be seen equations 1 and 2 result-
ing from forcing of the diturbances are nonlinear, nonhomo-
geneous, first order differential equations. The
differential equations resulting from forcing of the

disturbances on other operating parameters are also
of the same type, and are also dicussed in the later
chapters. Approximate solution can be obtained for
such equations using standard analytical techniques by
first converting to a second order linear equation (3).
However the forcing of the step disturbance which can
be represented mathematically by Fourier Series expan-
sion makes the analytical approach highly complicated.
The approach used in the present work is to solve the
equation numerically on a RCA Spectra 70/35 digital
computer.

The method used for the solution of the differential
equation is of the predictor-corrector type, which offers
the following advantages :

1. The difference between the predicted and
   corrected values provides one measure of the
   error resulting at each step, and can be used
   to control the step size.

2. Only one, or at the most two evaluations of
   derivatives need be computed at each step
   (compared to four for the fourth order Runge-
   Kutta method) which results in a saving of com-
   puting time.

Compared to these advantages, the major disadvantage

of the method lies in the instability, or propagation

errors, that arises because the order of the approxi-

mating difference equation is higher than that of the

original differential euqation and hence the difference

equation possesses extraneous solution which in some

instances can dominate the solution so that the solution

of the differential equation bears little resemblance

to the true solution of the original differential equation.

Because of the range of the integration involved in the

present solution it is absolutely essential that the

method be stable or relatively stable to obtain an accurate

solution.

Selection of the Method

For the ordinary differential equation of the type

$$Y' = (dY/dt) = U(t, Y) \quad \ldots \quad (3)$$

the basic requirement for a stable method of solution

(when $\partial U/\partial Y < 0$) or one that is relatively stable

(when $\partial U/\partial Y > 0$) is that

$$\Delta t < h/ \ (\partial U/\partial Y)$$

where h is a constant depending both on the type of

the predictor-corrector method used, and on whether

both $\partial U/\partial Y$ is negative or positive.

For a concentration disturbance on a second-order,

irreversibly reacting system, the final differential

equation is given by Equation 1. Comparing Equation 1

with Equation 3 there is obtained

$$U(t,Y) = - (\ (Q/V) - 2kA_s\ )Y - kY^2 - (Q/V)F(t) \qquad \ldots (4)$$

Differentiating equation (4) with respect to Y results in

$$\partial U/\partial Y = - (Q/V) - 2kA_s - 2kY \qquad \ldots (5)$$

Therefore if values of the parameters are V=100;

$Q_s = 10$; k = 1.2 and $A_{os} = 1.0$ then $A_s = 0.25$.

Substituting these values in equation (5)

$$\partial U/\partial Y = -.1 - (2 \times 1.2 \times 0.25) - 2 \times 1.2Y$$
$$= -0.7 - 2.4Y \qquad \ldots (6)$$

Now since Y represents the change in exit reactor

concentration from the steady state value of A_s equal

to 0.25, Y can never be less than minus 0.25 under any

circumstances. Also since A_s, the inlet reactant con-

centration at steady state, is 1.0, Y could never be

greater than 0.75 (though in actuality it is not greater

than 0.25). Substituting this limit of Y, it can be

seen that for

$$Y = 0.75; \ \partial U/\partial Y = -0.7 - (2.4 \times 0.75) = -2.5 \quad \ldots (7)$$

$$Y = 0.25; \ \partial U/\partial Y = -0.7 - (2.4 \times 2.5) = -1.3 \quad \ldots (8)$$

and that for

$$Y = -0.25 \ \partial U/\partial Y = -.7 - (2.4 \times -.25) = -0.1 \quad \ldots (9)$$

Thus for all the possible values of Y, $\partial U/\partial Y$ is
always negative, and it is apparent that the method
will be stable. Distafano (10) has tabulated limit-
ing values of the constant h required for the various
methods to be stable.

Based on the tabulated values of h as reported by
Distafano (10), and also knowing that the truncation
error for a fourth order predictor-corrector method is
lower than that for a third order, a fourth order
Milne-Hamming (11-12) method was selected from the
various predictor-corrector methods available. It
should be noted that some other predictor-corrector
methods might have been used effectively without
sacrificing the accuracy since the Δt finally used
is much lower than that permitted by the limit imposed
by stability considerations.

The basics involved in any predictor-corrector
methods are that first the open end predictor equation
is used to extrapolate from Point Y_i to point Y_{i+1}.
By using the predicted Y_{i+1} value a closed end corrector
equation is next applied to interpolate for an improved
value of Y_{i+1}. A rigorous truncation error analysis then
follows to modify the corrected value or in some cases
both the predicted and corrected values. The predictor-
corrector method used thus requires two derivative
evaluations per increment.

For a fourth order method, the truncation error
term is given by

$$(E_5 \quad (\Delta t)^5 Y^5) \; / \; 5! \qquad \ldots \; (10)$$

Where E_5 for the Milne-Hamming (MH) method is
equal to negative three. The truncation error for
MH method is thus given by

$$- (1/40) \cdot (\Delta t)^5 Y^5 \qquad \ldots \; (11)$$

Now as the values of Y range between 0.25 and -0.25,
the per-step truncation errors for Y = 0.25 have
been calculated for various step sizes and are reported
in Table I. Keeping the truncation error low will
increase the accuracy of the solution and from Table I
it appears that any of the four values of step sizes
will give low truncation error values.

The fourth order MH method uses the same predictor-
equation as does the Milne method, which is then corrected.
Now, instead of iterating the corrector equation to
convergence Hamming (11) suggested an alternate way to
save iteration time. According to him, a study of
truncation error indicated that most of the error in the
predicted and corrected values can be eliminated by the
use of the modified predictor and corrector equation.
The equations for the fourth order MH method used for
calculation for the solution of equation 3 are shown
below in the order in which they are used. In the
following equations i + 1 represents the point at

Table I :   Truncation Error as a Function
            of Step Size Δt

Step Size	Truncation Error
0.4	2.50×10^{-7}
0.2	7.31×10^{-9}
0.1	2.44×10^{-10}
0.05	7.63×10^{-12}

$Y = |0.25|$

which the values are to be calculated and i, i-1, i-2, i-3, the previous points at which the values are assumed to be known.

Predictor :

$$P(Y_{i+1}) = \text{Predicted value of Y at point i-1}$$
$$= F(Y_{i-3}) + (2Y'_i - Y'_{i-1} + 2Y'_{i-2}) \ (4 \Delta t/3)$$

$$\ldots \quad (12)$$

Where $F(Y_{i-3})$ is the final value of the differential equation at the point i-3.

Modifier :

$$M(Y_{i+1}) = \text{Modified value of Y at point i+1}$$
$$= P(Y_{i+1}) - (P(Y_i) - C(Y_i)) \ (112/121)$$

$$\ldots \quad (13)$$

Differential Equation:

$$M(Y'_{i-1}) = U(t_{i+1}, \ M(Y_{i+1})) \qquad \ldots \ (14)$$

Corrector :

$$C(Y_i + 1) = \text{Corrected value of Y at point i+1}$$
$$= (1/8) \ (\ (9Y_i - Y_{i-2} + 3\Delta t \ (M(Y'_{i+1}) +$$
$$2Y'_i - Y'_{i-1})) \qquad \ldots \ (15)$$

Final value :

$$F(Y_{i+1}) = \text{Final value of Y at point i+1}$$
$$= C(Y_{i+1}) + (9/121) \ (\ P(Y_{i+1}) - C(Y_{i+1}))$$

Final form of Differential Equation :

$$(Y'_{i+1}) = U (t_{i+1}, F(Y_{i+1})) \qquad \cdots (16)$$

When the procedure involving the above equations is employed, the limiting value of Δt for stability is given by

$$\Delta t < 0.65/ (|\partial U/\partial Y|) \qquad \cdots (17)$$

Substituting these values of $\partial U/\partial Y$ obtained in equations 7 and 8.

$$\Delta t < 0.65/ |1.3| = 0.5 \qquad \cdots (18)$$

$$\Delta t < 0.65/ |0.1| = 6.5 \qquad \cdots (19)$$

Hence it is seen that for stability, the limiting step size should be less than 0.50.

The study of equation 16 shows that the fourth order MH method is not self starting as it requires a knowledge of the values at four previous points. If knowledge of the initial condition represents the value at the first starting point, the value of the second, third and fourth (i-2, i-1, i) points may be obtained by using the fourth order Runge Kutta method (13). This method involved the use of

$$Y_{i+1} = Y_1 + (L_0 + 2L_1 + 2L_2 + L_3) (1/6) \qquad \cdots (20)$$

where the respective L values are determined by

substituting the following appropriate L values in the above question.

$$L_0 = \Delta t \cdot U (t_i, Y_i)$$

$$L_1 = \Delta t \cdot U (t_i + (t/2), Y_i + L_0/2))$$

$$L_2 = \Delta t \cdot U (t_i + (t/2), Y_i + L_1/2))$$

$$L_3 = \Delta t \cdot U (t_i + \Delta t, Y_i + L_2) \quad \ldots (21)$$

By employing the fourth order Runge Kutta method for the first three points and then using the fourth order MH predictor-corrector method for the remaining points, a time-versus-change in concentration profile and hence a reactor concentration, profile can be obtained. The results show that the concentration of the reactor exit stream due to forcing of the periodic disturbance, is also periodic in nature. This is true for any amplitude and frequency of the forced disturbance.

Now if Y is a function of time, or as a matter of choice of any other variable which is a periodic function of t, with period 2M, then the finite Fourier series based on 2M equidistant sample points, 0, 1, 2,........ (2M-2), (2M-1) is given by

$$Y(t) = (\overline{A}_0/2) + \sum_{K-1}^{M-1} \overline{A}_k \cdot \cos(\pi Kt/M) +$$

$$(\sum_{K-1}^{M-1} \overline{B}_K \cdot \sin(\pi Kt/M)) + (\overline{A}_M/2) \cos(\pi t) \quad \ldots (22)$$

Where $\overline{A}_K = (1/M) \sum_{t=0}^{2M-1} Y(t) \, \cos \, (\pi Kt/M)$

And $\overline{B}_K = (1/M) \sum_{t=0}^{2M-1} Y(t) \, \sin \, (\pi Kt/M)$ ... (23)

The coefficient $\overline{A}_o/2$ is zero for a periodic function which is symmetrical about the t axis; for any nonsymmetrical function it represents the mean value of the function over the period. It is given by

$$\overline{A}_o/2 = (1/2M) \sum_{t=0}^{2M-1} Y(t) \qquad \text{... (24)}$$

For 2M+1 points which represents an odd number of equidistant points

$$\overline{A}_o/2 = (1/(2M+1)) \sum_{t=0}^{2M} Y(t) \quad \text{... (24a)}$$

In the present work since the objective is to determine the performance of the reactor over an extended period of time, all that is required is the average value of the function Y given by $\overline{A}_o/2$.

Series of average values of Y given by $\overline{A}_o/2$ are found for a number of consecutive periods and the mean of this average value is used to evaluate the reactor performance. It should be noted here that before starting to calculate $\overline{A}_o/2$, the system is allowed to reach a state where the negative exponential effect of time on the reactor exit concentration has died out.

The average value of Y, then, for a particular system is given by

$$Y_{av} = \underset{\text{Period} = 1}{\overset{P}{\sum}} (\bar{A}_o/2) / P \qquad \ldots (25)$$

Where P is the number of periods over which $(\bar{A}_o/2)$ is averaged out and

$$A_{av} = A_s + Y_{av} \qquad \ldots (25a)$$

This value of A_{av} is then substituted in Equation 32 for calculation of reactor performance when a periodic disturbance is forced on the inlet reactant concentration. For periodic disturbances of feed flow rate and simultaneous feed flow rate and concentration type, an additional profile of time versus QA $=Q$ ($A_s + Y$) is obtained. Since it is found that QA is also periodic in nature, a procedure for averaging QA similar to that for averaging Y is employed. This QA is then substituted in Equation 7 for the evaluation of the reactor performance.

Selection of the Step Size

The choice of the step size involves consideration of numerical stability, truncation error and the roundoff error. Truncation error and numerical stability have already been discussed under "Selection of the Method" and needs no further elaboration here.

The roundoff error was kept at a minimum level
by running the solution on the computer in double
precision arithmetic. Also it was found that running
the problem in single precision arithmetic gave identical
results to that in double precision arithmetic up to
five significant digits of Y for all the step sizes
considered.

On the basis of this study involving these three errors
in the solution of the differential equation for the cal-
culation of various Y values one can conclude that keeping
the step size under 0.5 will ensure the accuracy of the
solution.

However because of the nature of the periodic
disturbances and the manner in which the average value
of Y per cycle ($\overline{A}_o/2$) is calculated, it is imperative
that the value of Δt shall be as low as possible. This
can be easily seen by referring to Table II where are
tabulated the values of time and the reactor concentra-
tion at the beginning of each period, the total time
per period, and the average concentration change per period
as a function of step size. It will be seen that with
increasing Δt, the total time per period for a given
Δt varies widely, which results in wide variation of
average values of Y. Table III shows the percentage error
in average Y, (Y_{av}), for the reactor system for the

TABLE II : Effect of Step Size Δt on Y_{av}
For Step Concentration Disturbance.

Step Size	t, Times at the Start of each Period	Total Time Per Period	Y, Reactor concentration change corresponding to time t.	$\frac{\overline{A_o}}{2}$, Average Y per cycle	Y_{av}, Average bracketed $\frac{\overline{A_o}}{2}$
0.4	53.2	–	-.024523	–	
	74.4	21.2	-.024523	-.02970522	
	95.2	20.8	-.024523	-.02670413	-.02770449
	116.0	20.8	-.024523	-.02670413	
0.2	53.2	–	-.0057532	–	
	74.2	21.0	-.0057533	-.02659093	
	95.2	21.0	-.0057515	-.02379241	-.02514892
	116.0	20.8	-.0057532	-.02506342	
	137.0	21.0	-.0057533	-.02659093	

(continued)

TABLE II : Effect of Step Size Δt on Y$_{av}$

For Step Concentration Disturbance.

Step Size	t, Times at the start of each period	Total Time Per Period	Y, Reactor concentration change corresponding to time t.	$\overline{A_0}/2$ Average Y per cycle	Y$_{av}$, Average bracketed $\overline{A_0}/2$
0.1	53.2	-	-.00011276	-	
	74.2	21.0	-.00011277	-.02499819	
	95.1	20.9	-.00011276	-.02423102	
	116.0	20.9	-.00011373	-.02563652	-.02496600
	137.0	21.0	-.00011276	-.02499829	
0.05	32.30	-	-.0022292	-	
	53.25	20.95	-.0022287	-.02459102	
	74.20	20.95	-.0022287	-.02459102	
	95.10	20.90	-.0022292	-.02490921	-.02493514
	116.05	20.95	-.0022292	-.02529223	
	137.00	20.95	-.0022292	-.02529223	

Frequency of Disturbance = 0.3   Amplitude of Disturbance = 0.9

TABLE III : Comparison of Y_{av} in Table II

Δt	Y_{av}	$\dfrac{(Y_{av})_{\Delta t} - (Y_{av})_{\Delta t = 0.1}}{(Y_{av})_{\Delta t = 0.1}} \times 100$
0.4	$-.02770449$	10.900
0.2	$-.02514892$	0.609
0.1	$-.02496600$	$-$
0.05	$-.02493514$	0.123

different step size Δt with reference to $\Delta t = 0.1$.

As the average value of Y is obtained by summation of individual Y values, lowering the step size Δt, will increase the number of intervals in any given cycle. This will result in a higher number of Y values to be summed up per cycle leading to higher roundoff errors. Table IV shows the Y_{av} obtained for different step sizes using double and single precision arithmetic. From this Table IV it is seen that the effect of roundoff error even for the smallest step size condisered is only 0.018 percent, which is quite insignificant.

Coupling of the above effects as shown in Tables III and IV, with the availability of computer time, it appears that the optimum step size to use is 0.1 for the parameters involved and accordingly computer calculations were carried out using $\Delta t = 0.1$ as a step size.

The computer programs for the calculation of average exit concentration due to the forcing of step disturbances on concentration, feed flow rate and both the concentration and the feed flow rate are shown in the Appendix. Also shown in the Appendix is a complete printout of a time versus concentration change profile for step concentration disturbance.

TABLE IV : Comparison of Y_{av} from Double
and Single Precision Arithmetic

Δt	Y_{av} double precision	$\overline{Y}_{av}$ single precision	$\dfrac{Y_{av} - \overline{Y}_{av}}{Y_{av}}$ x 100
0.4	-0.02770449	-0.02770394	0.0020
0.2	-0.02514892	-0.02514795	0.0039
0.1	-0.02496600	-0.02496418	0.0073
0.05	-0.02493510	-0.02493069	0.0180

CHAPTER 3

DISTURBANCES IN REACTOR FEED CONCENTRATION

The various types of concentration upsets considered
are sine, ramp and step disturbances. These are dia-
grammed in Figure 1. All the disturbances are symmetrical
about a mean value which corresponds to the steady state
concentration so that over a given period, the net input
of the reactant remains constant and averages out to steady
state operation.

Consider a second order irreversible reaction of
the type

$$2A \rightarrow Products$$
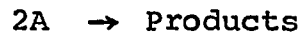
taking place in a single, isothermal CSTR, with such
disturbances applied on the inlet reactant concentration.
Let A_0 be the inlet reactant concentration at any time t,
and A can be the concentration of the reactant in the
reactor, which is the same as the exit concentration for
an ideal CSTR. By material balance, accumulation of A
in the reactor equals the net rate of flow of A in, less
the rate at which A is converted to products, as formulated
by

$$V(dA/dt) = Q (A_0 - A) - kVA^2 \quad \ldots \text{(26)}$$

Here, V is the volume of the reactor, Q is the volu-
metric flow rate and k is the specific reaction rate con-
stant. If A_s represents the steady state exit concentration

23.

FIGURE 1: Types of Concentration Disturbance Forced on the System.

1a: Sine

1b: Ramp

1c: Step

1d: Step

1e: Step

1f: Full Step

1g: Ramp
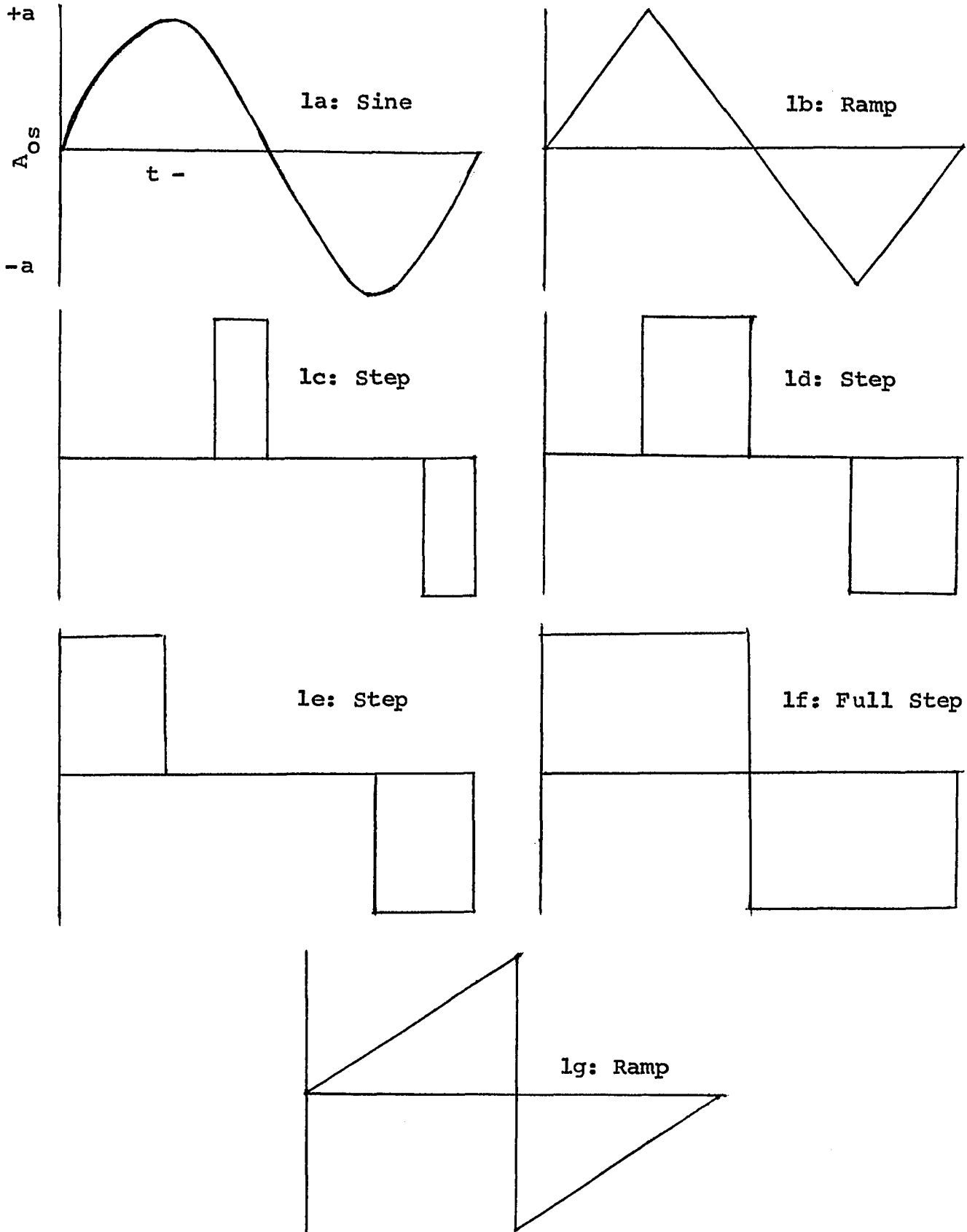
of reactant A, and Q_s denotes the steady state flow

rate, then at the steady state, equation 26 reduces to

$$V(dA_s/dt) = Q_s (A_{os} - A_s) - kVA_s^2 = 0 \qquad \ldots \quad (27)$$

If we now let Y represent any deviation in the

exit concentration from A_s, then, by definition

$$A = A_s + Y \qquad \ldots \quad (28)$$

By subtracting equation 27 from equation 26 and elimi-

nating A with the help of equation 28, there is obtained

$$dY/dt + ((Q_s/V) + 2kA_s) Y + kY^2 =$$

$$(Q_s/V) (A_o - A_{os}) \qquad \ldots \quad (29)$$

where Q_s is the constant flow rate of the steady state.

Now, A_o itself is a function of time and can be rewritten

as

$$A_o = A_{os} + F(t) \qquad \ldots \quad (30)$$

where F(t) depends on the type of disturbance being

forced. Models of these disturbances are listed in

Table V. Substitution of F(t) in equation 29 finally

results in

$$(dY/dt + Q/V + 2kA_s) Y + kY^2 =$$

$$(Q/V) F(t) \qquad \ldots \quad (31)$$

Differential equation 31 is nonlinear and nonhomogeneous.

It is solved numerically on a digital computer using the

fourth order Milne-Hamming predictor-corrector method

(10, 11, 12) to give $(QA)_{av}$, the time average flow rate

of reactant A out of the reactor. For the numerical

calculations, the values of the parameters used were

$V = 100$; $Q_s = 10$; $k = 1.2$ and $A_{os} = 1.0$. Substituting

these values in equation 27 results in

$$10(1-A_s) - 1.2 \times 100A_s^2 = 0$$

$$12 A_s^2 + A_s - 1 = 0$$

$$A_s = \frac{-1 \pm \sqrt{1+48}}{24}$$

$$= + 0.25 \text{ or } -0.333$$

Neglecting the negative value, which is physically

meaningless,

$$A_s = 0.25$$

The steady state rate of production may be measured

by the change in concentration of A. By material balance,

this is $QA_{os} - QA_s$. A net change in the production rate

attributable to a disturbance can conveniently be repre-

sented by the change in the output rate of reagent A,

which is given by $(QA)_{av} - (QA)_s$. If this difference is

negative in value, more A has been converted and the pro-

duction rate has been improved. Conversely, a positive

value of the difference indicates deterioration of the

productivity of the reactor. Of greater significance to

the designer is the effect of the periodic disturbance

relative to the steady state performance of the reactor.

This can be formulated into a figure of merit, symbolized by

TABLE V : F(t) For Disturbances
Shown in Figure 1.

Refer To Figure	Periodic Disturbance	F(t)	Z_1	Z_2
1a	Sine	$a \sin \omega t$	–	–
1b	Ramp	$a(t - mT) / (T/4)$	0	1/4
		$a(t - (m+\frac{1}{2})T) / (T/4)$	1/4	1/2
		$-a((m+\frac{1}{2})T - t) / (T/4)$	1/2	3/4
		$-a((m+1)T - t) / (T/4)$	3/4	1
1c	Step	0	0	3/8
		+a	3/8	1/2
		0	1/2	7/8
		-a	3/4	1
1d	Step	0	0	1/4
		+a	1/4	1/2
		0	1/2	3/4
		-a	3/4	1
1e	Step	+a	0	1/4
		0	1/4	3/4
		-a	3/4	1
1f	Step	+a	0	1/2
		-a	1/2	1
1g	Ramp	$a(t-mT) / (T/2)$	0	1/2
		$a((m+1)T - t) / (T/2)$	1/2	1

$$\Delta = (\ (\ (QA)_{av} - (QA)_s \ ) \ /$$
$$(\ (QA_o)_s - (QA)_s \ ) \ ) \ \times \ 100 \qquad \ldots \ (32)$$

A negative value of the figure of merit, Δ , indicates improved productivity of the reactor relative to the steady state performance. Figures of merit have been calculated for a range of frequencies and amplitudes, not all of which are necessarily practicable, for the different types of disturbances. The results are plotted in Figure 2. All the results plotted in Figure 2 and in the subsequent figures have been tabulated separately and are listed in Appendix A.

The periodic disturbance of the feed concnetration, of whatever form, leads to definite improvement in the reactor performance. An examination of the results indicates, however, that the relative improvements vary with both frequency and amplitude of a given form of disturbance. This variation is best generalized by noting that the relative improvement in performance is proportional to the absolute area included under the cover of the concentration disturbance,

$$(Area) \ = \ 2m \int_0^{T/2} F(t) \ dt \qquad \ldots \ (33)$$

where m is the integral number of cycles in time t, or $m = t/T$ as long as t is an integral multiple of T. For a given amplitude, a, and frequency, these areas are at for the step disturbance, $0.63\ldots$at for the sinusoidal disturbance and $\frac{1}{2}$at for the ramp disturbance. Thus it

FIGURE 2 : Effect of Concentration Disturbances of
Various Functions.
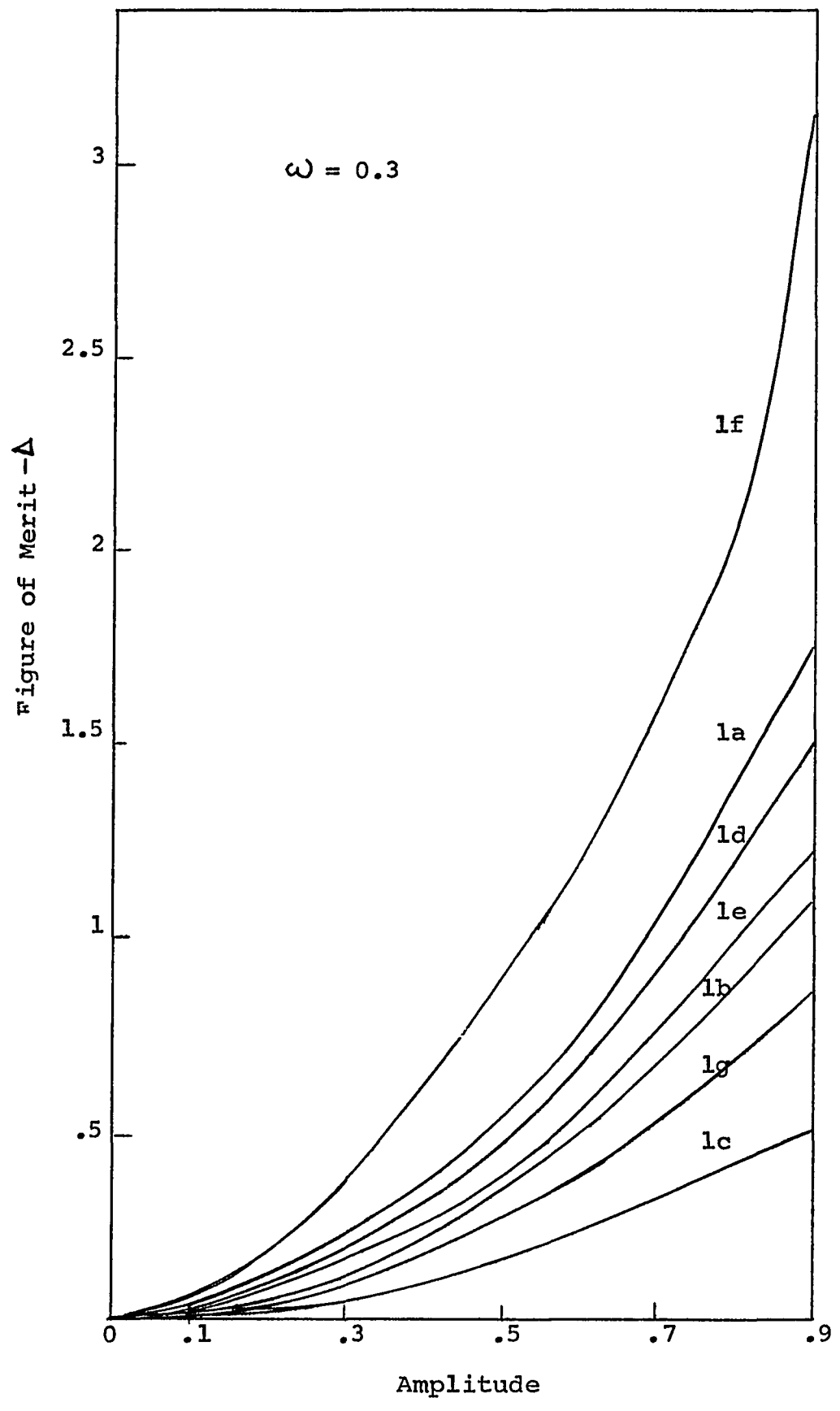
is expected that the change in performance will be maximized by the step disturbance and least for a ramp disturbance. This is confirmed by the results summarized in Table VI.

The step disturbances modelled in Figures 1b, 1d and 1e, with the same amplitude and frequency, have exactly the same areas, yet the relative change in performance, Δ , is different for each of them. This difference can be qualitatively correlated with the number of times in a cycle the slope of the disturbance curve undergoes a change, as shown in Table VII. The results clearly indicate the trend toward decreasing values of Δ as the number of slope changes increases. For a given included area under the curve, it would be expected that a sinusoidal disturbance, with constantly changing slope would be a preferred form of feed concentration disturbance. Given the same amplitude and frequency, however, in a sinusoidal and a step disturbance, the former includes only about 0.63 times the area of the step disturbance. This areal difference outweighs the effect of continuous slope change enjoyed by the sine disturbance. To include the same included area with a sinusoidal disturbance as with a step necessitates operating at a higher amplitude for the former. If such an amplitude is indeed achievable, in practice it would be better processing strategy to force the step disturbance to take advantage of the improved performance which the step would provide.

TABLE VI: Effect of Area Under the Disturbance
Curve on Reactor Performance.

Refer to Figure	Form	Area	Δ	Amplitude a
1f	Step	at	.89	.5
1a	Sine	0.63 at	.51	.5
1b	Ramp	0.50 at	.33	.5

TABLE VII: Effect of Slope Changes
on Reactor Performance

Disturbance Model, Fig.	Slope Changes Per Cycle	Δ
1b	2	.33
1d	4	.45
1e	3	.36
1g	1	.26

CHAPTER 4

STEP DISTURBANCE ON CONCENTRATION
AND FLOW RATE

Frequency Effects in Step
Disturbances of Concentration

Because the step disturbance of feed concentration
appears to provide the best operating strategy, a detailed
study was made of the effect of step frequency the results
of which are presented in Figure 3. For all cases, the
figure of merit, Δ, is a negative quantity, and for a
given amplitude of the disturbance, decreases with increa-
sing frequency. At lower frequencies, the system approaches
zero frequency effect conditions. However, at higher
frequencies, the system cannot respond to infinitely fast
switching and it tends to operate closer to a steady state
condition of concentration which is the mean of the upper
and lower bounds of the disturbance and which, for a
symmetrical disturbance corresponds to the original steady
state inlet concentration. This is more readily explained
by reference to Figure 4 which represents the steady state
response curve for various inlet concentrations. This response
surface is the locus of points obtained by solving for A_s
in equation 27 for various values of inlet feed concen-
tration. This means that any point on the surface represents
a reactor exit concentration for a corresponding inlet feed
concentration for a second order irreversible reaction. For

FIGURE 3 : Full Step Concentration Disturbances
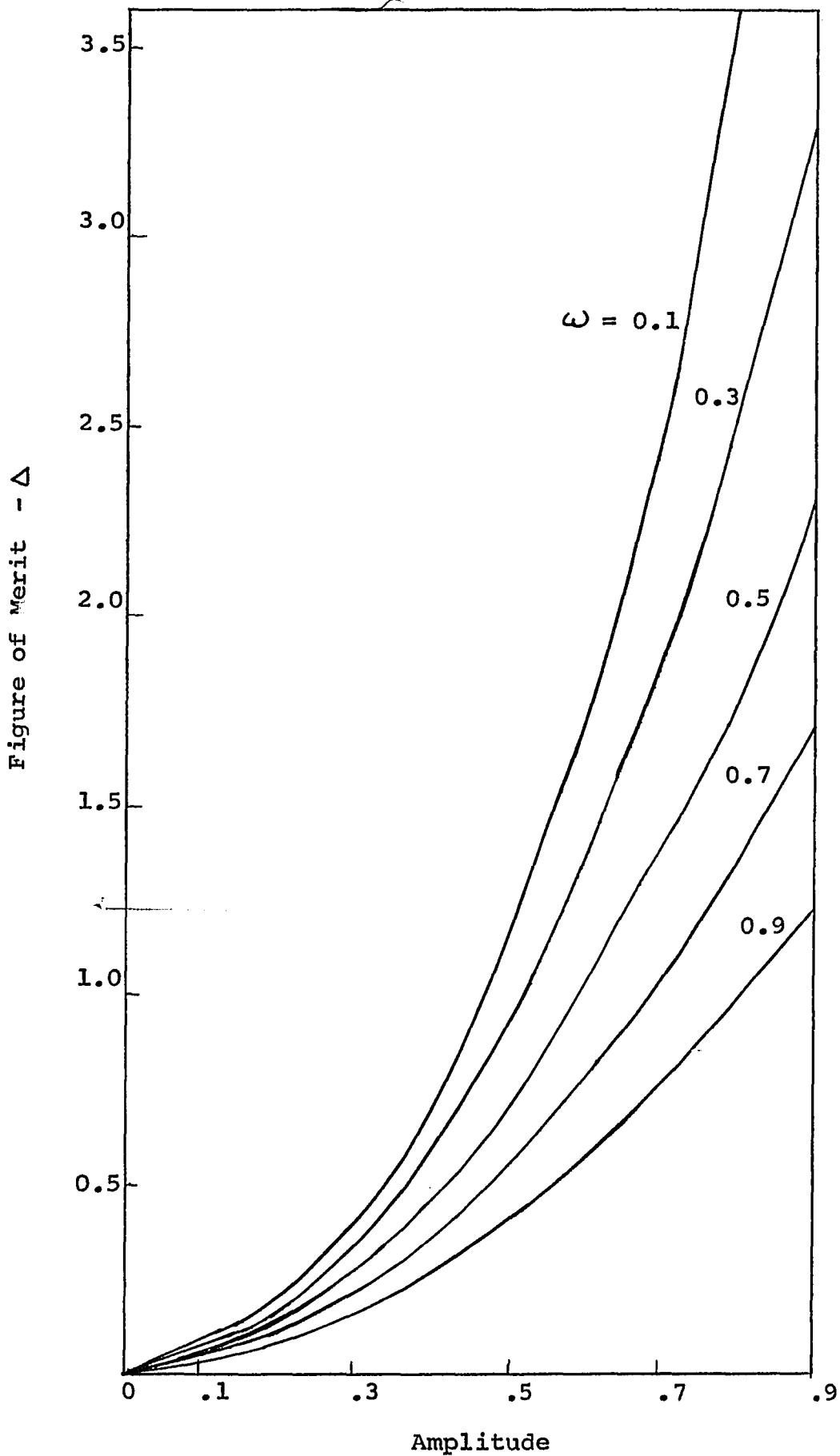
example, consider an exaggerated disturbance of amplitude

0.7, symmetrically imposed on a steady state inlet con-

centration of 1.0. This results in an inlet feed concentra-

tion of 0.3 for one half of the disturbance cycle and 1.7

for the other half of the cycle. For zero frequency effect,

the exit concentration can be approximated by operation under

steady state for two different inlet concentrations of 0.3

and 1.7; the final exit concentration is then given by the

mid-point of the chord joining these two points. For very high

frequency the disturbances are too fast for the system to

respond and the system behaves as if it were operating at an

inlet feed concentration value 1.0 which is the mean of 0.3 and

1.7. This mean value is nothing but the steady state opera-

tion value of the inlet feed concentration and hence the

exit concentration is a point on the steady state response

curve for a mean inlet concentration of 1.0. Between these

two points is the locus for the exit concentrations for other,

intermediate frequencies obtained by solving for Y in

equation 31 for step concentration disturbance of amplitude

0.7. It can also be appreciated that if the steady state

response curvature had been opposite to that shown in

Figure 4, there would have been experienced a deterioration

in performance rather than an improvement.

Figure 5 provides a comparison between the performance

of step and sine concentration disturbances for an otherwise

identical system. It is seen that even for low amplitudes,

FIGURE 4: Effect of Frequency on the Concentration Disturbance.

Amplitude = 0.7

Very fast freq.
0.9
0.7
0.5
0.3
0.1
very slow

Steady state response surface

Concentration of Reactant in the Exit Stream, A

Steady State Feed Concentration, A_{os}

FIGURE 5: Performance Improvement of Full Step
Disturbance in Concentration Compared
to Sinusoidal Disturbance.
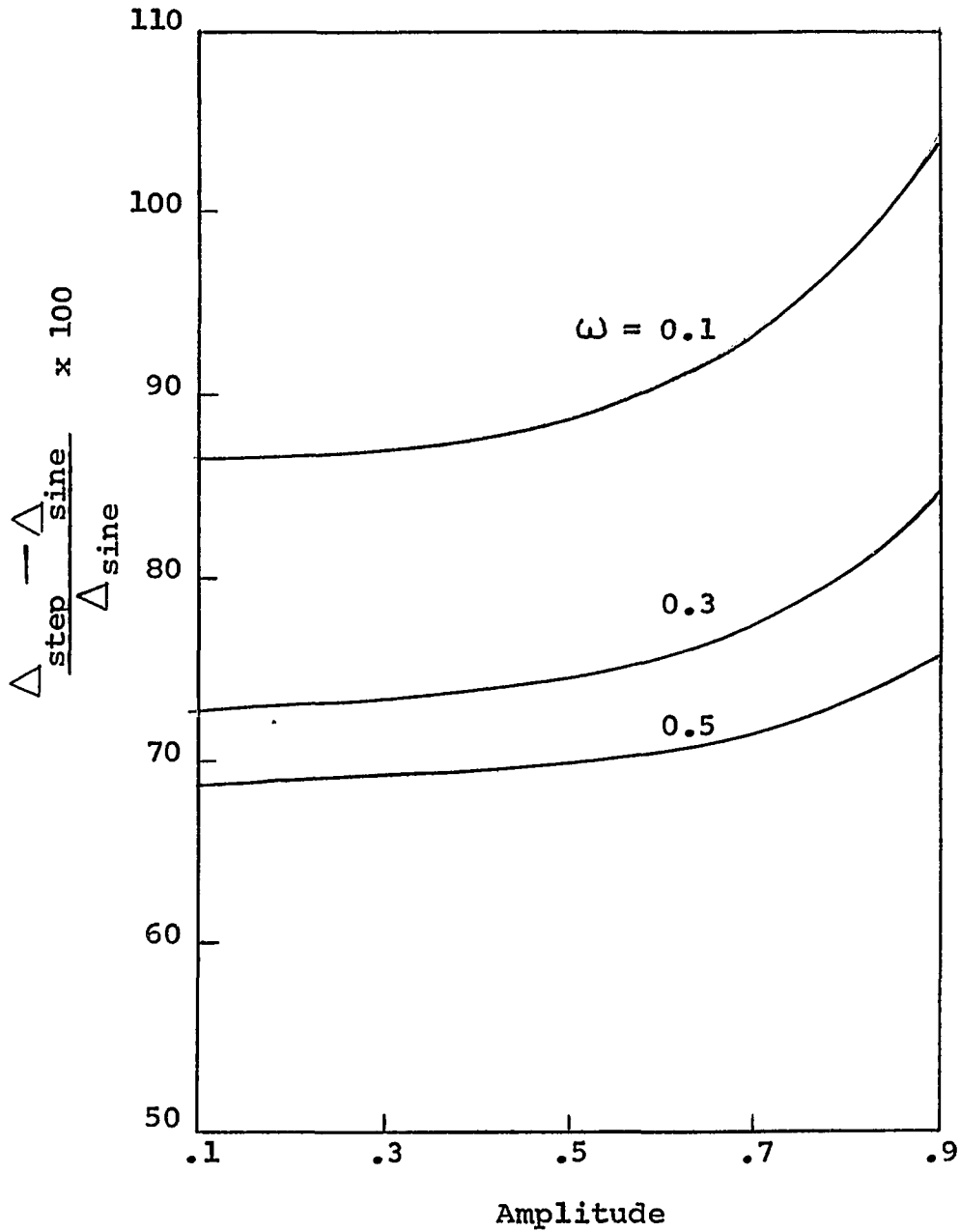
the percentage improvement in performance brought about
by the step disturbance is in the range of 170 to 185
percent of the improvement due to a sinusoidal distur-
bance, a significant improvement.

Step Disturbances in Feed Flow Rate

For the same reactor system, if a step disturbance
is forced on the inlet flow rate, it may be modelled by
the equation

$$Q = Q_s + F_1 (t) \qquad \qquad \ldots \ (34)$$

where the flow disturbance F_1 (t) has an amplitude
b, and F_1 (t) and b have the same significance as F_1 (t)
and in Table V, except that they apply to flow rate
instead of concentration. The material balance for such
a system gives

$$V \ (dA/dt) = (\ Q_s + F_1 \ (t) \ ) \ \varkappa \ (A_{os} - A) - kVA^2$$

$$\ldots \ (35)$$

subtracting equation 27 from equation 35 results in

$$V \ (dY/dt) = F_1(t)A_{os} - (\ (Q_s + F_1(t) \ )A)$$

$$ + Q_sA_s - kV \ (A - A_s) \ (A + A_s) \qquad \ldots \ (36)$$

Substituting equation 28 into 36 and rearranging leads to

$$dY/dt = F_1(t) \ (A_{os} - A_s) \ / \ V$$

$$ - (\ (\ (Q_s + F_1(t) \ ) / \ V \ ) + 2kA_s)Y - kY^2 \qquad \ldots \ (37)$$

For a sinusoidal flow disturbance it was shown by Douglas
(1) that the resulting effect would be opposite to that
obtained by concentration disturbances. The data plotted

in Figure 6, resulting from the numerical solution of
differential equation 37 shows that Δ is positive,
indicating that flow disturbances result in deterioration
of reactor performance in the present case of a second
order reaction. Step disturbances of the feed flow
rate produce greater deterioration in performance than
do sinusoidal disturbances of the same amplitude and
frequency.

FIGURE 6: Effect of Full Step Flow Disturbances on Performance.
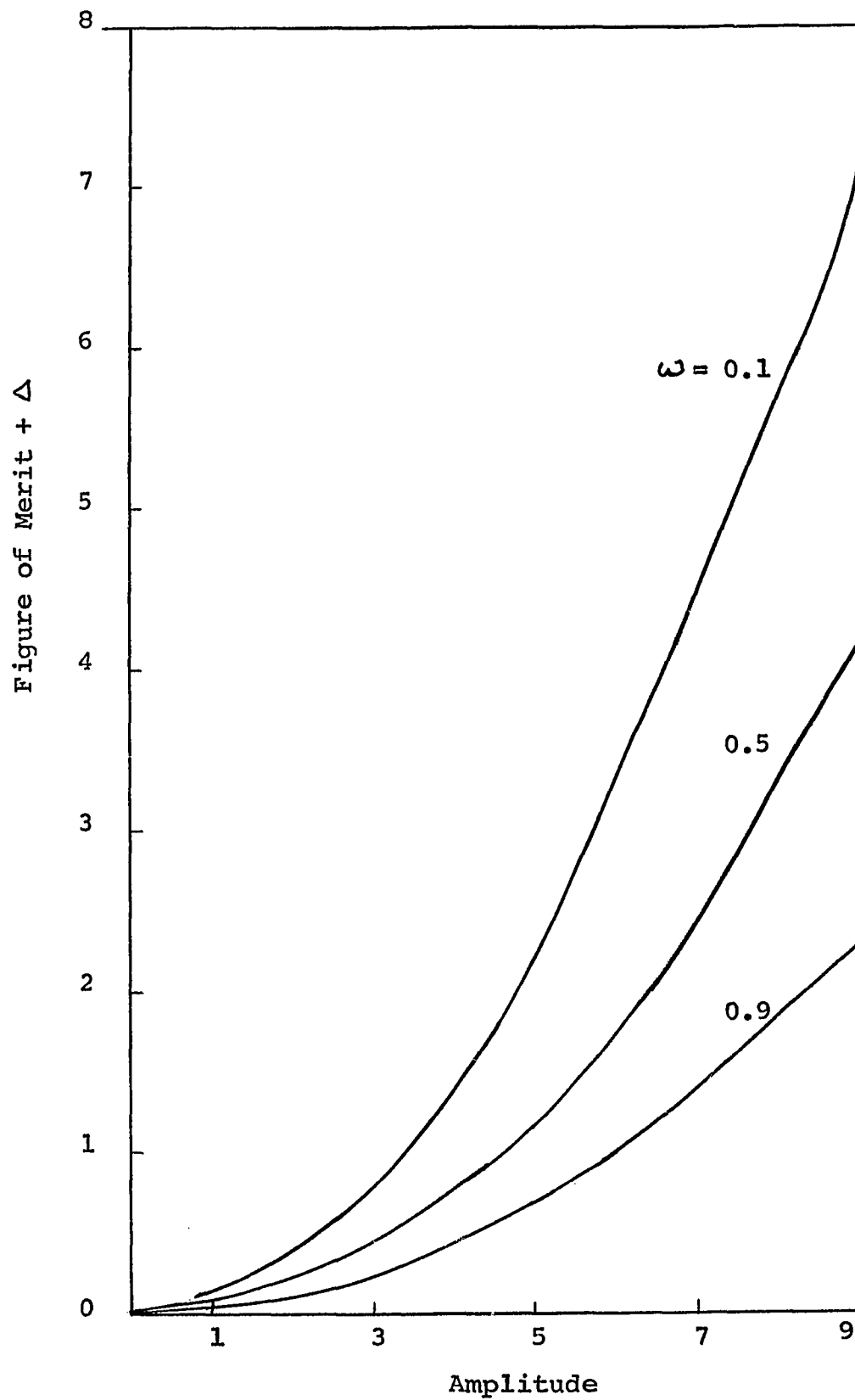
CHAPTER   5

SIMULTANEOUS STEP DISTURBANCES IN FEED CONCENTRATION AND FLOW RATE

The effect on reactor performance due to coupled disturbances in feed composition and flow rate was investigated. In addition to the amplitude and frequency variables in both kinds of disturbances, it is necessary to consider the phase lag between the two disturbances. If the flow rate disturbance given in equation 34 lags behind the concentration disturbance of equation 5 by an angle ϕ, then substitution of equations 23 and 30 in equation 26 and subtraction of equation 27 from this results in

$$V(dY/dt) = Q \; (A_{os} + F_1(t) - A_s - Y) - Q_s$$
$$(A_{os} - A_s) - kV(A - A_s) \; (A + A_s) \qquad \ldots \text{(38)}$$

Rearranging equation 38 leads to

$$V \; dY/dt = (Q - Q_s) \; (A_{os} - A_s) + Q \; (F(t)-Y) -$$
$$kVY \; (2A_s + Y) \qquad \ldots \text{(39)}$$

and finally substitution of 34 for Q produces

$$V \; dY/dt = F_1(t) \; (A_{os} - A_s) +$$
$$(Q + F_1(t) \;) \; (F(t) - Y) - kVY(2A_s + Y) \qquad \ldots \text{(40)}$$

The difference in performance resulting from the forcing of step and sine wave types of disturbances follow the patterns previously described for the individual variations. The absolute value of Δ is higher for the step disturbance, indicating the greater effec-

tiveness of the latter.

The application of equation 32 for the calculation of Δ would be quite misleading in studying the performance of the reactors with combined disturbances since the amount of reactant A fed into the reactor for disturbances of the same frequency depends on the phase lag ϕ and can differ from the steady state value of $Q_s A_{os}$. For example, for simultaneous sine wave disturbances, the average amount of reactant A into the reactor is

$$(QA_o) = (\int_0^T (A_{os} + a \sin\omega t)$$

$$(Q_s + b \sin(\omega t - \phi)) dt. \ ) / (\int_0^T dt) \qquad \ldots (41)$$

Noting that sine and cosine are orthogonal and periodic in nature, equation 41 reduces to

$$(QA_o) = Q_s A_{os} + \tfrac{1}{2} ab \cos\phi \qquad \ldots (42)$$

For simultaneous step disturbances, euqation 41 can be rewritten as follows

$$(QA_o) = (\int_0^T (A_{os} + F(t))$$

$$(Q_s + F_1(t)) dt) / (\int_0^T dt) \qquad \ldots (43)$$

which, after some manipulation reduces to

$$(QA_o) = Q_s A_{os} + ab \ G(\phi) \qquad \ldots (44)$$

where, if ϕ is in radians

$$G(\phi) = (-4\phi \ / \ 2\pi) + 1; \quad (0<\phi<\pi)$$

and $\quad G(\phi) = (\ 4\phi \ / \ 2\pi) - 3; \quad (\pi<\phi/<2\pi)$

$$\ldots \ (45)$$

The function, $G(\phi)$ is shown in Figure 7.

The amount of reactant A fed into the reactor is thus higher than, equal to or lower than the steady state value, $Q_s A_{os}$, depending on the value of phas angle ϕ. Values of $(QA)_{av} - (QA)_s$ are shown in Figure 8 as a function of different amplitudes and frequencies of the oscillatory disturbances.

The question arises: what would happen if the process were to run at a new equivalent steady state condition, with the new reactant feed concentration given by

$$A'_{os} = (Q_s A_{os} + (ab/2) \cos \phi \ )/ \ Q_s \qquad \ldots \ (46)$$

for sinusoidal disturbances and

$$A'_{os} = (Q_s A_{os} + ab \ G \ (\phi) \ ) \ /Q_s \qquad \ldots \ (47)$$

for step disturbances. Equations 44 and 45 show that the reactant feed concentration does not vary from the old steady state value for phase angles of 90° and 270° and has a maximum deviation for 0° and 180°. Table VIII demonstrates that for a phase angle of 0°, which represents the highest inlet concentration, the new equivalent steady state operation appears to be more favourable than does

FIGURE 7 : Function G(∅) for Simultaneous Full Step
Concentration and Flow Rate Disturbances.
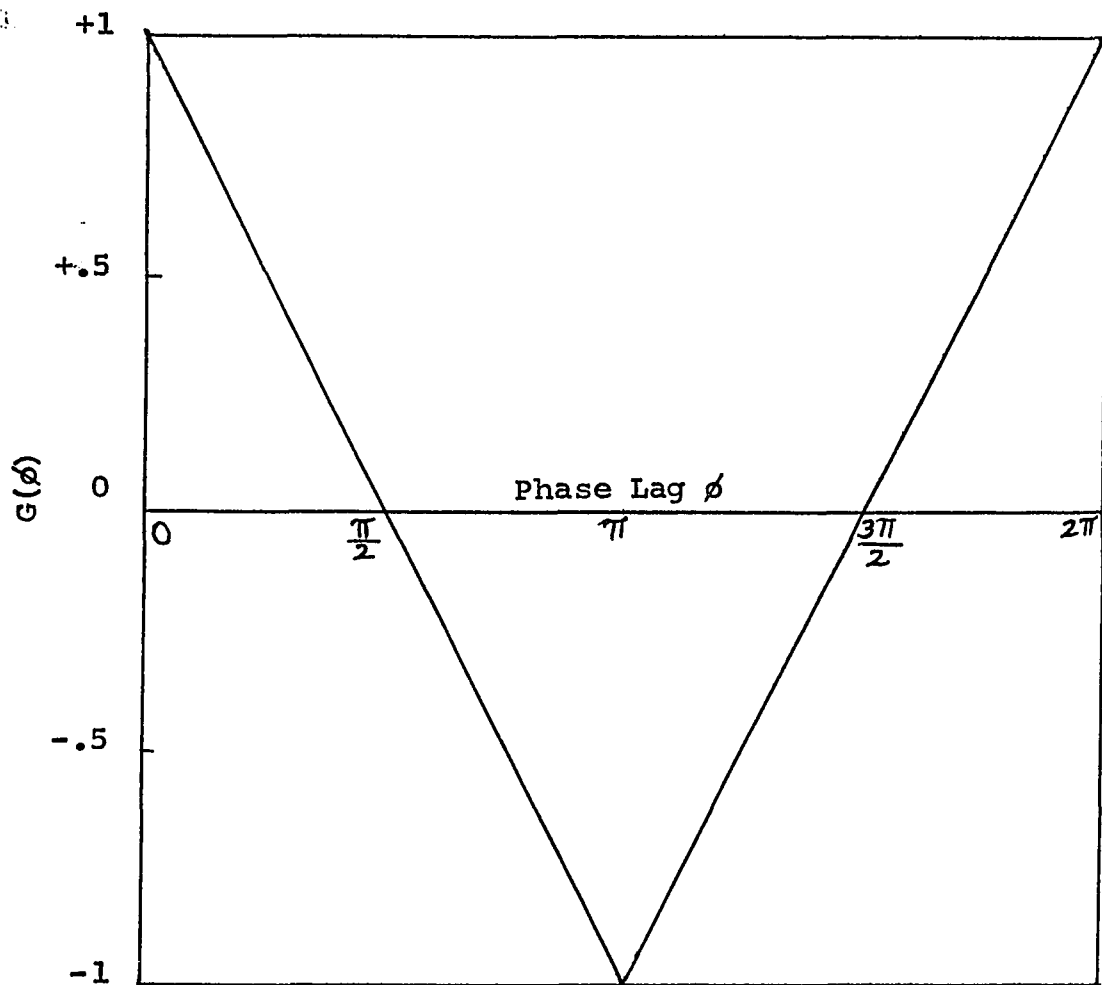
FIGURE 8: Simultaneous Full Step Disturbances on Concentration and Flow Rate
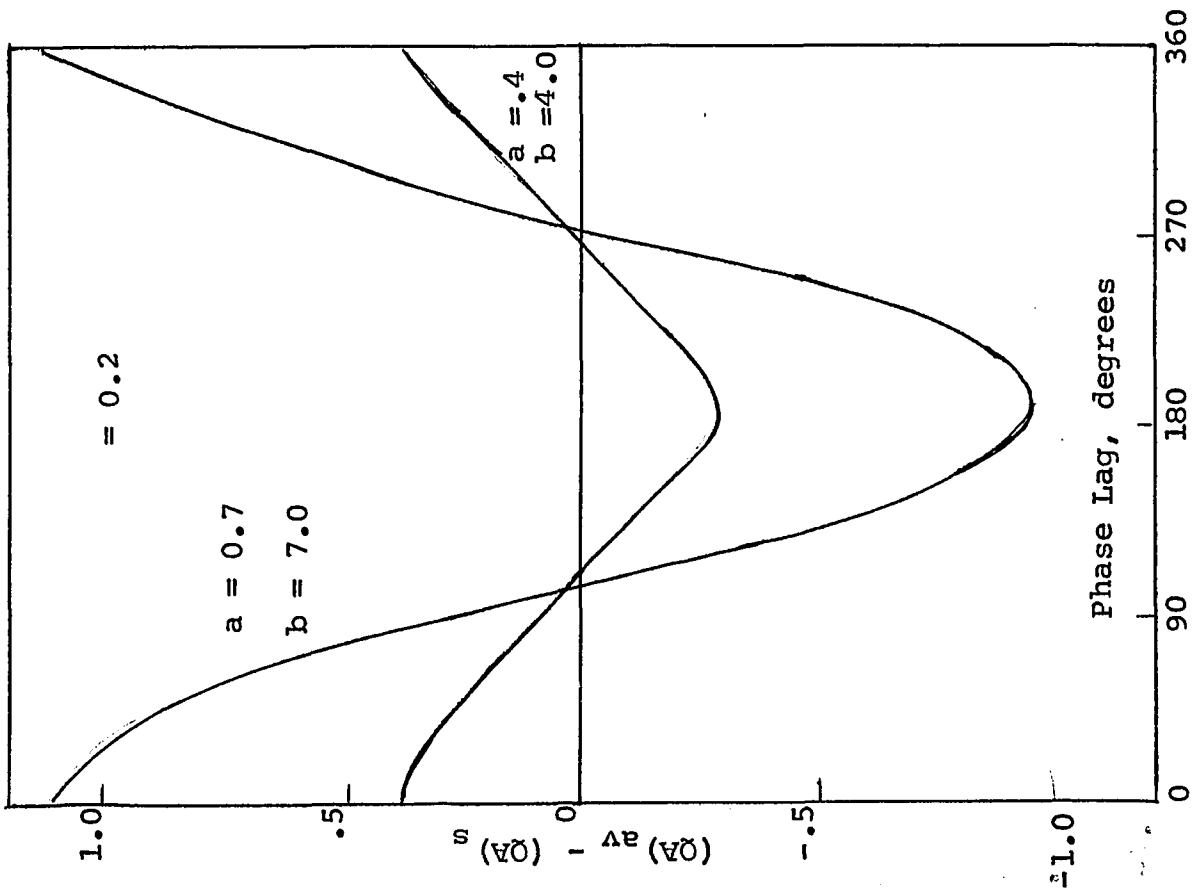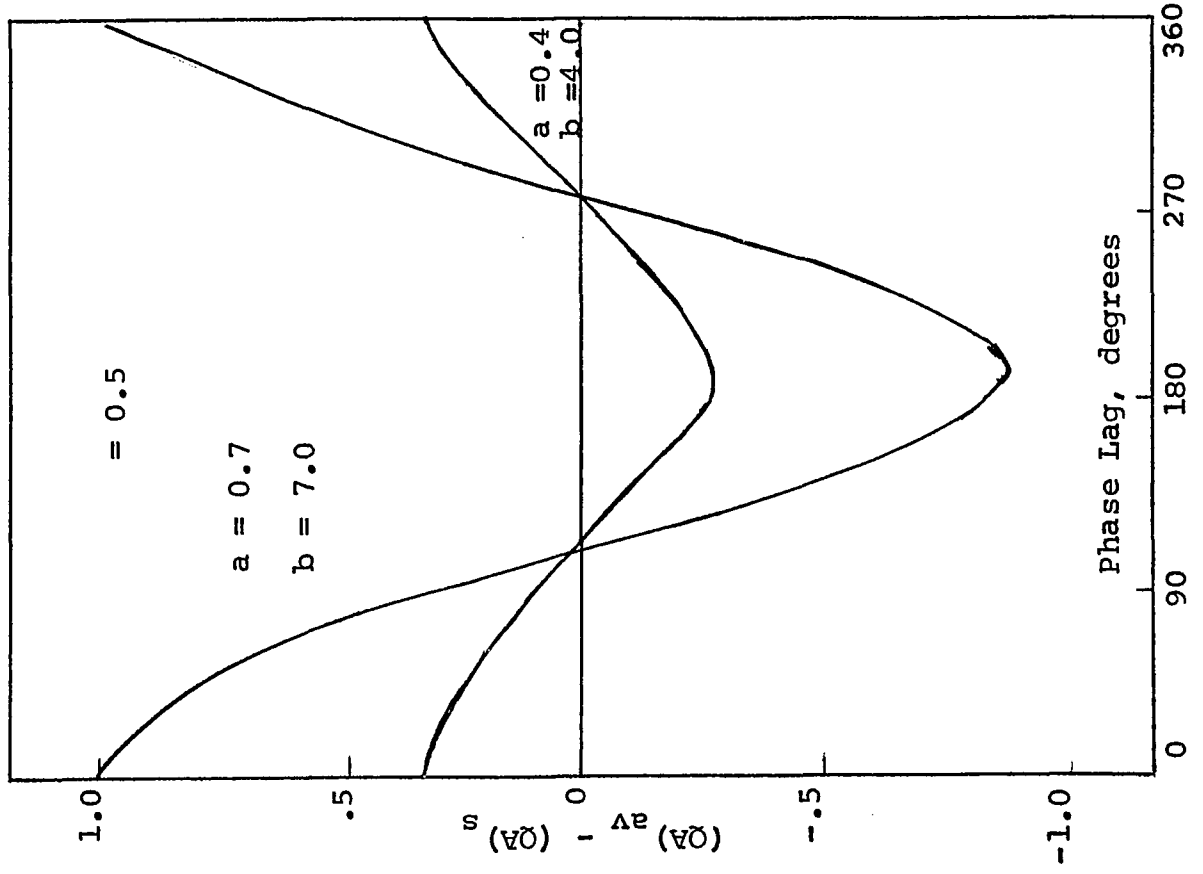
TABLE VIII : Comparison Between Simultaneous Step
Disturbance and the Equivalent Steady
State Operation

Distur. Freq.	Phase Lag	a	b	abG(ϕ) #	(QA$_o$)*	(QA$_{av}$)	Reactant Convd.	A'$_{os}$	(QA'$_{os}$)	A'$_s$	(QA'$_s$)	Reactant Convd.
0.2	0	.4	.4	1.6	11.6	2.868	8.732					
0.5	0	.4	.4	1.6	11.6	2.827	8.773					
0.8	0	.4	.4	1.6	11.6	2.776	8.824	1.16	11.6	.2720	2.720	8.800
0.2	0	.7	.7	4.9	14.9	3.617	11.283					
0.5	0	.7	.7	4.9	14.9	3.485	11.415					
0.8	0	.7	.7	4.9	14.9	3.352	11.548	1.49	14.9	.3132	3.132	11.768
0.2	π	.4	.4	-1.6	8.4	2.221	6.179					
0.5	π	.4	.4	-1.6	8.4	2.233	6.167					
0.8	π	.4	.4	-1.6	8.4	2.250	6.150	0.84	8.4	.2262	2.262	6.138
0.2	π	.7	.7	-4.9	5.1	1.578	3.522					
0.5	π	.7	.7	-4.9	5.1	1.624	3.476					
0.8	π	.7	.7	-4.9	5.1	1.659	3.441	0.51	5.1	.1687	1.687	3.413

Equation 45

* Equation 44

periodic operation. For a phase lag of 180°, although
periodic operation appears to give performance which
is superior to that produced by the new equivalent steady
state value, it still operates at a disadvantage when
compared to the old steady state. Since either the feed
rate or the product capacity of the reactor is pretty
well fixed, the best operating strategy would be to run
as close as possible to phase lag of 90° or 270° .
However, Figure 8 shows that $(QA)_{av} - (QA)_s$ is positive,
indicating deteriorating reactor performance. This leaves
the region around the 270° phase lag, for which $(QA)_{av} - (QA)_s$ is negative. For the step disturbance, a comparison
of Δ for the 270° phase lag shows that somewhat better
performance results when a disturbance is forced only on
the concentration. These considerations indicate a
useful strategy which might be followed in operating a
reactor where the feed concentration alone cannot be
changed periodically without disturbing the steady state
flow, thus involving in addition the forcing of the
flow disturbance.

CHAPTER 6

THE INFLUENCE OF KINETIC PARAMETERS

The effect of the residence time, τ , on Δ for periodic step disturbances was briefly investigated for the irreversible second order reaction. The results are plotted in Figure 9. In essence, at a given amplitude and frequency of the periodic disturbance, Δ increases with decreasing residence time. This corresponds to a closer approach to the zero-frequency case which produces the greatest effect on Δ , as we have already noted. The effect is a considerable one. For example, for a frequency of 0.1 radians per hour, and concentration amplitude varying between 0.1 to 0.9, at τ of 10 hours, Δ varies from -0.05% to -4.75%. With the same disturbance parameters, at τ of 1.0 hour, Δ ranged from 0.2% to 20.5%, greater than a fourfold increase in effectiveness.

The effect of a periodic disturbance depends essentially on the non-linearity of the kinetic system. For a first order system, which is linear, disturbances symmetrical about a mean steady state have no net effect on the system productivity, and Δ is invariably zero-valued. As the reaction order increases, for a given disturbance, the change in performance is amplified. For example, Figure 10 shows $|\Delta|$ for a third order reaction to be higher than for a second order reaction with a corresponding disturbance. As the order of reaction falls below first, the sign of Δ for a particular kind of disturbance changes. Thus, for a half order reaction, we should find $\Delta < 0$ for cyclic flow disturbances, and $\Delta > 0$ for feed concentration, optimum strategy would be to force

FIGURE 9 : Effect of Full Step Concentration
            Disturbance for a Third Order Reaction.
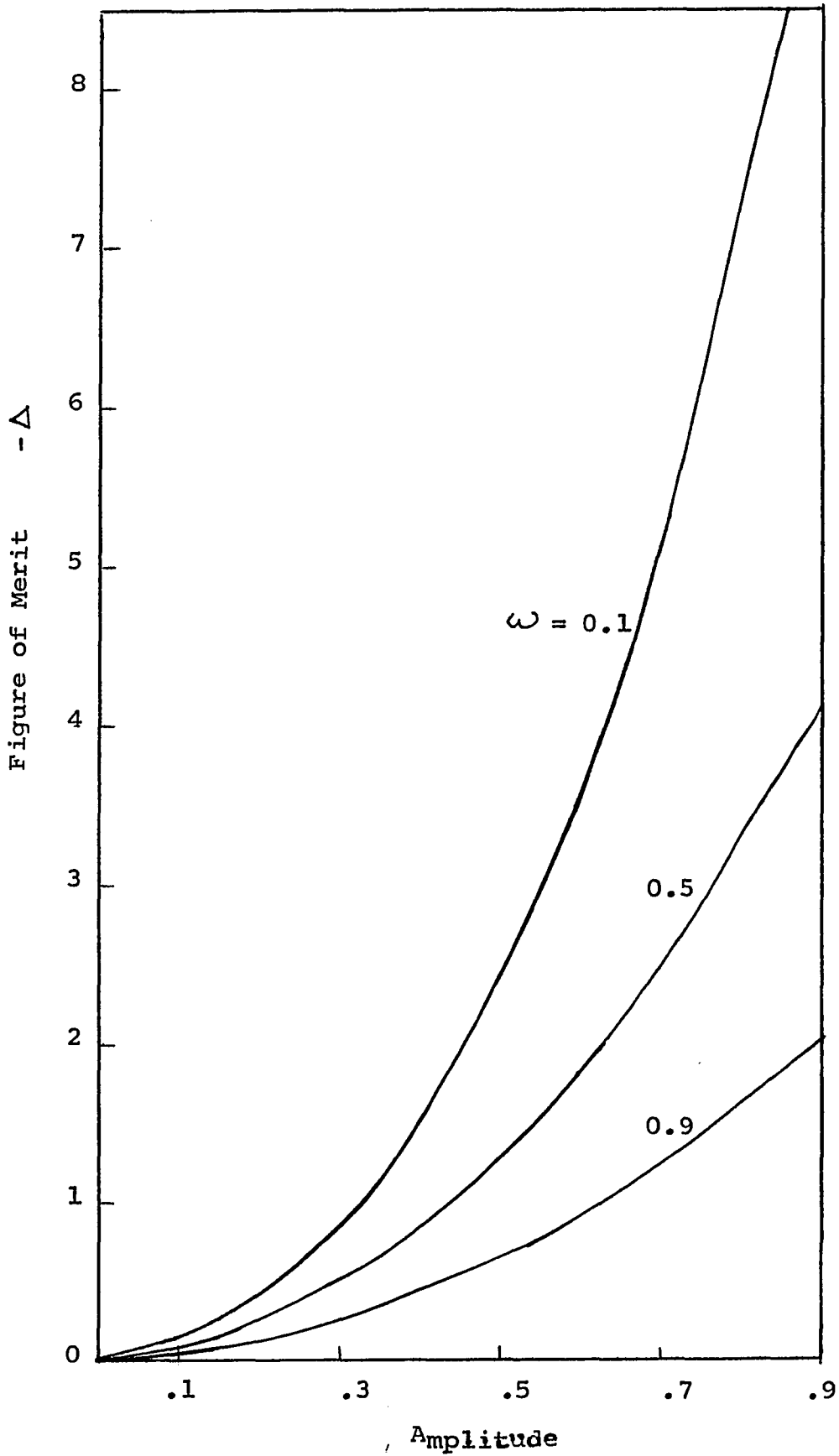
FIGURE 10: Effect of Residence Time

49.
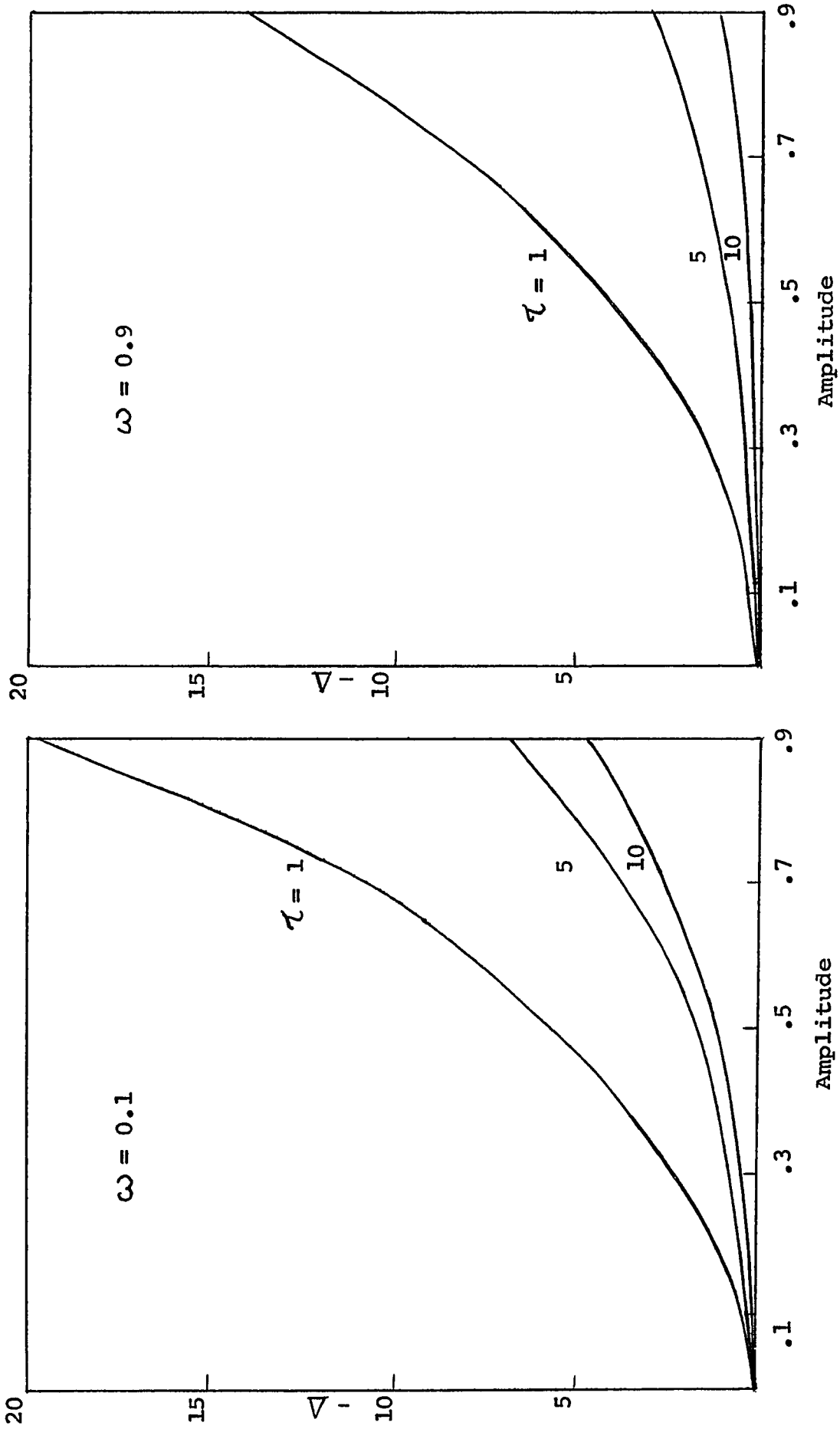
cyclic feed flow disturbances without changing the feed concentration.

A very brief study was made of the effect of temperature disturbance on the reactor system. Since the rate constant is an exponential function of the temperature, a very slight change in temperature should result in a substantial change in rate constant. It is assumed that the two are related by the equation

$$k = E_0 \exp (- E_1 / Rx \text{ Temp}) \qquad \text{...} \qquad (47a)$$

where E_0 is 1.08713×10^{14} cu. ft. / lb. mole $-$ hr and E_1 is 44700 B.T.U. / lb. mole and R is the Universal constant equal to 1.987 B.T.U. per lb. mole $-$ ^{O}R.

Substitution of the above constants and the temperature of 700°R in equation 47a results in value of k equal to 1.2, which is the same as the one used all along in this work. Amplitude variation of ten percent in temperature from the steady state value of 700 ^{O}R leads to ;

$$k = 0.376 \text{ for } 630 \text{ } ^O\text{R}$$

and

$$k = 22.285 \text{ for } 770 \text{ } ^O\text{R}$$

When substituted in equation 27, these result in steady state value of A, as noted by A_s, of 0.7745 and 0.06478 respectively.

For zero frequency effect due to the full step disturbance, the exit concentration can be approximated by equal steady state operation for k = 0.376 and 22.285, and is given by A_s of 0.41964 which is the average of the above two values

of A_s and indicates a deterioration in performance. For

very high frequency, the system should behave as if it

were operating at a temperature of $700^{\circ}R$ and $k = 1.2$,

because the disturbances are too fast for the system to

respond and should approach a value of A_s equal to 0.25.

Actual calculations confirm the zero frequency effect,

but at high frequency it was found that Y_{av} approaches

zero at about a frequency of 0.4 and then undergoes a reversal

in sign and approaches a value of about minus 0.09. Before

any conclusions can be made about this contradicting behaviour

at high frequency, it is suggested that a detail separate study

be made of the temperature effects.

CHAPTER 7

SERIES REACTORS AND THE INLET
CONCENTRATION DISTURBANCE

The results outlined in the previous chapters show
that the forcing of a periodic disturbance on the feed
concentration results in the improvement of the reactor
performance and also that reactor exit concentration
stream concentration is periodic in nature. Based on this,
the concept of forcing periodic step disturbances on the
feed concentration has been extended to a series of
backmix reactors.

Consider a second order irreversible reaction of
the type

$$2A \rightarrow products$$

taking place in a series of N isothermal CSTR of volumes
V_1 , V_2, V_3 .....V_N.

Let the subscripts 1, 2, 3 ..... N in the concentration
terms refer to the streams coming out of the reactor
number 1, 2, 3 ..... N respectively. Then by definition
A_{1s}, A_{2s}, ...A_{Ns} represent the steady state exit concentration
of reactant A from the reactor number 1, 2, ... N respectively
and Y_1, Y_2 ... Y_N the deviation in the exit concentration
from A_{1s}, A_{2s}, ...A_{Ns} respectively.

Based on this notation, equation 28 can be rewritten as :

$$A_1 = A_{1s} + Y_1 \quad \text{for reactor number 1} \qquad \ldots \quad (48a)$$

$$A_2 = A_{2s} + Y_2 \quad \text{for reactor number 2} \qquad \ldots \quad (48b)$$

$$\vdots$$

$$A_N = A_{Ns} + Y_N \quad \text{for reactor number 3} \qquad \ldots \quad (48N)$$

Since the exit stream for reactor number 1(2, 3, ... N-1) is fed in toto into the reactor number 2 (3, 4, ... N), the concentration of the stream entering any reactor is same as the concentration of the stream leaving the previous reactor, equation 30 too can be rewritten as :

$$A_O = A_{Os} + F(t) \qquad \ldots \quad (49a)$$

$$A_1 = A_{1s} + Y_1 \qquad \ldots \quad (49b)$$

$$A_2 = A_{2s} + Y_2 \qquad \ldots \quad (49c)$$

$$A_{N-1} = A_{(N-1)s} + Y_{N-1} \qquad \ldots \quad (49N)$$

By material balance on the reactant A around reactor number 1, equations 26, 27, 29 and 31 can be rewritten as follows :

$$V_1 (dA_1/dt) = Q (A_o + A_1) - kV_1A_1^2 \qquad \ldots (50)$$

$$V_1 (dA_{2s}/dt) = Q_s (A_{os} - A_{1s}) - kV_1A_{1s}^2 = 0 \qquad \ldots (51)$$

$$dY_1/dt + ((Q_s/V_1) + 2kA_{1s}) Y_1 + kY_1^2 =$$
$$(Q_s/V_1) (A_o - A_{os}) \qquad \ldots (52)$$

$$dY_1/dt + ((Q/V_1) + 2kA_{1s}) Y_1 + kY_1^2 =$$
$$(Q/V_1) F(t) \qquad \ldots (53)$$

Similarly for reactor number 2, the equations are :

$$V_2 (dA_2/dt) = Q (A_1 - A_2) - kV_2A_2^2 \qquad \ldots (54)$$

$$V_2 (dA_{2s}/dt) = Q_s (A_1 - A_{2s}) - kV_2A_{2s}^2 = 0 \qquad \ldots (55)$$

$$dY_2/dt + ((Q_s/V_2) + 2kA_{2s}) Y_2 + kY_2^2 =$$
$$(Q_s/V_2) (A_1 - A_{1s}) \qquad \ldots (56)$$

$$(dY_2/dt) + ((Q/V_2) + 2kA_{2s}) Y_2 + kY_2^2 =$$
$$(Q/V_2) Y_1 \qquad \ldots (57)$$

The same procedure can be repeated for any number of reactors. For the Nth reactor the final differential equation is given by

$$(dY_N/dt) + ((Q/V_N) + 2kA_{Ns}) Y_{N-1} + kY_N^2 =$$
$$(Q/V_N) Y_{N-1} \qquad \ldots (58)$$

These differentials have been solved by the method previously
used on the digital computer and the results are plotted in
Figure 11 . As may be expected $\left|\Delta\right|$, the figure of merit,
decreases with increasing number of reactors. This arises
because the reactor exit stream, even though periodic in
nature will be of relatively lower amplitude compared
to the inlet periodic concentration disturbance because
of the damping effect resulting from the holding time of
the reactor. This in turn will affect the figure of merit,
Δ , because Δ itself is a function of amplitude.

Also since a plug flow reactor system can be approxi-
mated by an infinite number of backmix reactors in series,
the results can be expected in the limit to predict the
behaviour of a plug flow system under forced inlet concen-
tration disturbance condition.

FIGURE 11: Effect of Full Step Concentration
Disturbance for a Series of Reactors
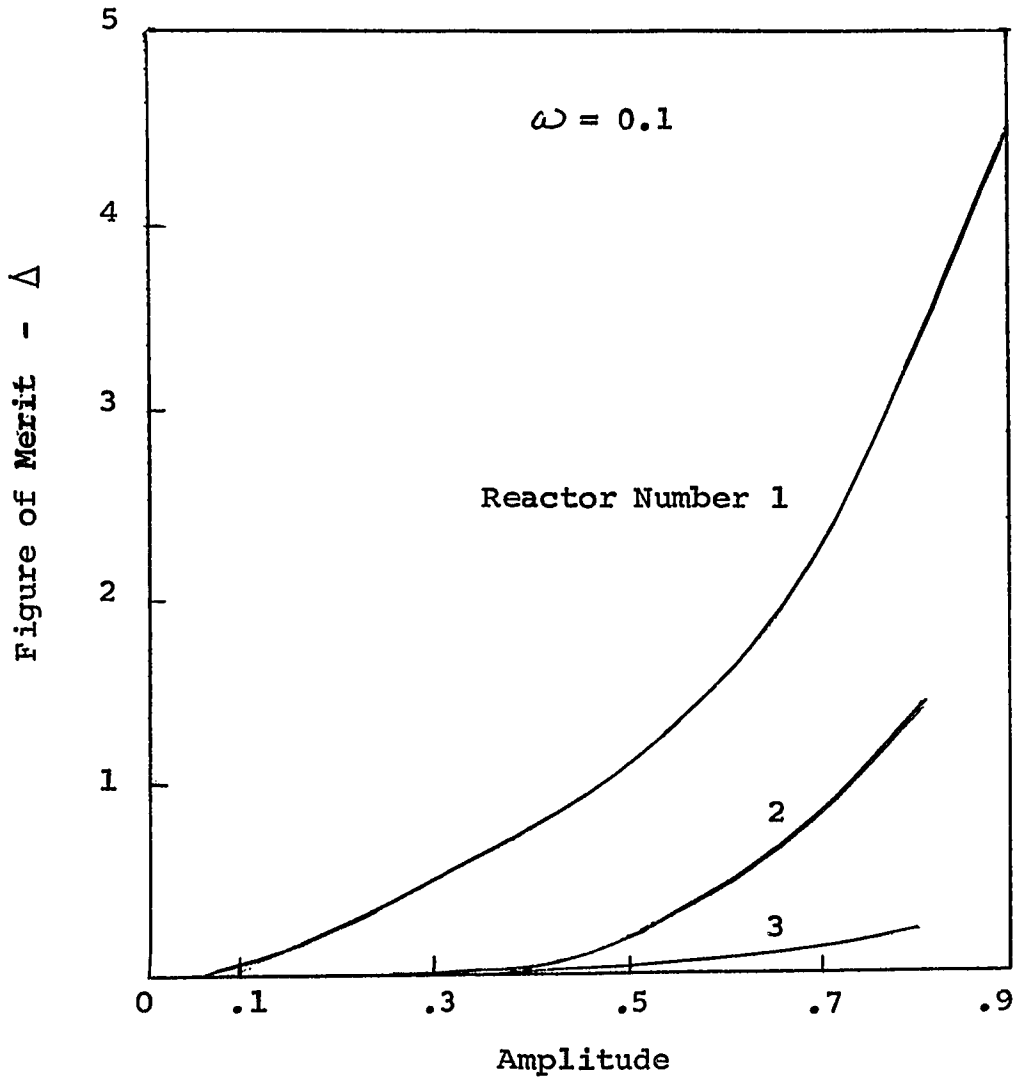
NOMENCLATURE

A = reactant concentration

a = amplitude of oscillations of feed composition disturbances.

b = amplitude of oscillations of flow rate disturbances.

G = functional variattion of phase lag of simultaneous disturbances.

k = specific rate constant.

N = number of reactors

Q = volumetric flow rate

T = period of oscillation

t = real time

V = reactor volume

Y = deviation from steady state reactor composition of reactant A.

Z = fraction of period of oscillation.

Greek Letters

Δ = percentage change in production relative to the steady state.

τ = residence time in the reactor.

ϕ = phase angle or lag between disturbances in feed composition and flow rate.

ω = frequency of the disturbance

Superscripts and Subscripts

av = average value

o = feed condition

s = steady state condition

' = equivalent steady state operation

1,2,N = number of the reactor.

APPENDIX A

Tabulation of Results, Obtained Through

Computer, Which are Used for Plotting

of the Various Figures.

TABLE A-I$_a$: Y$_{av}$ for Different <u>Concentration</u> Disturbance
Shown in Figure 1.

Type of Disturbance	Sine (Figure 1a)			Ramp (Figure 1b)			Ramp (Figure 1g)		
Frequency Amplitude	0.3	0.5	0.9	0.3	0.5	0.9	0.3	0.5	0.9
0.1	-.00015	-.00012	-.00006	-.00010	-.00007	-.00004	-.00007	-.00005	-.00003
0.5	-.00381	-.00294	-.00164	-.00250	-.00193	-.00109	-.00281*	-.00200*	-.00116*
0.9	-.01350	-.00997	-.00541	-.00859	-.00646	-.00357	-.00640	-.00459	-.00258

*Represents values for amplitude of 0.6

Order of the Reaction : <u>Second</u>

V = 100   k = 1.2   A$_{os}$ = 1.0
Q = 10   N = 1   A$_s$ = 0.25

TABLE A-TB : Δ for Different Concentration Disturbance
Shown in Figure 1.

Type of Disturbance	Sine (Figure 1a)			Ramp (Figure 1b)			Ramp (Figure 1g)		
Frequency	0.3	0.5	0.9	0.3	0.5	0.9	0.3	0.5	0.9
Amplitude									
0.1	-0.020	-0.015	-0.009	-0.013	-0.010	-0.006	-0.010	-0.007	-0.004
0.5	-0.508	-0.392	-0.219	-0.333	-0.258	-0.145	-0.374*	-0.267*	-0.155*
0.9	-1.800	-1.329	-0.721	-1.146	-0.861	-0.475	-0.861	-0.612	-0.344

*Represents values for amplitude of 0.6

60.

TABLE A–IIa : Y_{av} for Different Concentration
Disturbance shown in Figure 1

Type of Disturbance	Step (Figure 1c)		Step (Figure 1d)		Step (Figure 1e)		Full Step (Figure 1f)	
Frequency Amplitude	0.3	0.7	0.3	0.7	0.3	0.7	0.3	0.7
0.5	-.00109	-.00089	-.00329	-.00187	-.00272	-.00149	-.00669	-.00390
0.9	-.00380	-.00199	-.01159	-.00613	-.00945	-.00459	-.02494	-.01290

Order of the Reaction : Second

V = 100 k = 1.2 A_{os} = 1.0

Q = 10 N = 1 A_s = 0.25

TABLE AIIb : Δ for Different Concentration Disturbance

shown in Figure 1

Type of Disturbance	Step (Figure 1c)		Step (Figure 1d)		Step (Figure 1e)		Full Step (Figure 1f)	
Frequency Amplitude	0.3	0.7	0.3	0.7	0.3	0.7	0.3	0.7
0.5	-0.145	-0.119	-0.439	-0.249	-0.363	-0.198	-0.892	-0.521
0.9	-0.507	-0.265	-1.545	-0.818	-1.260	-0.612	-3.325	-1.719

62.

TABLE A-III : Y_{av} and Δ for Full Step Concentration
Disturbance of Figure 1f

Frequency	0.1		0.3		0.5		0.7		0.9	
Amplitude	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ
0.1	-.00032	-0.042	-.00025	-0.034	-.00020	-0.026	-.00019	-0.025	-.00011	-0.015
0.3	-.00294	-0.391	-.00233	-0.311	-.00177	-0.236	-.00144	-0.192	-.00099	-0.132
0.5	-.00856	-1.141	-.00669	-0.892	-.00500	-0.669	-.00390	-0.521	-.00276	-0.368
0.7	-.01830	-2.439	-.01385	-1.847	-.01010	-1.350	-.00768	-1.024	-.00547	-0.730
0.9	-.03556	-4.741	-.02494	-3.325	-.01749	-2.332	-.01290	-1.719	-.00918	-1.223

Order of the Reaction : Second

$V = 100$ $k = 1.2$ $A_{os} = 1.0$

$Q_s = 10$ $N = 1$ $A_s = 0.25$

TABLE A-IV : Y_{av} and Δ for Sine Concentration Disturbance of Figure 1a.

Frequency	0.1		0.3		0.5		0.7		0.9	
Amplitude	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ
0.1	-.00017	-0.023	-.00015	-0.020	-.00012	-0.015	-.00009	-0.012	-.00006	-0.009
0.3	-.00157	-0.210	-.00134	-0.179	-.00104	-0.139	-.00078	-0.104	-.00059	-0.078
0.5	-.00453	-0.604	-.00381	-0.508	-.00294	-0.392	-.00219	-0.292	-.00164	-0.219
0.7	-.00946	-1.261	-.00980	-1.040	-.00587	-0.783	-.00435	-0.580	-.00324	±0.432
0.9	-.01739	-2.319	-.01350	-1.800	-.0097	-1.329	-.00730	-0.973	-.00541	-0.721

Order of the Reaction : Second A_{os} = 1.0

V = 100   k = 1.2 A_s = 0.25

Q_s = 10   N = 1

TABLE A-V : $(QA)_{av}$ and Δ for Full Step Flow Rate Disturbance.

Frequency	0.1		0.3		0.5		0.7		0.9	
Amplitude	$(QA)_{av}$		$(QA)_{av}$		$(QA)_{av}$		$(QA)_{av}$		$(QA)_{av}$	
1.0	2.50656	0.087	2.50525	0.070	2.50400	0.053	2.50200	0.027	2.50220	0.030
3.0	2.55942	0.791	2.54730	0.63	2.53610	0.481	2.52395	0.319	2.52024	0.270
5.0	2.66710	2.230	2.63183	1.756	2.58980	1.197	2.56943	0.926	2.55567	0.743
7.0	2.83413	4.450	2.75900	3.450	2.69110	2.546	2.63755	1.833	2.60843	1.447
9.0	3.06870	7.573	2.92695	5.680	2.81690	4.220	2.72655	3.023	2.67694	2.356

Order of the Reaction : Second

V = 100   k = 1.2 A_{os} = 1.0

Q_s = 10   N = 1 A_s = 0.25

τ = 10

TABLE A-VI : $(QA)_{av}$ and Δ for <u>Sine Flow Rate Disturbance</u>

Frequency	0.1		0.3		0.5		0.7		0.9	
Amplitude	$(QA)_{av}$	Δ	$(QA)_{av}$	Δ	$(QA)_{av}$	Δ	$(QA)_{av}$	Δ	$(QA)_{av}$	Δ
1.0	2.50354	0.047	2.50307	0.041	2.50239	0.032	2.50178	0.024	2.50142	0.019
3.0	2.53198	0.426	2.52755	0.367	2.52149	0.287	2.51615	0.215	2.51238	0.165
5.0	2.58977	1.197	2.57663	1.022	2.55958	0.794	2.54479	0.597	2.53410	0.455
7.0	2.67877	2.384	2.65057	2.008	2.61640	1.552	2.58741	1.165	2.56476	0.864
9.0	2.80248	4.033	2.74947	3.326	2.69138	2.552	2.64353	1.914	2.60674	1.423

Order of Reaction :   <u>Second</u>

V = 100 k = 1.2 A_{os} = 1.0

Q_s = 10 N = 1 A_s = 0.25

τ = 10

66.

TABLE A-VII : $(QA)_{av}$ and Amount A Converted for Simultaneous

Full Step Concentration and Flow Rate Disturbance

Frequency of Concentration and Flow Rate Disturbances	Amplitude of Concentration Disturbances		Phase Lag of Flow Rate Disturbances in Degrees ϕ							
			0°		90°		180°		270°	
	Concentration a	Flow Rate b	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted
0.2	0.1	1.0	2.5230	7.5766	2.5050	7.4950	2.4830	7.4170	2.5010	7.4990
	0.4	4.0	2.8675	8.7325	2.5794	7.4206	2.2206	6.1794	2.5064	7.4936
	0.5	5.0	3.0731	9.4269	2.6217	7.3783	2.0555	5.4445	2.5124	7.4876
	0.7	7.0	3.6169	11.2831	2.7243	7.2757	1.5783	3.5217	2.4937	7.5063
	0.9	9.0	4.3284	13.7716	2.8271	7.1729	0.7955	1.1045	2.4275	7.5725

(continued)

TABLE A-VII : $(QA)_{av}$ and Amount A Converted for Simultaneous

Full Step Concentration and Flow Rate Disturbance

Frequency of Concentration and Flow Rate Disturbances	Amplitude of Disturbances		Phase Lag of Flow Rate Disturbances in Degrees ϕ							
			0°		90°		180°		270°	
	Concentration Rate	Flow Rate	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted
	a	b								
0.5	0.1	1.0	2.5250	7.5751	2.5057	7.4943	2.4834	7.4166	2.4987	7.5013
	0.4	4.0	2.8266	8.7735	2.5978	7.4022	2.2334	6.1666	2.4681	7.5319
	0.5	5.0	3.0094	9.4906	2.6508	7.3492	2.0761	5.4239	2.4470	7.5530
	0.7	7.0	3.4852	11.4148	2.7857	7.2143	1.6238	3.4762	2.3840	7.6160
	0.9	9.0	4.1076	13.9924	2.9428	7.0572	0.8264	1.0377	2.8224	7.1776

(Continued)

68.

TABLE A-VII : $(QA)_{av}$ abd Amount A Converted for Simultaneous

Full Step Concentration and Flow Rate Disturbance

Frequency of Concentration and Flow Rate Disturbances	Amplitude of Disturbances		Phase Lag of Flow Rate Disturbances in Degrees ϕ							
			0°		90°		180°		270°	
	Concentration a	Flow Rate b	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted	$(QA)_{av}$	Amount A Converted
0.8	0.1	1.0	2.5150	7.5851	2.5048	7.4952	2.4859	7.4141	2.4947	7.5053
	0.4	4.0	2.7760	8.8240	2.5901	7.4099	2.2499	6.1501	2.4422	7.5578
	0.5	5.0	2.9341	9.5659	2.6563	7.3437	2.0995	5.4005	2.4046	7.5954
	0.7	7.0	3.3520	11.5480	2.7678	7.2322	1.6586	3.4414	2.3245	7.6755
	0.9	9.0	3.8953	14.2047	2.9323	7.0677	0.8917	1.0083	2.2403	7.7597

Amount A Converted $= (QA_{os}) + ab \, \text{Cos} \, \phi \, - \, (QA)_{av}$

Order of the Reaction : Second

V = 100   k = 1.2 A_{os} = 1.0

Q_s = 10   N = 1 A_s = 0.25

τ = 10

69.

TABLE A-VIII: $(QA)_{av}$ and Amount A Converted for Simultaneous Sine Concentration and Flow Rate Disturbances

Frequency of Concentration and Flow Rate Disturbances	Amplitude of Disturbances		Phase Lab of Flow Rate Disturbance in Degrees ϕ							
	Concentration	Flow Rate	$0°$		$90°$		$180°$		$270°$	
			$(QA)_{av}$	Amount A* Converted	$(QA)_{av}$	Amount A* Converted	$(QA)_{av}$	Amount A* Converted	$(QA)_{av}$	Amount A* Converted
0.2	0.1	1.0	2.5121	7.5379	2.5033	7.4967	2.4913	7.4587	2.5001	7.4999
	0.5	5.0	2.8013	8.4489	2.5831	7.4169	2.2763	6.4737	2.4991	7.5009
	0.9	9.0	3.4659	10.5841	2.7654	7.2346	1.7022	4.2478	2.4623	7.5377
0.5	0.1	1.0	2.5107	7.5393	2.5041	7.4959	2.4918	7.4582	2.4983	7.5017
	0.5	5.0	2.7666	8.4834	2.6024	7.3976	2.2889	6.4611	2.4567	7.5433
	0.9	9.0	3.3575	10.6925	2.8251	7.1749	1.7650	4.1856	2.3459	7.6541
0.9	0.1	1.0	2.5095	7.5405	2.5038	7.4962	2.4921	7.4579	2.4978	7.5022
	0.5	5.0	2.7368	8.5132	2.5952	7.4048	2.2986	6.4514	2.4444	7.5556
	0.9	9.0	3.2632	10.7868	2.8018	7.1982	1.8005	4.1495	2.3143	7.6857

*Amount A Converted = (QA_{os}) + 1/2 ab C_{os} ϕ - $(QA)_{av}$

Order of the Reaction: Second

$V = 100 \quad K = 1.2 \quad A_{os} = 1.0$

$Q_s = 10 \quad N = 1 \quad A_s = 0.25$

$\tau = 1.0$

70.

TABLE A-IX : Y_{av} and Δ for <u>Full Step Concentration Disturbance</u>

Frequency	0.1		0.5		0.9	
Amplitude	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ
0.1	-.00054	-.0086	-.00030	-0.048	-.00016	-0.026
0.3	-.00508	-.0.811	-.00276	-0.441	-.00142	-0.227
0.5	-.01506	-2.405	-.00773	-1.234	-.00395	-0.631
0.7	-.03297	-5.265	-.01552	-2.478	-.00776	-1.240
0.9	-.06517	-.0.407	-.02627	-4.195	-.01289	-2.059

Order of the Reaction : <u>Third</u>

$V = 100$ $k = 1.2$ $A_{os} = 1.0$

$Q_s = 10$ $N = 1$ $A_s = 0.3738$

$\tau = 10$

TABLE A-X : $(QA)_{av}$ and Δ for <u>Full Step Flow</u>

<u>Rate Disturbance</u>

Frequency	0.1		0.5		0.9	
Amplitude	$(QA)_{av}$	Δ	$(QA)_{av}$	Δ	$(QA)_{av}$	Δ
1.0	3.74380	0.093	3.74110	0.050	3.73963	0.026
3.0	3.78934	0.820	3.76580	0.444	3.75242	0.230
5.0	3.8820	2.303	3.81472	1.225	3.77770	0.634
7.0	4.02694	4.614	3.88242	2.306	3.81822	1.281
9.0	4.23090	7.871	3.97933	3.853	3.86345	2.003

Order of the Reaction: <u>Third</u>

$V = 100$ $k = 1.2$ $A_{os} = 1.0$

$Q_s = 10$ $N = 1$ $A_s = 0.3738$

$\tau = 10$

TABLE A-XI ; Comparison Between Half Order and Second Order

Reaction Y_{av} and Δ for Full Step Concentration Disturbance

Order of the Reaction	Half Order				Second Order			
Frequency	0.3		0.5		0.3		0.5	
Amplitude	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ	Y_{av}	Δ
0.1	.00040	0.059	.00024	0.036	-.00028	-0.068	-.00015	-0.035
0.5	.00657	0.965	.00354	0.521	-.00706	-1.708	-.00280	-0.678
0.9	.02454	3.608	.01117	1.543	-.02329	-5.638	-.00993	-2.405

Q	10		10
V	100		100
τ	10		10
N	1		1
k	0.12		0.12
A_{os}	1.0		1.0
A_s	0.320		0.320

TABLE A-XIIa : Y_{av} for Full Step Concentration

Disturbance for Different Residence Time.

Frequency Amplitude	τ = 1.0			τ = 5.0		
	0.1	0.6	0.9	0.3	0.3	0.9
0.1	-.00084	-.00073	-.00066	-.00039	-.00033	-.00022
0.6	-.03270	-.02791	-.02505	-.01527	-.01258	-.00821
0.9	-.08430	-.06971	-.06126	-.03976	-.03105	-.01919

V	10	50
Q	10	10
k	1.2	.12
N	1	1
A_{os}	1	1
A_s	0.5870	0.3333

TABLE A-XII b : Δ for Full Step Concentration Disturbance

for Different Residence Time

Frequency Amplitude	τ = 1.0			τ = 5.0			τ = 10.0		
	0.1	0.6	0.9	0.3	0.5	0.9	0.1	0.5	0.9
0.1	-0.201	-0.176	-0.162	-0.058	-0.049	-0.033	-0.042	-0.026	-0.015
0.6(0.5)*	-8.070	-6.770	-6.060	-2.290	-1.887	-1.232	-1.141	-0.669	-0.368
0.9	-20.400	-16.900	-14.850	-5.964	-4.657	-2.879	-4.741	-2.232	-1.223

* 0.5 for residence time τ = 10.0

TABLE A-XIIIa : Y_{av} for Full Step Concentration Disturbance

For Series of Reactors.

Frequency	0.1			0.5			0.9		
Amplitude	Reactor Number			Reactor Number			Reactor Number		
	1	2	3	1	2	3	1	2	3
0.1	-.00032	-.0000091	-.0000008	-.00020	-.0000045	-.0000004			
0.5	-.00856	-.00147	-.00074	-.00500	-.00073	-.00032	-.00276	-.00043	-.00012
0.9	-.03556	-.01377	-.00248	-.01749	-.00506	-.00417	-.00918	-.00258	-.00159

Order of the Reaction : Second

Q_s = 10 k = 1.2 N = 3 A_{os} = 1.0

V_1 = 100 V_2 = 100 V_3 = 100

A_{1s} = 0.25 A_{2s} = 0.1086 A_{3s} = 0.0062

τ_1 = 10 τ_2 = 10 τ_3 = 10

TABLE A-XIIIb: Δ for Full Step Concentration Disturbance
for Series of Reactors

Frequency	0.1			0.5			0.9		
	Reactor Number			Reactor Number			Reactor Number		
Amplitude	1	2	3	1	2	3	1	2	3
0.1	-0.042	-0.001	-0.00008	-0.026	-0.00050	-0.00004	-0.015		
0.5	-1.141	-0.165	-0.074	-0.669	-0.082	-0.032	-0.368	-0.049	-0.012
0.9	-4.741	-1.545	-0.249	-2.232	-0.568	-0.420	-1.223	-0.290	-0.160

$\tau_1 = 10$ $\tau_2 = 10$ $\tau_3 = 10$

TABLE A-XIVa : Y_{av} for Full Step Concentration Disturbance
for Series of Reactors.

Frequency	0.1			0.5			0.9		
	Reactor Number			Reactor Number			Reactor Number		
Amplitude	1	2	3	1	2	3	1	2	3
0.1	-.00084	-.0000450	-.0000026	-.00065	-.0000355	-.0000021	-.00066	-.0000443	-.0000026
0.5	-.02207	-.00745	-.00236	-.01937	-.00641	-.00201	-.01846	-.00584	-.00179
0.9	-.08430	-.06624	-.04528	-.07274	-.05424	-.03554	-.06126	-.04461	-.02762

Order of the Reaction: Second

$Q_s = 10$ $k = 1.2$ $N = 3$ $A_{os} = 1.0$

$V_1 = 10$ $V_2 = 10$ $V_3 = 10$

$A_{1s} = 0.5868$ $A_{2s} = 0.3973$ $A_{3s} = 0.2938$

$\tau_1 = 1$ $\tau_2 = 1$ $\tau_3 = 1$

TABLE A-XIVb : Δ for Full Step Concentration Disturbance
for series of Reactors.

Frequency	0.1			0.5			0.9		
	Reactor Number			Reactor Number			Reactor Number		
Amplitude	1	2	3	1	2	3	1	2	3
0.1	-0.201	-0.00740	-0.00037	-0.158	-0.0059	-0.00030	-0.162	-0.00735	-0.00037
0.5	-5.341	-1.236	-0.334	-4.687	-1.063	-0.284	-4.466	-0.968	-0.2544
0.9	-20.400	-10.990	-6.412	-17.603	-8.990	-5.033	-14.850	-7.402	-3.911

$\tau_1 = 1 \qquad \tau_2 = 1 \qquad \tau_3 = 1$

79.

APPENDIX B

COMPUTER PROGRAMS USED IN THE SOLUTION

OF THE DIFFERENTIAL

EQUATIONS

COMPUTER PROGRAM 1

Computer Program for Simulation of Periodic Tank Reactor
under Forced Concentration Disturbance Conditions.

SYMBOL	DEFINITION
LW	Number of frequencies for which computation is performed.
L	Number of amplitudes for which computation is performed.
TIME 1	Initial time at which the disturbance is forced.
DELTT 1	Initial step size.
DELTPR	Interval at which the results are printed.
FREQ	Frequency of the disturbance.
AMP	Amplitude of the disturbance.
Q	Inlet Volumetric flow rate.
V	Volume of the reactor.
AS	Steady state, reactant A exit concentration.
RK	Specific rate constant.
Q1	Reciprocal of residence time.
Q1A, Q2	Dummy Variables.
DELTT	Additional step size for which the computations can be repeated.
Y1	Change in reactant A exit concentration from the steady state value.
YID	Difference between YI values at time t and time t plus delta t.
TIME	Total Time at a particular instance since the initial forcing of the disturbance.
TPR	Time at which the results are printed.
YD	Value of the concentration change at the point i-3.

SYMBOL	DEFINITION
YA	Summation of YI values calculated by the Runge-Kutta method.
DY ( )	L values in the Runge-Kutta equation Concentration change of A as represented by YI plus some value of L in the Runge-Kutta equation.
ARG	Step function of concentration disturbance.
YR ( )	First three final YI values as calculated by the Runge-Kutta method.
DYF ( )	First three final values of the differential equation (Equation 30) as calculated by Runge-Kutta method.
YDD1, YDD2, YDD3	Final value of the differential equation (Equation 30) at the points i-2, i-1 and i respectively as calculated by the Milne-Hamming method.
YD1, YD2, YD3	Final values of YI at the points i-2, i-1 and i respectively as calculated by Milne-Hamming method.
YD3P, YD3C	Predicted and corrected values respectively of YI at the point i.
KS, SK	Number of steps representing negative values of YI in a cycle.
KP, PK	Number of steps representing positive values of YI in a cycle.
YA1	Summation of the positive values of YI in a cycle.
YA2	Summation of the negative values of YI in a cycle.
YD4P, YD4M, YD4C	Predicted modified and corrected values respectively of YI at the point i + 1.
T1	Time for completion of one cycle of the disturbance.
SN1	Time for completion of integral number of cycles.

SYMBOL	DEFINITION
YDD4	Value of the differential equation (Equation 30) based on the modified and the final values of YI at the point i + 1.
YD4F	Final value of YI at the point i + 1.
YAVG	Average value of exit concentration change of reactant A per cycle.

FORTRAN IV017 SOURCE PROGRAM

```
 1          PROGRAM PALHAM
 2          IMPLICIT REAL*8(A-H,O-Z)
 3          DIMENSIONDY%5<, YP%5<, DYF%5<     ,AMP%10<  ,FREQ%12<
 4 C  SECOND ORDER IRREVERSIBLE STEP FUCT ON FEED CONC
 5 C   REFER JAMES ,SMITH , MULFORD ,PP 380
 6 C  DATA PRINTED IN READ ORDER
 7 C   CONC REPRESENTS VARIATION FROM STEADY STATE VALUE
 8          READ 2,IW,  L
 9          READ  3, TIME1,  DELTT1 ,DELTPR
10         READ 4, Q, V, AS, RK
11          READ  41, % FREQ%NW<, NW # 1,  LW  <
12          READ  41, % AMP%N< ,  N # 1, L <
13    41   FORMAT %7F10.4 <
14     2   FORMAT %2I2 <
15     3   FORMAT % 3F10.4 <
16     4  FORMAT %4F10.4<
17          PRINT  203
18   2030 FORMAT % 813, /// 20X,  @CALCULATIONS FOR STEP@,
19      1 1X, @CONCENTRATION DISTURBANCE@  <
20          PRINT 204
21    204  FORMAT % /// 12X, @SECOND ORDER IRREVERSIBLE REACTION@<
22          PRINT  78
23    78   FORMAT %   ////// 12X, @DATA USED IS AS FOLLOWS@ <
24          PRINT 79, LW
25    79   FORMAT %          // 12X,@CALC. FOR NO. OF FREQ #@, I2<
26          PRINT 80 , L
27    80   FORMAT %         / 12X,@CALC. FOR NO. OF AMPL #@, I2<
28          PRINT  81, TIME1
29    81   FORMAT %/12X, @INITIAL TIME #@, F5.2 <
30          PRINT 82, DELTT1
31    82   FORMAT %/12X, @STEP SIZE #@, F5.2 <
32          PRINT  87, DELTPR
33    87   FORMAT %  / 12X, @PRINT STEP SIZE #@, F5.2 <
34          PRINT 83, Q
35    83   FORMAT %/12X, @INLET FLOW RATE #@, F5.1 <
36          PRINT 84, V
37    84   FORMAT %/12X,  @REACTOR VOLUME #@, F6.1  <
38          PRINT 85 , AS
39    85   FORMAT %/12X, @STEADY STATE REACTOR/CONC. #@, F5.2<
40          PRINT 86, RK
41    86  FORMAT %/12X, @RATE CONSTANT #@, F5.2 <
42          DO 33 JW # 1, LW
43          W # FREQ%JW<
44          DO 32  J # 1, L
45          AM # AMP%J<
46          PRINT  42, AMP%J< ,FREQ%JW<
47   420 FORMAT%813,/// 12X,  @AMPLITUDE #@, F6.2,  7X,
48      1@FREQUENCY #@,  F6.2 ////  <
49       Q1 # Q/V
50       Q1A # Q1*AM
```

FORTRAN IV017 SOURCE PROGRAM PALHAM   PROGRAM

```
51          Q2    #   Q1  &  ~ 2.*RK*AS<
52          DELTT   #   DELTTI
53      1   YI   #   0.0
54          YID   #   0.0
55          TIME   #   TIME1
56          TPR   #   DELTPR
57          PRINT 6
58      60 FORMAT % /// 16X,   @TIME@,  10X,  @EXIT CONC CHANGE@
59       1 ,  9X,  @STEP DISTURB.@ <
60          PRINT 201
61     201 FORMAT % 56X, @AMPLITUDE@ <
62          PRINT 7,  TIME,YI
63      7  FORMAT % / 12X, F9.3,  8X,  F15.5 / <
64          YD   #   YI
65          YA   #   YD
66          DY%1<   #   0.0
67          DO  18  K  #  1, 3
68          DO  19  N  #  2, 5
69          GO  TO %11, 12, 13, 12, 13 < , N
70      13  TIME   #   TIME  &% DELTT/2.0 <
71      12  Y   #   YI  &  %DY%N-1<  /2.0  <
72          IF  %N.LE. 4<  GO TO119
73          Y   #   Y &   % DY %N-1 < / 2.0 <
74     119  CONTINUE
75          ARG  # 1.0
76          ARG1  #   AM*ARG
77      19  DY%N<  #% %Q1A* ARG         < -  %RK*Y*Y<  -Q2*Y<*DELTT
78          YID  #  %1./6.0<*%%DY%2<&% 2.*%DY%3< & DY%4<<< & DY%5<<
79          YI  #   YI & YID
80          YR%K<   #   YI
81          YA  #   YA  &  YR%K<
82          PRINT  9, TIME, YI, ARG1
83          ARG  # 1.0
84          ARG1  #   AM*ARG
85     180 DYF%K<  #   %Q1A*   ARG        < -%RK* YR%K<*YR%K< <
86       1 - % Q2* YR%K< <
87          YDD1  #   DYF%1<
88          YDD2  #   DYF%2<
89          YDD3  #   DYF%3<
90          YD1  #   YR%1<
91          YD2  #   YR%2<
92          YD3  #   YR%3<
93          PRINT  8
94      80 FORMAT %//12X,  @THE FOLLOWING VALUES CALCULATED@
95       1 , @ BY HAMMING EQUATION @/<
96          TIME   # 4.0*DELTT
97          YD3P  #YD3
98          YD3C  #   YD3
99          KS  #   0
100         KP  #   0
```

FORTRAN IV017 SOURCE PROGRAM RATHAR   PROGRAM

```
101          YA1  #  0.0
102          YA2  #  0.0
103          DO  31  I  #  5,  20000
104    100 YD4P# YD &%"4./3.<*%%2.*YDD1<- YDD2 &  %2.*YDD3 <<
105      1 * DELTT <
106          YD4M  # YD4P -%112./121.< *%YD3P -YD3C<
107          T1  #  %  2.0* 3.1415927 < / W
108          DO  129  NS  #  1 , 10
109          SN  #  NS
110          SN1  #  SN*T1
111          IF % TIME  .LT.  SN1 < GO TO 121
112    129 CONTINUE
113    121 CONTINUE
114          QN  #  SN  -  1.0
115          IF % TIME .LE. % T1 * % QN& % 1./2. <<< < GO TO 142
116          IF % TIME .LE. % T1 * % QN& % 4./4. <<< < GO TO 143
117    141 ARG  #  0.0
118          ARG1  #   AM*ARG
119          GO TO 151
120    142 ARG  #  1.0
121          ARG1  #   AM*ARG
122          GO TO 151
123    143 ARG  # -1.0
124          ARG1  #   AM*ARG
125          GO TO 151
126    151 CONTINUE
127          YDD4 #%Q1A*  ARG        < -%RK*YD4M*YD4M< -%Q2*YD4M<
128       0 YD4C # %.125< *%%9.*YD3< -YD1 & %% 3.*DELTT<*%YDD4
129       1 & %2.*YDD3 < - YDD2 < < <
130          YD4F  #   YD4C & %9./121.< *%YD4P - YD4C <
131       0 YDD4  #  %Q1A*  ARG        < - %RK*%YD4F*YD4F<<
132       1 - % Q2*YD4F <
133          IF % TIME .LE. %8.1/W< <  GO TO 23
134          IF % YD4F  - 0.0 < 75, 71, 71
135     71 IF % KP - 2 < 23, 72, 72
136     75 IF % KS - 1 < 74, 74, 73
137     74 YA2  #  YA2  &  YD4F
138          KP  #  KP  &  1
139          GO TO 23
140     72 YA1  #  YA1  &  YD4F
141          KS  #  KS & 1
142          GO TO 23
143     73 SK  #  KS
144          PK  #  KP
145          YAVG  #  %  YA1  &  YA2        < / % SK & PK       <
146          PRINT 14, TIME, YD4F,  YAVG
147    140 FORMAT%//12X,F9.3,8X, E15.5, 4X,@AVERAGE CONCENTRATION@
148       1 , /49X, @CHANGE#@,  E14.6 <
149          PRINT 17, SK , YA1
150    170 FORMAT% / 12X,  @NO. OF -VE PTS. #@, F7.1 ,
```

```
151         1 @   AND ITS TOTAL #@, E16.6 <
152           PRINT  91, PK , YA2
153     910 FORMAT@    12X,  @NO. OF EVE PTS. #@, F7.1 ,
154         1 @   AND ITS TOTAL #@, E16.6 // <
155           KP  #  1
156           KS  #  0
157           YA1  #  0.0
158           YA2  #  YD4F
159           GO  TO  23
160      23 IF % TIME - TPK < 26, 25, 25
161      25 PRINT 9,TIME, YD4F  ,  ARG1
162       9 FORMAT %        12X, F9.3,   8X,  E15.5  ,  7X, E15.5 <
163      27 TPK  #  TPR  &  DELTPR
164      26 IF %TIME  - % % 6.3/W<*6.9< < 20,21,21
165      20 A  #  I
166         TIME  #  A*DELTT
167         YD  #  YD1
168         YD1  #  YD2
169         YD2  #  YD3
170         YD3  #  YD4F
171         YD3P #  YD4P
172         YD3C #  YD4C
173         YDD1  #  YDD2
174         YDD2  #  YDD3
175         YDD3  #  YDD4
176      31 CONTINUE
177         PRINT  43
178      43 FORMAT%///@ AVG. CHANGE IN CONC. IS@<
179      21 IF  % DELTT  .GE.  0.110 <  GO  TO  22
180            IF  % DELTT  .LE.  0.110 <  GO  TO  11
181         GO  TO  11
182      22 DELTT  #  DELTT/2.0
183         TIME  #  TIME1
184         PRINT  24  ,  DELTT
185     240 FORMAT %///@ ANOTHER CASE WITH DIFFERENT DELTT  #@
186        1 ,  F5.3 <
187         GO  TO  1
188      11 CONTINUE ,
189      32 CONTINUE
190       ( DELTT  #  DELTT1
191         TIME  #  TIME1
192      33 CONTINUE
193         STOP
194         END
```

CALCULATIONS FOR STEP CONCENTRATION DISTURBANCE

SECOND ORDER IRREVERSIBLE REACTION

DATA USED IS AS FOLLOWS

CALC. FOR NO. OF FREQ = 1

CALC. FOR NO. OF AMPL = 1

INITIAL TIME = 0.00

STEP SIZE = 0.10

PRINT STEP SIZE = 2.00

INLET FLOW RATE = 10.0

REACTOR VOLUME = 100.0

STEADY STATE REACTOR CONC. = 0.25

RATE CONSTANT = 1.20

AMPLITUDE = 0.90   FREQUENCY = 0.10

TIME	EXIT CONC CHANGE	STEP DISTURB. AMPLITUDE
0.000	0.00000D 00	
0.100	0.96892D-02	0.90000D 00
0.200	0.16774D-01	0.90000D 00
0.300	0.24283D-01	0.90000D 00

THE FOLLOWING VALUES CALCULATED BY HAMMING EQUATION

2.100	0.92065D-01	0.90000D 00
4.100	0.10598D 00	0.90000D 00
6.100	0.10806D 00	0.90000D 00
8.100	0.10837D 00	0.90000D 00
10.100	0.10841D 00	0.90000D 00
12.100	0.10842D 00	0.90000D 00
14.100	0.10842D 00	0.90000D 00
16.100	0.10842D 00	0.90000D 00
18.100	0.10842D 00	0.90000D 00
20.100	0.10842D 00	0.90000D 00
22.100	0.10842D 00	0.90000D 00
24.100	0.10842D 00	0.90000D 00
26.100	0.10842D 00	0.90000D 00
28.100	0.10842D 00	0.90000D 00
30.100	0.10842D 00	0.90000D 00
32.100	0.19229D-01	-0.90000D 00
34.100	-0.98480D-01	-0.90000D 00
36.100	-0.14259D 00	-0.90000D 00
38.100	-0.16377D 00	-0.90000D 00
40.100	-0.17515D 00	-0.90000D 00
42.100	-0.18163D 00	-0.90000D 00
44.100	-0.18544D 00	-0.90000D 00
46.100	-0.18773D 00	-0.90000D 00
48.100	-0.18912D 00	-0.90000D 00
50.100	-0.18996D 00	-0.90000D 00
52.100	-0.19048D 00	-0.90000D 00
54.100	-0.19080D 00	-0.90000D 00
56.100	-0.19100D 00	-0.90000D 00
58.100	-0.19112D 00	-0.90000D 00
60.100	-0.19120D 00	-0.90000D 00
62.100	-0.19125D 00	-0.90000D 00
64.100	-0.13088D-01	0.90000D 00

66.100	0.87 07E-01	0.000000 00
68.100	0.10533D 00	0.000000 00
70.100	0.107970 00	0.000000 00
72.100	0.10835D 00	0.000000 00
74.100	0.10841D 00	0.000000 00
76.100	0.10842D 00	0.000000 00
78.100	0.10842D 00	0.000000 00
80.100	0.10842D 00	0.000000 00
82.100	0.10842D 00	0.000000 00
84.100	0.10842D 00	0.000000 00
86.100	0.10842D 00	0.000000 00
88.100	0.10842D 00	0.000000 00
90.100	0.10842D 00	0.000000 00
92.100	0.10842D 00	0.000000 00
94.100	0.10842D 00	0.000000 00
96.100	-0.66484D-01	-0.000000 00
98.100	-0.12902D 00	-0.000000 00
100.100	-0.15691D 00	-0.000000 00
102.100	-0.17137D 00	-0.000000 00
104.100	-0.17945D 00	-0.000000 00
106.100	-0.18415D 00	-0.000000 00
108.100	-0.18695D 00	-0.000000 00
110.100	-0.18864D 00	-0.000000 00
112.100	-0.18967D 00	-0.000000 00
114.100	-0.19031D 00	-0.000000 00
116.100	-0.19070D 00	-0.000000 00
118.100	-0.19093D 00	-0.000000 00
120.100	-0.19108D 00	-0.000000 00
122.100	-0.19117D 00	-0.000000 00
124.100	-0.19123D 00	-0.000000 00
126.100	-0.11578D 00	0.900000 00
128.100	0.45268D-01	0.900000 00
130.100	0.101790 00	0.900000 00
132.100	0.10744D 00	0.900000 00
134.100	0.10828D 00	0.900000 00
136.100	0.10840D 00	0.900000 00
138.100	0.10842D 00	0.900000 00
140.100	0.10842D 00	0.900000 00
142.100	0.10842D 00	0.900000 00
144.100	0.10842D 00	0.900000 00
146.100	0.10842D 00	0.900000 00
148.100	0.10842D 00	0.900000 00
150.100	0.10842D 00	0.900000 00
152.100	0.10842D 00	0.900000 00
154.100	0.10842D 00	0.900000 00
156.100	0.10842D 00	0.900000 00

157.900	-0.10326D-03	AVERAGE CONCENTRATION CHANGE= -0.355659D-01

NO. OF -VE PTS. = 308.0 AND ITS TOTAL =   0.317235D 02
NO. OF +VE PTS. = 320.0 AND ITS TOTAL = -0.540588D 02

158.100	-0.10967D-01	-0.90000D 00
160.100	-0.11944D 00	-0.90000D 00
162.100	-0.14903D 00	-0.90000D 00
164.100	-0.16461D 00	-0.90000D 00
166.100	-0.17474D 00	-0.90000D 00
158.100	-0.18256D 00	-0.90000D 00
170.100	-0.18600D 00	-0.90000D 00
172.100	-0.18906D 00	-0.90000D 00
174.100	-0.18932D 00	-0.90000D 00
176.100	-0.19009D 00	-0.90000D 00
178.100	-0.19056D 00	-0.90000D 00
180.100	-0.19085D 00	-0.90000D 00
182.100	-0.19103D 00	-0.90000D 00
184.100	-0.19114D 00	-0.90000D 00
186.100	-0.19121D 00	-0.90000D 00
188.100	-0.19125D 00	-0.90000D 00
190.100	0.20950D-01	0.90000D 00
192.100	0.94265D-01	0.90000D 00
194.100	0.10431D 00	0.90000D 00
196.100	0.10811D 00	0.90000D 00
198.100	0.10837D 00	0.90000D 00
200.100	0.10841D 00	0.90000D 00
202.100	0.10842D 00	0.90000D 00
204.100	0.10842D 00	0.90000D 00
206.100	0.10842D 00	0.90000D 00
208.100	0.10842D 00	0.90000D 00
210.100	0.10842D 00	0.90000D 00
212.100	0.10842D 00	0.90000D 00
214.100	0.10842D 00	0.90000D 00
216.100	0.10842D 00	0.90000D 00
218.100	0.10842D 00	0.90000D 00
220.100	0.81771D-01	-0.90000D 00

220.800	-0.10326D-03	AVERAGE CONCENTRATION
		CHANGE= -0.35336D-01

```
NO. OF -VE PTS. =  309.0   AND ITS TOTAL =   0.318319D 02
NO. OF +VE PTS. =  320.0   AND ITS TOTAL =  -0.540588D 02
```

222.100	-0.80011D-01	-0.90000D 00
224.100	-0.13459D 00	-0.90000D 00
226.100	-0.15969D 00	-0.90000D 00
228.100	-0.17289D 00	-0.90000D 00
230.100	-0.18032D 00	-0.90000D 00
232.100	-0.18466D 00	-0.90000D 00
234.100	-0.18726D 00	-0.90000D 00
236.100	-0.18883D 00	-0.90000D 00

238.100	-0.16170D 00	-0.00000D 00
240.100	-0.19033D 00	-0.00000D 00
242.100	-0.13474D 00	-0.00000D 00
244.100	-0.19096D 00	-0.00000D 00
246.100	-0.19110D 00	-0.00000D 00
248.100	-0.19115D 00	-0.00000D 00
250.100	-0.19124D 00	-0.00000D 00
252.100	-0.72237D-01	0.00000D 00
254.100	0.75625D-01	0.00000D 00
256.100	0.10344D 00	0.00000D 00
258.100	0.10769D 00	0.00000D 00
260.100	0.10831D 00	0.00000D 00
262.100	0.10340D 00	0.00000D 00
264.100	0.10842D 00	0.00000D 00
266.100	0.10342D 00	0.00000D 00
268.100	0.10842D 00	0.90000D 00
270.100	0.10842D 00	0.00000D 00
272.100	0.10842D 00	0.00000D 00
274.100	0.10842D 00	0.00000D 00
276.100	0.10942D 00	0.00000D 00
278.100	0.10842D 00	0.90000D 00
280.100	0.10842D 00	0.00000D 00
282.100	0.10842D 00	0.00000D 00

283.600	-0.10326D-03	AVERAGE CONCENTRATION
		CHANGE= -0.355659D-01

NO. OF -VE PTS. = 308.0   AND ITS TOTAL =   0.317235D 02
NO. OF +VE PTS. = 320.0   AND ITS TOTAL =   -0.540588D 02

284.100	-0.38331D-01	-0.00000D 00
286.100	-0.11814D 00	-0.90000D 00
288.100	-0.15164D 00	-0.90000D 00
290.100	-0.16253D 00	-0.90000D 00
292.100	-0.17783D 00	-0.00000D 00
294.100	-0.18319D 00	-0.90000D 00
296.100	-0.18638D 00	-0.90000D 00
298.100	-0.18829D 00	-0.90000D 00
300.100	-0.18946D 00	-0.90000D 00
302.100	-0.19018D 00	-0.90000D 00
304.100	-0.19061D 00	-0.90000D 00
306.100	-0.19089D 00	-0.90000D 00
308.100	-0.19105D 00	-0.90000D 00
310.100	-0.19115D 00	-0.90000D 00
312.100	-0.19122D 00	-0.90000D 00
314.100	-0.19126D 00	-0.90000D 00
316.100	0.40919D-01	0.90000D 00
318.100	0.97761D-01	0.90000D 00
320.100	0.10684D 00	0.90000D 00

322.100	0.10410D 00	0.00000D 00
324.100	0.10739D 00	0.00000D 00
326.100	0.10742D 00	0.00000D 00
328.100	0.10842D 00	0.00000D 00
330.100	0.10842D 00	0.00000D 00
332.100	0.10842D 00	0.00000D 00
334.100	0.10842D 00	0.00000D 00
336.100	0.10842D 00	0.00000D 00
338.100	0.10842D 00	0.00000D 00
340.100	0.10842D 00	0.00000D 00
342.100	0.10842D 00	0.00000D 00
344.100	0.10842D 00	0.00000D 00
346.100	0.30045D-01	-0.00000D 00

346.400	-0.10326D-03	AVERAGE CONCENTRATION CHANGE= -0.355659D-01

NO. OF -VE PTS. = 308.0   AND ITS TOTAL =   0.317235D 02
NO. OF +VE PTS. = 320.0   AND ITS TOTAL = -0.540588D 02

348.100	-0.95133D-01	-0.00000D 00
350.100	-0.14110D 00	-0.00000D 00
352.100	-0.16300D 00	-0.00000D 00
354.100	-0.17472D 00	-0.00000D 00
356.100	-0.18138D 00	-0.00000D 00
358.100	-0.18529D 00	-0.00000D 00
360.100	-0.18764D 00	-0.00000D 00
362.100	-0.18906D 00	-0.00000D 00
364.100	-0.18993D 00	-0.00000D 00
366.100	-0.19046D 00	-0.00000D 00
368.100	-0.19079D 00	-0.00000D 00
370.100	-0.19099D 00	-0.00000D 00
372.100	-0.19112D 00	-0.00000D 00
374.100	-0.19120D 00	-0.00000D 00
376.100	-0.19124D 00	-0.00000D 00
378.100	-0.24172D-01	0.00000D 00
380.100	0.85789D-01	0.00000D 00
382.100	0.10502D 00	0.00000D 00
384.100	0.10792D 00	0.00000D 00
386.100	0.10935D 00	0.00000D 00
388.100	0.10841D 00	0.00000D 00
390.100	0.10842D 00	0.00000D 00
392.100	0.10842D 00	0.00000D 00
394.100	0.10842D 00	0.00000D 00
396.100	0.10842D 00	0.00000D 00
398.100	0.10842D 00	0.00000D 00
400.100	0.10842D 00	0.00000D 00
402.100	0.10842D 00	0.00000D 00
404.100	0.10842D 00	0.00000D 00

```
406.100                 0.10742D 00           0.90000D 00
408.100                 0.10742D 00           0.90000D 00


409.300                -0.10326D-03      AVERAGE CONCENTRATION
                                         CHANGE= -0.353369D-01

NO. OF -VE PTS. =  309.0   AND ITS TOTAL =   0.318319D 02
NO. OF +VE PTS. =  320.0   AND ITS TOTAL =  -0.540588D 02


410.100                -0.56176D-01          -0.90000D 00
412.100                -0.12492D 00          -0.90000D 00
414.100                -0.15491D 00          -0.90000D 00
416.100                -0.17029D 00          -0.90000D 00
418.100                -0.17983D 00          -0.90000D 00
420.100                -0.18378D 00          -0.90000D 00
422.100                -0.18473D 00          -0.90000D 00
424.100                -0.18951D 00          -0.90000D 00
426.100                -0.18959D 00          -0.90000D 00
428.100                -0.19026D 00          -0.90000D 00
430.100                -0.19066D 00          -0.90000D 00
432.100                -0.19092D 00          -0.90000D 00
434.100                -0.19107D 00          -0.90000D 00
```

COMPUTER PROGRAM 2

Computer Program for Simulation of Periodic Tank Reactor under Forced Flow Rate Disturbance conditions.

SYMBOL	DEFINITION
LW	Number of frequencies for which computation is performed.
L	Number of amplitudes for which computation is performed.
TIME 1	Initial time at which the disturbance is forced.
DELTT 1	Initial step size.
DELTPR	Interval at which the results are printed.
FREQ	Frequency of the disturbance.
AMP	Amplitude of the disturbance.
Q	Inlet steady state volumetric flow rate.
V	Volume of the reactor.
AS	Steady state reactant A exit concentration.
RK	Specific rate constant.
AFS	Steady state reactant A inlet concentration.
Q1, Q1A, Q2	Dummy variables.
DELTT	Additional step size for which the computation can be repeated.
YI	Change in reactant A exit concentration from the steady state value.
YID	Difference between YI values at time t and time t plus delta, t.
TIME	Total time at a particular instance since the initial forcing of the disturbance.
TPR	Time at which the results are printed.

SYMBOL	DEFINITION
YD	Value of the concentration change at the point i – 3.
YA	Summation of YI values calculated by the Runge Kutta method.
DY ( )	L values in the Runge Kutta equation.
Y	Concentration change of A as represented by YI plus some value of L in the Runge-Kutta equation.
YR ( )	First three final YI values as calculated by the Runge-Kutta method.
DYF ( )	First three final values of the differential equation (Equation 37) as calculated by the Runge-Kutta method.
ARG	Step function of flow rate disturbance.
YDD1, YDD2 YDD3.	Final value of the differential equation. (Equation 37) at the points i-2, i-1, and i respectively as calculated by the Milne-Hamming method.
YD1, YD2, YD3.	Final values of YI at the points i-2, i-1, and i respectively as calculated by Milne-Hammingmethod.
YD3P, YD3C	Predicted and corrected values respectively of YI at the point.
KS, SK	Number of steps representing positive values of YI in a cycle.
KP, PK	Number of steps representing negative values of YI in a cycle.
QA1, QA2	Summation of all QUS1 values corresponding to positive and negative YI values respectively.
YA1, YA2	Dummy variables.
PA1	Summation of all the positive values of YI.
PA2	Summation of all the negative values of YI.

SYMBOL	DEFINITION
YD4P, YD4M, YD4C	Predicted, modified and corrected values respectively of YI at the point i + 1 as calculated by Milne-Hamming equation.
T1	Time for completion of one cycle of the disturbance.
SN1	Time for completion of integral number of cycles.
YDD4	Value of the differential equation (Equation 37) based on the modified and the final values of YI at the point i + 1.
YD4F	Final value of YI at the point i + 1.
AM4	Magnitude of the disturbance at any given time t.
QUS	Volumetric flow rate at any given time t.
YD4FA	Product of QUS and YI.
QUS1	Exit molar flow rate of reactant A.
PAVG	Average value of exit concentration change of reactant A per cycle.
QAVG	Average value of QUS 1 per cycle.

FORTRAN IV017 SOURCE PROGRAM

```
1          PROGRAM PALITAL
2          IMPLICIT REAL*8%A-H,O-Z<
3          DIMENSIONDY%5<, YR%5<, DYF%5<    ,AMP%10<   ,FREQ%12<
4  C SECOND ORDER IRREVERSIBLE STEP FUCTION FEED FLOW
5  C  REFER JAMES ,SMITH , WULFORD ,&& 380
6  C DATA PRINTED IN READ ORDER
7  C  CONC REPRESENTS VARIATION FROM STEADY STATE VALUE
8          READ 2,LW, L
9          READ  3, TIME1,  DELTT1  ,DFLTPR
10         READ 4, O, V, AS, RK
11         READ  41, % FREQ%NW<, NW  #.1, LW  <
12         READ  41, % AMP%N< ,  N  # 1, L <
13    41   FORMAT %7F10.4 <
14     2   FORMAT %2I2 <
15     3   FORMAT % 3F10.4 <
16     4  FORMAT %4F10.4<
17         PRINT 2,LW, L
18         PRINT  3,  TIME1, DELTT1
19         PRINT  4,  O,V,AS,RK
20          P  #  0.0
21         DO  33  JW  #  1,  LW
22          W  #  FREQ%JW<
23         DO  32   J  # 1,  L
24         AM  #  AMP%J<
25         PRINT 42,  AMP%J< ,FREQ%JW<
26   420 FORMAT %a1a,7X,  11HAMPLITUDE #, F6.2, 11HFREQUENCY #
27      1 ,  F6.2 <
28         AFS  #  1.0
29         Q1  #  AM/V
30         Q1A  #  Q1* % AFS - AS <
31         Q2  # % %O/V< & %2.0*RK*AS < <
32         PRINT  44
33    44  FORMAT%/a    Q1           Q1A          Q2       a<
34         DELTT  #  DELTT1
35     1 YI  #  0.0
36       YID  #  0.0
37        TIME  #  TIME1
38        TPR  #  DELTPR
39       PRINT 6
40     6  FORMAT %///10X,9HTIME%HRS<,  10X,  15HCONC%MOLES/CUFT<
41       PRINT 5, Q1, Q1A,  Q2
42     5  FORMAT%   3E12.4///<
43       PRINT 7,  TIME,YI
44     7  FORMAT% //7X, F9.3, 10X,  E15.5 //<
45       YD  #  YI
46       YA  #  YD
47       DY%1<  #  0.0
48       DO  18  K # 1, 3
49      DO  19  N  #  2, 5
50       GO  TO %11, 12, 13, 12, 13 < , N
```

FORTRAN IV017 SOURCE PROGRAM BALHAM   PROGRAM

```
51      13  TIME  #  TIME  &% DELTT/2.0 <
52      12  Y  #  YT  &  %DY%N-1<  /2.0  <
53          IF %N.LE. 4<  GO TO119
54          Y  #  Y &  % DY %N-1 < / 2.0 <
55     119  ARG  #  1.0
56     190  DY%"<  #% %Q1A* ARG         < -  %RK*Y*Y< -%Q2*Y <
57       1  - % Q1*ARG*Y < < * DELTT
58          YID  #  %1./6.0<*%%DY%2<&% 2.*%DY%3< & DY%4<<< & DY%5<<
59          YI  #  YI & YID
60          YR%K<  #  YI
61          YA  #  YA  & YP%K<
62          PRINT 9, TIME, YI
63          ARG  #  1.0
64     180  DYF%K<  #  %Q1A*  ARG        < -%RK* YR%K<*YR%K< <
65       1  - % Q2*YR%K< <
66       2  -  % Q1 * ARG * YR%K< <
67          YDD1  #  DYF%1<
68          YDD2  #  DYF%2<
69          YDD3  #  DYF%3<
70          YD1  #  YR%1<
71          YD2  #  YR%2<
72          YD3  #  YR%3<
73          PRINT 8
74      80  FORMAT %//@        THE FOLLOWING VALUES CALCULATED
75       1  HAMMING  EQUATION @ <
76          TIME  # 4.0*DELTT
77          YD3P  #YD3
78          YD3C  #  YD3
79          KS . #  0
80          KP  #  0
81          QA1  #  0.0
82          QA2  #  0.0
83          YA1  #  0.0
84          YA2  #  0.0
85          PA1  #  0.0
86          PA2  #  0.0
87          DO 31  I  #  5,  20000
88     100  YD4P# YD, &%%4./3.<*%%2.*YDD1<- YDD2 &  %2.*YDD3<<
89       1  * DELTT <
90          YD4M  #  YD4P -%112./121.< **%YD3P -YD3C<
91          T1  #  % 2.0* 3.1415927 < / W
92          DO 129 NS  #  1 , 30
93          SN  #  NS
94          SN1  #  SN*T1
95          IF % TIME  .LT.  SN1 < GO TO 121
96     129  CONTINUE
97     121  CONTINUE
98          QN  #  SN  - 1.0
99          IF % TIME  .LE. % T1*% QN &% 1./ 2. <<< < GO TO 142
100         IF % TIME  .LE. % T1*% QN &% 4./ 4. <<< < GO TO 143
```

```
FORTAN IV017 SOURCE PROGRAM   RALHAM    PROGRAM

101    141   ARG  #  0.0
102          GO TO 151
103    142   ARG  #  1.0
104          GO TO 151
105    143   ARG  # -1.0
106          GO TO  151
107    151   CONTINUE
108        0 YDD4  #%Q1A*   ARG         < -%RK*YD4M*YD4M< -%Q2*YD4M<
109        1  - % Q1*ARG*YD4M<
110        0 YD4C # %.125< *%%9.*YD3< -YD1 & %% 3.*DELTT<*%YDD4
111        1 & %2. *YDD3 <  - YDD2 < < <
112          YD4F #   YD4C & %9./121.< **YD4D - YD4C <
113        0 YDD4  #  %Q1A*   ARG        < - %RK*%YD4F*YD4F<<
114        1 - % Q2*YD4F < - % Q1* ARG * YD4F <
115          AM4  #  AM * ARG
116          QUS  #  Q & AM4
117          YD4FA  #  QUS * YD4F
118          QUS1  #  QUS * % AS & YD4F <
119          IF % TIME .LE. %8.1/W< <  GO TO 23
120          IF % YD4F  - 0.0 <  75, 71, 71
121    71    IF % KP - 2 < 23, 72, 72
122    75    IF % KS - 1 < 74, 74, 73
123    74    PA2  #  PA2  & YD4F
124          QA2  #  QA2 &  QUS1
125          KP  #  KP  & 1
126          GO TO  23
127    72    PA1  #  PA1  &   YD4F
128          QA1  #  QA1  &  QUS1
129          KS  #  KS & 1
130          GO TO  23
131    73    SK  #  KS
132          PK  #  KP
133          PAVG  #  %  PA1  & PA2        < / % SK & PK      <
134          QAVG  #  %  QA1  & QA2        < / % SK & PK      <
135          PRINT  14,  TIME , YD4F ,  QUS1
136    14    FORMAT%//10X,F9.3,10X,E15.5, 7X,     E15.5  <
137          PRINT  95,  PAVG
138    95    FORMAT %/35X, a AVG. CONC. ALONE #a,  E15.7 //<
139          PRINT  79,  QAVG
140    79    FORMAT %/35X, a AVERAGE % CONC*QS<      #a, E15.7 /<
141          PRINT  93, QA1,  QA2
142    93     FORMAT %/ E15.5,  7X,  E15.5/<
143          PRINT  17, SK,  PK
144    17    FORMAT % 2X, aNO. OF PTS. #a , F10.4,  10X, F10.4/<
145          KP  #  1
146          KS  #  0
147          QA1  #  0.0
148          QA2  #  QUS1
149          PA1  #  0.0
150          PA2  #  YD4F
```

```
FORTRAN IVO17 SOURCE PROGRAM   BAIHAM    PROGRAM

151          YA1  #   0.0
152          YA2  #   YD4FA
153          GO   TO   23
154  C       YD4F REPRESENTS AVERAGE CHANGE IN CONCENTRATION
155  C       FROM  THE  STEADY  STATE  WITH  NO FEED  CONCENTRATION
156  C       DISTURBANCE
157     23   IF % TIME - TPR < 26, 25, 25
158     25   PRINT91,TIMF, YD4F   ,  OUS   ,   QUS1    .  , YD4FA
159    910   FORMAT "        10X,  F9.3,  10X,   E15.5  ,   10X,   E15.5,
160       1  10X,   E15.5 ,  10X,   E15.5  <
161      9   FORMAT "        10X, F9.3, 10X,   E15.5  <
162     27   TPR  #   TPR  &  DELTPR
163     26       IF STIME  - % % 6.3/W<*31.<  <   20,21,21
164     20   A   #   I
165          TIME  #   A*DELTT
166          YD   #  YD1
167          YD1  #  YD2
168          YD2  #  YD3
169          YD3  #  YD4F
170          YD3P #  YD4P
171          YD3C #  YD4C
172          YDU1  #   YDD2
173          YDD2  #   YDD3
174          YDU3  #   YDD4
175     31   CONTINUE
176          PRINT  43
177     43   FORMAT%///@ AVG. CHANGE IN CONC. IS@<
178     21   IF % DELTT  .GE.  0.110 <  GO   TO   22
179          IF % DELTT  .LE.  0.110 <  GO   TO   11
180          GO  TO  11
181     22   DELTT  #  DELTT/2.0
182          TIME  #  TIME1
183          PRINT  24   ,  DELTT
184    240   FORMAT %///@ ANOTHER CASE WITH DIFFERENT 4ELTT  #@,
185       1  F5.3 <
186          GO  TO  1
187     11   CONTINUE
188     32   CONTINUE
189          DELTT  #  DELTT1
190          TIME  #  TIME1
191     33   CONTINUE
192          STOP
193          END
```

COMPUTER PROGRAM 3

Computer Program for Simulation of Periodic Tank Reactor under simultaneous forced concentration and Flow Rate Disturbances.

SYMBOL	DEFINITION
LW	Number of frequencies for which computation is performed.
L	Number of amplitudes for which computation is performed.
LP	Number of phase lag for which computation is performed.
TIME 1	Initial time at which the disturbance is forced.
DELTT 1	Initial step size.
DELTPR	Interval at which the results are printed.
Q	Inlet steady state volumetric flow rate.
V	Volume of the reactor.
AS	Steady state reactant A exit concentration.
RK	Specific rate constant.
FREQ	Frequency of the concentration disturbance.
AMP, AM	Amplitude of the concentration disturbance.
PHP	Phase lag between two disturbances in degrees.
AM2	Amplitude of the flow rate disturbance.
AFS	Steady state reactant A inlet concentration.
Q1, Q1A, Q2	Dummy variables.
Q6	Rate of unconverted reactant A in the exit stream at steady state.
P	Phase lag between two disturbances in radians.
P1	Dummy variable.

SYMBOL	DEFINITION
DELTT	Additional step size for which the computation can be repeated.
YI	Change in reactant A exit concentration from the steady state value.
YID	Difference between YI values at time t and time t plus delta t.
TIME	Total time at a particular instance since the initial forcing of the disturbance.
TPR	Time at which the results are printed.
YD	Value of the concentration change at the point i-3.
YA	Summation of YI values calculated by the Runge Kutta method.
DY ( )	L values in the Runge Kutta equation.
Y	Concentration change of A as represented by YI plus some value of L in the Runge-Kutta equation.
YR ( )	First three final YI values as calculated by the Runge-Kutta method.
DYF ( )	First three final values of the differential equation (Equation 40) as calculated by the Runge-Kutta method.
YDD1, YDD2, YDD3	Final value of the differential equation (Equation 40) at the points i-2, i-1 and i respectively as calculated by the Milne-Hamming method.
YD1, YD2, YD3	Final values of YI at the points i-2, i-1 and i respectively as calculated by the Milne-Hamming method.
YD3P, YD3C	Predicted and corrected values respectively of YI at the point.
KS, SK	Number of steps representing positive values of YI in a cycle.

SYMBOL	DEFINITION
KP, PK	Number of steps representing negative values of YI in a cycle.
QA1, QA2	Summation of all QUS1 values corresponding to positive and negative YI values respectively.
YA1, YA2	Dummy variables.
PA1	Summation of all the positive values of YI.
PA2	Summation of all the negative values of YI.
YD4P, YD4M, YD4C	Predicted, modified and corrected values respectively of YI at the point i + 1 as calculated by Milne-Hamming equation.
T1	Time for completion of one cycle of the disturbance.
SN1	Time for completion of integral number of cycles.
YDD4	Value of the differential equation (Equation 37) based on the modified and the final values of YI at the point i + 1.
YD4F	Final value of YI at the point i + 1.
AM4	Magnitude of the disturbance at any given time t.
QUS	Volumetric flow rate at any given time t.
YD4FA	Product of QUS and YI
QUS1	Exit molar flow rate of reactant A.
PAVG	Average value of exit concentration change of reactant A per cycle.
QAVG	Average value of QUS1 per cycle.

FORTRAN IV017 SOURCE PROGRAM

```
 1          PROGRAM BALHAM
 2          IMPLICIT REAL*8%A-H,O-Z<
 3          DIMENSION DY%5<, YP%5<, DYF%5<    ,AMP%10<  ,FREQ%12<
 4          DIMENSION  PHP%12<           , AMPB%10<
 5  C       SECOND ORDER IRREVERSIBLE SINGLE C.S.T.R.
 6  C       COMBINE STEP DISTURBANCES ON FEED  FLOW AND FEED CONC.
 7  C       FOR A GIVEN CASE BOTH HAVE SAME FREQUENCY BUT THE
 8  C       AMPLITUDES VARY BY A FACTOR OF TEN
 9  C       FLOW DISTURBANCE LAGS BEHIND CONC. DISTURBANCE BY
10  C       PHASE LAG IN DEGREES
11  C  REFER JAMES ,SMITH , WULFORD ,&& 380
12  C  DATA PRINTED IN READ ORDER
13  C  CONC REPRESENTS VARIATION FROM STEADY STATE VALUE
14          READ 2, LW, L,  LP
15          READ  3, TIME1,  DELTT1  ,DELTPR
16         READ 4, Q, V, AS, RK
17          READ  41, % FREQ%NW<, NW  # 1,  LW  <
18          READ  41, % AMP%N< ,   N  # 1,  L <
19          READ  41,% PHP%NP< ,   NP # 1,  LP <
20     41   FORMAT %7F10.4 <
21      2   FORMAT %3I2  <
22      3   FORMAT % 3F10.4 <
23      4   FORMAT %4F10.4<
24          PRINT 2,  LW, L, LP
25          PRINT  3,  TIME1, DELTT1
26          PRINT  4,  Q,V,AS,RK
27          DO 33  JW  # 1,  LW
28          W  #  FREQ%JW<
29          DO  32   J  # 1,  L
30          AM  #  AMP%J<
31          AM2  #  AM* 10.0
32          DO  34  NP  # 1,  LP
33          P2  #  PHP%NP<
34          PRINT  42,  AMP%J<  ,FREQ%JW<  ,  PHP%NP<
35     420  FORMAT %10,7X,  11HAMPLITUDE #, F6.2, 11HFREQUENCY #
36        1 ,F6.2,5X,19H PHASE LAG DEGREE #,  F8.2 <
37          PRINT 46 , AM2
38     460  FORMAT %/@           FLOW DISTURBANCE AMPLITUDE  #@,
39        1 F6.2 <
40          AFS  #  1.0
41          Q1  #  AM2 / V
42          Q1A  #  Q1* % AFS - AS <
43          Q2  #  Q/V
44          Q6  #  Q * AS
45          P  #  % 2.0* 3.1415927* P2 < / % 360.0 <
46          P1  #  % P2  / 360.0 <
47          PRINT  44
48     44   FORMAT%/@   Q1           Q1A           Q2       @<
49          DELTT  #  DELTT1
50      1  YI  #  0.0
```

```
51          YIP  #  0.0
52          TIME  #  TIMLI
53          TPK  #  DELTPR
54          PRINT 6
55     6 FORMAT %///10X,9HTIME%HRS<,  10X,  15HCONC%MOLES/CUFT<
56          PRINT 5, Q1, Q1A,  Q2
57     5 FORMAT%    3F12.4///<
58          PRINT 7,  TIME,YI
59     7 FORMAT% //7X, F9.3, 10X,  E15.5 //<
60          YD  #  YI
61          YA  #  YD
62          DY%1<  #  0.0
63          DO 18  K  #  1, 3
64          DO 19  N  #  2, 5
65          GO TO %11, 12, 13, 12, 13 < , N
66    13 TIME  #  TIME  6% DELTT/2.0 <
67    12 Y  #  YT  6  %DY%N-1<  /2.0  <
68          IF %N.LE. 4< GO TO119
69          Y  #  Y 6  % DY %N-1 < / 2.0 <
70   119 ARG  #  1.0
71          IF % P1 .LE. 0.0 < GO TO 115
72          IF % P1 .LE.4./8.< GO TO 116
73          IF % P1 .LE.8./8.< GO TO 115
74   115 ARG1# 1.0
75          GO TO 117
76   116 ARG1  #  -1.0
77          GO TO 117
78   117 CONTINUE
79   190 DY%N< # % % Q1A * ARG1 <  6 % % Q2 6 % Q1* ARG1 < <*
80     1  %% AM*ARG< -     Y<< - %% RK*     Y< * %% 2.0*AS< 6
81     2 Y<< < * DELTT
82          YID  #  %1./6.0<*%%DY%2<6% 2.*%DY%3< 6 DY%4<<< 6 DY%5< <
83          YI  #  YI 6 YID
84          YR%K<  #  YI
85          YA  #  YA  6  YR%K<
86          PRINT 9,  TIME, YI
87   180 DYF%K< #  % Q1A * ARG1 <  6 % % Q2 6 % Q1* ARG1 < <*
88     1  %% AM*ARG< - YR%K<<< - %% RK*YR%K<< * %% 2.0*AS< 6
89     2 YR%K< <<
90          YDD1  #  DYF%1<
91          YDD2  #  DYF%2<
92          YDD3  #  DYF%3<
93          YD1  #  YR%1<
94          YD2  #  YR%2<
95          YD3  #  YR%3<
96          PRINT 8
97    08 FORMAT %//a        THE FOLLOWING VALUES CALCULATED BY
98     1 HAMMING EQUATION a <
99          TIME  #  4.0*DELTT
100         YD3P  #YD3
```

.

FORTRAN IV G17 SOURCE PROGRAM PALHAM   PROGRAM

```
101          YD3C    #   YD3
102          KS    #    0
103          KD    #    0
104          KU    #    0
105          KX    #    0
106          QA1    #    0.0
107          QA2    #    0.0
108          YA1    #    0.0
109          YA2    #    0.0
110          PA1    #    0.0
111          PA2    #    0.0
112          DO   31   I   #   5,   20000
113     100 YD4P#  YD  &%%4./3.<*%%2.*YDD1<-  YDD2 &   %2.*YDD3 <<*
114       1 DELTT   <
115          YD4N   #  YD4P -%112./121.<  *%YD3P -YD3C<
116          T1   #   ~ 2.0*  3.1415927  <  /  W
117          DO   129   NS   #   1 ,  10
118          SN   #   NS
119          SN1   #   SN*T1
120          IF % TIME  .LT.   SN1 < GO TO 121
121     129  CONTINUE
122     121  CONTINUE
123          QN  #   SN  -   1.0
124          IF % P1  .LE.%0.0     <   <  GO TO    130
125          IF % P1  .LE.%1.0/8.0<   <  GO TO    131
126          IF % P1  .LE.%2.0/8.0<   <  GO TO    132
127          IF % P1  .LE.%3.0/8.0<   <  GO TO    133
128          IF % P1  .LE.%4.0/8.0<   <  GO TO    134
129          IF % P1  .LE.%5.0/8.0<   <  GO TO    135
130          IF % P1  .LE.%6.0/8.0<   <  GO TO    136
131          IF % P1  .LE.%7.0/8.0<   <  GO TO    137
132          IF % P1  .LE.%8.0/8.0<   <  GO TO    138
133     130  CONTINUE
134          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TO 142
135          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TO 144
136     131  CONTINUE
137          IF % TIME   .LE. % T1*% ON &% 1./ 8. <<< < GO TO 141
138          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TO 142
139          IF % TIME   .LE. % T1*% ON &% 5./ 8. <<< < GO TO 143
140          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TO 144
141     132  CONTINUE
142          IF % TIME   .LE. % T1*% ON &% 2./ 8. <<< < GO TO 141
143          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TO 142
144          IF % TIME   .LE. % T1*% ON &% 6./ 8. <<< < GO TO 143
145          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TO 144
146     133  CONTINUE
147          IF % TIME   .LE. % T1*% ON &% 3./ 8. <<< < GO TO 141
148          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TO 142
149          IF % TIME   .LE. % T1*% ON &% 7./ 8. <<< < GO TO 143
150          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TO 144
```

FORTRAN IV017 SOURCE PROGRAM PAIHAM   PROGRAM

```
151    134   CONTINUE
152          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TU 141
153          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TU 143
154    135   CONTINUE
155          IF % TIME   .LE. % T1*% ON &% 1./ 8. <<< < GO TU 142
156          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TU 141
157          IF % TIME   .LE. % T1*% ON &% 5./ 8. <<< < GO TU 144
158          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TU 143
159    136   CONTINUE
160          IF % TIME   .LE. % T1*% ON &% 2./ 8. <<< < GO TU 142
161          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TU 141
162          IF % TIME   .LE. % T1*% ON &% 6./ 8. <<< < GO TU 144
163          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TU 143
164    137   CONTINUE
165          IF % TIME   .LE. % T1*% ON &% 3./ 8. <<< < GO TU 142
166          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TU 141
167          IF % TIME   .LE. % T1*% ON &% 7./ 8. <<< < GO TU 144
168          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TU 143
169    138   CONTINUE
170          IF % TIME   .LE. % T1*% ON &% 4./ 8. <<< < GO TU 142
171          IF % TIME   .LE. % T1*% ON &% 8./ 8. <<< < GO TU 144
172    141   ARG # 1.0
173          ARG1 # -1.0
174          GO TU 151
175    142   ARG # 1.0
176          ARG1 # 1.0
177          GO TU 151
178    143   ARG # -1.0
179          ARG1 # 1.0
180          GO TU 151
181    144   ARG # -1.0
182          ARG1 # -1.0
183          GO TU 151
184    151   CONTINUE
185     0    YD4  # % Q1A * ARG1 < & %% Q2 & % Q1* ARG1 < <*
186     1    %% AM*ARG< - YD4M<< - %% RK* YD4M< * %% 2.0*AS< &
187     2    YD4M  <<
188     0    YD4C # %.125< *%%9.*YD3< -YD1 & %% 3.*DELTT<*%YDD4 &
189     1    %2.*YDD3 < - YDD2 < < <
190          YD4F  #  YD4C & %9./121.< *%YD4P - YD4C <
191     0    YD4  # % Q1A * ARG1 < & %% Q2 & % Q1* ARG1 < <*
192     1    %% AM*ARG< - YD4F<< - %% RK* YD4F< * %% 2.0*AS< &
193     2    YD4F < <
194          AM4  #  AM2 * ARG1
195          QUS # Q & AM4
196          YD4FA  #  QUS * YD4F
197          QUS1  #  QUS * % AS & YD4F <
198          IF % TIME .LE. % 5.1/W < < GO TO 23
199          IF % QUS1 - Q6 < 64, 65, 65
200    64    KU # 5
```

FORTRAN IV017 SOURCE PROGRAM RADHAN   PROGRAM

```
201          IF % KX - 5 < 23, 72, 23
202    65    IF % KU - 5 < 23, 71, 23
203    71    IF % KS - 2 < 75, 75, 73
204    75    IF % KP - 0 < 11, 76, 74
205    76    PRINT 14, TIME , YD4F , QUS1
206    74    PA2  #  PA2  &  YD4F
207          QA2  #  QA2  &  QUS1
208          KP   #  KP  &  1
209          KX   #  5
210          GO  TO  23
211    72    PA1  #  PA1  &  YD4F
212          QA1  #  QA1  &  QUS1
213          KS   #  KS  &  1
214          GO  TO  23
215    73    SK   #  KS
216          PK   #  KP
217          PAVG  #  %  PA1  &  PA2      < / % SK & PK        <
218          QAVG  #  %  QA1  &  QA2      < / % SK & PK        <
219          PRINT  14,  TIME , YD4F , QUS1
220    14    FORMAT%//10X,F9.3,10X,E15.5, 7X,        E15.7 / <
221          PRINT  95,  PAVG
222    95    FORMAT %/35X, a AVG. CONC. ALONE #a,   E15.7 //<
223          PRINT  79,  QAVG
224    79    FORMAT %/35X, a AVERAGE % CONC*0S<         #a, E15.7 /<
225          PRINT  93,  QA1,  QA2
226    93    FORMAT %/ E15.5,  7X,  E15.5/<
227          PRINT  17,  SK,  PK
228    17    FORMAT % 2X, aNO. OF PTS. #a  , F10.4,  10X,  F10.4/<
229          KP   #  1
230          KS   #  0
231          QA1  #  0.0
232          QA2  #  QUS1
233          PA1  #  0.0
234          PA2  #  YD4F
235          YA1  #  0.0
236          YA2  #  YD4FA
237          GO  TO  23
238    23    IF % TIME - TPR < 26, 25, 25
239    25    PRINT91,TIME, YD4F    , OUS   ,  QUS1        , YD4FA
240    910   FORMAT %       10X, F9.3, 10X,  E15.5  ,  10X,  E15.5,
241     1    10X,  E15.5 , 10X,  E15.5  <
242     9    FORMAT %       10X, F9.3, 10X,  E15.5  <
243    27    TPR  #  TPR  &  DELTPR
244    26    IF % TIME - % % 6.3/ W < * 6.4 < < 20, 21, 21
245    20    A   #  1
246          TIME  #  A*DELTT
247          YD   #  YD1
248          YD1  #  YD2
249          YD2  #  YD3
250          YD3  #  YD4F
```

FORTRAN IV017 SOURCE PROGRAM   RATHAM   PROGRAM

```
251          YD3P # YD4P
252          YD3C # YD4C
253          YD01 #  YD02
254          YD02 #  YD03
255          YD03 #  YD04
256     31   CONTINUE
257          PRINT  43
258     43   FORMATS///@ AVG. CHANGE IN CONC. IS?<
259     21   IF  % DELTT  .GE.  0.110 <  GO  TO  22
260          IF  % DELTT  .LE.  0.110 <  GO  TO  11
261          GO  TO  11
262     22   DELTT #  DELTT/2.0
263          TIME # TIME1
264          PRINT  24   ,  DELTT
265    240 FORMAT %///@ ANOTHER CASE WITH DIFFERENT DELTT  #@  ,
266      1 F5.3 <
267          GO  TO  1
268     11   CONTINUE
269     34   CONTINUE
270          DELTT #  DELTT1
271          TIME # TIME1
272     32   CONTINUE
273     33   CONTINUE
274          STOP
275          END
```

COMPUTER PROGRAM 4

Computer Program for Simulation of Series of Periodic Tank
Reactors under Forced Concentration Disturbance Conditions.

SYMBOL	DEFINITION
NR	Number of reactors connected in series.
LW	Number of frequencies for which computation is performed.
LA	Number of amplitudes for which computation is performed.
TIME1	Initial time at which the disturbance is forced.
DELTT1	Initial step size.
DELTPR	Interval at which the results are printed.
Q	Inlet volumetric flow rate.
RK	Specific rate constant.
V ( )	Volume of the individual reactors.
FREQ	Frequency of the disturbance.
AMP	Amplitude of the disturbance
AS ( )	Steady state reactant A exit concentration for each reactor.
YI ( )	Change in reactant A exit concentration from the steady state for each reactor.
Q1A ( ) Q2 ( )	Dummy variables.
DELTT	Additional step size for which the computation can be repeated.

SYMBOL	DEFINITION
TIME	Total time at a particular instance since the initial forcing of the disturbance.
TPR	Time at which the results are printed.
DY ( )	L values in the Runge-Kutta equation.
YID	Difference between YI ( ) values at time t and time t plus delta t.
Y ( )	Concentration change of A as represented by YI ( ) plus some value of L in the Runge-Kutta equation for each reactor.
YIP ( )	Dummy variables.
DYF ( )	First three final values of the differential equation (Equations 53, 57, 58) as calculated by the Runge-Kutta method.
YDD1 ( ) YDD2 ( ) YDD3 ( )	Final value of the differential equation (Equations 53, 57, 58) at the points i-2, i-1, and i respectively as calculated by the Milne-Hamming method for each reactor.
YD1 ( ), YD2 ( ) YD3 ( )	Final values of YI at the points, i-2, i-1 and i respectively as calculated by Milne-Hamming for each reactor.
YD3P ( ), YD3C ( )	Predicted and corrected values respectively of Yl at the point i.
YD ( )	Value of the concentration change at the point i-3 for each reactor.
YA1 ( )	Summation of the positive values of Yl ( ) in a cycle for each reactor.
YA2 ( )	Summation of the negative values of YI ( ) in a cycle of each reactor.
KS, SK	Number of steps representing negative values of YI in a cycle for the first reactor.
KP, PK	Number of steps representing positive values of YI in a cycle for the first reactor.

SYMBOL   DEFINITION

YD4P (   )   Predicted, modified and corrected values
YD4M (   )   respectively of Yl at the point i + 1 for each
YD4C (   )   reactor.

Tl   Time for completion of one cycle of the
                 disturbance.

SN1   Time for completion of integral number of cycles.

D4F(1)   Step function of concentration disturbance into
                 the first reactor.

YARG   Magnitude of the concentration disturbance into
                 the first reactor.

YDD4 (   )   Value of the differential equation (Equations 53,
                 57, 58) based on the modified and the final
                 values of Yl at the point i + 1 for each reactor.

YD4F (   )   Final value of YI at the point i + 1 for each
                 reactor.

YAVG (   )   Average value of exit concentration change of
                 reactant A per cycle for each reactor.

```
 1          PROGRAM PALHAM
 2          IMPLICIT REAL*8 A-H,O-Z)
 3          DIMENSION  FREQ(10) , AMP(10)
 4          DIMENSION DY(9) , Y(9) , DARG(9) , DYF(9)
 5          DIMENSION V(9) , AS(9) , Q1A(9) , Q2(9)
 6          DIMENSION YI(9) , YD(9) , YIP(9)
 7          DIMENSION YD1(9) , YD2(9) , YD3(9)
 8          DIMENSION YDD1(9) , YDD2(9) , YDD3(9) , YDD4(9)
 9          DIMENSION YD3P(9) , YD4P(9) , YD3C(9) , YD4C(9)
10          DIMENSION YA1(9) , YA2(9) , YAVG(9)
11          DIMENSION YD4M(9) , YD4F(9) , D4F(9)
12  C       SECOND ORDER IRREVERSIBLE REACTION
13  C       SERIES OF STIRRED TANK REACTORS
14  C       DATA PRINTED IN READ ORDER
15  C       SQUARE WELL TYPE DIST. ON FEED CONC.
16  C       NUMBER OF REACTORS IN SERIES IS REPRESENTED BY NR
17  C       REFER JAMES , SMITH , WOLFORD ,  PP 380
18  C       CONC. REPRESENTS VARIATION FROM STEADY STATE VALUE
19          READ 1, NR
20          READ 2, LW , LA
21      1   FORMAT ( I2)
22      2   FORMAT (2I2)
23          READ 3, TIME1, DELTT1, DELTPR
24          READ 4, Q, RK
25      3   FORMAT  ( 3F10.4)
26      4   FORMAT( 2F10.4)
27          NR2 = MR & 1
28          READ 5, ( V(NV) , NV = 1, NR )
29          READ 5, ( FREQ(NW), NW = 1, LW )
30          READ 5, ( AMP(N) , N = 1, LA)
31          READ 5, ( AS(NS) , NS = 2, NR2 )
32      5   FORMAT ( 7F10.4 )
33          PRINT 1, NR
34          PRINT 2, LW, LA
35          PRINT 3, TIME1 , DELTT1, DELTPR
36          PRINT 4, Q , RK
37          PRINT 6, ( AS(NS) , NS = 2, NR2 )
38          PRINT 6, ( V(NV) , NV = 1, NR )
39      6   FORMAT ( / 7F10.4 / )
40          DO 10 JW = 1, LW
41          W = FREQ(JW)
42          DO 11 JA = 1, LA
43          AM = AMP(JA)
44          PRINT 7, NR
45      70  FORMAT ( @1@ , 20X, @ NUMBER OF REACTORS IN SERIES #@
46      1 , I2 )
47          PRINT 8, AMP(JA) , FREQ(JW)
48      80  FORMAT (/ 7X, @AMPLITUDE #@,F6.2,  7X, @FREQUENCY #@,
49      1 F6.2 )
50          YI(1) = 0.0
```

FORTRAN IVO17 SOURCE PROGRAM   PALHAM   PROGRAM

```
51              DO 12   J # 2, NR2
52              YI%J<   # 0.0
53              Q1A%J-1<   # %0*AH< / V%J-1<
54       12     Q2%J<   # % 0/V%J-1< < & % 2.0*RK* AS%J< <
55              PRINT 9, % Q1A%J-1< , J # 2, NR2  <
56              PRINT 13, % Q2%J< , J # 2, NR2 <
57        9     FORMAT % /@ Q1A-S #@)  5E15.4 <
58       13     FORMAT % / @ O2-S #@) 5E15.4 <
59              DELTT   # DELTT1
60       67     TIME # TIME1
61              TPR # DELTPR
62              PRINT  14
63      140     FORMAT % /// 10X, 9HTIME%HRS<,  10X,
64        1     @ CONC.%MOLES/CU.FT.< @ <
65              PRINT 15, TIME , % YI%J< , J # 2, NR2 <
66       15     FORMAT % //10X, F9.3,  10X,  4% E15.5 , 5X < <
67              DO 20  K # 1, 3
68              DO 21  J # 2,  NR2
69              IF %K-1< 22, 22, 23
70       22     TIME  # TIME1
71              YI%J< #  0.0
72              DY%1<  #  0.0
73              YID #  0.0
74       23     DO 24  N # 2, 5
75              GO TO % 100, 26, 27, 26, 27 <,N
76       27     TIME # TIME & %DELTT/2.0 <
77       26     Y%N< # YI%J< & %DY%N-1</2.0<
78              IF % N .LE. 4 < GO TO 28
79              Y%N< # Y%N< & % DY%N-1</2.0 <
80       28     CONTINUE
81              IF %J-2< 29,29, 24
82       29     DARG%3< # 1.0
83              DARG%4< # 1.0
84              DARG%5<  # 1.0
85   C      0 THE ABOVE THREE VALUES OF DARG VARY DEPENDING ON TYPE
86   C      1 OF  DISTURBANCE
87              IF %K-1< 30, 30, 31
88       30     DARG%2< # 0.0
89              GO TO 24
90       31     DARG%2< #1.0
91   C      0 THE ABOVE TWO   VALUES OF DARG VARY DEPENDING ON TYPE
92   C      1 OF  DISTURBANCE
93              GO TO 24
94      240     DY%N< #%% Q1A%J-1<*DARG%N<< - % RK*Y%N<*Y%N< <
95        1     -% Q2%J<*Y%N<< < * DELTT
96        0 YID # %1./6.0<* % DY%2< & % 2.0 * %DY%3< & DY%4< < <
97        1 &  DY%5< <
98              YI%J<  # YI%J< & YID
99              DARG%2<  # Y%2<
100             DARG%3<  # Y%3<
```

FORTRAN IV017 SOURCE PROGRAM   RALHAM   PROGRAM

```
101            DARG%4<   #  Y%4<
102            DARG%5<   #  Y%5<
103            IF % J-2 < 32, 32, 33
104      32    YIP%J-1<  #  1.0
105  C         THE ABOVE THREE VALUES OF DARG VARY DEPENDING ON TYPE
106  C         OF DISTURBANCE <
107            GO TO 34
108      33    YIP%J-1<  #    YI%J-1<
109            GO TO 34
110     340    DYF%K<    #   % Q1A%J-1<*YIP%J-1< < - % RK*YI%J<*YI%J< <
111       1    - % Q2%J< * YI%J<  <
112            GO TO % 35, 36, 37 <,K
113      35    YD01%J<   #  DYF%1<
114            YD1%J<    #   YI%J<
115            GO TO 38
116      36    YD02%J<   #   DYF%2<
117            YD2%J<    #  YI%J<
118            GO TO 38
119      37    YD03%J<   #   DYF%3<
120            YD3%J<    #   YI%J<
121            GO TO 38
122      38    BK  #  K
123      21    TIME  #  BK* DELTT
124            PRINT 15, TIME, % YI%J< , J # 2, NR2  <
125      20    CONTINUE
126            PRINT 39
127     390    FORMAT % // @    THE FOLLOWING VALUES CALCD. BY
128       1 HAMMING EQUATION @ <
129            TIME  #  4.0 * DELTT
130            DO 40  J  # 2, NR2
131            YD3P%J<   #   YD3%J<
132            YD3C%J<   #   YD3%J<
133            YD%J<  #  0.0
134            YA1%J<  #  0.0
135      40    YA2%J<  #  0.0
136            KS  # 0
137            KP  # 0
138            DO 41  I  # 5, 20000
139            DO 42  J  # 2, NR2
140       0 YD4P%J<  #  YD%J<  & % %4.0/3.0< * % %2.0*YD01%J< <
141       1  - YD02%J<
142       2   & % 2.0*YD03%J< < < *DELTT <
143       0 YD4M%J<  #  YD4P%J<  - % %112.0/121.0< * %YD3P%J<
144       1  - YD3C%J< < <
145            IF % J .GE. 3 < GO TO 43
146            T1  #  % 2.0* 3.1415927 < / W
147            DO  44  NS  # 1 , 10
148            SN  #  NS
149            SN1  #  SN*T1
150            IF % TIME .LT.  SN1 < GO TO 45
```

```
151    44   CONTINUE
152    45   CONTINUE
153         QN  #  SN  -  1.0
154         IF % TIME .LT. % T1*% QN & %1./4.<<<<GO TO 46
155         IF % TIME .LE. % T1*% QN & %1./2.<<<<GO TO 46
156         IF % TIME .LT. % T1*% QN & %3./4.<<<<GO TO 47
157         IF % TIME .LE. % T1*% QN & %4./4.<<<<GO TO 47
158    46   D4F%1<  #  1.0
159         YAKG  #   D4F%1<*AM
160         GO TO 49
161    47   D4F%1<  #  -1.0
162         YAKG  #   D4F%1<*AM
163         GO TO 48
164    48   CONTINUE
165   430   YDD4%J<  #% Q1A%J-1<* D4F%J-1<  < - % RK*YD4M%J<*
166     1   YD4M%J< <
167     2   - % Q2%J< * YD4M%J< <
168     0   YD4C%J<  #  %0.125 < * % % 9.0 * YD3%J< < - YD1%J<
169     1   & %% 3.* DELTT <
170     2     * % YDD4%J< & % 2.0*YDD3%J< <  - YDD2%J<<< <
171     0   YD4F%J<  #  YD4C%J<  & % %9./121.< * %YD4P%J<
172     1   - YD4C%J<<<
173     0   YDD4%J<  #  % Q1A%J-1< * D4F%J-1< <  - % RK*YD4F%J<
174     1   * YD4F%J< < -
175     2   % Q2%J< * YD4F%J< <
176         IF % TIME .LE. % 8.1/W < <  GO TO 50
177         IF % YD4F%2< - 0.0 < 49, 51, 51
178    51   IF % KP - 2 < 50,52, 52
179    49   IF % KS - 1 < 54, 54 , 53
180    54   IF % J .GE. 3 < GO TO 55
181         KP  #  KP  & 1
182    55   YA2%J<  #  YA2%J<  & YD4F%J<
183         GO TO 50
184    52   IF % J .GE. 3 < GO  TO 56
185         KS  #  KS  & 1
186    56   YA1%J<  #  YA1%J<  & YD4F%J<
187         GO TO 50
188    53   IF % J .GE.3<  GO  TO  57
189         SK  #  KS
190         PK  #  KP
191    57   YAVG%J<  #  % YA1%J< & YA2%J< < / % SK & PK <
192         JY  #  J - 1
193         PRINT  58, TIME, YD4F%J<, YA1%J<, YA2%J<, YAVG%J<,JY
194   580   FORMAT % // 10X, F9.3, 5X, F15.5, 5X, E11.4, 3X,
195     1   E11.4 , 7X,
196     2   @ AVERAGE CONC. #@,E15.7, @   IN REACTOR NUMBER @, I2 <
197         YA1%J<  #  0.0
198         YA2%J<  #  YD4F%J<
199         IF % J .LT. NR2 < GO TO  50
200         PRINT  59, SK, PK
```

FORTRAN IV017 SOURCE PROGRAM RALHAM   PROGRAM

```
201    59   FORMAT " / 2X,    NO. OF PUINTS # a, F10.4, 10X,F10.4<
202         KP   #   1
203         KS   #   0
204    50   CONTINUE
205         YD%J<   # YD1%J<
206         YD1%J<  #   YD2%J<
207         YD2%J<  #   YD3%J<
208         YD3%J<     #   YD4F%J<
209         YD3P%J<  #   YD4P%J<
210         YD3C%J<  #   YD4C%J<
211         YDU1%J<  #   YDD2%J<
212         YDU2%J<     #   YDD3%J<
213         YDD3%J<  #   YDD4%J<
214         D4F%J<   #   YD4F%J<
215    42   CONTINUE
216         IF% TIME - TPR < 61,  60, 60
217    60   PRINT 62, TIME , YAPG      , % YD4F%J< , J # 2 , NR2<
218    62   FORMAT % 10X, F9.3, 5X, E15.5 , 5% 5X, E15.5 < <
219         TPR   #   TPR   & DELTPR
220    61   IF % TIME - % % 6.3/W<#6.9< < 63, 64, 64
221    63   A  #   I
222         TIME   #   A * DELTT
223    41   CONTINUE
224    64   IF % DELTT .GE. 0.110 < GO TO 65
225         IF % DELTT .LE. 0.110 < GO TO 100
226         GO TO 100
227    65   DELTT #   DELTT / 2.0
228         TIME   #   TIME1
229         PRINT 66,  DELTT
230   660   FORMAT % /// a    ANOTHER CASE WITH DIFFERENY DELTT #a
231     1 , F5.3 <
232         GO TO 67
233   100   CONTINUE
234    11   CONTINUE
235         DELTT   #   DELTT1
236         TIME   #   TIME1
237    10   CONTINUE
238         STOP
239         END
```

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